



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2026 – 09:13 pm BST

PDB ID : 2W55 / pdb_00002w55
Title : Crystal Structure of Xanthine Dehydrogenase (E232Q variant) from Rhodobacter capsulatus in Complex with Hypoxanthine
Authors : Doebbler, J.A.; Truglio, J.J.; Leimkuhler, S.; Kisker, C.
Deposited on : 2008-12-04
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

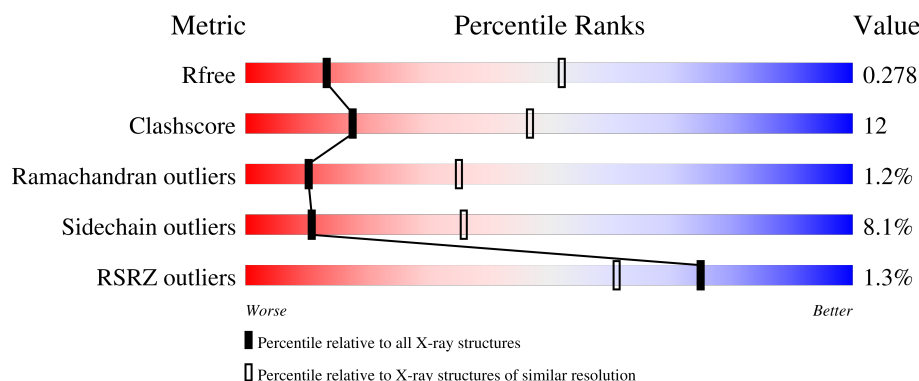
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	462	2% 68% 27% • •
1	C	462	0% 70% 24% • •
1	E	462	2% 68% 26% • •
1	G	462	3% 65% 29% • •
2	B	777	0% 69% 26% • •

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Mol	Chain	Length	Quality of chain
2	D	777	
2	F	777	
2	H	777	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	XAX	B	1778	X	-	-	-
5	XAX	D	1778	X	-	-	-
5	XAX	F	1778	X	-	-	-
5	XAX	H	1778	X	-	-	-
7	HPA	H	1780	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 36807 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called XANTHINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3375	2115	608	627	25			
1	C	450	Total	C	N	O	S	0	0	0
			3375	2115	608	627	25			
1	E	450	Total	C	N	O	S	0	0	0
			3375	2115	608	627	25			
1	G	450	Total	C	N	O	S	0	0	0
			3375	2115	608	627	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	TRP	LEU	conflict	UNP O54050
C	26	TRP	LEU	conflict	UNP O54050
E	26	TRP	LEU	conflict	UNP O54050
G	26	TRP	LEU	conflict	UNP O54050

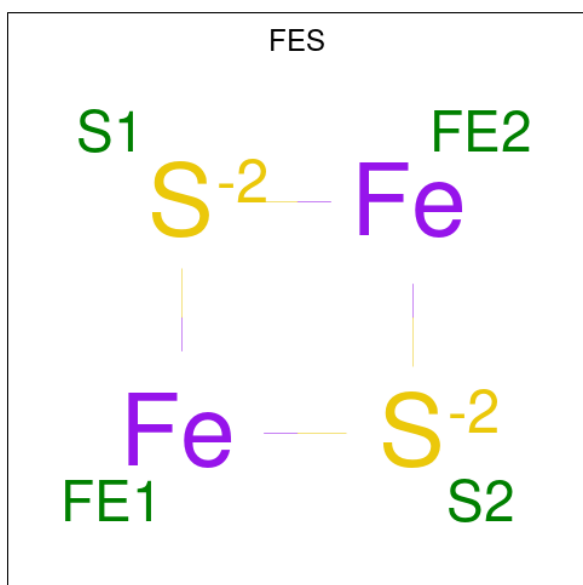
- Molecule 2 is a protein called XANTHINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	760	Total	C	N	O	S	0	0	0
			5716	3581	1057	1052	26			
2	D	760	Total	C	N	O	S	0	0	0
			5716	3581	1057	1052	26			
2	F	760	Total	C	N	O	S	0	0	0
			5716	3581	1057	1052	26			
2	H	760	Total	C	N	O	S	0	0	0
			5716	3581	1057	1052	26			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	232	GLN	GLU	engineered mutation	UNP O54051
B	772	ARG	GLY	conflict	UNP O54051
D	232	GLN	GLU	engineered mutation	UNP O54051
D	772	ARG	GLY	conflict	UNP O54051
F	232	GLN	GLU	engineered mutation	UNP O54051
F	772	ARG	GLY	conflict	UNP O54051
H	232	GLN	GLU	engineered mutation	UNP O54051
H	772	ARG	GLY	conflict	UNP O54051

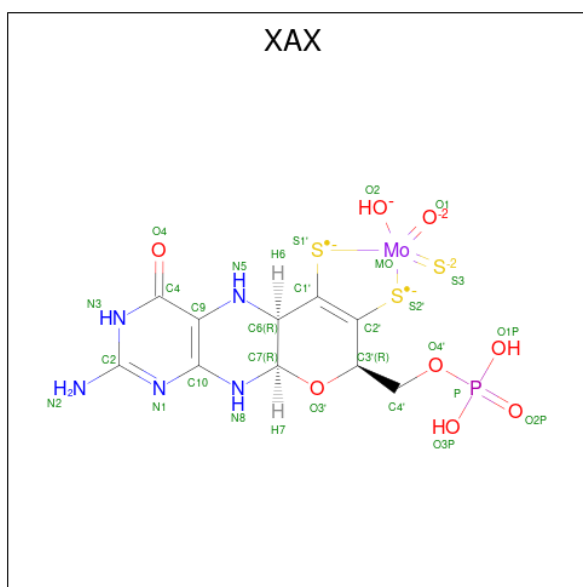
- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		

- # FAD
-
- The image displays the chemical structure of Flavin Adenine Dinucleotide (FAD), a crucial coenzyme. The structure is composed of several interconnected components:
- Flavin Mononucleotide (FMN) moiety:** This includes the isoalloxazine ring system (colored blue and purple) and the ribityl side chain (colored red). The ribityl chain consists of three carbon atoms, with the terminal carbon being a primary alcohol group.
 - Phosphate groups:** Two phosphate groups (colored red) are attached to the ribityl chain, linking it to the adenine base. The first phosphate is attached to the second carbon of the ribityl chain, and the second phosphate is attached to the third carbon.
 - Adenine base:** The adenine base (colored blue and purple) is attached to the second phosphate group. It is a purine derivative, consisting of a fused pyrimidine and imidazole ring system.
- The structure is shown in a 3D representation, with atoms labeled with their respective element symbols (C, N, O, P) and bond types (single, double, triple). The overall structure is a complex molecule that plays a central role in many biological processes, particularly in energy metabolism.

- Molecule 5 is {[(5aR,8R,9aR)-2-amino-4-oxo-6,7-di(sulfanyl-kappaS)-3,5,5a,8,9a,10-hexahydro-4H-pyrano[3,2-g]pteridin-8-yl)methyl dihydrogenato(2-) phosphate} (hydroxy)oxo(thio) molybdenum (CCD ID: XAX) (formula: $C_{10}H_{13}MoN_5O_8PS_3$).

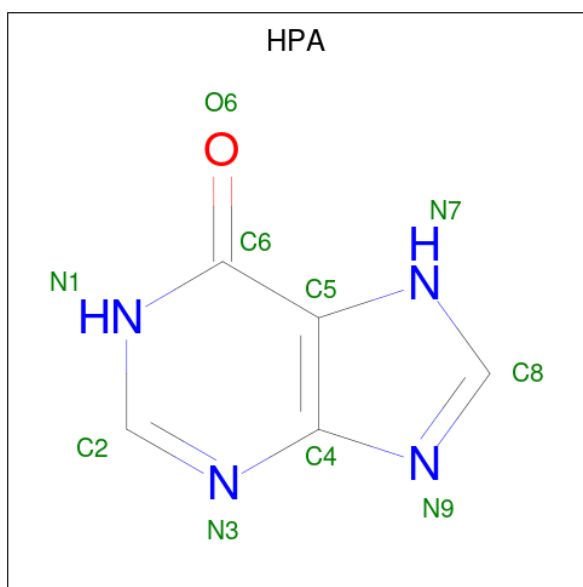


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	B	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		
5	D	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		
5	F	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		
5	H	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		

- Molecule 6 is BARIUM ION (CCD ID: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ba	0	0
			1	1		
6	D	1	Total	Ba	0	0
			1	1		
6	F	1	Total	Ba	0	0
			1	1		
6	H	1	Total	Ba	0	0
			1	1		

- Molecule 7 is HYPOXANTHINE (CCD ID: HPA) (formula: C₅H₄N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			10	5	4	1		
7	D	1	Total	C	N	O	0	0
			10	5	4	1		
7	F	1	Total	C	N	O	0	0
			10	5	4	1		
7	H	1	Total	C	N	O	0	0
			10	5	4	1		

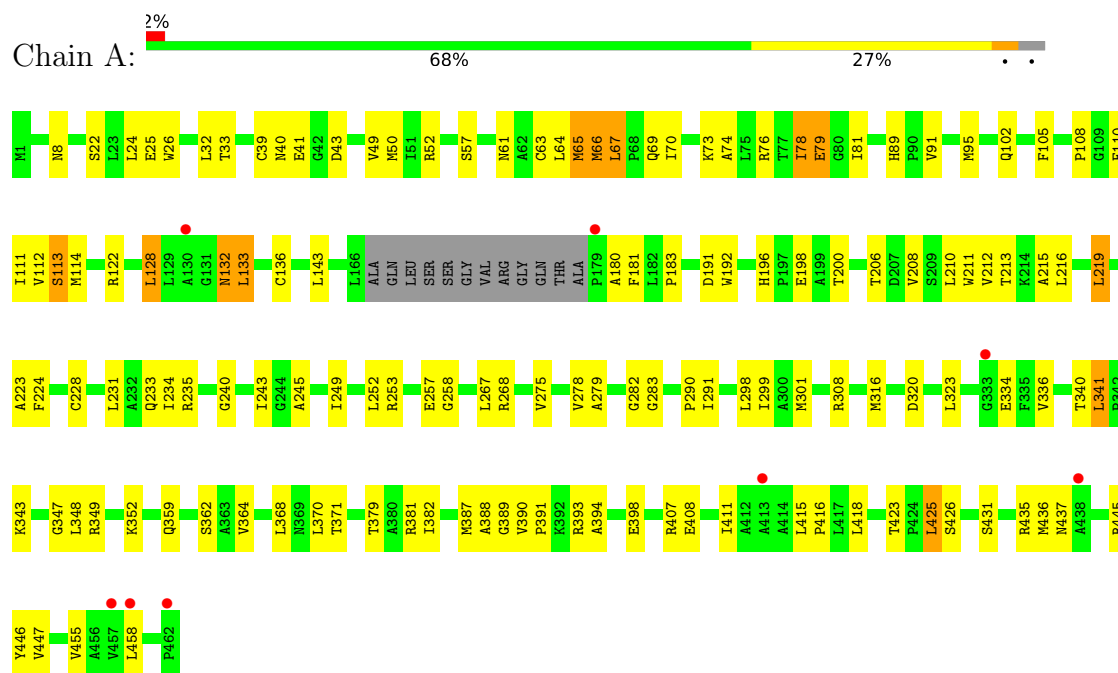
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total	O	0	0
			4	4		
8	B	8	Total	O	0	0
			8	8		
8	C	3	Total	O	0	0
			3	3		
8	D	11	Total	O	0	0
			11	11		
8	E	1	Total	O	0	0
			1	1		
8	F	12	Total	O	0	0
			12	12		
8	G	1	Total	O	0	0
			1	1		
8	H	3	Total	O	0	0
			3	3		

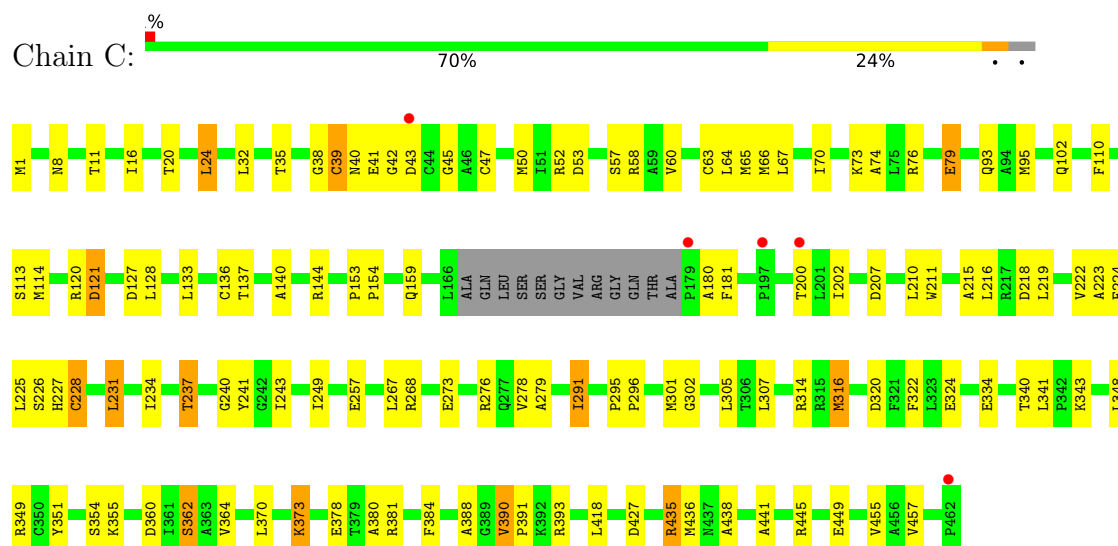
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

