Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 04:06 PM EDT

PDB ID	:	1YCF / pdb_00001ycf
Title	:	Oxidized (di-ferric) FprA from Moorella thermoacetica
Authors	:	Silaghi-Dumitrescu, R.; Kurtz, D.M.; Lanzilotta, W.N.
Deposited on	:	2004-12-22
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