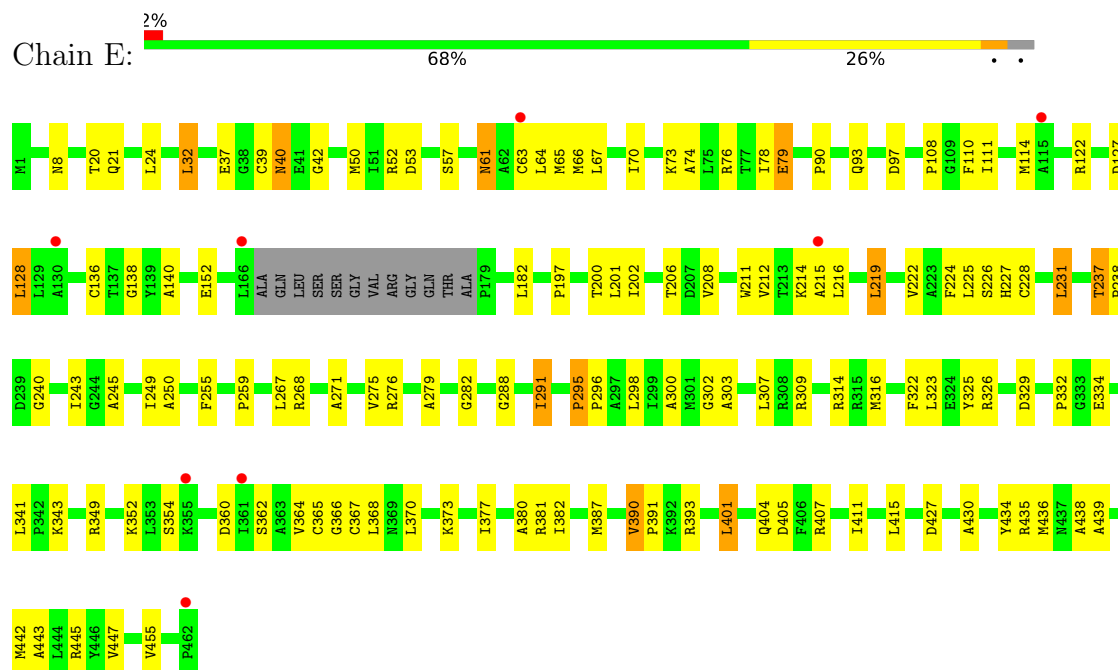
• Molecule 1: XANTHINE DEHYDROGENASE

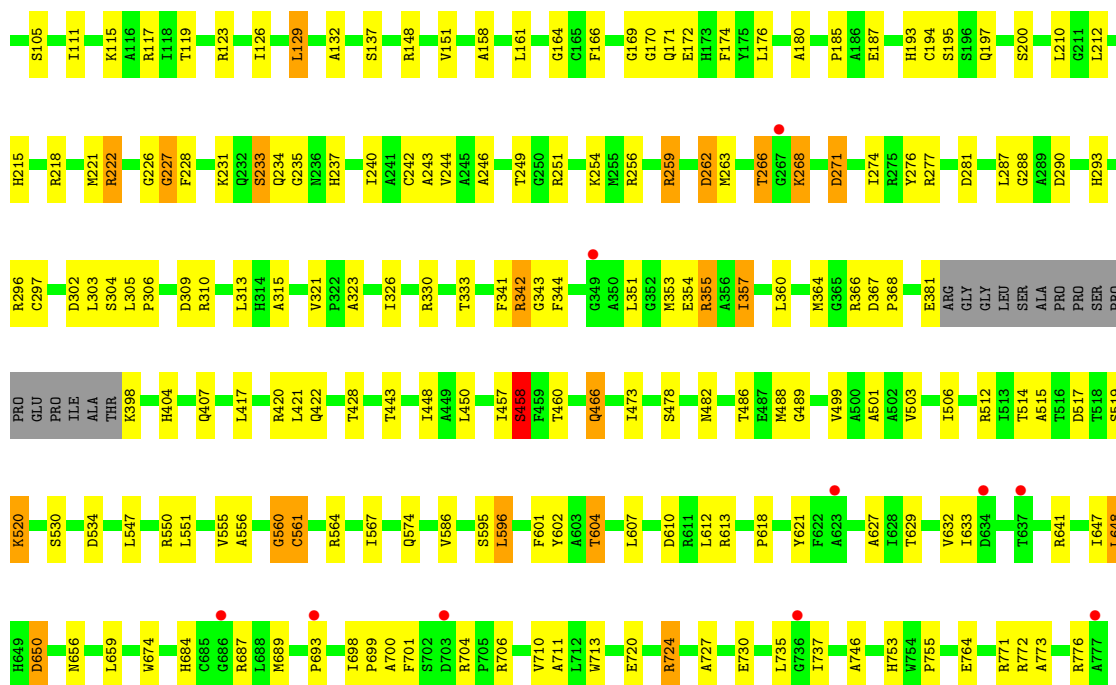


• Molecule 1: XANTHINE DEHYDROGENASE

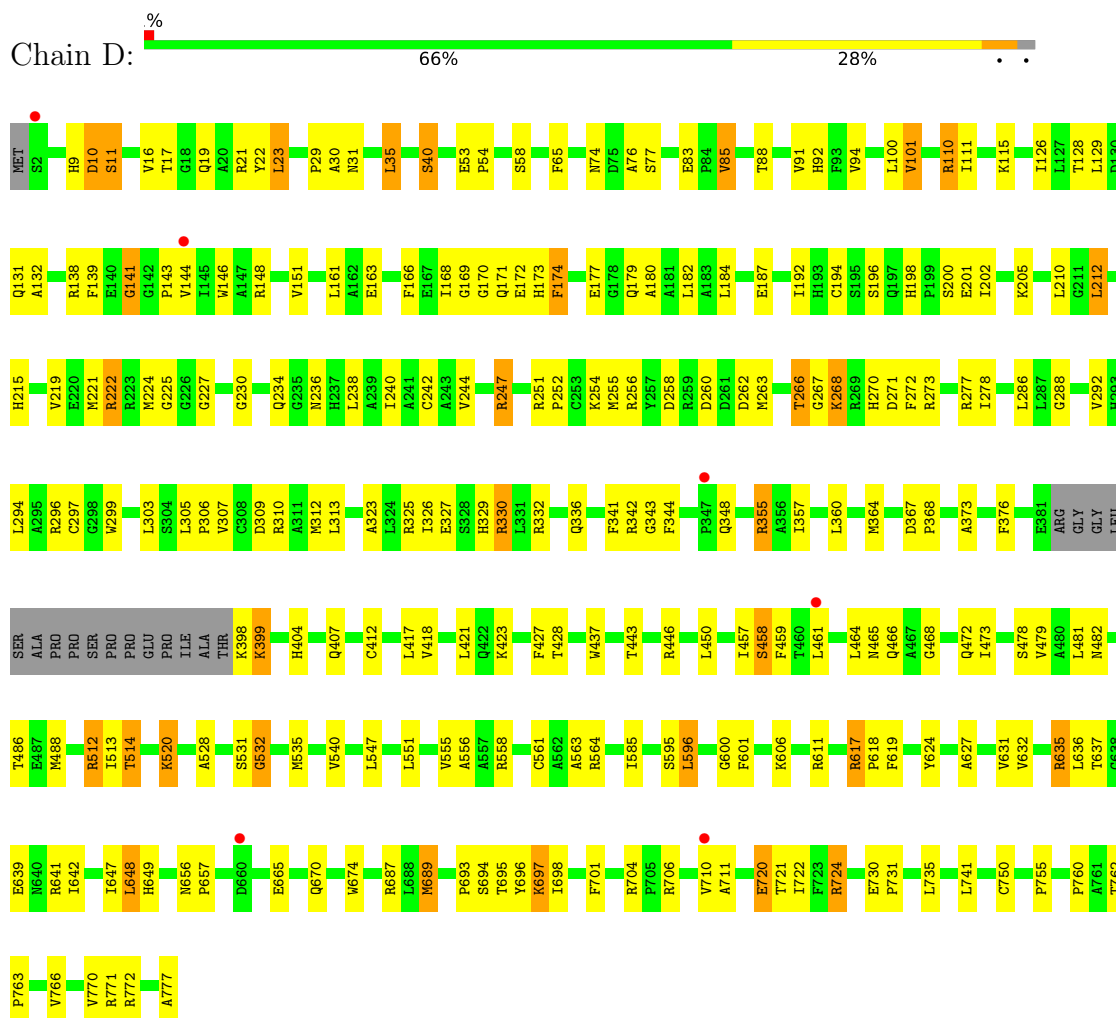


• Molecule 1: XANTHINE DEHYDROGENASE

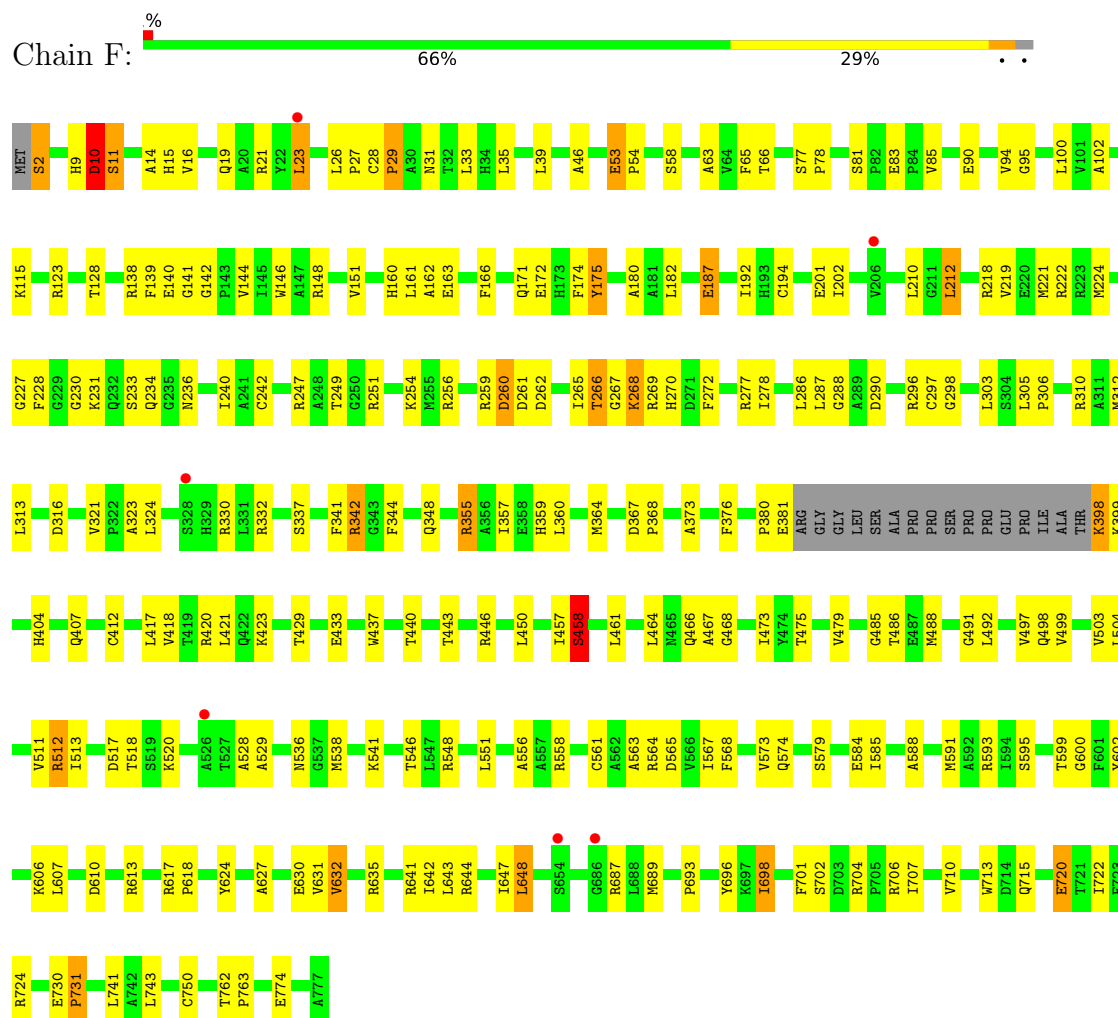




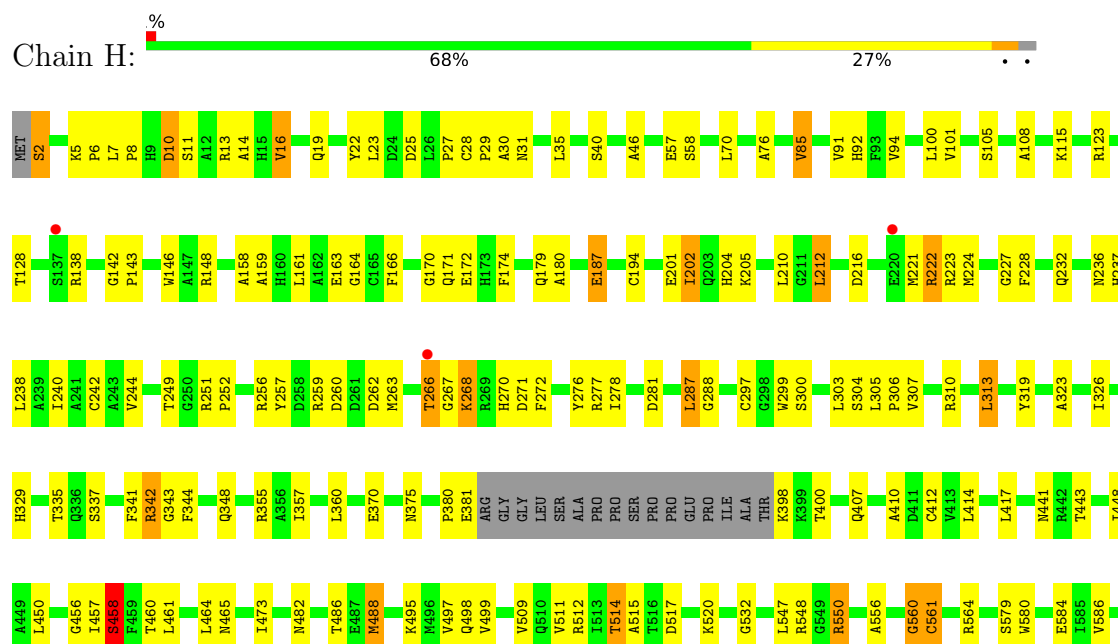
• Molecule 2: XANTHINE DEHYDROGENASE

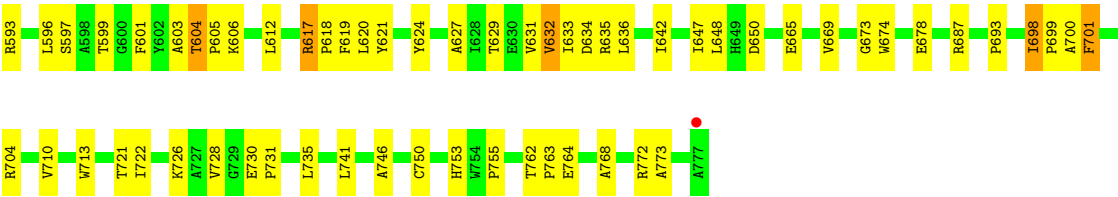


- Molecule 2: XANTHINE DEHYDROGENASE



• Molecule 2: XANTHINE DEHYDROGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.74Å 140.57Å 157.61Å 109.45° 106.10° 101.09°	Depositor
Resolution (Å)	50.00 – 3.40 50.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	93.7 (50.00-3.40) 77.8 (50.00-3.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.40Å)	Xtrriage
Refinement program	REFMAC 5.5.0055	Depositor
R, R_{free}	0.221 , 0.270 0.225 , 0.278	Depositor DCC
R_{free} test set	3708 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	79.0	Xtrriage
Anisotropy	0.037	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	36807	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7034e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XAX, HPA, BA, FES, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/3438	0.85	3/4658 (0.1%)
1	C	0.48	0/3438	0.84	3/4658 (0.1%)
1	E	0.48	0/3438	0.84	2/4658 (0.0%)
1	G	0.50	0/3438	0.85	6/4658 (0.1%)
2	B	0.47	0/5844	0.85	3/7941 (0.0%)
2	D	0.48	0/5844	0.87	1/7941 (0.0%)
2	F	0.48	0/5844	0.88	8/7941 (0.1%)
2	H	0.48	0/5844	0.85	1/7941 (0.0%)
All	All	0.48	0/37128	0.86	27/50396 (0.1%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	CYS	N-CA-C	6.58	119.43	111.40
1	E	136	CYS	N-CA-C	5.77	118.68	111.24
2	F	81	SER	CA-C-N	5.77	125.77	119.89
2	F	81	SER	C-N-CA	5.77	125.77	119.89
2	B	85	VAL	N-CA-C	-5.53	106.42	111.67
1	G	258	GLY	CA-C-N	5.38	124.83	119.24
1	G	258	GLY	C-N-CA	5.38	124.83	119.24
1	C	384	PHE	N-CA-C	5.35	117.13	108.41
2	B	65	PHE	N-CA-C	5.33	118.18	109.59
2	F	28	CYS	CA-C-N	5.32	126.49	119.84
2	F	28	CYS	C-N-CA	5.32	126.49	119.84
1	G	136	CYS	N-CA-C	5.29	117.62	110.06
2	F	731	PRO	CA-C-N	-5.22	114.66	120.45
2	F	731	PRO	C-N-CA	-5.22	114.66	120.45
1	G	423	THR	CA-C-N	5.16	125.89	120.11
1	G	423	THR	C-N-CA	5.16	125.89	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	237	HIS	N-CA-C	5.15	116.58	111.07
1	C	237	THR	CA-C-N	5.11	126.23	119.84
1	C	237	THR	C-N-CA	5.11	126.23	119.84
2	F	715	GLN	CA-C-N	5.11	125.10	119.89
2	F	715	GLN	C-N-CA	5.11	125.10	119.89
2	D	427	PHE	N-CA-C	5.11	116.92	111.36
2	H	237	HIS	N-CA-C	5.10	116.92	111.36
1	G	295	PRO	N-CA-C	5.09	116.92	110.70
1	E	271	ALA	CB-CA-C	-5.08	110.69	116.54
1	A	258	GLY	CA-C-N	5.05	124.49	119.24
1	A	258	GLY	C-N-CA	5.05	124.49	119.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3375	0	3368	77	0
1	C	3375	0	3368	72	0
1	E	3375	0	3369	75	0
1	G	3375	0	3371	94	0
2	B	5716	0	5633	137	0
2	D	5716	0	5633	166	0
2	F	5716	0	5633	150	0
2	H	5716	0	5633	151	0
3	A	8	0	0	0	0
3	C	8	0	0	0	0
3	E	8	0	0	0	0
3	G	8	0	0	1	0
4	A	53	0	31	6	0
4	C	53	0	31	5	0
4	E	53	0	31	2	0
4	G	53	0	31	7	0
5	B	28	0	8	4	0
5	D	28	0	8	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	28	0	8	7	0
5	H	28	0	8	4	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
7	B	10	0	4	0	0
7	D	10	0	4	3	0
7	F	10	0	4	1	0
7	H	10	0	4	7	0
8	A	4	0	0	0	0
8	B	8	0	0	1	0
8	C	3	0	0	1	0
8	D	11	0	0	0	0
8	E	1	0	0	0	0
8	F	12	0	0	0	0
8	G	1	0	0	0	0
8	H	3	0	0	0	0
All	All	36807	0	36180	906	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (906) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:1778:XAX:O1	7:F:1780:HPA:H2	1.49	1.12
2:D:179:GLN:HB3	2:D:238:LEU:HD11	1.45	0.99
1:C:445:ARG:HG3	1:C:455:VAL:HG11	1.50	0.94
2:H:457:ILE:O	2:H:458:SER:HB2	1.62	0.93
2:F:138:ARG:HD3	2:F:142:GLY:H	1.34	0.92
1:E:387:MET:CE	1:E:439:ALA:HB2	1.99	0.91
1:A:24:LEU:HD12	1:A:63:CYS:HB3	1.53	0.91
1:G:243:ILE:HD13	1:G:341:LEU:HD21	1.52	0.91
2:F:407:GLN:OE1	2:F:618:PRO:HD2	1.71	0.91
2:D:77:SER:HB2	2:D:83:GLU:HB3	1.53	0.90
1:E:295:PRO:HB2	1:E:296:PRO:HD3	1.55	0.89
1:C:40:ASN:ND2	1:C:63:CYS:HB2	1.87	0.88
2:D:179:GLN:HB3	2:D:238:LEU:CD1	2.04	0.87
2:F:210:LEU:HB3	2:F:212:LEU:HD21	1.58	0.85
2:F:224:MET:HE3	2:F:488:MET:HB3	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:457:ILE:O	2:B:458:SER:HB2	1.75	0.85
2:H:755:PRO:O	2:H:772:ARG:HD2	1.76	0.85
2:B:701:PHE:O	2:B:704:ARG:HG2	1.76	0.84
2:H:465:ASN:HB3	2:H:604:THR:OG1	1.77	0.84
1:E:237:THR:OG1	1:E:238:PRO:HD2	1.78	0.83
2:D:247:ARG:HG2	2:D:247:ARG:HH11	1.41	0.83
2:H:701:PHE:O	2:H:704:ARG:HG2	1.79	0.82
2:B:129:LEU:HD12	2:B:129:LEU:H	1.44	0.82
2:F:360:LEU:HG	2:F:364:MET:HE3	1.61	0.82
2:F:488:MET:HE3	5:F:1778:XAX:H4'	1.59	0.81
2:D:443:THR:HG23	2:D:636:LEU:HD13	1.61	0.81
1:E:249:ILE:HG23	1:E:267:LEU:HD22	1.63	0.80
1:C:200:THR:HB	1:C:222:VAL:HG12	1.63	0.80
2:D:701:PHE:O	2:D:704:ARG:HG2	1.84	0.78
1:C:249:ILE:HG23	1:C:267:LEU:HD22	1.65	0.78
2:H:259:ARG:HG2	2:H:693:PRO:HD3	1.65	0.78
2:D:31:ASN:HB2	2:D:251:ARG:HD3	1.66	0.77
1:C:133:LEU:HD13	2:D:698:ILE:HD11	1.67	0.77
2:F:272:PHE:CD2	2:F:348:GLN:HG2	2.21	0.76
2:D:151:VAL:HG21	2:D:325:ARG:HB2	1.67	0.76
2:D:360:LEU:HG	2:D:364:MET:HE3	1.68	0.76
1:G:41:GLU:HA	1:G:210:LEU:HD21	1.67	0.76
1:C:322:PHE:HB3	1:C:390:VAL:HG22	1.67	0.75
1:G:24:LEU:HD12	1:G:63:CYS:HB3	1.69	0.75
2:B:75:ASP:OD2	2:B:82:PRO:HA	1.87	0.74
1:G:455:VAL:HG13	2:H:443:THR:HG21	1.69	0.74
2:F:288:GLY:HA2	2:F:323:ALA:O	1.87	0.74
1:C:279:ALA:HB1	4:C:1465:FAD:H4'	1.70	0.74
2:F:305:LEU:HB3	2:F:306:PRO:HD3	1.70	0.73
2:F:497:VAL:HG13	2:F:511:VAL:HB	1.70	0.73
2:F:457:ILE:O	2:F:458:SER:HB2	1.85	0.73
2:B:360:LEU:HG	2:B:364:MET:HE3	1.71	0.73
1:G:352:LYS:HG3	1:G:362:SER:HB3	1.71	0.72
2:D:637:THR:OG1	2:D:639:GLU:HG3	1.89	0.72
1:A:411:ILE:HG13	1:A:447:VAL:HG21	1.71	0.71
1:C:40:ASN:HD22	1:C:63:CYS:HB2	1.52	0.71
1:A:65:MET:HE1	1:A:278:VAL:HG11	1.72	0.71
1:A:133:LEU:HD13	2:B:698:ILE:HD11	1.71	0.71
2:H:163:GLU:HG2	2:H:277:ARG:HG2	1.71	0.71
1:A:394:ALA:O	1:A:398:GLU:HB2	1.90	0.71
2:B:305:LEU:HB3	2:B:306:PRO:HD3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:31:ASN:HB2	2:F:251:ARG:HD3	1.73	0.70
2:D:23:LEU:HD22	2:D:180:ALA:HB1	1.71	0.70
1:E:455:VAL:HG13	2:F:443:THR:HG21	1.73	0.70
1:A:298:LEU:HD13	1:A:301:MET:HE3	1.71	0.70
2:F:58:SER:HB2	2:F:115:LYS:HD2	1.73	0.70
2:H:13:ARG:HG2	2:H:13:ARG:HH11	1.55	0.70
2:D:224:MET:HE3	2:D:488:MET:HB3	1.74	0.70
1:E:279:ALA:HB1	4:E:1465:FAD:H4'	1.73	0.70
2:H:232:GLN:HE22	7:H:1780:HPA:H2	1.56	0.70
1:A:110:PHE:HB3	1:A:114:MET:HE2	1.72	0.69
2:H:753:HIS:HB2	2:H:773:ALA:HA	1.73	0.69
1:G:382:ILE:HD12	1:G:398:GLU:HG3	1.73	0.69
1:E:387:MET:HE2	1:E:439:ALA:HB2	1.74	0.69
2:F:144:VAL:CG2	2:F:330:ARG:HH12	2.05	0.69
1:A:455:VAL:HG13	2:B:443:THR:HG21	1.74	0.69
2:B:720:GLU:HA	2:B:724:ARG:NH2	2.08	0.69
2:F:701:PHE:O	2:F:704:ARG:HG2	1.93	0.68
2:B:610:ASP:HB3	2:B:613:ARG:HB2	1.75	0.68
2:F:303:LEU:O	2:F:306:PRO:HD2	1.92	0.68
2:H:482:ASN:HD22	2:H:514:THR:HB	1.57	0.68
2:F:641:ARG:NH2	2:F:706:ARG:HD3	2.09	0.68
2:B:755:PRO:O	2:B:772:ARG:HD2	1.93	0.68
1:A:26:TRP:CD1	1:A:67:LEU:HD11	2.29	0.68
2:B:77:SER:HB2	2:B:83:GLU:HB3	1.75	0.68
2:D:23:LEU:HD13	2:D:194:CYS:HA	1.76	0.68
5:F:1778:XAX:S3	5:F:1778:XAX:MO	2.04	0.68
2:B:259:ARG:HG2	2:B:693:PRO:HD3	1.76	0.67
2:H:11:SER:OG	2:H:223:ARG:NH2	2.27	0.67
1:E:24:LEU:HD21	1:E:37:GLU:HG2	1.77	0.67
2:B:70:LEU:HD23	2:B:244:VAL:HG11	1.77	0.67
5:D:1778:XAX:S3	5:D:1778:XAX:MO	2.05	0.67
2:F:635:ARG:NH1	2:F:750:CYS:HB3	2.10	0.66
1:A:105:PHE:O	1:A:108:PRO:HD2	1.95	0.66
5:H:1778:XAX:S3	5:H:1778:XAX:MO	2.06	0.66
1:E:322:PHE:HB3	1:E:390:VAL:HG22	1.77	0.66
2:F:9:HIS:CD2	2:F:15:HIS:HE1	2.13	0.66
2:F:27:PRO:HB2	2:H:29:PRO:HG3	1.76	0.66
1:A:234:ILE:HD13	1:A:243:ILE:HG13	1.76	0.66
5:B:1778:XAX:MO	5:B:1778:XAX:S3	2.06	0.66
2:H:23:LEU:HD13	2:H:194:CYS:HA	1.78	0.66
2:B:650:ASP:HA	2:B:713:TRP:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ARG:HB3	1:A:128:LEU:HD21	1.76	0.65
1:A:352:LYS:HG3	1:A:362:SER:HB3	1.77	0.65
2:B:641:ARG:HH21	2:B:706:ARG:HH21	1.43	0.65
2:H:92:HIS:HB2	2:H:299:TRP:CE3	2.30	0.65
1:G:183:PRO:HG3	1:G:189:LEU:HD13	1.77	0.65
2:F:29:PRO:HG3	2:H:27:PRO:HB2	1.78	0.65
2:D:163:GLU:HG2	2:D:277:ARG:HG2	1.79	0.65
2:D:305:LEU:HB3	2:D:306:PRO:HD3	1.79	0.65
2:B:586:VAL:HG13	2:B:596:LEU:HD22	1.77	0.64
1:C:322:PHE:HB3	1:C:390:VAL:CG2	2.27	0.64
2:H:380:PRO:O	2:H:381:GLU:HB2	1.96	0.64
1:A:50:MET:HE2	1:A:57:SER:HB2	1.78	0.64
2:F:144:VAL:HG22	2:F:330:ARG:HH12	1.63	0.64
2:B:78:PRO:HD2	2:B:302:ASP:HA	1.80	0.64
2:F:420:ARG:HE	2:F:713:TRP:HZ3	1.46	0.64
2:D:341:PHE:HD2	2:D:342:ARG:H	1.44	0.64
2:D:247:ARG:HG2	2:D:247:ARG:NH1	2.08	0.64
1:A:243:ILE:HD13	1:A:341:LEU:HD21	1.80	0.63
2:D:179:GLN:NE2	2:D:234:GLN:HB2	2.13	0.63
4:G:1465:FAD:N1	4:G:1465:FAD:H2'	2.12	0.63
1:C:1:MET:HE2	1:C:16:ILE:HG13	1.78	0.63
1:C:360:ASP:OD1	2:D:697:LYS:HE3	1.98	0.63
2:B:720:GLU:HA	2:B:724:ARG:HH21	1.62	0.63
2:F:9:HIS:HD2	2:F:15:HIS:HE1	1.46	0.63
2:F:556:ALA:HB2	2:F:563:ALA:HA	1.81	0.63
2:D:689:MET:HE3	2:D:689:MET:HA	1.80	0.63
2:B:262:ASP:O	2:B:266:THR:HG23	1.99	0.63
1:G:364:VAL:HG22	1:G:435:ARG:HG3	1.79	0.63
1:G:371:THR:HB	1:G:378:GLU:HB3	1.81	0.63
2:F:148:ARG:HD2	2:F:404:HIS:HA	1.81	0.63
2:D:341:PHE:HD2	2:D:342:ARG:N	1.96	0.63
1:A:382:ILE:HD12	1:A:398:GLU:HG3	1.80	0.62
5:H:1778:XAX:MO	5:H:1778:XAX:O2	1.70	0.62
2:D:418:VAL:HG13	2:D:450:LEU:HD11	1.82	0.62
2:D:730:GLU:H	2:D:731:PRO:HD2	1.64	0.62
5:F:1778:XAX:MO	5:F:1778:XAX:O2	1.71	0.62
5:D:1778:XAX:MO	5:D:1778:XAX:O2	1.70	0.62
2:F:467:ALA:HB1	2:F:536:ASN:OD1	1.99	0.62
1:C:39:CYS:SG	1:C:41:GLU:HB2	2.40	0.62
1:E:211:TRP:HA	1:E:215:ALA:HB3	1.81	0.62
1:G:8:ASN:HA	1:G:76:ARG:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1778:XAX:MO	5:B:1778:XAX:O2	1.71	0.61
4:C:1465:FAD:H2'	4:C:1465:FAD:N1	2.15	0.61
2:D:210:LEU:HD22	2:D:247:ARG:HD3	1.81	0.61
2:D:461:LEU:HD12	7:D:1780:HPA:H8	1.82	0.61
1:E:445:ARG:HG3	1:E:455:VAL:HG11	1.82	0.61
2:H:7:LEU:HB3	2:H:8:PRO:HD2	1.81	0.61
1:A:426:SER:H	2:F:574:GLN:HE22	1.47	0.61
2:D:201:GLU:HG2	2:D:236:ASN:HD21	1.66	0.61
1:E:240:GLY:HA2	1:E:343:LYS:HG2	1.82	0.61
2:F:210:LEU:HB3	2:F:212:LEU:CD2	2.29	0.61
5:D:1778:XAX:O1	7:D:1780:HPA:H2	2.01	0.61
1:A:22:SER:OG	1:A:25:GLU:HG2	2.00	0.61
2:D:512:ARG:HE	2:D:512:ARG:HA	1.64	0.61
2:F:35:LEU:HD11	2:F:242:CYS:HA	1.81	0.61
1:A:216:LEU:HD13	2:B:111:ILE:HG13	1.83	0.61
2:B:46:ALA:HB2	2:B:123:ARG:HH21	1.66	0.61
1:C:234:ILE:HD13	1:C:243:ILE:HG13	1.82	0.61
2:F:23:LEU:HD22	2:F:180:ALA:HB1	1.82	0.61
2:H:310:ARG:HD2	2:H:344:PHE:HB3	1.81	0.61
2:D:179:GLN:CB	2:D:238:LEU:HD11	2.27	0.61
2:D:417:LEU:HG	2:D:648:LEU:HD23	1.82	0.60
2:D:730:GLU:N	2:D:731:PRO:HD2	2.16	0.60
1:A:52:ARG:HB3	1:A:74:ALA:HB3	1.84	0.60
1:C:373:LYS:HB2	1:C:378:GLU:HG3	1.82	0.60
2:D:482:ASN:HD22	2:D:514:THR:HB	1.65	0.60
2:H:457:ILE:O	2:H:458:SER:CB	2.43	0.60
2:B:227:GLY:HA2	2:B:231:LYS:HG3	1.84	0.60
2:B:422:GLN:HE21	2:B:450:LEU:HD13	1.66	0.60
1:A:283:GLY:HA2	4:A:1465:FAD:C8A	2.32	0.60
2:D:459:PHE:H	2:D:465:ASN:HD21	1.50	0.60
2:H:297:CYS:SG	2:H:304:SER:HB3	2.42	0.60
2:H:560:GLY:O	2:H:561:CYS:HB3	2.00	0.60
1:C:32:LEU:HD12	1:C:79:GLU:HG3	1.84	0.60
1:C:302:GLY:HA2	1:C:381:ARG:NH1	2.16	0.60
1:C:427:ASP:OD1	1:C:435:ARG:NH2	2.35	0.59
2:F:144:VAL:HG22	2:F:330:ARG:NH1	2.17	0.59
2:F:269:ARG:HD3	2:F:348:GLN:HE22	1.67	0.59
2:D:240:ILE:O	2:D:244:VAL:HG23	2.01	0.59
2:D:648:LEU:HD12	2:D:711:ALA:HB3	1.84	0.59
2:B:23:LEU:HD22	2:B:180:ALA:HB1	1.84	0.59
2:B:720:GLU:HG2	2:B:724:ARG:HH22	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:PHE:HB3	1:C:114:MET:HE2	1.85	0.59
1:A:70:ILE:HA	1:A:73:LYS:HG3	1.84	0.59
2:B:28:CYS:HB2	2:B:29:PRO:CD	2.32	0.59
2:B:49:GLY:HA3	2:B:119:THR:OG1	2.01	0.59
2:D:35:LEU:HD11	2:D:242:CYS:HA	1.84	0.59
2:H:550:ARG:HH12	2:H:597:SER:H	1.49	0.59
1:A:245:ALA:HB2	1:A:336:VAL:HG12	1.85	0.59
1:G:245:ALA:HB1	1:G:282:GLY:HA3	1.84	0.59
2:D:77:SER:HB2	2:D:83:GLU:CB	2.30	0.59
2:F:201:GLU:HG2	2:F:236:ASN:HD21	1.68	0.59
2:H:460:THR:H	7:H:1780:HPA:H8	1.67	0.59
2:D:421:LEU:HD13	2:D:648:LEU:HB2	1.84	0.58
1:C:390:VAL:HG22	1:C:391:PRO:HD2	1.85	0.58
2:D:94:VAL:HG11	2:D:687:ARG:HG2	1.85	0.58
1:E:201:LEU:HD22	1:E:225:LEU:HD21	1.84	0.58
2:F:262:ASP:O	2:F:266:THR:HG23	2.03	0.58
2:F:528:ALA:HA	5:F:1778:XAX:S2'	2.42	0.58
2:F:606:LYS:O	2:F:617:ARG:HD2	2.03	0.58
2:H:698:ILE:HB	2:H:699:PRO:HD2	1.86	0.58
2:B:70:LEU:CD2	2:B:244:VAL:HG11	2.33	0.58
1:A:445:ARG:HG3	1:A:455:VAL:HG11	1.83	0.58
2:B:310:ARG:HD2	2:B:344:PHE:HB3	1.86	0.58
1:C:52:ARG:HB3	1:C:74:ALA:HB3	1.86	0.58
1:C:301:MET:HB3	1:C:348:LEU:HD22	1.85	0.58
2:D:58:SER:HB2	2:D:115:LYS:HD2	1.86	0.58
2:D:17:THR:OG1	2:D:19:GLN:HG3	2.03	0.58
1:G:266:LEU:HD13	1:G:350:CYS:HB3	1.85	0.58
2:B:753:HIS:HB2	2:B:773:ALA:HA	1.85	0.58
1:E:250:ALA:HB2	1:E:276:ARG:HB3	1.85	0.58
1:G:138:GLY:HA2	2:H:669:VAL:HG21	1.84	0.58
2:H:143:PRO:HB3	2:H:329:HIS:CE1	2.39	0.58
2:D:54:PRO:HB2	2:D:115:LYS:O	2.04	0.57
2:B:11:SER:HB2	2:B:15:HIS:CD2	2.39	0.57
2:D:262:ASP:O	2:D:266:THR:HG23	2.04	0.57
1:G:415:LEU:N	1:G:416:PRO:HD2	2.19	0.57
1:A:206:THR:HG21	1:A:275:VAL:HG13	1.86	0.57
2:F:9:HIS:HD2	2:F:15:HIS:CE1	2.22	0.57
1:G:445:ARG:HE	1:G:455:VAL:HG12	1.69	0.57
2:D:407:GLN:OE1	2:D:618:PRO:HD2	2.05	0.57
2:F:54:PRO:HB2	2:F:115:LYS:O	2.05	0.57
2:H:148:ARG:O	2:H:323:ALA:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:547:LEU:HD23	2:B:550:ARG:HH11	1.69	0.57
2:D:310:ARG:HD2	2:D:344:PHE:HB3	1.86	0.57
2:F:2:SER:HB3	2:F:498:GLN:HG2	1.86	0.57
1:G:22:SER:OG	1:G:25:GLU:HG2	2.04	0.57
2:B:601:PHE:CG	2:D:595:SER:HB2	2.40	0.57
2:D:40:SER:HB2	2:D:91:VAL:HG11	1.86	0.57
2:H:262:ASP:O	2:H:266:THR:HG23	2.04	0.57
2:F:473:ILE:HG23	2:F:479:VAL:HG12	1.87	0.57
2:H:460:THR:H	7:H:1780:HPA:C8	2.18	0.57
2:H:161:LEU:HD21	2:H:163:GLU:OE2	2.04	0.57
1:G:330:ARG:HH21	4:G:1465:FAD:C2A	2.18	0.56
2:D:65:PHE:HB2	2:D:100:LEU:HB3	1.86	0.56
2:F:730:GLU:N	2:F:731:PRO:HD2	2.20	0.56
2:B:171:GLN:O	2:B:268:LYS:HB3	2.05	0.56
2:D:556:ALA:HB1	2:D:561:CYS:O	2.05	0.56
1:E:295:PRO:HB2	1:E:296:PRO:CD	2.31	0.56
1:E:387:MET:HE3	1:E:439:ALA:HB2	1.83	0.56
2:F:46:ALA:HB2	2:F:123:ARG:HH21	1.69	0.56
2:H:23:LEU:HD22	2:H:180:ALA:HB1	1.86	0.56
2:H:35:LEU:HB3	2:H:100:LEU:HD11	1.86	0.56
2:H:232:GLN:NE2	7:H:1780:HPA:H2	2.20	0.56
2:B:221:MET:HE2	2:B:486:THR:HB	1.87	0.56
2:D:459:PHE:HB2	2:D:465:ASN:ND2	2.21	0.56
2:H:170:GLY:N	2:H:271:ASP:HB3	2.21	0.56
2:D:76:ALA:HA	2:D:205:LYS:HD2	1.87	0.56
1:E:8:ASN:HA	1:E:76:ARG:HD2	1.86	0.56
1:E:427:ASP:OD1	1:E:435:ARG:NH2	2.39	0.56
2:H:46:ALA:HB2	2:H:123:ARG:HH21	1.71	0.56
2:F:417:LEU:HD21	2:F:648:LEU:O	2.06	0.55
2:F:163:GLU:HG2	2:F:277:ARG:HG2	1.88	0.55
2:F:573:VAL:HB	2:F:585:ILE:HG13	1.88	0.55
1:C:305:LEU:HD21	1:C:307:LEU:HD21	1.89	0.55
2:F:77:SER:HB2	2:F:83:GLU:HB3	1.87	0.55
1:G:299:ILE:HG13	1:G:318:LEU:HD23	1.88	0.55
2:B:28:CYS:HB2	2:B:29:PRO:HD2	1.89	0.55
2:B:51:ASP:HB3	2:B:117:ARG:HB3	1.88	0.55
2:D:309:ASP:CG	2:D:611:ARG:HE	2.14	0.55
2:D:35:LEU:HA	2:D:101:VAL:O	2.07	0.55
2:B:148:ARG:HD2	2:B:404:HIS:HA	1.89	0.55
2:F:9:HIS:ND1	2:F:491:GLY:HA2	2.21	0.55
1:A:233:GLN:HG3	1:A:235:ARG:HH22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:ASP:O	2:B:266:THR:CG2	2.55	0.55
1:E:228:CYS:HB3	1:E:231:LEU:HB2	1.89	0.55
2:F:224:MET:CE	2:F:488:MET:HB3	2.35	0.55
2:B:151:VAL:HG11	2:B:290:ASP:HB2	1.89	0.55
2:B:560:GLY:O	2:B:561:CYS:HB3	2.07	0.55
2:F:720:GLU:HG3	2:F:724:ARG:NH2	2.22	0.55
2:F:94:VAL:HG11	2:F:687:ARG:HG2	1.88	0.54
2:D:148:ARG:HD2	2:D:404:HIS:HA	1.89	0.54
2:D:221:MET:HE2	2:D:486:THR:HB	1.88	0.54
2:F:210:LEU:HD22	2:F:247:ARG:HD3	1.88	0.54
5:H:1778:XAX:S3	5:H:1778:XAX:O1	2.65	0.54
1:C:249:ILE:CG2	1:C:267:LEU:HD22	2.34	0.54
2:F:270:HIS:CD2	2:F:297:CYS:HA	2.43	0.54
2:H:58:SER:HB2	2:H:115:LYS:HD2	1.89	0.54
2:B:197:GLN:HG3	2:B:231:LYS:HB2	1.88	0.54
2:B:277:ARG:HB2	2:B:290:ASP:HB3	1.90	0.54
1:E:200:THR:HB	1:E:222:VAL:HG12	1.89	0.54
2:H:35:LEU:HA	2:H:101:VAL:O	2.07	0.54
2:B:517:ASP:HB3	2:B:520:LYS:HB2	1.89	0.54
2:H:665:GLU:O	2:H:669:VAL:HG23	2.08	0.54
2:B:194:CYS:O	2:B:221:MET:HG2	2.07	0.54
2:D:138:ARG:HA	2:D:332:ARG:H	1.72	0.54
2:D:169:GLY:HA3	2:D:760:PRO:HD3	1.89	0.54
1:E:307:LEU:HB2	1:E:314:ARG:HB2	1.88	0.54
2:F:162:ALA:HB1	2:F:359:HIS:CD2	2.43	0.54
5:B:1778:XAX:S3	5:B:1778:XAX:O2	2.66	0.54
2:B:417:LEU:HG	2:B:648:LEU:HD23	1.90	0.54
1:C:370:LEU:HD22	1:C:380:ALA:HA	1.90	0.54
2:F:174:PHE:HZ	2:F:693:PRO:HB3	1.73	0.54
1:G:371:THR:OG1	1:G:379:THR:HB	2.07	0.54
1:G:444:LEU:O	1:G:448:ARG:HG3	2.07	0.54
2:H:586:VAL:HG13	2:H:596:LEU:HD22	1.90	0.54
1:G:134:CYS:SG	1:G:137:THR:HG23	2.48	0.53
2:H:370:GLU:HA	2:H:370:GLU:OE2	2.08	0.53
2:B:129:LEU:H	2:B:129:LEU:CD1	2.20	0.53
5:D:1778:XAX:S3	5:D:1778:XAX:O2	2.66	0.53
1:G:70:ILE:HA	1:G:73:LYS:HG3	1.90	0.53
2:D:177:GLU:HB3	2:D:225:GLY:HA3	1.90	0.53
2:D:310:ARG:HD2	2:D:344:PHE:HD2	1.73	0.53
2:D:627:ALA:HB2	2:D:735:LEU:HD22	1.90	0.53
2:H:166:PHE:CZ	2:H:355:ARG:HG3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:184:LEU:HD23	2:D:252:PRO:HB3	1.91	0.53
2:D:288:GLY:HA2	2:D:323:ALA:O	2.07	0.53
2:D:468:GLY:HA2	2:D:600:GLY:O	2.08	0.53
2:D:556:ALA:HB2	2:D:563:ALA:HA	1.89	0.53
2:H:580:TRP:HB3	2:H:584:GLU:HB2	1.89	0.53
1:A:290:PRO:HA	1:A:391:PRO:HD3	1.91	0.53
2:D:457:ILE:O	2:D:458:SER:HB2	2.08	0.53
1:E:405:ASP:HB3	1:E:407:ARG:HG2	1.89	0.53
2:F:321:VAL:HB	2:F:324:LEU:HD12	1.91	0.53
1:G:207:ASP:HB2	4:G:1465:FAD:H52A	1.90	0.53
1:A:200:THR:HG21	1:A:219:LEU:HD13	1.91	0.53
2:F:698:ILE:HD13	2:F:698:ILE:H	1.73	0.53
1:G:234:ILE:HD13	1:G:243:ILE:HG13	1.91	0.53
2:H:2:SER:HB3	2:H:498:GLN:O	2.08	0.53
2:D:143:PRO:HB3	2:D:329:HIS:ND1	2.24	0.53
2:D:171:GLN:O	2:D:268:LYS:HB3	2.09	0.53
2:H:547:LEU:HD23	2:H:550:ARG:HH11	1.74	0.53
2:B:771:ARG:HG3	2:B:776:ARG:HB2	1.89	0.53
2:D:771:ARG:NH2	2:D:777:ALA:HB2	2.24	0.53
1:G:111:ILE:HD11	2:H:16:VAL:HG22	1.91	0.53
2:D:23:LEU:CD2	2:D:180:ALA:HB1	2.39	0.52
1:G:441:ALA:HB1	2:H:636:LEU:HB3	1.91	0.52
1:G:460:VAL:HG11	2:H:632:VAL:HG11	1.91	0.52
2:H:461:LEU:HB2	2:H:464:LEU:HD12	1.89	0.52
2:B:228:PHE:O	2:B:341:PHE:HA	2.09	0.52
2:F:78:PRO:HG3	2:F:233:SER:HB2	1.91	0.52
2:F:146:TRP:CZ3	2:F:312:MET:HB3	2.44	0.52
2:F:218:ARG:NH2	2:F:517:ASP:OD1	2.43	0.52
2:B:23:LEU:HD13	2:B:194:CYS:HA	1.91	0.52
2:F:221:MET:HE2	2:F:486:THR:HB	1.92	0.52
1:G:206:THR:HG21	1:G:275:VAL:HG13	1.91	0.52
1:C:316:MET:HG3	1:C:320:ASP:HB2	1.92	0.52
2:B:218:ARG:CD	8:B:2004:HOH:O	2.58	0.52
2:D:128:THR:HG23	2:D:131:GLN:H	1.74	0.52
2:D:720:GLU:HG3	2:D:724:ARG:NH2	2.24	0.52
1:E:390:VAL:HG22	1:E:391:PRO:HD2	1.91	0.52
2:F:174:PHE:CZ	2:F:693:PRO:HB3	2.45	0.52
2:B:341:PHE:O	2:B:342:ARG:C	2.52	0.52
2:F:65:PHE:HB2	2:F:100:LEU:HB3	1.92	0.52
2:B:421:LEU:HD13	2:B:648:LEU:HB2	1.92	0.51
2:D:641:ARG:HH21	2:D:706:ARG:HH21	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:171:GLN:O	2:F:268:LYS:HB3	2.10	0.51
2:F:398:LYS:N	2:F:398:LYS:HE3	2.24	0.51
1:A:43:ASP:OD2	2:B:693:PRO:HG2	2.10	0.51
1:E:200:THR:HG21	1:E:219:LEU:HD13	1.92	0.51
1:G:164:PHE:O	1:G:165:THR:HG22	2.10	0.51
1:C:314:ARG:HD3	1:C:334:GLU:OE1	2.11	0.51
2:H:11:SER:HB2	2:H:14:ALA:HB3	1.93	0.51
2:H:232:GLN:HE22	7:H:1780:HPA:C2	2.22	0.51
1:C:120:ARG:O	1:C:121:ASP:C	2.53	0.51
1:E:32:LEU:HD12	1:E:79:GLU:HG3	1.92	0.51
1:E:111:ILE:HA	1:E:114:MET:HE3	1.93	0.51
2:F:21:ARG:HD3	2:F:26:LEU:HD23	1.93	0.51
2:H:473:ILE:HB	2:H:596:LEU:HB3	1.91	0.51
2:H:617:ARG:HD3	2:H:619:PHE:O	2.11	0.51
1:C:144:ARG:NH2	2:D:665:GLU:OE2	2.41	0.51
1:G:351:TYR:CE2	1:G:445:ARG:HD3	2.46	0.51
2:H:40:SER:HB2	2:H:91:VAL:HG11	1.93	0.51
2:D:762:THR:HB	2:D:763:PRO:HD2	1.93	0.51
2:F:192:ILE:HB	2:F:219:VAL:HG22	1.92	0.51
2:H:417:LEU:HD21	2:H:648:LEU:O	2.10	0.51
2:F:227:GLY:HA2	2:F:231:LYS:HG3	1.93	0.51
1:C:140:ALA:O	1:C:144:ARG:HG3	2.11	0.51
2:D:399:LYS:C	2:D:399:LYS:HD2	2.36	0.51
1:E:53:ASP:HB3	1:E:73:LYS:HD3	1.93	0.51
1:G:201:LEU:HD12	1:G:330:ARG:HH22	1.75	0.51
2:B:586:VAL:HG13	2:B:596:LEU:CD2	2.41	0.51
1:C:216:LEU:HD13	2:D:111:ILE:HG12	1.92	0.51
1:C:351:TYR:CE2	1:C:445:ARG:HD3	2.46	0.51
2:D:443:THR:HG23	2:D:636:LEU:CD1	2.38	0.51
2:F:151:VAL:HG11	2:F:290:ASP:HB2	1.91	0.51
1:C:95:MET:SD	1:C:114:MET:HE1	2.52	0.50
2:D:182:LEU:HD13	2:D:254:LYS:HB2	1.92	0.50
2:D:457:ILE:O	2:D:458:SER:CB	2.59	0.50
2:F:730:GLU:H	2:F:731:PRO:HD2	1.76	0.50
2:B:226:GLY:O	2:B:231:LYS:HE3	2.10	0.50
2:B:627:ALA:HB2	2:B:735:LEU:HD22	1.91	0.50
1:C:43:ASP:HB3	2:D:693:PRO:HB2	1.92	0.50
1:C:70:ILE:HA	1:C:73:LYS:HG3	1.93	0.50
1:E:302:GLY:HA2	1:E:381:ARG:NH1	2.27	0.50
1:G:122:ARG:HB3	1:G:128:LEU:HD21	1.92	0.50
1:A:111:ILE:HD11	2:B:16:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:THR:O	1:G:112:VAL:HB	2.11	0.50
2:H:13:ARG:HH11	2:H:13:ARG:CG	2.22	0.50
2:H:412:CYS:HA	2:H:624:TYR:CZ	2.47	0.50
2:B:604:THR:HB	2:B:607:LEU:HD11	1.94	0.50
2:D:360:LEU:HG	2:D:364:MET:CE	2.41	0.50
1:G:52:ARG:HB3	1:G:74:ALA:HB3	1.93	0.50
1:A:183:PRO:HD2	1:A:224:PHE:O	2.11	0.50
1:A:316:MET:HE2	1:A:320:ASP:HB3	1.92	0.50
1:G:368:LEU:HG	1:G:382:ILE:HG23	1.93	0.50
2:B:315:ALA:O	2:B:353:MET:HE2	2.12	0.50
2:D:551:LEU:HD22	2:D:585:ILE:HG22	1.94	0.50
1:G:394:ALA:O	1:G:398:GLU:HB2	2.11	0.50
2:B:132:ALA:HA	2:B:137:SER:HB3	1.93	0.50
1:E:302:GLY:CA	1:E:381:ARG:HH11	2.25	0.50
2:F:249:THR:C	2:F:251:ARG:H	2.19	0.50
2:F:647:ILE:HB	2:F:710:VAL:HG22	1.94	0.50
2:H:341:PHE:O	2:H:342:ARG:C	2.54	0.50
2:B:499:VAL:O	2:B:503:VAL:HG23	2.12	0.50
2:F:551:LEU:HD22	2:F:585:ILE:HG22	1.94	0.50
2:B:473:ILE:HB	2:B:596:LEU:HB3	1.94	0.49
2:F:418:VAL:HG13	2:F:450:LEU:HD11	1.93	0.49
2:B:633:ILE:HG12	2:B:746:ALA:HB1	1.94	0.49
2:D:9:HIS:CD2	2:D:11:SER:H	2.30	0.49
2:D:171:GLN:NE2	2:D:674:TRP:HB2	2.26	0.49
2:H:171:GLN:O	2:H:268:LYS:HB3	2.12	0.49
2:F:11:SER:HB2	2:F:14:ALA:HB3	1.94	0.49
2:F:412:CYS:HA	2:F:624:TYR:CZ	2.47	0.49
1:A:8:ASN:HA	1:A:76:ARG:HD2	1.95	0.49
2:B:78:PRO:HG3	2:B:233:SER:HB2	1.94	0.49
1:C:66:MET:HG3	1:C:224:PHE:HE2	1.77	0.49
2:D:210:LEU:HB3	2:D:212:LEU:HD21	1.93	0.49
1:E:90:PRO:HB3	1:E:152:GLU:HB2	1.95	0.49
1:E:368:LEU:HG	1:E:382:ILE:HG23	1.94	0.49
2:F:380:PRO:HD3	2:F:412:CYS:O	2.12	0.49
1:G:433:ALA:O	1:G:437:ASN:HB2	2.12	0.49
2:H:158:ALA:HA	2:H:287:LEU:HD22	1.93	0.49
2:H:407:GLN:OE1	2:H:618:PRO:HD2	2.13	0.49
1:C:302:GLY:HA2	1:C:381:ARG:HH11	1.76	0.49
1:G:431:SER:OG	2:H:764:GLU:OE1	2.28	0.49
1:C:211:TRP:HA	1:C:215:ALA:HB3	1.95	0.49
5:D:1778:XAX:S3	5:D:1778:XAX:O1	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:302:GLY:HA2	1:E:381:ARG:HH11	1.78	0.49
1:A:436:MET:HE3	1:A:436:MET:O	2.13	0.48
2:B:174:PHE:HZ	2:B:693:PRO:HB3	1.78	0.48
1:E:430:ALA:HB1	1:E:434:TYR:HD2	1.78	0.48
2:H:166:PHE:HB3	2:H:355:ARG:NH2	2.28	0.48
1:A:206:THR:OG1	4:A:1465:FAD:O1P	2.28	0.48
1:C:354:SER:HB3	1:C:362:SER:HA	1.94	0.48
1:E:354:SER:HB2	1:E:360:ASP:OD2	2.13	0.48
5:F:1778:XAX:S3	5:F:1778:XAX:O2	2.71	0.48
2:H:267:GLY:HA2	2:H:268:LYS:HE2	1.96	0.48
2:F:172:GLU:HB3	2:F:696:TYR:CZ	2.49	0.48
2:B:171:GLN:NE2	2:B:674:TRP:HB2	2.29	0.48
2:B:417:LEU:HD21	2:B:648:LEU:O	2.13	0.48
2:D:310:ARG:NH2	2:D:619:PHE:HE2	2.11	0.48
2:D:85:VAL:HG21	2:D:240:ILE:HG21	1.94	0.48
2:D:128:THR:HG22	2:D:131:GLN:CD	2.39	0.48
2:D:278:ILE:HD11	2:D:286:LEU:HD22	1.95	0.48
2:F:23:LEU:CD2	2:F:180:ALA:HB1	2.42	0.48
1:G:299:ILE:O	1:G:381:ARG:NH1	2.39	0.48
1:G:388:ALA:C	1:G:390:VAL:H	2.21	0.48
2:H:221:MET:HE2	2:H:486:THR:HB	1.95	0.48
2:B:698:ILE:HB	2:B:699:PRO:HD2	1.96	0.48
2:D:110:ARG:HH22	2:D:260:ASP:HB2	1.78	0.48
2:D:482:ASN:ND2	2:D:514:THR:HB	2.29	0.48
4:A:1465:FAD:N1	4:A:1465:FAD:H2'	2.29	0.48
2:B:148:ARG:O	2:B:323:ALA:HA	2.14	0.48
1:C:8:ASN:HA	1:C:76:ARG:HD2	1.96	0.48
2:D:531:SER:HB2	2:D:535:MET:HG3	1.96	0.48
1:A:50:MET:CE	1:A:57:SER:HB2	2.44	0.48
1:C:66:MET:HE2	1:C:202:ILE:HD13	1.94	0.48
1:E:300:ALA:HB2	1:E:367:CYS:HB3	1.95	0.48
2:H:547:LEU:HD23	2:H:550:ARG:HD3	1.95	0.48
2:H:673:GLY:O	2:H:678:GLU:HB2	2.14	0.48
2:D:144:VAL:HG11	2:D:312:MET:HE1	1.96	0.48
2:D:641:ARG:NH2	2:D:706:ARG:HE	2.12	0.48
1:E:42:GLY:HA3	1:E:64:LEU:HD11	1.95	0.48
2:F:46:ALA:HB2	2:F:123:ARG:NH2	2.29	0.48
2:F:138:ARG:HD3	2:F:142:GLY:N	2.16	0.48
2:H:497:VAL:HG13	2:H:511:VAL:HB	1.96	0.48
2:B:448:ILE:HA	2:B:629:THR:O	2.14	0.48
2:H:762:THR:HB	2:H:763:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:SER:N	2:F:574:GLN:HE22	2.12	0.47
2:B:530:SER:O	2:B:727:ALA:HB1	2.13	0.47
1:C:50:MET:HE3	1:C:57:SER:HB2	1.96	0.47
2:D:292:VAL:HG22	2:D:327:GLU:HB3	1.96	0.47
2:H:76:ALA:HA	2:H:205:LYS:HD2	1.95	0.47
2:D:481:LEU:HD11	2:D:540:VAL:HG22	1.95	0.47
1:G:245:ALA:HB2	1:G:336:VAL:HG12	1.96	0.47
1:G:346:PRO:O	1:G:349:ARG:NH2	2.46	0.47
2:H:631:VAL:HG12	2:H:642:ILE:HA	1.95	0.47
1:E:237:THR:OG1	1:E:238:PRO:CD	2.57	0.47
1:E:322:PHE:HB3	1:E:390:VAL:CG2	2.44	0.47
2:F:635:ARG:NH1	2:F:774:GLU:OE2	2.47	0.47
2:B:94:VAL:HG11	2:B:687:ARG:HG2	1.96	0.47
2:B:567:ILE:HG13	2:B:574:GLN:HB2	1.94	0.47
1:C:41:GLU:HA	1:C:210:LEU:HD21	1.95	0.47
1:C:127:ASP:OD1	1:C:268:ARG:HD3	2.14	0.47
2:D:306:PRO:HB2	2:D:344:PHE:CZ	2.50	0.47
2:F:85:VAL:HG21	2:F:240:ILE:HG21	1.96	0.47
1:G:26:TRP:CD1	1:G:67:LEU:HD11	2.49	0.47
1:G:445:ARG:HG3	1:G:455:VAL:HG11	1.96	0.47
1:G:113:SER:HB2	1:G:132:ASN:HD21	1.79	0.47
2:H:28:CYS:HB2	2:H:29:PRO:HD2	1.95	0.47
2:H:179:GLN:HB2	2:H:257:TYR:CD1	2.49	0.47
2:H:380:PRO:O	2:H:381:GLU:CB	2.61	0.47
1:A:347:GLY:O	1:A:446:TYR:OH	2.23	0.47
2:H:22:TYR:O	2:H:25:ASP:HB2	2.14	0.47
2:H:70:LEU:HD22	2:H:244:VAL:HG11	1.97	0.47
2:B:34:HIS:HD2	2:B:105:SER:HA	1.80	0.47
1:C:38:GLY:O	1:C:39:CYS:HB3	2.14	0.47
1:G:66:MET:HG3	1:G:224:PHE:HE2	1.79	0.47
1:G:316:MET:HE2	1:G:320:ASP:HB2	1.97	0.47
2:H:201:GLU:HG2	2:H:236:ASN:HD21	1.80	0.47
2:H:300:SER:HB2	2:H:337:SER:HB2	1.97	0.47
2:H:460:THR:OG1	7:H:1780:HPA:H8	2.14	0.47
1:C:42:GLY:HA3	1:C:64:LEU:HD11	1.95	0.47
1:E:70:ILE:HA	1:E:73:LYS:HG3	1.96	0.47
1:E:245:ALA:HB1	1:E:282:GLY:HA3	1.97	0.47
2:F:9:HIS:O	2:F:10:ASP:C	2.58	0.47
2:F:316:ASP:HB3	2:F:404:HIS:ND1	2.29	0.47
2:F:473:ILE:HG12	2:F:479:VAL:HG12	1.96	0.47
1:G:108:PRO:O	1:G:112:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:605:PRO:HB2	2:H:606:LYS:HG3	1.97	0.47
2:B:501:ALA:HB1	2:B:506:ILE:O	2.15	0.47
5:B:1778:XAX:S3	5:B:1778:XAX:O1	2.72	0.47
1:C:35:THR:CG2	1:C:47:CYS:HB2	2.45	0.47
1:E:401:LEU:O	1:E:404:GLN:HB2	2.15	0.47
1:G:228:CYS:HB3	1:G:231:LEU:HB2	1.97	0.47
2:D:606:LYS:O	2:D:617:ARG:HD2	2.14	0.47
2:H:448:ILE:HA	2:H:629:THR:O	2.15	0.47
1:A:252:LEU:HD23	1:A:267:LEU:HD11	1.96	0.46
2:D:551:LEU:O	2:D:555:VAL:HG23	2.16	0.46
1:G:45:GLY:N	3:G:1464:FES:S2	2.87	0.46
1:G:155:ALA:HB3	1:G:158:LEU:HD12	1.97	0.46
1:A:49:VAL:HA	1:A:112:VAL:HG11	1.97	0.46
1:C:225:LEU:C	1:C:227:HIS:H	2.24	0.46
2:D:196:SER:O	2:D:221:MET:HG3	2.14	0.46
2:D:312:MET:HE2	2:D:330:ARG:HH12	1.80	0.46
1:E:370:LEU:HD23	1:E:380:ALA:HA	1.98	0.46
2:H:35:LEU:HD11	2:H:242:CYS:HA	1.97	0.46
2:H:105:SER:OG	2:H:108:ALA:HB2	2.15	0.46
2:H:303:LEU:O	2:H:307:VAL:HG23	2.15	0.46
2:B:185:PRO:HG3	2:B:246:ALA:HB1	1.97	0.46
1:G:347:GLY:O	1:G:446:TYR:OH	2.26	0.46
2:B:351:LEU:HD13	2:B:737:ILE:HG12	1.97	0.46
2:D:412:CYS:HA	2:D:624:TYR:CZ	2.50	0.46
1:G:352:LYS:HE3	1:G:362:SER:HB3	1.98	0.46
1:G:427:ASP:OD1	1:G:435:ARG:NH2	2.48	0.46
1:A:249:ILE:HG23	1:A:267:LEU:HD22	1.96	0.46
1:A:418:LEU:HB3	1:A:436:MET:HE1	1.98	0.46
4:A:1465:FAD:H9	4:A:1465:FAD:H1'2	1.84	0.46
2:B:520:LYS:HE2	2:D:520:LYS:HD2	1.98	0.46
2:F:14:ALA:HA	2:F:19:GLN:HB2	1.98	0.46
2:F:635:ARG:HD3	2:F:750:CYS:SG	2.56	0.46
2:H:249:THR:C	2:H:251:ARG:H	2.24	0.46
1:G:250:ALA:HB2	1:G:276:ARG:HB3	1.98	0.46
2:D:547:LEU:HD21	2:D:596:LEU:C	2.39	0.46
2:F:266:THR:O	2:F:268:LYS:HE2	2.15	0.46
1:A:95:MET:SD	1:A:114:MET:HE1	2.56	0.46
1:E:24:LEU:CD1	1:E:63:CYS:HB3	2.46	0.46
1:E:110:PHE:HB3	1:E:114:MET:HE2	1.97	0.46
1:G:11:THR:HG22	1:G:164:PHE:HE1	1.81	0.46
2:D:166:PHE:CZ	2:D:168:ILE:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:488:MET:CE	5:D:1778:XAX:H4'	2.46	0.46
1:E:377:ILE:HD13	1:E:401:LEU:HG	1.98	0.46
1:A:113:SER:HB2	1:A:132:ASN:HD21	1.79	0.45
2:B:215:HIS:ND1	2:D:478:SER:HB2	2.31	0.45
2:B:233:SER:C	2:B:235:GLY:H	2.24	0.45
2:B:240:ILE:O	2:B:244:VAL:HG23	2.16	0.45
2:D:267:GLY:HA2	2:D:336:GLN:HB3	1.97	0.45
1:G:136:CYS:HB3	2:H:228:PHE:CZ	2.51	0.45
2:B:169:GLY:C	2:B:271:ASP:HB3	2.42	0.45
2:D:473:ILE:HG23	2:D:479:VAL:HG12	1.98	0.45
1:G:211:TRP:HA	1:G:215:ALA:HB3	1.98	0.45
2:B:158:ALA:HA	2:B:287:LEU:HD22	1.97	0.45
2:D:31:ASN:ND2	2:D:252:PRO:CD	2.80	0.45
5:F:1778:XAX:O1	5:F:1778:XAX:S3	2.75	0.45
1:A:41:GLU:HA	1:A:210:LEU:HD21	1.99	0.45
1:A:370:LEU:HA	1:A:379:THR:O	2.16	0.45
2:B:647:ILE:HD12	2:B:710:VAL:HG22	1.98	0.45
2:D:262:ASP:O	2:D:266:THR:CG2	2.63	0.45
1:E:366:GLY:HA3	1:E:442:MET:SD	2.57	0.45
2:B:274:ILE:HG12	2:B:293:HIS:HD2	1.81	0.45
1:E:206:THR:HG21	1:E:275:VAL:HG13	1.98	0.45
2:F:341:PHE:O	2:F:342:ARG:C	2.59	0.45
2:H:288:GLY:HA2	2:H:323:ALA:O	2.17	0.45
2:B:23:LEU:HA	2:B:26:LEU:HD12	1.97	0.45
2:B:366:ARG:HH11	2:B:366:ARG:HB3	1.82	0.45
2:B:482:ASN:HD22	2:B:514:THR:HB	1.82	0.45
2:B:551:LEU:O	2:B:555:VAL:HG23	2.16	0.45
2:B:595:SER:HB2	2:D:601:PHE:CG	2.52	0.45
2:H:174:PHE:CZ	2:H:693:PRO:HB3	2.52	0.45
2:H:621:TYR:HE1	2:H:726:LYS:HG2	1.81	0.45
2:F:599:THR:HG23	2:H:599:THR:HG23	1.98	0.45
1:G:113:SER:CB	1:G:132:ASN:HD21	2.30	0.45
2:H:517:ASP:HB3	2:H:520:LYS:HB2	1.99	0.45
2:B:172:GLU:HG2	2:B:263:MET:HE2	1.99	0.45
2:F:9:HIS:CD2	2:F:15:HIS:CE1	2.99	0.45
2:F:182:LEU:HD13	2:F:254:LYS:HB2	1.98	0.45
2:F:641:ARG:HH22	2:F:706:ARG:HD3	1.79	0.45
2:H:224:MET:HE3	2:H:488:MET:HG2	1.98	0.45
2:H:460:THR:N	7:H:1780:HPA:H8	2.31	0.45
2:H:650:ASP:HA	2:H:713:TRP:HB3	1.99	0.45
1:E:50:MET:CE	1:E:57:SER:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:267:GLY:HA3	2:F:337:SER:O	2.17	0.45
2:F:538:MET:HE3	2:F:602:TYR:CE1	2.52	0.45
2:F:631:VAL:HG12	2:F:642:ILE:HA	1.98	0.45
1:G:330:ARG:HH21	4:G:1465:FAD:H2A	1.82	0.45
2:H:281:ASP:HB3	2:H:287:LEU:HD11	1.97	0.45
2:H:635:ARG:HH11	2:H:750:CYS:HB3	1.82	0.45
2:F:166:PHE:CZ	2:F:355:ARG:HG3	2.51	0.45
2:H:556:ALA:HB1	2:H:561:CYS:O	2.17	0.45
1:A:211:TRP:HA	1:A:215:ALA:HB3	1.99	0.44
1:A:388:ALA:O	1:A:390:VAL:N	2.36	0.44
2:B:288:GLY:HA2	2:B:321:VAL:HG13	1.99	0.44
2:D:74:ASN:ND2	2:D:88:THR:HG23	2.32	0.44
2:D:341:PHE:HE2	2:D:670:GLN:HE22	1.65	0.44
2:D:343:GLY:H	2:D:730:GLU:HG2	1.82	0.44
1:G:61:ASN:ND2	1:G:61:ASN:H	2.15	0.44
1:G:66:MET:O	1:G:69:GLN:HB2	2.17	0.44
5:H:1778:XAX:S3	5:H:1778:XAX:O2	2.75	0.44
1:A:181:PHE:O	1:A:223:ALA:HA	2.17	0.44
1:C:1:MET:CE	1:C:16:ILE:HG13	2.47	0.44
1:E:309:ARG:HB2	1:E:334:GLU:HG2	1.99	0.44
2:F:278:ILE:HD11	2:F:286:LEU:HD22	1.98	0.44
2:F:485:GLY:HA3	2:F:492:LEU:HD21	1.98	0.44
1:A:66:MET:H	1:A:66:MET:HG2	1.65	0.44
2:B:478:SER:HB2	2:D:215:HIS:ND1	2.32	0.44
4:C:1465:FAD:H9	4:C:1465:FAD:H1'2	1.76	0.44
2:D:92:HIS:HB2	2:D:299:TRP:CE3	2.52	0.44
2:D:649:HIS:CE1	2:D:731:PRO:HB2	2.53	0.44
1:G:134:CYS:SG	1:G:137:THR:CG2	3.06	0.44
1:A:425:LEU:HG	2:F:579:SER:HB2	1.99	0.44
2:B:38:GLY:HA3	2:B:99:PHE:CE2	2.53	0.44
2:F:144:VAL:CG2	2:F:330:ARG:NH1	2.77	0.44
2:F:306:PRO:HB2	2:F:344:PHE:CZ	2.52	0.44
2:H:319:TYR:HA	2:H:375:ASN:O	2.18	0.44
2:H:650:ASP:OD2	2:H:726:LYS:NZ	2.41	0.44
2:B:222:ARG:HD2	2:B:222:ARG:HA	1.82	0.44
2:B:556:ALA:HB1	2:B:561:CYS:O	2.18	0.44
2:D:303:LEU:O	2:D:307:VAL:HG23	2.18	0.44
2:D:635:ARG:NH1	2:D:750:CYS:HB3	2.32	0.44
1:E:66:MET:HE3	1:E:202:ILE:HG21	1.99	0.44
2:F:373:ALA:HA	2:F:376:PHE:CE1	2.52	0.44
2:H:92:HIS:HB2	2:H:299:TRP:HE3	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:164:GLY:HA3	2:H:276:TYR:CZ	2.53	0.44
1:A:8:ASN:OD1	1:A:76:ARG:HA	2.17	0.44
1:A:64:LEU:HD13	1:A:206:THR:HG22	1.99	0.44
1:A:253:ARG:HH21	1:A:268:ARG:HG3	1.83	0.44
2:D:173:HIS:HA	2:D:341:PHE:CZ	2.53	0.44
1:A:240:GLY:HA2	1:A:343:LYS:HG2	1.99	0.44
2:F:35:LEU:HB3	2:F:100:LEU:HD11	1.99	0.44
2:F:446:ARG:HD3	2:F:630:GLU:OE2	2.18	0.44
1:G:36:LYS:HB3	1:G:105:PHE:CZ	2.52	0.44
1:G:110:PHE:HB3	1:G:114:MET:HE2	1.99	0.44
1:G:318:LEU:O	1:G:321:PHE:HB3	2.18	0.44
2:H:305:LEU:HB3	2:H:306:PRO:CD	2.48	0.44
1:A:245:ALA:HB1	1:A:282:GLY:HA3	1.99	0.44
2:B:35:LEU:HD11	2:B:242:CYS:HA	2.00	0.44
2:B:195:SER:O	2:B:231:LYS:HD2	2.17	0.44
1:E:182:LEU:HG	1:E:224:PHE:HB2	2.00	0.44
1:G:284:ASN:OD1	1:G:295:PRO:HD3	2.18	0.44
2:H:7:LEU:HB3	2:H:8:PRO:CD	2.47	0.44
2:H:29:PRO:HG2	2:H:252:PRO:HG3	1.99	0.44
2:D:266:THR:O	2:D:268:LYS:HE2	2.18	0.43
2:D:528:ALA:HA	5:D:1778:XAX:S2'	2.58	0.43
2:D:755:PRO:O	2:D:772:ARG:HD2	2.18	0.43
1:G:149:ALA:O	1:G:152:GLU:HB2	2.18	0.43
2:H:700:ALA:O	2:H:701:PHE:C	2.60	0.43
2:B:656:ASN:HB3	2:B:659:LEU:HB2	2.00	0.43
1:C:24:LEU:HD12	1:C:63:CYS:HB3	2.01	0.43
1:C:291:ILE:H	1:C:291:ILE:HG12	1.69	0.43
1:E:127:ASP:OD2	1:E:268:ARG:HD3	2.18	0.43
2:H:29:PRO:C	2:H:31:ASN:H	2.26	0.43
2:B:126:ILE:HG22	2:B:333:THR:HG22	1.99	0.43
2:D:192:ILE:HB	2:D:219:VAL:HG22	2.00	0.43
2:H:194:CYS:O	2:H:221:MET:HG2	2.17	0.43
2:H:222:ARG:HD2	2:H:515:ALA:HA	2.01	0.43
2:D:31:ASN:ND2	2:D:252:PRO:HD3	2.34	0.43
1:G:8:ASN:OD1	1:G:80:GLY:HA3	2.18	0.43
1:G:50:MET:HE3	1:G:57:SER:HB2	1.99	0.43
1:G:110:PHE:C	1:G:114:MET:HE2	2.44	0.43
1:C:102:GLN:HB2	1:C:136:CYS:HB3	2.00	0.43
2:D:272:PHE:CD2	2:D:348:GLN:HG2	2.54	0.43
1:E:225:LEU:C	1:E:227:HIS:H	2.27	0.43
4:E:1465:FAD:H2'	4:E:1465:FAD:N1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:GLU:O	1:A:198:GLU:HG3	2.17	0.43
1:C:364:VAL:HG21	1:C:438:ALA:HB3	1.98	0.43
2:D:648:LEU:HA	2:D:711:ALA:O	2.18	0.43
1:E:407:ARG:O	1:E:411:ILE:HG12	2.18	0.43
1:G:109:GLY:O	1:G:113:SER:HB2	2.19	0.43
2:H:278:ILE:HG23	2:H:360:LEU:HD13	2.00	0.43
1:A:102:GLN:O	2:B:489:GLY:HA2	2.18	0.43
2:D:9:HIS:HD2	2:D:11:SER:H	1.66	0.43
1:E:78:ILE:HD13	1:E:108:PRO:HA	2.00	0.43
2:F:261:ASP:HB3	2:F:265:ILE:CD1	2.48	0.43
1:G:181:PHE:O	1:G:223:ALA:HA	2.17	0.43
1:G:279:ALA:HB1	4:G:1465:FAD:H4'	1.99	0.43
2:H:94:VAL:HG11	2:H:687:ARG:HG2	2.01	0.43
2:D:656:ASN:HA	2:D:657:PRO:HD2	1.90	0.43
2:F:53:GLU:HB3	2:F:54:PRO:HD3	2.00	0.43
2:F:641:ARG:HH21	2:F:706:ARG:HD3	1.84	0.43
1:G:240:GLY:HA2	1:G:343:LYS:HG3	2.00	0.43
1:G:298:LEU:HD13	1:G:301:MET:HE3	2.01	0.43
1:G:316:MET:HE2	1:G:320:ASP:CB	2.48	0.43
2:H:270:HIS:CD2	2:H:297:CYS:HA	2.54	0.43
1:A:32:LEU:HD12	1:A:79:GLU:HG3	2.00	0.43
2:B:281:ASP:HB3	2:B:287:LEU:HD11	2.00	0.43
1:C:65:MET:HE1	1:C:278:VAL:HG11	2.01	0.43
1:C:441:ALA:O	2:D:636:LEU:HD23	2.19	0.43
4:C:1465:FAD:N1	4:C:1465:FAD:C2'	2.81	0.43
2:D:631:VAL:HG12	2:D:642:ILE:HA	2.01	0.43
2:D:730:GLU:N	2:D:731:PRO:CD	2.82	0.43
2:F:261:ASP:HB3	2:F:265:ILE:HD12	2.01	0.43
2:F:556:ALA:HB1	2:F:561:CYS:O	2.19	0.43
1:A:299:ILE:O	1:A:381:ARG:NH1	2.45	0.43
2:B:297:CYS:SG	2:B:304:SER:HB3	2.59	0.43
1:C:388:ALA:C	1:C:390:VAL:H	2.26	0.43
2:D:166:PHE:CZ	2:D:355:ARG:HG3	2.54	0.43
2:D:437:TRP:CZ3	2:D:446:ARG:HG3	2.54	0.43
2:F:23:LEU:HD13	2:F:194:CYS:HA	2.01	0.43
1:G:44:CYS:HA	1:G:133:LEU:HG	2.01	0.43
2:H:172:GLU:HG2	2:H:263:MET:HE2	2.00	0.43
1:A:364:VAL:HG22	1:A:435:ARG:HG2	2.00	0.42
2:B:170:GLY:N	2:B:271:ASP:HB3	2.34	0.42
2:B:309:ASP:OD1	2:B:330:ARG:NH2	2.52	0.42
1:C:207:ASP:HB2	4:C:1465:FAD:O1A	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:528:ALA:O	2:F:529:ALA:HB3	2.19	0.42
1:G:307:LEU:HB2	1:G:314:ARG:HB2	2.01	0.42
2:H:450:LEU:HD23	2:H:450:LEU:C	2.44	0.42
1:A:431:SER:OG	2:B:764:GLU:OE1	2.30	0.42
2:B:164:GLY:HA3	2:B:276:TYR:CZ	2.54	0.42
2:B:648:LEU:HD12	2:B:711:ALA:HB3	2.01	0.42
2:D:367:ASP:HA	2:D:368:PRO:HD3	1.90	0.42
1:E:316:MET:HE1	1:E:329:ASP:OD2	2.19	0.42
2:F:631:VAL:HG21	2:F:743:LEU:HA	2.01	0.42
2:H:456:GLY:HA3	2:H:619:PHE:CD1	2.54	0.42
1:A:89:HIS:ND1	1:A:91:VAL:HB	2.35	0.42
1:A:368:LEU:HG	1:A:382:ILE:HG23	2.01	0.42
2:B:519:SER:O	2:D:472:GLN:NE2	2.50	0.42
1:C:1:MET:N	8:C:2001:HOH:O	2.53	0.42
2:D:174:PHE:CE1	2:D:263:MET:HE1	2.54	0.42
1:E:249:ILE:CG2	1:E:267:LEU:HD22	2.42	0.42
2:F:298:GLY:HA3	2:F:337:SER:HA	2.00	0.42
4:G:1465:FAD:H1'2	4:G:1465:FAD:H9	1.77	0.42
2:H:272:PHE:CD2	2:H:348:GLN:HG2	2.54	0.42
2:H:159:ALA:HB3	2:H:281:ASP:HA	2.01	0.42
2:B:420:ARG:HD2	2:B:648:LEU:HD21	2.02	0.42
2:B:422:GLN:NE2	2:B:450:LEU:HD13	2.34	0.42
1:E:24:LEU:HD13	1:E:40:ASN:HD21	1.82	0.42
1:G:443:ALA:O	1:G:447:VAL:HG23	2.18	0.42
1:A:40:ASN:HD22	1:A:213:THR:CG2	2.33	0.42
1:A:415:LEU:N	1:A:416:PRO:CD	2.83	0.42
2:B:22:TYR:CD1	2:B:22:TYR:N	2.88	0.42
2:D:222:ARG:C	2:D:222:ARG:HE	2.26	0.42
1:E:415:LEU:HD21	1:E:443:ALA:HB3	2.02	0.42
2:F:39:LEU:HB3	2:F:95:GLY:HA2	2.01	0.42
2:F:595:SER:HB2	2:H:601:PHE:CG	2.54	0.42
2:B:700:ALA:O	2:B:701:PHE:C	2.63	0.42
1:C:228:CYS:HB3	1:C:231:LEU:HB2	2.01	0.42
2:D:29:PRO:O	2:D:30:ALA:C	2.63	0.42
2:D:170:GLY:N	2:D:271:ASP:HB3	2.34	0.42
2:D:641:ARG:HH21	2:D:706:ARG:HE	1.67	0.42
1:E:122:ARG:HG2	1:E:128:LEU:HD11	2.02	0.42
2:F:437:TRP:HA	2:F:440:THR:HG22	2.00	0.42
2:F:588:ALA:O	2:F:591:MET:HB2	2.20	0.42
1:A:40:ASN:HD22	1:A:213:THR:HG21	1.85	0.42
1:A:78:ILE:HA	1:A:81:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ARG:O	1:A:334:GLU:HA	2.19	0.42
2:B:24:ASP:HA	2:B:254:LYS:NZ	2.35	0.42
2:D:35:LEU:HB2	2:D:255:MET:HE3	2.02	0.42
2:D:179:GLN:NE2	2:D:230:GLY:O	2.53	0.42
2:F:23:LEU:HD11	2:F:182:LEU:HB3	2.02	0.42
2:F:138:ARG:HA	2:F:332:ARG:H	1.84	0.42
2:F:512:ARG:HG3	2:F:513:ILE:N	2.35	0.42
2:F:722:ILE:HG23	2:F:722:ILE:O	2.20	0.42
2:H:146:TRP:CZ3	2:H:313:LEU:HD13	2.54	0.42
2:H:228:PHE:O	2:H:341:PHE:HA	2.20	0.42
2:B:302:ASP:OD1	2:B:303:LEU:N	2.53	0.42
1:C:240:GLY:HA2	1:C:343:LYS:HG2	2.01	0.42
1:E:364:VAL:HG21	1:E:438:ALA:HB3	2.01	0.42
1:G:65:MET:CE	1:G:278:VAL:HG11	2.50	0.42
2:B:684:HIS:HE2	2:F:565:ASP:HA	1.85	0.42
2:D:179:GLN:HE22	2:D:234:GLN:HB2	1.84	0.42
2:D:309:ASP:O	2:D:313:LEU:HB2	2.19	0.42
2:D:721:THR:O	2:D:722:ILE:C	2.63	0.42
2:F:139:PHE:C	2:F:141:GLY:H	2.28	0.42
2:F:468:GLY:HA2	2:F:600:GLY:O	2.20	0.42
2:H:495:LYS:O	2:H:499:VAL:HG23	2.19	0.42
1:A:41:GLU:HA	1:A:210:LEU:CD2	2.50	0.41
1:C:354:SER:O	1:C:355:LYS:C	2.62	0.41
2:D:172:GLU:HB3	2:D:696:TYR:CZ	2.55	0.41
2:F:63:ALA:HB3	2:F:102:ALA:HB3	2.02	0.41
1:G:67:LEU:C	1:G:69:GLN:H	2.28	0.41
2:H:85:VAL:HG21	2:H:240:ILE:HG21	2.01	0.41
2:H:627:ALA:HB2	2:H:735:LEU:HD22	2.02	0.41
2:B:42:GLU:HG2	2:B:45:ALA:HB2	2.01	0.41
2:B:66:THR:HG22	2:B:68:ALA:H	1.85	0.41
1:C:241:TYR:O	1:C:340:THR:HA	2.20	0.41
2:D:110:ARG:HH21	2:D:258:ASP:HB2	1.85	0.41
2:D:270:HIS:CD2	2:D:297:CYS:HA	2.55	0.41
2:D:461:LEU:CD1	7:D:1780:HPA:H8	2.49	0.41
1:E:61:ASN:ND2	1:E:61:ASN:H	2.17	0.41
1:G:183:PRO:HD2	1:G:224:PHE:O	2.19	0.41
2:H:380:PRO:HD3	2:H:412:CYS:O	2.20	0.41
2:D:22:TYR:O	2:D:23:LEU:C	2.62	0.41
2:D:139:PHE:C	2:D:141:GLY:H	2.28	0.41
2:D:146:TRP:CZ3	2:D:312:MET:HB3	2.55	0.41
1:E:291:ILE:HD13	1:E:291:ILE:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:360:LEU:O	2:F:364:MET:HG2	2.20	0.41
2:F:762:THR:O	2:F:763:PRO:C	2.62	0.41
1:G:119:ASP:C	1:G:121:ASP:H	2.28	0.41
1:G:314:ARG:NH1	1:G:334:GLU:OE2	2.53	0.41
2:H:606:LYS:HE3	2:H:617:ARG:HH22	1.86	0.41
1:C:295:PRO:HB2	1:C:296:PRO:HD3	2.01	0.41
2:D:126:ILE:HG21	2:D:132:ALA:HA	2.01	0.41
2:D:766:VAL:O	2:D:770:VAL:HG23	2.19	0.41
2:F:166:PHE:CE1	2:F:355:ARG:HG3	2.56	0.41
2:F:610:ASP:HB3	2:F:613:ARG:HB2	2.01	0.41
1:G:49:VAL:HG23	1:G:60:VAL:HG23	2.01	0.41
2:H:171:GLN:CD	2:H:674:TRP:HB2	2.46	0.41
2:H:560:GLY:O	2:H:561:CYS:CB	2.67	0.41
1:A:387:MET:HE1	1:A:436:MET:HA	2.03	0.41
2:B:564:ARG:H	2:B:564:ARG:HG3	1.65	0.41
1:C:45:GLY:C	1:C:47:CYS:H	2.28	0.41
2:D:310:ARG:HD2	2:D:344:PHE:CD2	2.54	0.41
2:D:373:ALA:HA	2:D:376:PHE:CE1	2.56	0.41
2:F:421:LEU:HD13	2:F:648:LEU:HB2	2.01	0.41
2:H:647:ILE:HD12	2:H:710:VAL:HG22	2.00	0.41
2:B:23:LEU:CD1	2:B:193:HIS:O	2.68	0.41
2:B:407:GLN:OE1	2:B:618:PRO:HD2	2.21	0.41
2:B:534:ASP:OD2	2:B:621:TYR:OH	2.30	0.41
1:C:153:PRO:HA	1:C:154:PRO:HD3	1.96	0.41
1:E:52:ARG:HB3	1:E:74:ALA:HB3	2.03	0.41
1:E:352:LYS:HG3	1:E:362:SER:HB3	2.01	0.41
1:E:352:LYS:HE3	1:E:362:SER:HB3	2.01	0.41
2:H:204:HIS:CD2	2:H:204:HIS:C	2.98	0.41
2:H:414:LEU:HG	2:H:624:TYR:CD2	2.55	0.41
2:H:465:ASN:HB3	2:H:604:THR:HG1	1.82	0.41
2:H:730:GLU:O	2:H:731:PRO:C	2.63	0.41
2:B:53:GLU:HB3	2:B:54:PRO:HD3	2.01	0.41
2:B:266:THR:O	2:B:268:LYS:HE2	2.21	0.41
2:D:177:GLU:CB	2:D:225:GLY:HA3	2.51	0.41
2:D:531:SER:O	2:D:532:GLY:C	2.64	0.41
2:F:175:TYR:HE2	2:F:230:GLY:HA3	1.84	0.41
2:F:450:LEU:HD23	2:F:450:LEU:C	2.46	0.41
2:F:450:LEU:HA	2:F:627:ALA:O	2.21	0.41
1:G:140:ALA:N	1:G:141:PRO:CD	2.84	0.41
1:G:351:TYR:CZ	1:G:445:ARG:HG2	2.56	0.41
2:H:174:PHE:HZ	2:H:693:PRO:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:179:GLN:HB3	2:H:238:LEU:HD11	2.02	0.41
2:H:212:LEU:CD1	2:H:216:ASP:HB3	2.50	0.41
2:H:400:THR:HG21	2:H:410:ALA:HB2	2.02	0.41
2:H:633:ILE:HG12	2:H:746:ALA:HB1	2.03	0.41
1:A:67:LEU:C	1:A:69:GLN:H	2.29	0.41
1:A:111:ILE:HD11	2:B:16:VAL:CG2	2.51	0.41
1:C:53:ASP:OD2	1:C:58:ARG:NH2	2.54	0.41
2:F:499:VAL:O	2:F:503:VAL:HG23	2.21	0.41
1:G:136:CYS:HB3	2:H:228:PHE:HZ	1.84	0.41
2:B:166:PHE:CE1	2:B:355:ARG:HG3	2.55	0.41
2:B:210:LEU:HD11	2:B:243:ALA:HB1	2.01	0.41
2:B:233:SER:O	2:B:235:GLY:N	2.54	0.41
2:B:343:GLY:H	2:B:730:GLU:HG2	1.86	0.41
1:C:60:VAL:HG11	1:C:278:VAL:HG13	2.03	0.41
1:C:102:GLN:HG3	1:C:137:THR:HG22	2.03	0.41
1:C:181:PHE:O	1:C:223:ALA:HA	2.21	0.41
1:C:237:THR:HG23	1:C:240:GLY:H	1.86	0.41
2:D:278:ILE:HG23	2:D:360:LEU:HD13	2.02	0.41
1:E:202:ILE:HG12	1:E:208:VAL:HG11	2.03	0.41
1:E:214:LYS:HD2	2:F:260:ASP:OD1	2.21	0.41
1:E:436:MET:HA	1:E:436:MET:HE3	2.03	0.41
2:F:269:ARG:HB2	2:F:341:PHE:CD1	2.56	0.41
1:G:206:THR:OG1	4:G:1465:FAD:O2P	2.38	0.41
2:H:138:ARG:HD3	2:H:142:GLY:H	1.86	0.41
2:H:635:ARG:HD3	2:H:750:CYS:SG	2.61	0.41
2:B:367:ASP:HA	2:B:368:PRO:HD3	1.99	0.41
1:C:455:VAL:HG13	2:D:443:THR:HG21	2.02	0.41
2:F:632:VAL:HG13	2:F:643:LEU:HD11	2.02	0.41
2:B:249:THR:C	2:B:251:ARG:H	2.29	0.40
2:B:466:GLN:HA	2:B:602:TYR:O	2.22	0.40
1:C:418:LEU:HB3	1:C:436:MET:HE1	2.03	0.40
2:D:198:HIS:CD2	2:D:201:GLU:H	2.39	0.40
2:D:273:ARG:HB3	2:D:294:LEU:HD12	2.02	0.40
2:D:647:ILE:HB	2:D:710:VAL:HG22	2.03	0.40
1:E:138:GLY:C	1:E:140:ALA:H	2.29	0.40
2:F:160:HIS:CB	2:F:364:MET:HE2	2.51	0.40
2:F:644:ARG:HB2	2:F:707:ILE:HB	2.03	0.40
1:G:138:GLY:O	1:G:139:TYR:HB2	2.21	0.40
2:H:14:ALA:HA	2:H:19:GLN:HB2	2.03	0.40
2:H:341:PHE:HD2	2:H:342:ARG:N	2.19	0.40
2:H:768:ALA:O	2:H:772:ARG:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PRO:O	1:A:112:VAL:HG23	2.22	0.40
1:A:208:VAL:HG22	4:A:1465:FAD:H3B	2.03	0.40
1:A:279:ALA:HB1	4:A:1465:FAD:H4'	2.03	0.40
2:B:222:ARG:HD2	2:B:515:ALA:HA	2.04	0.40
1:E:298:LEU:HB3	1:E:303:ALA:HB3	2.03	0.40
2:F:466:GLN:NE2	2:H:593:ARG:HG2	2.37	0.40
2:H:212:LEU:HD13	2:H:216:ASP:HB3	2.04	0.40
1:A:192:TRP:O	1:A:196:HIS:HD2	2.04	0.40
1:E:243:ILE:HD11	1:E:255:PHE:CE2	2.55	0.40
1:E:255:PHE:O	1:E:259:PRO:HD2	2.21	0.40
2:F:33:LEU:HG	2:F:251:ARG:HD2	2.02	0.40
2:F:53:GLU:HA	2:F:53:GLU:OE1	2.21	0.40
2:F:367:ASP:HA	2:F:368:PRO:HD2	1.78	0.40
2:F:593:ARG:HD2	2:H:603:ALA:HB1	2.04	0.40
1:G:111:ILE:HA	1:G:114:MET:HE3	2.03	0.40
2:H:5:LYS:HA	2:H:6:PRO:HD3	1.97	0.40
2:H:222:ARG:HD2	2:H:222:ARG:HA	1.88	0.40
2:F:310:ARG:HD2	2:F:344:PHE:HB3	2.04	0.40
2:F:504:LEU:O	2:F:568:PHE:HB3	2.22	0.40
1:G:44:CYS:O	1:G:46:ALA:N	2.55	0.40
1:G:269:ARG:HH12	1:G:352:LYS:HB3	1.86	0.40
2:H:194:CYS:SG	2:H:202:ILE:HD12	2.61	0.40
2:B:354:GLU:HA	2:B:357:ILE:HG22	2.03	0.40
2:B:478:SER:HB2	2:D:215:HIS:CE1	2.56	0.40
1:C:273:GLU:OE1	1:C:276:ARG:NH1	2.51	0.40
1:E:288:GLY:HA2	1:E:322:PHE:HE2	1.86	0.40
1:E:325:TYR:CZ	1:E:326:ARG:HD2	2.57	0.40
2:H:262:ASP:O	2:H:266:THR:CG2	2.68	0.40
2:H:343:GLY:H	2:H:730:GLU:HG2	1.86	0.40
2:H:473:ILE:HD11	2:H:547:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/462 (96%)	394 (88%)	47 (10%)	5 (1%)	11	38
1	C	446/462 (96%)	405 (91%)	37 (8%)	4 (1%)	14	42
1	E	446/462 (96%)	406 (91%)	34 (8%)	6 (1%)	9	33
1	G	446/462 (96%)	393 (88%)	47 (10%)	6 (1%)	9	33
2	B	756/777 (97%)	707 (94%)	39 (5%)	10 (1%)	9	33
2	D	756/777 (97%)	685 (91%)	65 (9%)	6 (1%)	16	44
2	F	756/777 (97%)	690 (91%)	58 (8%)	8 (1%)	11	38
2	H	756/777 (97%)	699 (92%)	46 (6%)	11 (2%)	8	30
All	All	4808/4956 (97%)	4379 (91%)	373 (8%)	56 (1%)	10	35

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	458	SER
1	C	39	CYS
2	D	187	GLU
2	D	458	SER
2	D	532	GLY
2	F	10	ASP
2	F	187	GLU
2	H	187	GLU
2	H	458	SER
1	A	39	CYS
1	A	389	GLY
2	B	73	ASP
2	B	187	GLU
2	B	234	GLN
2	B	342	ARG
1	C	121	ASP
2	D	10	ASP
1	E	39	CYS
2	F	342	ARG
2	F	458	SER
1	G	45	GLY
2	H	10	ASP
2	H	560	GLY
2	H	561	CYS

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Mol	Chain	Res	Type
1	A	257	GLU
2	B	561	CYS
1	C	180	ALA
1	E	197	PRO
1	E	226	SER
2	F	29	PRO
2	F	140	GLU
2	F	228	PHE
2	H	342	ARG
2	H	701	PHE
1	A	180	ALA
1	C	226	SER
2	D	227	GLY
1	E	323	LEU
1	G	39	CYS
2	B	115	LYS
2	B	560	GLY
1	E	332	PRO
2	F	260	ASP
1	G	359	GLN
2	H	30	ALA
1	A	359	GLN
2	B	233	SER
1	E	295	PRO
1	G	180	ALA
2	B	227	GLY
2	H	722	ILE
2	D	141	GLY
1	G	302	GLY
2	H	532	GLY
2	H	227	GLY
1	G	197	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/347 (98%)	308 (91%)	31 (9%)	9	30
1	C	339/347 (98%)	313 (92%)	26 (8%)	12	37
1	E	339/347 (98%)	314 (93%)	25 (7%)	13	38
1	G	339/347 (98%)	311 (92%)	28 (8%)	10	35
2	B	571/584 (98%)	532 (93%)	39 (7%)	14	40
2	D	571/584 (98%)	520 (91%)	51 (9%)	9	31
2	F	571/584 (98%)	518 (91%)	53 (9%)	8	29
2	H	571/584 (98%)	530 (93%)	41 (7%)	13	39
All	All	3640/3724 (98%)	3346 (92%)	294 (8%)	11	36

All (294) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	THR
1	A	61	ASN
1	A	65	MET
1	A	66	MET
1	A	67	LEU
1	A	78	ILE
1	A	79	GLU
1	A	113	SER
1	A	128	LEU
1	A	132	ASN
1	A	133	LEU
1	A	143	LEU
1	A	191	ASP
1	A	212	VAL
1	A	219	LEU
1	A	228	CYS
1	A	231	LEU
1	A	291	ILE
1	A	323	LEU
1	A	340	THR
1	A	341	LEU
1	A	348	LEU
1	A	349	ARG
1	A	371	THR
1	A	393	ARG
1	A	407	ARG
1	A	408	GLU

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Mol	Chain	Res	Type
1	A	423	THR
1	A	425	LEU
1	A	437	ASN
1	A	458	LEU
2	B	10	ASP
2	B	16	VAL
2	B	19	GLN
2	B	21	ARG
2	B	85	VAL
2	B	129	LEU
2	B	161	LEU
2	B	176	LEU
2	B	200	SER
2	B	212	LEU
2	B	222	ARG
2	B	256	ARG
2	B	259	ARG
2	B	262	ASP
2	B	266	THR
2	B	268	LYS
2	B	271	ASP
2	B	296	ARG
2	B	313	LEU
2	B	326	ILE
2	B	355	ARG
2	B	357	ILE
2	B	381	GLU
2	B	398	LYS
2	B	428	THR
2	B	458	SER
2	B	460	THR
2	B	466	GLN
2	B	488	MET
2	B	512	ARG
2	B	520	LYS
2	B	596	LEU
2	B	604	THR
2	B	612	LEU
2	B	632	VAL
2	B	648	LEU
2	B	650	ASP
2	B	689	MET

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Mol	Chain	Res	Type
2	B	724	ARG
1	C	11	THR
1	C	20	THR
1	C	24	LEU
1	C	67	LEU
1	C	79	GLU
1	C	93	GLN
1	C	113	SER
1	C	128	LEU
1	C	159	GLN
1	C	218	ASP
1	C	219	LEU
1	C	228	CYS
1	C	231	LEU
1	C	257	GLU
1	C	291	ILE
1	C	316	MET
1	C	324	GLU
1	C	341	LEU
1	C	349	ARG
1	C	362	SER
1	C	373	LYS
1	C	390	VAL
1	C	393	ARG
1	C	435	ARG
1	C	449	GLU
1	C	457	VAL
2	D	10	ASP
2	D	11	SER
2	D	16	VAL
2	D	21	ARG
2	D	23	LEU
2	D	35	LEU
2	D	40	SER
2	D	53	GLU
2	D	85	VAL
2	D	101	VAL
2	D	110	ARG
2	D	129	LEU
2	D	161	LEU
2	D	174	PHE
2	D	200	SER

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Mol	Chain	Res	Type
2	D	202	ILE
2	D	212	LEU
2	D	222	ARG
2	D	247	ARG
2	D	256	ARG
2	D	266	THR
2	D	268	LYS
2	D	296	ARG
2	D	326	ILE
2	D	330	ARG
2	D	355	ARG
2	D	357	ILE
2	D	398	LYS
2	D	399	LYS
2	D	423	LYS
2	D	428	THR
2	D	464	LEU
2	D	466	GLN
2	D	512	ARG
2	D	513	ILE
2	D	514	THR
2	D	520	LYS
2	D	558	ARG
2	D	564	ARG
2	D	596	LEU
2	D	617	ARG
2	D	632	VAL
2	D	635	ARG
2	D	648	LEU
2	D	689	MET
2	D	694	SER
2	D	695	THR
2	D	697	LYS
2	D	720	GLU
2	D	724	ARG
2	D	741	LEU
1	E	20	THR
1	E	21	GLN
1	E	32	LEU
1	E	40	ASN
1	E	61	ASN
1	E	65	MET

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Mol	Chain	Res	Type
1	E	67	LEU
1	E	79	GLU
1	E	93	GLN
1	E	97	ASP
1	E	128	LEU
1	E	212	VAL
1	E	216	LEU
1	E	219	LEU
1	E	231	LEU
1	E	237	THR
1	E	291	ILE
1	E	341	LEU
1	E	349	ARG
1	E	365	CYS
1	E	373	LYS
1	E	390	VAL
1	E	393	ARG
1	E	401	LEU
1	E	447	VAL
2	F	2	SER
2	F	10	ASP
2	F	11	SER
2	F	16	VAL
2	F	23	LEU
2	F	53	GLU
2	F	66	THR
2	F	90	GLU
2	F	128	THR
2	F	161	LEU
2	F	175	TYR
2	F	187	GLU
2	F	202	ILE
2	F	212	LEU
2	F	222	ARG
2	F	234	GLN
2	F	256	ARG
2	F	259	ARG
2	F	266	THR
2	F	268	LYS
2	F	287	LEU
2	F	296	ARG
2	F	313	LEU

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Mol	Chain	Res	Type
2	F	355	ARG
2	F	357	ILE
2	F	381	GLU
2	F	398	LYS
2	F	399	LYS
2	F	423	LYS
2	F	429	THR
2	F	433	GLU
2	F	458	SER
2	F	461	LEU
2	F	464	LEU
2	F	475	THR
2	F	512	ARG
2	F	518	THR
2	F	520	LYS
2	F	541	LYS
2	F	546	THR
2	F	548	ARG
2	F	558	ARG
2	F	564	ARG
2	F	567	ILE
2	F	584	GLU
2	F	607	LEU
2	F	632	VAL
2	F	648	LEU
2	F	689	MET
2	F	698	ILE
2	F	702	SER
2	F	720	GLU
2	F	741	LEU
1	G	24	LEU
1	G	33	THR
1	G	61	ASN
1	G	79	GLU
1	G	93	GLN
1	G	103	CYS
1	G	112	VAL
1	G	113	SER
1	G	122	ARG
1	G	128	LEU
1	G	137	THR
1	G	143	LEU

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Mol	Chain	Res	Type
1	G	208	VAL
1	G	228	CYS
1	G	231	LEU
1	G	291	ILE
1	G	327	LYS
1	G	341	LEU
1	G	349	ARG
1	G	364	VAL
1	G	382	ILE
1	G	393	ARG
1	G	408	GLU
1	G	409	ASP
1	G	417	LEU
1	G	423	THR
1	G	449	GLU
1	G	457	VAL
2	H	2	SER
2	H	10	ASP
2	H	16	VAL
2	H	57	GLU
2	H	85	VAL
2	H	128	THR
2	H	187	GLU
2	H	202	ILE
2	H	210	LEU
2	H	212	LEU
2	H	222	ARG
2	H	256	ARG
2	H	260	ASP
2	H	266	THR
2	H	268	LYS
2	H	287	LEU
2	H	313	LEU
2	H	326	ILE
2	H	335	THR
2	H	357	ILE
2	H	398	LYS
2	H	441	ASN
2	H	458	SER
2	H	488	MET
2	H	509	VAL
2	H	512	ARG

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Mol	Chain	Res	Type
2	H	514	THR
2	H	548	ARG
2	H	550	ARG
2	H	564	ARG
2	H	579	SER
2	H	604	THR
2	H	612	LEU
2	H	617	ARG
2	H	620	LEU
2	H	632	VAL
2	H	634	ASP
2	H	698	ILE
2	H	721	THR
2	H	728	VAL
2	H	741	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	61	ASN
1	A	69	GLN
1	A	93	GLN
1	A	132	ASN
1	A	196	HIS
1	A	227	HIS
1	A	328	GLN
1	A	359	GLN
1	A	440	GLN
2	B	193	HIS
2	B	198	HIS
2	B	208	HIS
2	B	236	ASN
2	B	237	HIS
2	B	293	HIS
2	B	338	ASN
2	B	422	GLN
2	B	510	GLN
2	B	572	GLN
2	B	640	ASN
2	B	744	HIS
1	C	40	ASN

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Mol	Chain	Res	Type
1	C	61	ASN
1	C	69	GLN
1	C	93	GLN
1	C	159	GLN
1	C	260	HIS
1	C	311	GLN
1	C	359	GLN
1	C	369	ASN
1	C	420	GLN
1	C	437	ASN
2	D	9	HIS
2	D	160	HIS
2	D	179	GLN
2	D	193	HIS
2	D	198	HIS
2	D	232	GLN
2	D	236	ASN
2	D	237	HIS
2	D	422	GLN
2	D	463	HIS
2	D	465	ASN
2	D	466	GLN
2	D	482	ASN
2	D	649	HIS
2	D	744	HIS
2	D	753	HIS
1	E	40	ASN
1	E	61	ASN
1	E	93	GLN
1	E	118	HIS
1	E	227	HIS
1	E	260	HIS
1	E	284	ASN
2	F	9	HIS
2	F	15	HIS
2	F	106	HIS
2	F	236	ASN
2	F	237	HIS
2	F	348	GLN
2	F	441	ASN
2	F	463	HIS
2	F	465	ASN

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Mol	Chain	Res	Type
2	F	466	GLN
2	F	482	ASN
2	F	574	GLN
2	F	649	HIS
1	G	61	ASN
1	G	69	GLN
1	G	93	GLN
1	G	99	HIS
1	G	132	ASN
1	G	227	HIS
1	G	260	HIS
1	G	328	GLN
1	G	359	GLN
2	H	106	HIS
2	H	232	GLN
2	H	236	ASN
2	H	237	HIS
2	H	293	HIS
2	H	338	ASN
2	H	441	ASN
2	H	466	GLN
2	H	482	ASN
2	H	744	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FES	A	1463	1	0,4,4	-	-	-		
3	FES	A	1464	1	0,4,4	-	-	-		
5	XAX	B	1778	-	20,31,31	4.02	4 (20%)	20,52,52	2.18	5 (25%)
3	FES	E	1464	1	0,4,4	-	-	-		
7	HPA	D	1780	-	10,11,11	1.75	1 (10%)	11,15,15	3.34	8 (72%)
3	FES	C	1464	1	0,4,4	-	-	-		
4	FAD	G	1465	-	56,58,58	1.33	6 (10%)	81,89,89	1.67	16 (19%)
5	XAX	F	1778	-	20,31,31	4.09	4 (20%)	20,52,52	1.85	6 (30%)
7	HPA	F	1780	-	10,11,11	1.86	2 (20%)	11,15,15	3.26	8 (72%)
3	FES	G	1463	1	0,4,4	-	-	-		
4	FAD	C	1465	-	56,58,58	1.27	4 (7%)	81,89,89	1.65	16 (19%)
5	XAX	H	1778	-	20,31,31	4.15	4 (20%)	20,52,52	2.06	4 (20%)
4	FAD	E	1465	-	56,58,58	1.29	4 (7%)	81,89,89	1.64	17 (20%)
3	FES	G	1464	1	0,4,4	-	-	-		
4	FAD	A	1465	-	56,58,58	1.36	6 (10%)	81,89,89	1.62	16 (19%)
7	HPA	B	1780	-	10,11,11	1.84	2 (20%)	11,15,15	3.56	9 (81%)
7	HPA	H	1780	-	10,11,11	1.76	1 (10%)	11,15,15	3.53	8 (72%)
3	FES	E	1463	1	0,4,4	-	-	-		
3	FES	C	1463	1	0,4,4	-	-	-		
5	XAX	D	1778	-	20,31,31	4.17	5 (25%)	20,52,52	1.74	4 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	A	1463	1	-	-	0/1/1/1
3	FES	C	1463	1	-	-	0/1/1/1
5	XAX	B	1778	-	1/1/7/9	3/6/46/46	0/4/4/4
3	FES	E	1464	1	-	-	0/1/1/1
7	HPA	D	1780	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	C	1464	1	-	-	0/1/1/1
4	FAD	G	1465	-	-	11/34/50/50	0/6/6/6
5	XAX	F	1778	-	1/1/7/9	2/6/46/46	0/4/4/4
7	HPA	F	1780	-	-	-	0/2/2/2
3	FES	G	1463	1	-	-	0/1/1/1
4	FAD	C	1465	-	-	10/34/50/50	0/6/6/6
5	XAX	H	1778	-	1/1/7/9	2/6/46/46	0/4/4/4
4	FAD	E	1465	-	-	10/34/50/50	0/6/6/6
3	FES	G	1464	1	-	-	0/1/1/1
4	FAD	A	1465	-	-	17/34/50/50	0/6/6/6
7	HPA	B	1780	-	-	-	0/2/2/2
7	HPA	H	1780	-	-	-	0/2/2/2
3	FES	E	1463	1	-	-	0/1/1/1
3	FES	A	1464	1	-	-	0/1/1/1
5	XAX	D	1778	-	1/1/7/9	2/6/46/46	0/4/4/4

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1778	XAX	C4'-C3'	-13.94	1.33	1.52
5	D	1778	XAX	C4'-C3'	-13.34	1.34	1.52
5	B	1778	XAX	C4'-C3'	-13.23	1.34	1.52
5	F	1778	XAX	C4'-C3'	-12.83	1.34	1.52
5	F	1778	XAX	C6-N5	-11.17	1.33	1.46
5	D	1778	XAX	C6-N5	-10.94	1.33	1.46
5	H	1778	XAX	C6-N5	-10.49	1.34	1.46
5	B	1778	XAX	C6-N5	-10.37	1.34	1.46
4	G	1465	FAD	C4X-N5	5.59	1.41	1.30
4	C	1465	FAD	C4X-N5	5.32	1.41	1.30
4	E	1465	FAD	C4X-N5	5.17	1.40	1.30
4	A	1465	FAD	C4X-N5	5.09	1.40	1.30
5	D	1778	XAX	C9-C10	5.07	1.47	1.38
5	H	1778	XAX	C9-C10	5.00	1.47	1.38
7	B	1780	HPA	C2-N3	4.97	1.39	1.30
7	F	1780	HPA	C2-N3	4.93	1.39	1.30
5	B	1778	XAX	C9-C10	4.89	1.47	1.38
7	H	1780	HPA	C2-N3	4.88	1.39	1.30
5	F	1778	XAX	C9-C10	4.74	1.46	1.38
7	D	1780	HPA	C2-N3	4.70	1.38	1.30
4	A	1465	FAD	C10-N1	3.99	1.41	1.33
4	G	1465	FAD	C10-N1	3.85	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1465	FAD	C10-N1	3.82	1.41	1.33
4	C	1465	FAD	C10-N1	3.76	1.40	1.33
4	A	1465	FAD	C5A-N7A	-3.07	1.33	1.39
4	G	1465	FAD	C5A-N7A	-3.05	1.33	1.39
4	E	1465	FAD	C5A-N7A	-2.91	1.33	1.39
4	C	1465	FAD	C5A-N7A	-2.74	1.33	1.39
5	D	1778	XAX	C7-C6	-2.71	1.51	1.53
4	E	1465	FAD	O4B-C1B	2.66	1.48	1.42
4	A	1465	FAD	C10-N10	2.41	1.42	1.37
4	A	1465	FAD	C1'-C2'	2.40	1.56	1.52
4	G	1465	FAD	O4B-C1B	2.35	1.47	1.42
5	F	1778	XAX	C9-C4	2.24	1.48	1.42
4	G	1465	FAD	C10-N10	2.24	1.42	1.37
5	B	1778	XAX	C9-C4	2.22	1.48	1.42
4	A	1465	FAD	O4B-C1B	2.20	1.47	1.42
5	H	1778	XAX	C9-C4	2.18	1.48	1.42
7	F	1780	HPA	C2-N1	2.17	1.39	1.35
4	C	1465	FAD	C4A-N9A	-2.11	1.33	1.37
7	B	1780	HPA	C2-N1	2.10	1.39	1.35
5	D	1778	XAX	C9-C4	2.09	1.47	1.42
4	G	1465	FAD	C8A-N9A	-2.04	1.33	1.37

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1465	FAD	C5A-C4A-N3A	-6.02	118.89	126.75
7	H	1780	HPA	C5-C6-N1	6.00	120.29	110.57
4	A	1465	FAD	C5A-C4A-N3A	-5.70	119.31	126.75
4	E	1465	FAD	C5A-C4A-N3A	-5.66	119.36	126.75
5	B	1778	XAX	O3'-C7-C6	5.59	112.69	108.96
7	B	1780	HPA	C5-C6-N1	5.56	119.58	110.57
7	F	1780	HPA	C5-C6-N1	5.51	119.50	110.57
7	D	1780	HPA	C5-C6-N1	5.48	119.46	110.57
5	H	1778	XAX	O3'-C7-C6	5.39	112.56	108.96
4	C	1465	FAD	C5A-C4A-N3A	-5.27	119.88	126.75
4	G	1465	FAD	N3A-C2A-N1A	-4.70	121.25	128.60
5	B	1778	XAX	C2-N1-C10	4.70	121.91	113.43
4	A	1465	FAD	N3A-C2A-N1A	-4.64	121.34	128.60
4	C	1465	FAD	N3A-C2A-N1A	-4.63	121.37	128.60
7	D	1780	HPA	N1-C2-N3	-4.59	120.50	125.57
7	H	1780	HPA	N1-C2-N3	-4.58	120.51	125.57
4	E	1465	FAD	N3A-C2A-N1A	-4.58	121.44	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1778	XAX	C2-N1-C10	4.51	121.58	113.43
7	B	1780	HPA	N7-C8-N9	-4.48	108.05	112.99
5	H	1778	XAX	C2-N1-C10	4.36	121.31	113.43
7	B	1780	HPA	N1-C2-N3	-4.34	120.77	125.57
5	D	1778	XAX	C2-N1-C10	4.31	121.20	113.43
7	B	1780	HPA	C2-N1-C6	-4.23	119.36	125.03
7	H	1780	HPA	C2-N1-C6	-4.17	119.43	125.03
7	F	1780	HPA	C2-N1-C6	-4.07	119.57	125.03
7	F	1780	HPA	N1-C2-N3	-4.05	121.10	125.57
4	G	1465	FAD	N3A-C4A-N9A	4.04	133.74	127.08
4	A	1465	FAD	N3A-C4A-N9A	4.03	133.73	127.08
4	G	1465	FAD	C2A-N3A-C4A	3.96	121.11	111.75
4	E	1465	FAD	N3A-C4A-N9A	3.95	133.59	127.08
4	E	1465	FAD	C2A-N3A-C4A	3.85	120.84	111.75
7	H	1780	HPA	C5-C4-N3	-3.80	120.18	124.44
4	C	1465	FAD	C2A-N3A-C4A	3.79	120.70	111.75
7	B	1780	HPA	C8-N9-C4	3.77	109.07	102.89
7	D	1780	HPA	C2-N1-C6	-3.75	120.00	125.03
4	A	1465	FAD	C2A-N3A-C4A	3.74	120.58	111.75
7	B	1780	HPA	C5-C4-N3	-3.72	120.26	124.44
7	D	1780	HPA	C5-C4-N3	-3.65	120.34	124.44
7	D	1780	HPA	N7-C8-N9	-3.62	109.00	112.99
7	F	1780	HPA	N7-C8-N9	-3.53	109.10	112.99
7	H	1780	HPA	C6-C5-C4	-3.51	119.21	121.61
4	C	1465	FAD	N3A-C4A-N9A	3.46	132.78	127.08
7	H	1780	HPA	N7-C8-N9	-3.41	109.23	112.99
4	G	1465	FAD	C5A-N7A-C8A	3.40	108.33	103.51
4	G	1465	FAD	N9A-C8A-N7A	-3.38	109.30	113.91
4	E	1465	FAD	N9A-C8A-N7A	-3.33	109.36	113.91
4	E	1465	FAD	C4-N3-C2	-3.32	119.50	125.64
4	A	1465	FAD	C4-N3-C2	-3.28	119.58	125.64
7	F	1780	HPA	C5-C4-N3	-3.28	120.75	124.44
7	H	1780	HPA	C8-N9-C4	3.27	108.24	102.89
7	H	1780	HPA	O6-C6-C5	-3.26	119.77	127.24
7	D	1780	HPA	C8-N9-C4	3.26	108.22	102.89
7	F	1780	HPA	C8-N9-C4	3.25	108.21	102.89
5	F	1778	XAX	O3'-C7-C6	3.24	111.12	108.96
4	C	1465	FAD	O4B-C1B-N9A	-3.22	101.71	108.06
7	B	1780	HPA	O6-C6-C5	-3.20	119.91	127.24
4	C	1465	FAD	C4-N3-C2	-3.11	119.89	125.64
4	E	1465	FAD	C5A-N7A-C8A	3.02	107.80	103.51
4	C	1465	FAD	N9A-C8A-N7A	-3.02	109.78	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	1780	HPA	O6-C6-C5	-3.01	120.33	127.24
7	D	1780	HPA	O6-C6-C5	-2.99	120.39	127.24
4	G	1465	FAD	C4-N3-C2	-2.97	120.16	125.64
4	G	1465	FAD	C4X-C10-N10	2.94	120.78	116.48
5	B	1778	XAX	C4-C9-N5	2.92	124.60	116.76
4	A	1465	FAD	C4X-C4-N3	2.90	120.56	113.19
4	C	1465	FAD	P-O3P-PA	-2.90	122.89	132.83
4	A	1465	FAD	P-O3P-PA	-2.89	122.91	132.83
4	A	1465	FAD	N9A-C8A-N7A	-2.88	109.97	113.91
7	D	1780	HPA	C6-C5-C4	-2.88	119.64	121.61
4	A	1465	FAD	C5A-N7A-C8A	2.87	107.58	103.51
7	F	1780	HPA	C6-C5-C4	-2.83	119.67	121.61
4	C	1465	FAD	C4X-C10-N10	2.83	120.62	116.48
4	G	1465	FAD	C4A-C5A-N7A	-2.80	107.21	110.62
5	D	1778	XAX	O4-C4-C9	-2.79	120.85	127.24
4	E	1465	FAD	C4X-C4-N3	2.78	120.25	113.19
4	G	1465	FAD	C10-C4X-N5	-2.78	118.96	124.86
5	F	1778	XAX	C4-C9-N5	2.74	124.11	116.76
7	B	1780	HPA	C6-C5-C4	-2.73	119.74	121.61
5	D	1778	XAX	C4-C9-N5	2.72	124.05	116.76
4	E	1465	FAD	P-O3P-PA	-2.71	123.53	132.83
4	C	1465	FAD	C10-C4X-N5	-2.70	119.13	124.86
5	B	1778	XAX	O4-C4-C9	-2.69	121.07	127.24
5	H	1778	XAX	C4-C9-N5	2.68	123.96	116.76
4	E	1465	FAD	C10-C4X-N5	-2.65	119.22	124.86
4	C	1465	FAD	C5A-N7A-C8A	2.65	107.27	103.51
4	G	1465	FAD	C4X-C4-N3	2.63	119.88	113.19
5	H	1778	XAX	O4-C4-C9	-2.63	121.22	127.24
4	A	1465	FAD	C4X-C10-N10	2.62	120.32	116.48
4	E	1465	FAD	C9A-C5X-N5	-2.60	119.60	122.43
4	C	1465	FAD	C4X-C4-N3	2.59	119.77	113.19
4	C	1465	FAD	C2B-C1B-N9A	2.58	119.85	113.30
4	A	1465	FAD	C4X-C10-N1	-2.52	118.87	124.73
4	A	1465	FAD	O4-C4-C4X	-2.46	120.08	126.60
4	G	1465	FAD	P-O3P-PA	-2.44	124.45	132.83
4	E	1465	FAD	C4A-C5A-N7A	-2.44	107.65	110.62
4	C	1465	FAD	C4A-C5A-N7A	-2.38	107.72	110.62
5	F	1778	XAX	O4-C4-C9	-2.36	121.83	127.24
4	E	1465	FAD	O4-C4-C4X	-2.35	120.36	126.60
5	B	1778	XAX	C9-C4-N3	2.30	119.17	112.31
7	B	1780	HPA	C8-N7-C5	2.29	108.72	106.61
4	E	1465	FAD	C4X-C10-N10	2.24	119.76	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1465	FAD	C4A-N9A-C8A	2.23	108.14	105.73
4	C	1465	FAD	C9A-C5X-N5	-2.21	120.03	122.43
4	E	1465	FAD	C4X-C10-N1	-2.21	119.60	124.73
4	A	1465	FAD	C10-C4X-N5	-2.21	120.17	124.86
4	C	1465	FAD	O4-C4-C4X	-2.20	120.75	126.60
4	A	1465	FAD	C4A-C5A-N7A	-2.20	107.94	110.62
4	G	1465	FAD	C4X-C10-N1	-2.16	119.71	124.73
4	G	1465	FAD	C9A-C5X-N5	-2.13	120.12	122.43
4	G	1465	FAD	C4-C4X-N5	2.11	121.23	118.23
4	A	1465	FAD	C4-C4X-C10	2.09	120.31	116.79
4	E	1465	FAD	C4-C4X-C10	2.09	120.30	116.79
5	D	1778	XAX	C9-C4-N3	2.06	118.44	112.31
5	F	1778	XAX	C2-N3-C4	-2.03	121.40	125.10
4	A	1465	FAD	C10-N1-C2	2.02	120.94	116.90
5	F	1778	XAX	C9-C4-N3	2.01	118.28	112.31
4	G	1465	FAD	C10-N1-C2	2.01	120.91	116.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1778	XAX	C3'
5	D	1778	XAX	C3'
5	F	1778	XAX	C3'
5	H	1778	XAX	C3'

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1465	FAD	N10-C1'-C2'-C3'
4	A	1465	FAD	C1'-C2'-C3'-O3'
4	A	1465	FAD	C1'-C2'-C3'-C4'
4	A	1465	FAD	C2'-C3'-C4'-O4'
4	A	1465	FAD	C2'-C3'-C4'-C5'
4	A	1465	FAD	O3'-C3'-C4'-O4'
4	A	1465	FAD	O3'-C3'-C4'-C5'
4	A	1465	FAD	C3'-C4'-C5'-O5'
4	A	1465	FAD	O4'-C4'-C5'-O5'
4	C	1465	FAD	C2'-C1'-N10-C10
4	C	1465	FAD	N10-C1'-C2'-O2'
4	C	1465	FAD	N10-C1'-C2'-C3'
4	C	1465	FAD	C2'-C3'-C4'-O4'
4	C	1465	FAD	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
4	C	1465	FAD	O3'-C3'-C4'-O4'
4	C	1465	FAD	O3'-C3'-C4'-C5'
4	C	1465	FAD	C3'-C4'-C5'-O5'
4	C	1465	FAD	O4'-C4'-C5'-O5'
4	E	1465	FAD	N10-C1'-C2'-O2'
4	E	1465	FAD	N10-C1'-C2'-C3'
4	E	1465	FAD	C2'-C3'-C4'-O4'
4	E	1465	FAD	O3'-C3'-C4'-O4'
4	G	1465	FAD	C2'-C1'-N10-C10
4	G	1465	FAD	N10-C1'-C2'-O2'
4	G	1465	FAD	N10-C1'-C2'-C3'
4	G	1465	FAD	C2'-C3'-C4'-O4'
4	G	1465	FAD	C2'-C3'-C4'-C5'
4	G	1465	FAD	O3'-C3'-C4'-O4'
4	G	1465	FAD	O3'-C3'-C4'-C5'
4	G	1465	FAD	C3'-C4'-C5'-O5'
4	G	1465	FAD	O4'-C4'-C5'-O5'
5	B	1778	XAX	O3'-C3'-C4'-O4'
5	D	1778	XAX	O3'-C3'-C4'-O4'
5	F	1778	XAX	O3'-C3'-C4'-O4'
5	H	1778	XAX	O3'-C3'-C4'-O4'
5	F	1778	XAX	C3'-C4'-O4'-P
4	E	1465	FAD	O3'-C3'-C4'-C5'
4	E	1465	FAD	C2'-C3'-C4'-C5'
4	E	1465	FAD	O4'-C4'-C5'-O5'
4	E	1465	FAD	C3'-C4'-C5'-O5'
4	A	1465	FAD	C2'-C1'-N10-C10
4	E	1465	FAD	C2'-C1'-N10-C10
4	A	1465	FAD	O2'-C2'-C3'-O3'
4	E	1465	FAD	O4B-C4B-C5B-O5B
4	A	1465	FAD	O2'-C2'-C3'-C4'
4	A	1465	FAD	N10-C1'-C2'-O2'
5	B	1778	XAX	C3'-C4'-O4'-P
5	H	1778	XAX	C3'-C4'-O4'-P
4	A	1465	FAD	C4'-C5'-O5'-P
4	G	1465	FAD	C4'-C5'-O5'-P
5	D	1778	XAX	C3'-C4'-O4'-P
5	B	1778	XAX	C4'-O4'-P-O3P
4	A	1465	FAD	C5B-O5B-PA-O3P
4	C	1465	FAD	PA-O3P-P-O1P
4	A	1465	FAD	C5B-O5B-PA-O1A
4	A	1465	FAD	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
4	G	1465	FAD	C1'-C2'-C3'-O3'

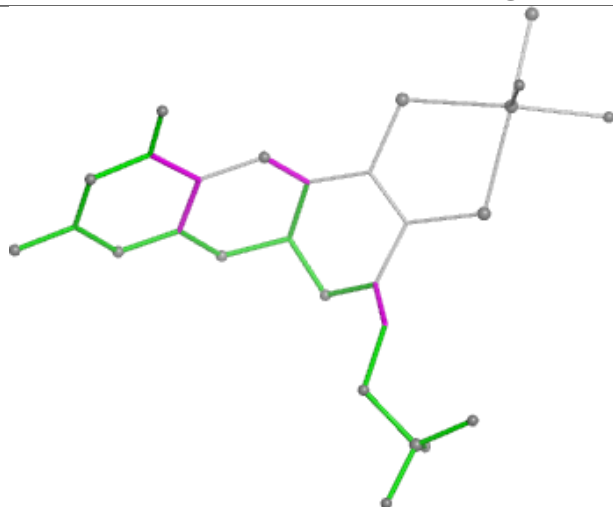
There are no ring outliers.

12 monomers are involved in 52 short contacts:

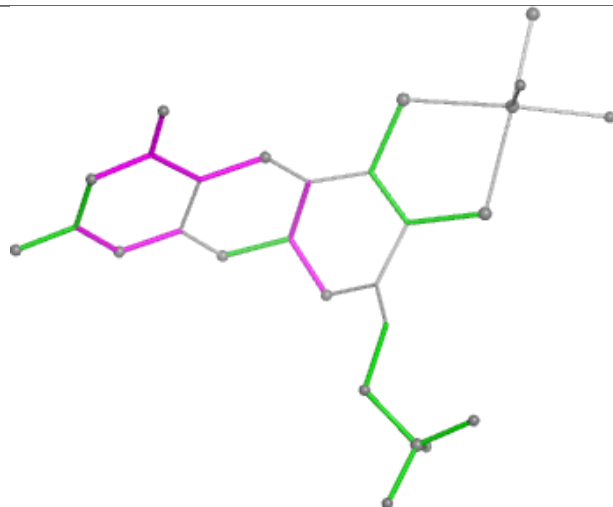
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1778	XAX	4	0
7	D	1780	HPA	3	0
4	G	1465	FAD	7	0
5	F	1778	XAX	7	0
7	F	1780	HPA	1	0
4	C	1465	FAD	5	0
5	H	1778	XAX	4	0
4	E	1465	FAD	2	0
3	G	1464	FES	1	0
4	A	1465	FAD	6	0
7	H	1780	HPA	7	0
5	D	1778	XAX	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

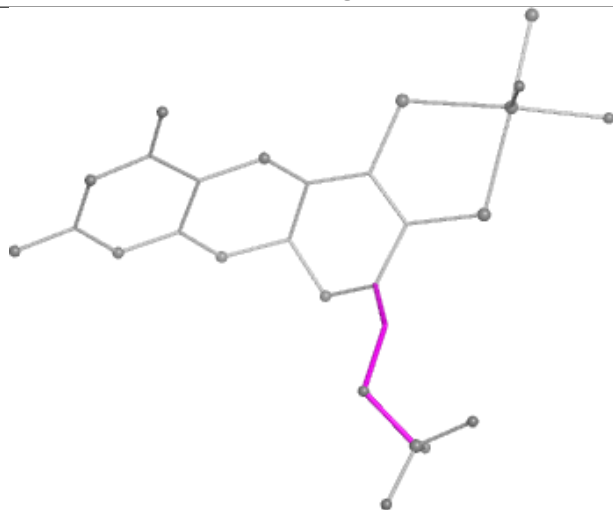
Ligand XAX B 1778



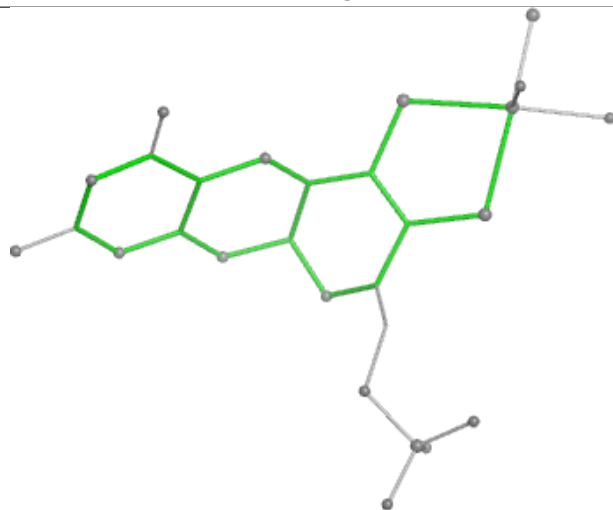
Bond lengths



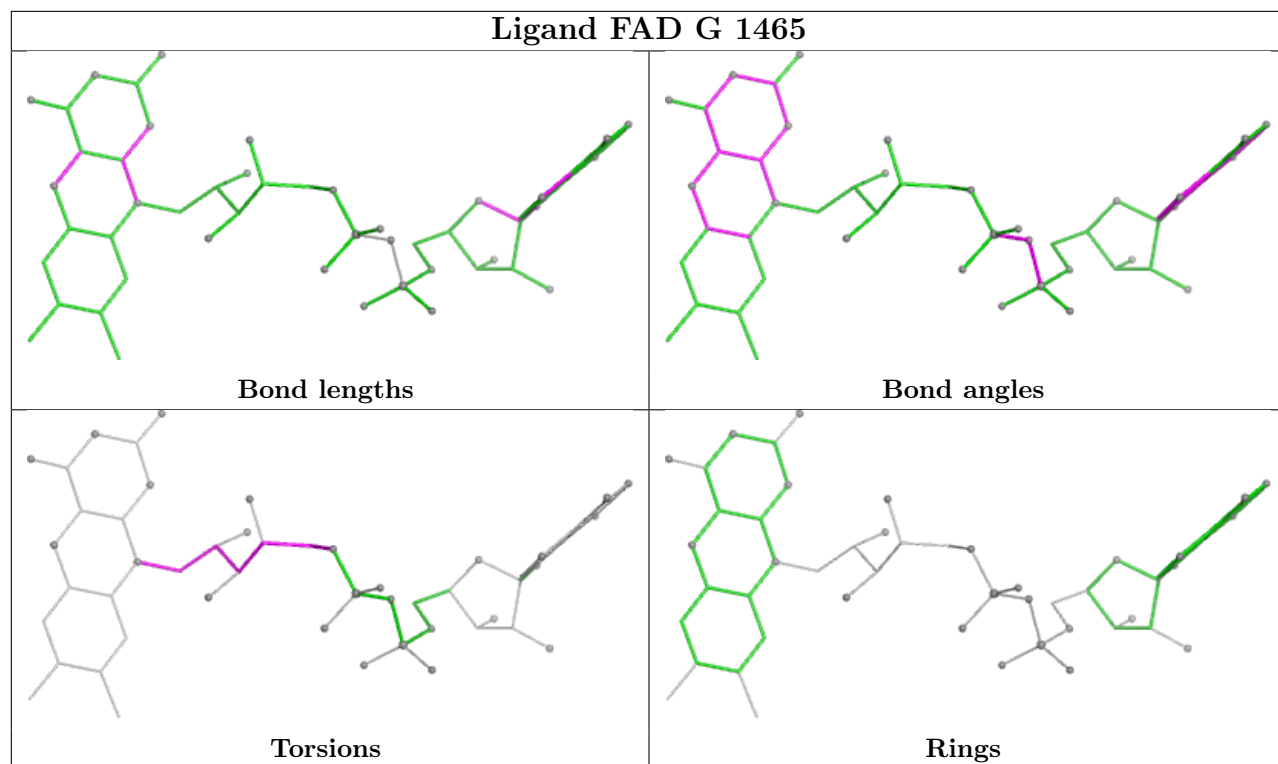
Bond angles



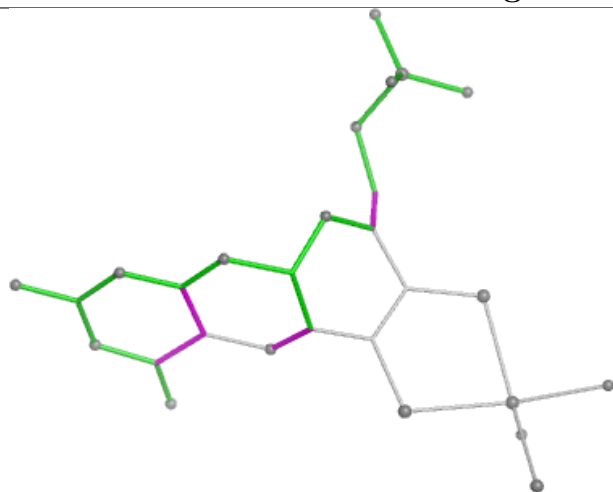
Torsions



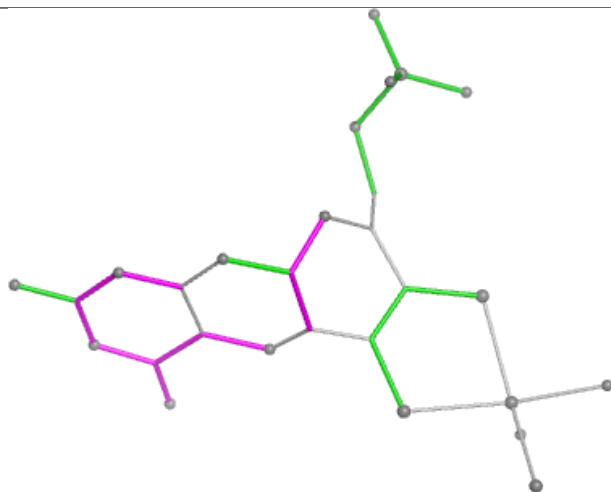
Rings



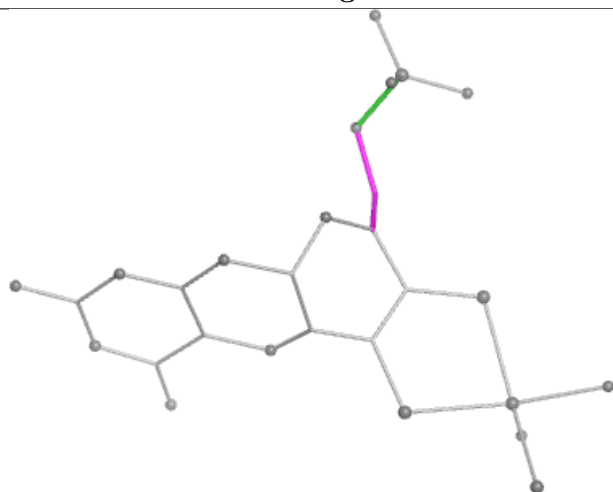
Ligand XAX F 1778



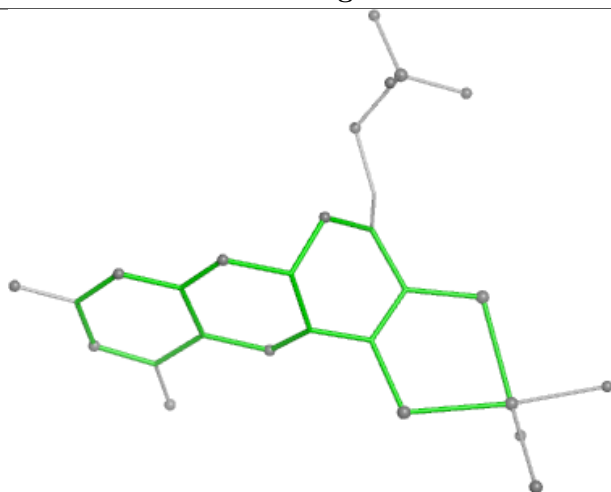
Bond lengths



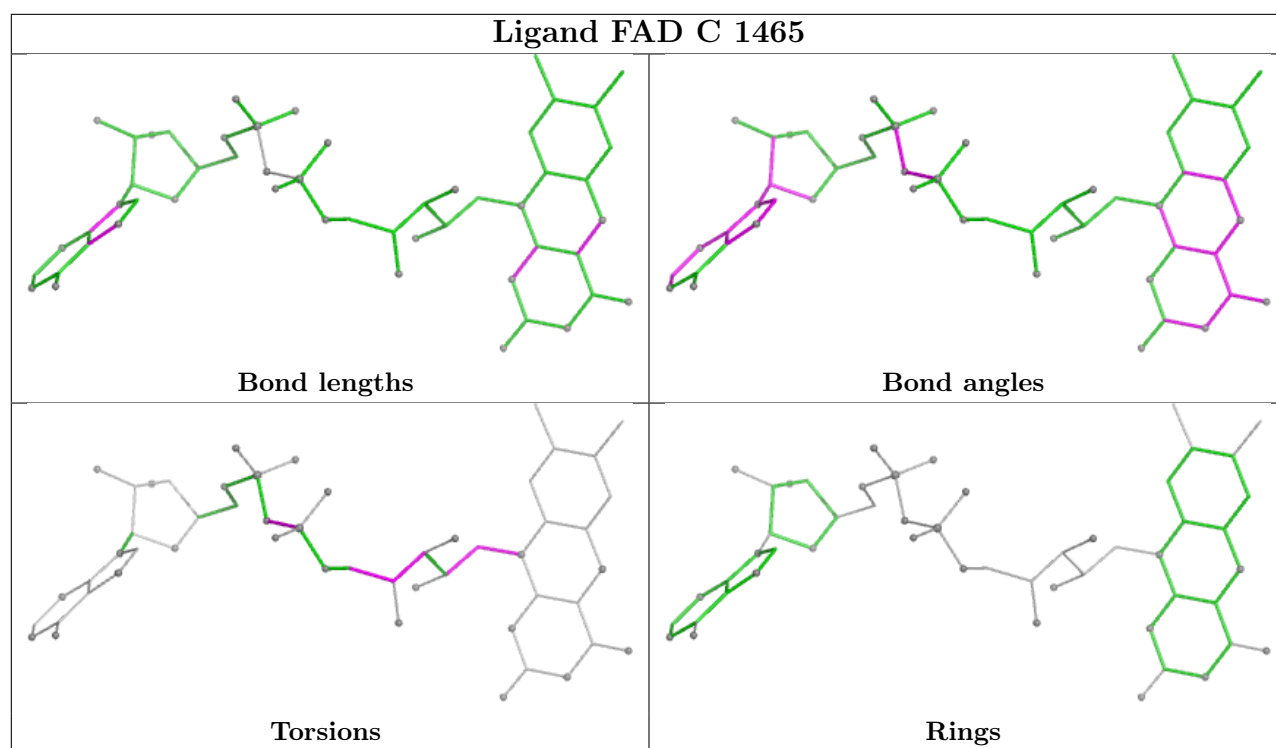
Bond angles

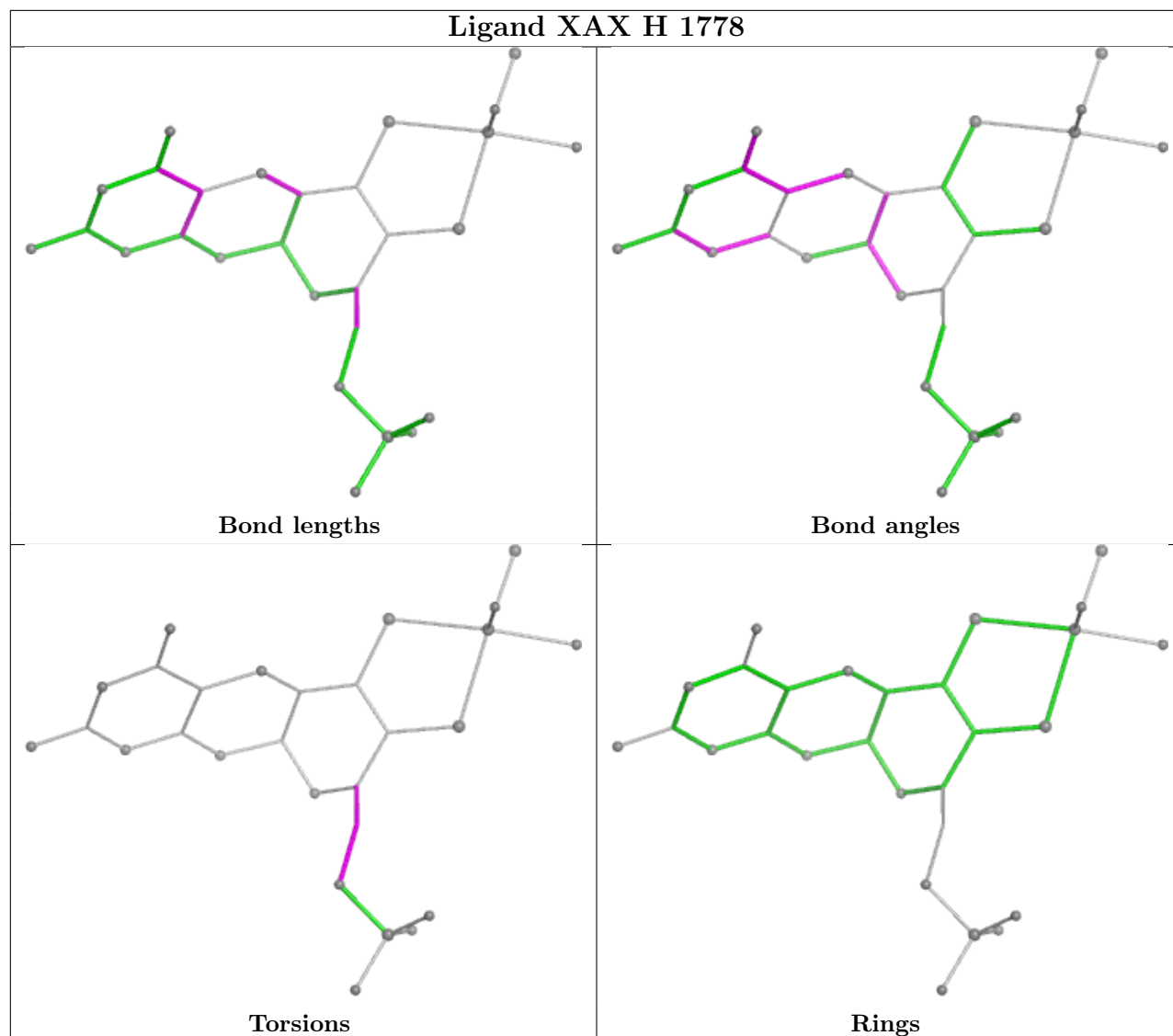


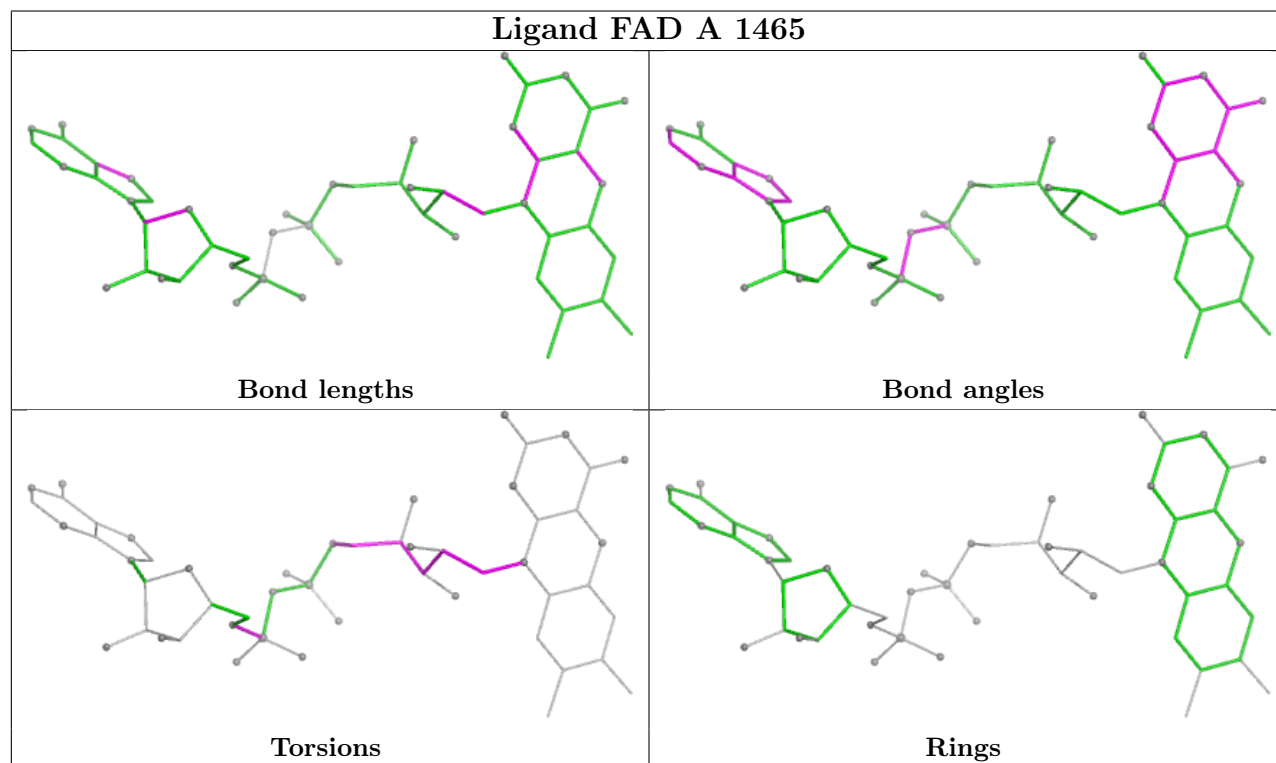
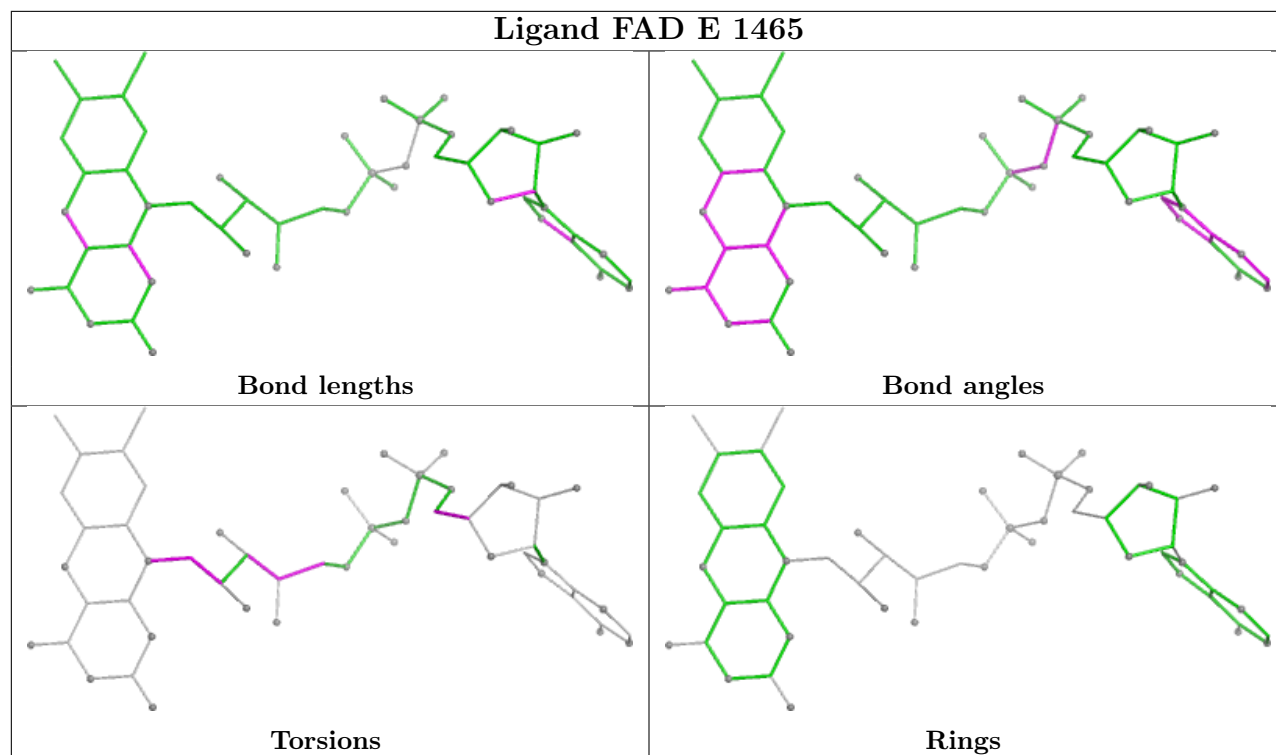
Torsions

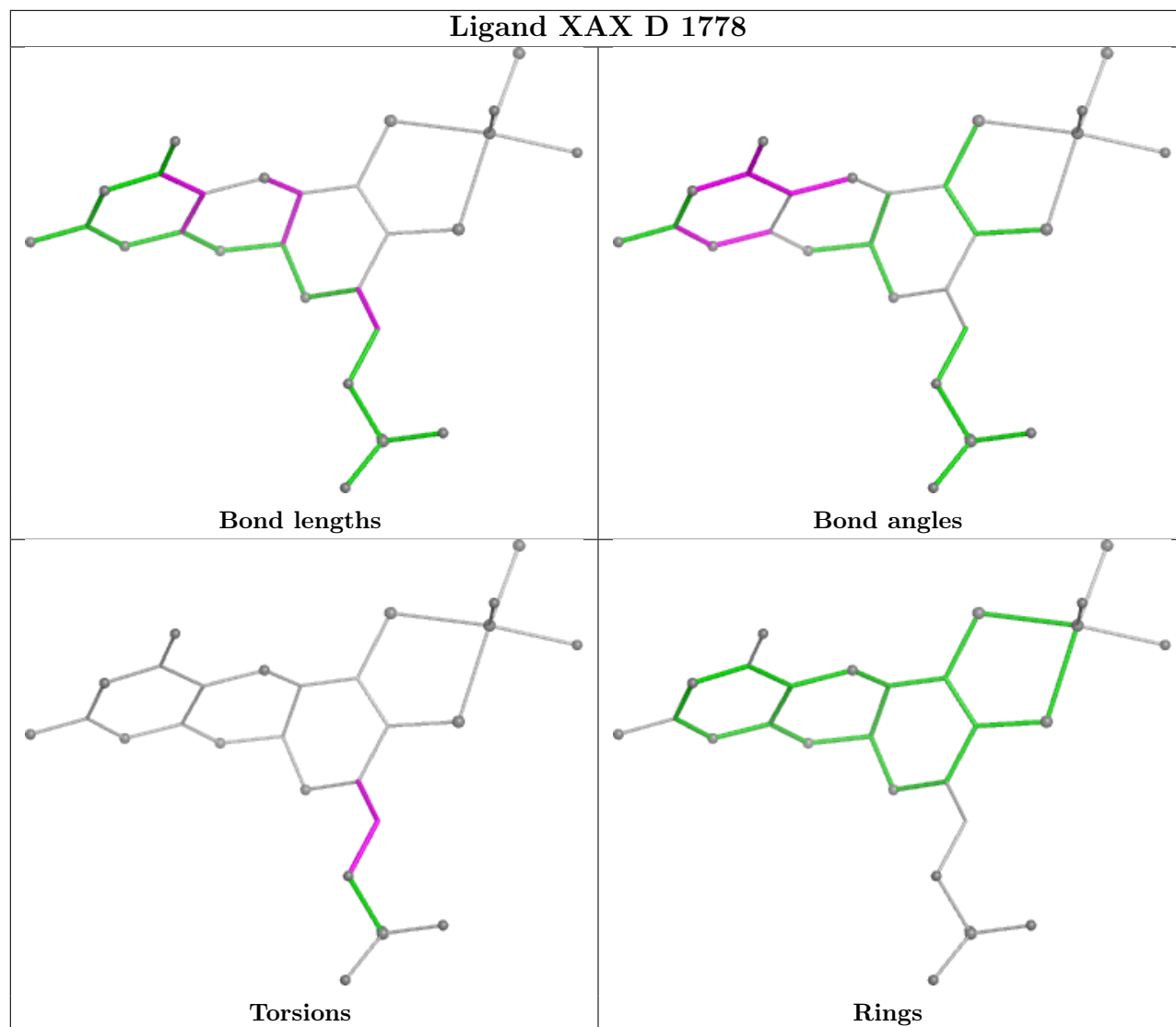


Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	450/462 (97%)	0.16	8 (1%) 67 53	41, 43, 44, 45	0
1	C	450/462 (97%)	0.01	5 (1%) 78 65	41, 43, 44, 45	0
1	E	450/462 (97%)	0.22	8 (1%) 67 53	41, 43, 44, 45	0
1	G	450/462 (97%)	0.26	16 (3%) 46 33	42, 43, 44, 45	0
2	B	760/777 (97%)	0.14	10 (1%) 75 61	40, 43, 44, 46	0
2	D	760/777 (97%)	-0.01	6 (0%) 82 71	41, 43, 44, 46	0
2	F	760/777 (97%)	-0.03	6 (0%) 82 71	41, 43, 44, 46	0
2	H	760/777 (97%)	-0.10	4 (0%) 87 78	41, 43, 44, 46	0
All	All	4840/4956 (97%)	0.06	63 (1%) 75 61	40, 43, 44, 46	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	462	PRO	6.4
1	E	462	PRO	6.4
2	H	137	SER	4.9
1	C	179	PRO	3.9
1	E	355	LYS	3.5
1	A	462	PRO	3.1
1	G	102	GLN	3.1
1	G	100	GLY	3.1
1	G	17	GLU	2.9
1	C	462	PRO	2.9
2	H	220	GLU	2.9
2	H	266	THR	2.8
1	E	115	ALA	2.8
2	B	777	ALA	2.8
1	G	20	THR	2.8
1	A	457	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	206	VAL	2.8
1	C	43	ASP	2.7
2	F	654	SER	2.7
1	G	19	PRO	2.7
2	D	461	LEU	2.6
1	G	101	SER	2.6
1	G	301	MET	2.6
1	A	130	ALA	2.6
2	H	777	ALA	2.6
1	A	413	ALA	2.5
2	F	686	GLY	2.5
1	E	215	ALA	2.4
2	B	623	ALA	2.4
1	A	438	ALA	2.4
2	F	328	SER	2.4
2	D	710	VAL	2.4
1	G	4	ALA	2.3
2	B	267	GLY	2.3
1	E	166	LEU	2.3
2	D	144	VAL	2.3
2	B	686	GLY	2.3
1	E	63	CYS	2.3
1	G	278	VAL	2.3
1	G	137	THR	2.3
2	F	23	LEU	2.3
1	G	222	VAL	2.3
1	E	130	ALA	2.2
1	G	136	CYS	2.2
2	B	703	ASP	2.2
1	A	179	PRO	2.2
2	B	634	ASP	2.2
1	G	275	VAL	2.2
1	G	70	ILE	2.2
2	D	2	SER	2.2
2	B	349	GLY	2.2
2	B	637	THR	2.1
2	F	526	ALA	2.1
2	D	347	PRO	2.1
1	C	200	THR	2.1
2	B	736	GLY	2.1
1	G	14	VAL	2.1
1	E	361	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	660	ASP	2.1
1	C	197	PRO	2.1
1	A	458	LEU	2.0
1	A	333	GLY	2.0
2	B	693	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

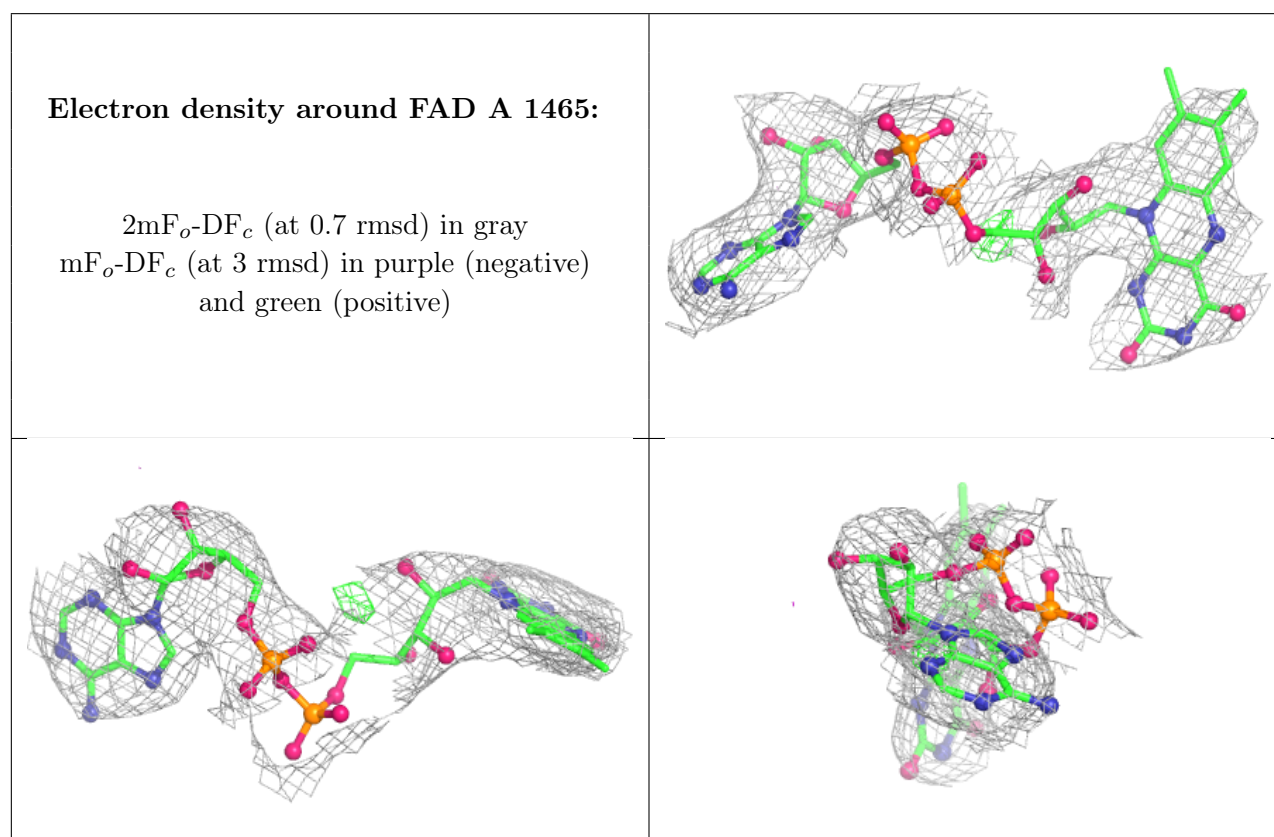
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	HPA	D	1780	10/10	0.83	0.14	43,43,43,43	0
7	HPA	B	1780	10/10	0.85	0.11	43,43,43,43	0
7	HPA	H	1780	10/10	0.89	0.12	43,43,43,43	0
4	FAD	A	1465	53/53	0.90	0.09	72,74,76,76	0
4	FAD	G	1465	53/53	0.91	0.09	74,76,79,80	0
7	HPA	F	1780	10/10	0.91	0.18	43,43,43,43	0
3	FES	E	1464	4/4	0.91	0.12	97,98,98,99	4
3	FES	G	1464	4/4	0.92	0.12	66,66,66,66	4
5	XAX	H	1778	28/28	0.93	0.15	52,55,62,63	28
5	XAX	B	1778	28/28	0.94	0.13	52,55,60,61	28
4	FAD	E	1465	53/53	0.94	0.09	62,66,78,78	0
3	FES	C	1464	4/4	0.94	0.08	107,108,108,108	4
5	XAX	F	1778	28/28	0.95	0.11	39,41,47,49	28
3	FES	A	1464	4/4	0.96	0.13	84,84,84,85	4
6	BA	H	1779	1/1	0.96	0.13	115,115,115,115	0
4	FAD	C	1465	53/53	0.96	0.07	46,51,55,55	0
6	BA	F	1779	1/1	0.97	0.14	98,98,98,98	0
5	XAX	D	1778	28/28	0.97	0.09	37,42,47,49	28

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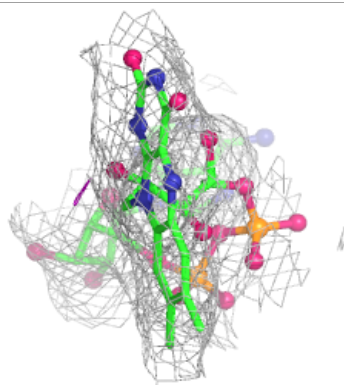
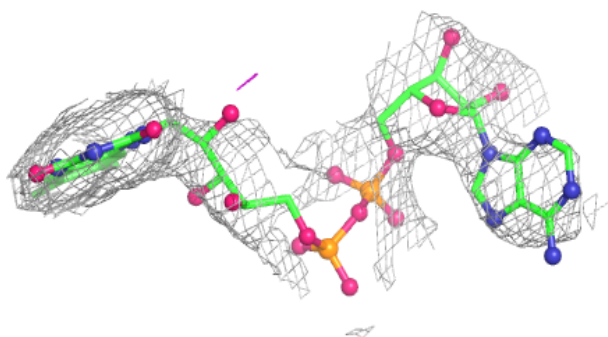
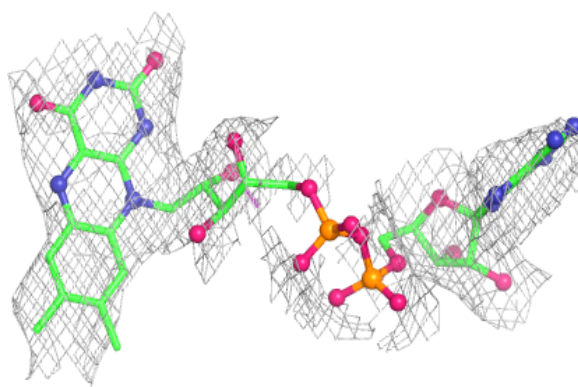
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BA	B	1779	1/1	0.97	0.15	108,108,108,108	0
3	FES	G	1463	4/4	0.98	0.10	44,45,45,46	4
6	BA	D	1779	1/1	0.98	0.13	105,105,105,105	0
3	FES	A	1463	4/4	0.99	0.09	29,30,30,30	4
3	FES	E	1463	4/4	0.99	0.10	32,32,32,33	4
3	FES	C	1463	4/4	0.99	0.10	24,25,25,25	4

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



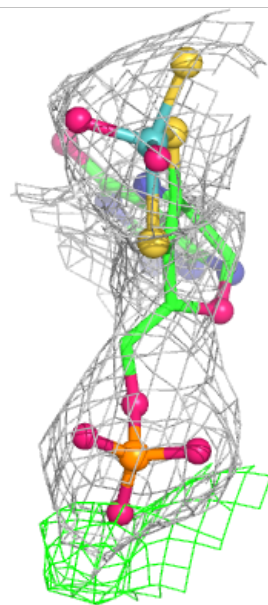
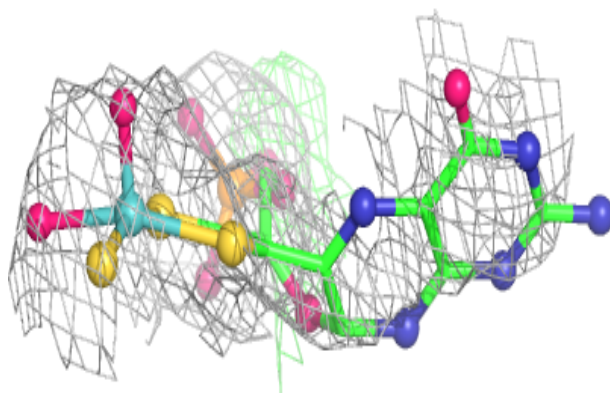
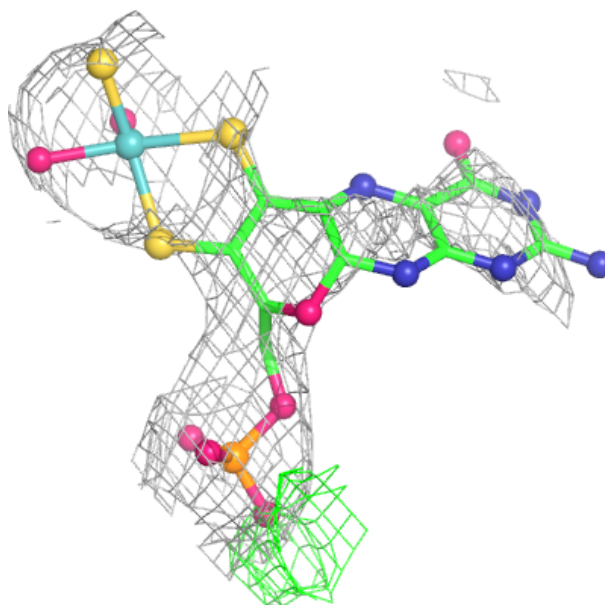
Electron density around FAD G 1465:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



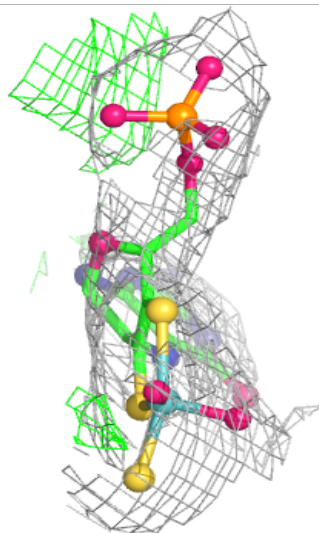
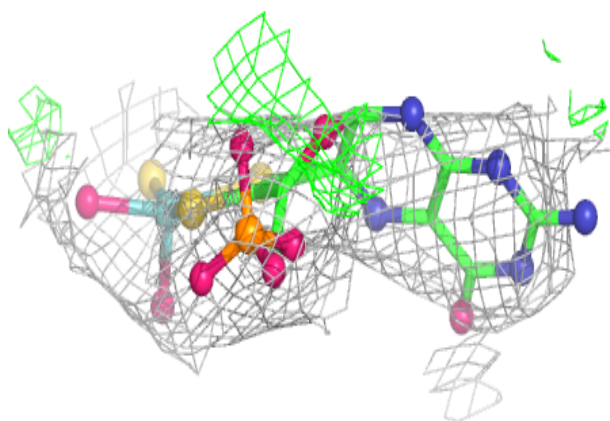
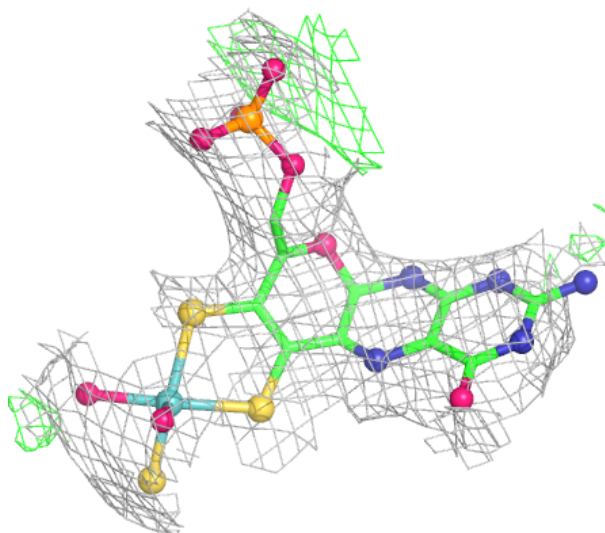
Electron density around XAX H 1778:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



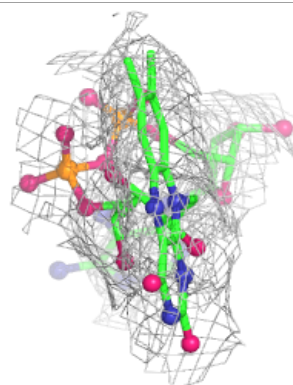
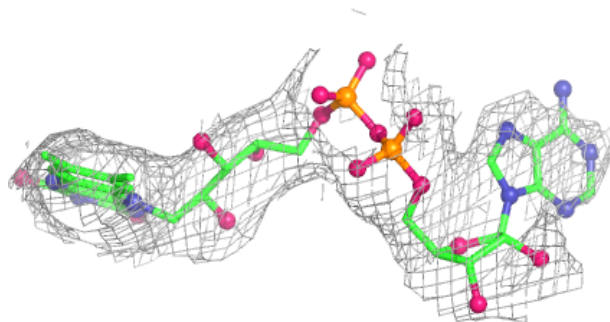
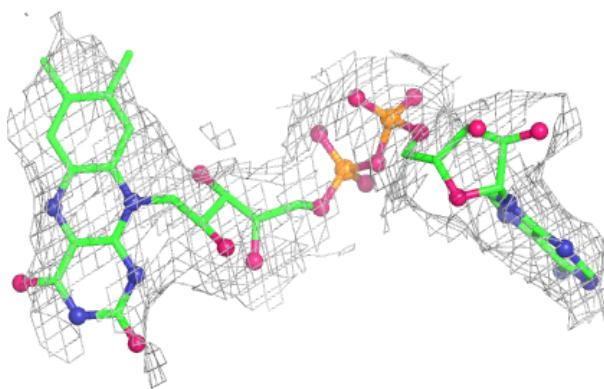
Electron density around XAX B 1778:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



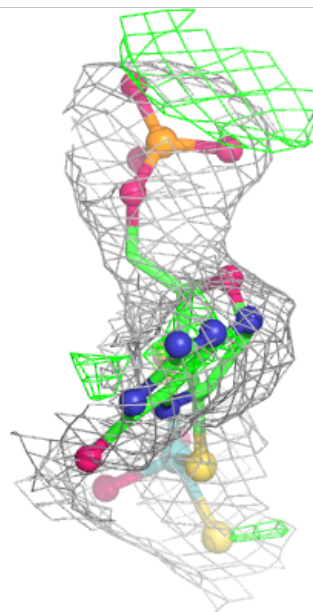
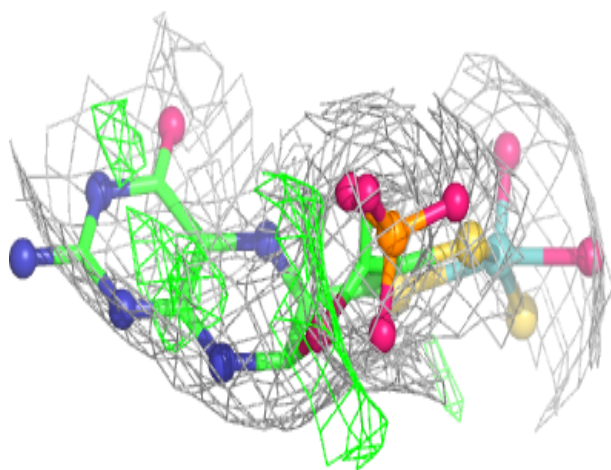
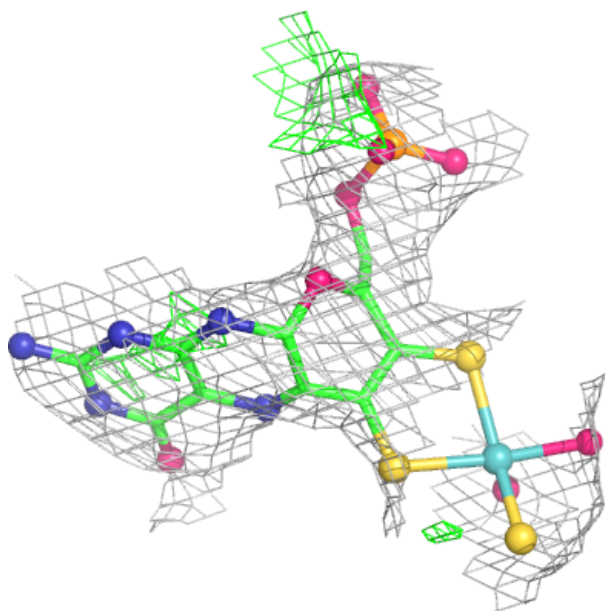
Electron density around FAD E 1465:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



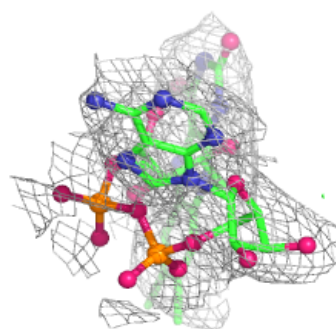
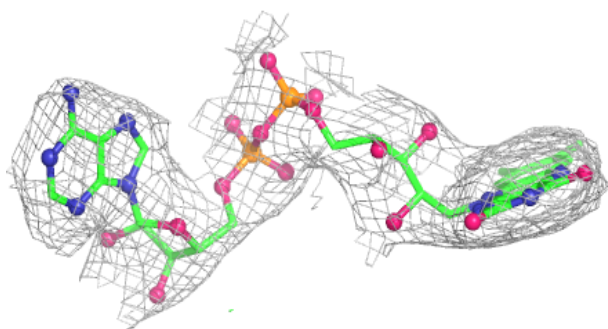
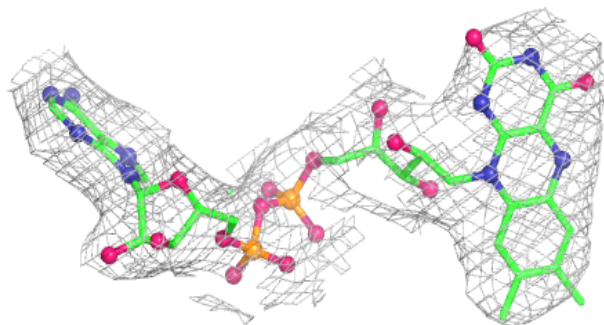
Electron density around XAX F 1778:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



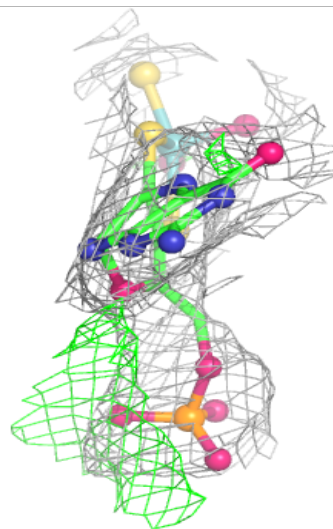
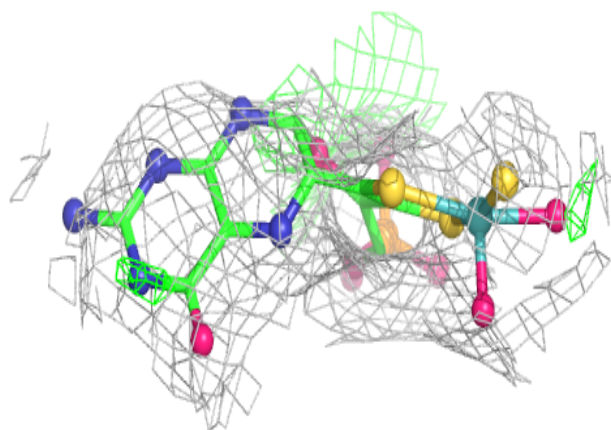
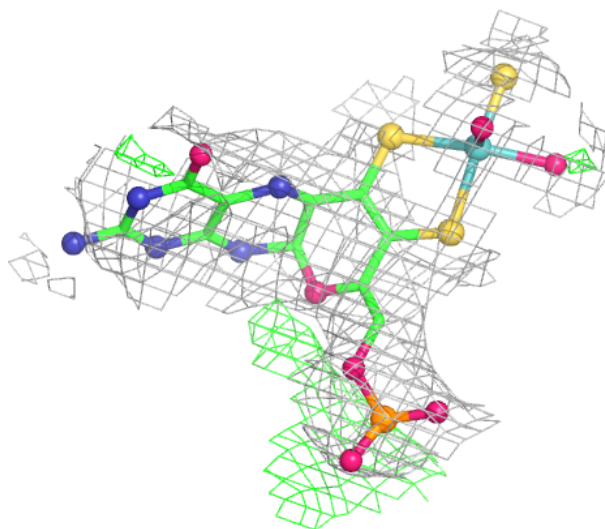
Electron density around FAD C 1465:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around XAX D 1778:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.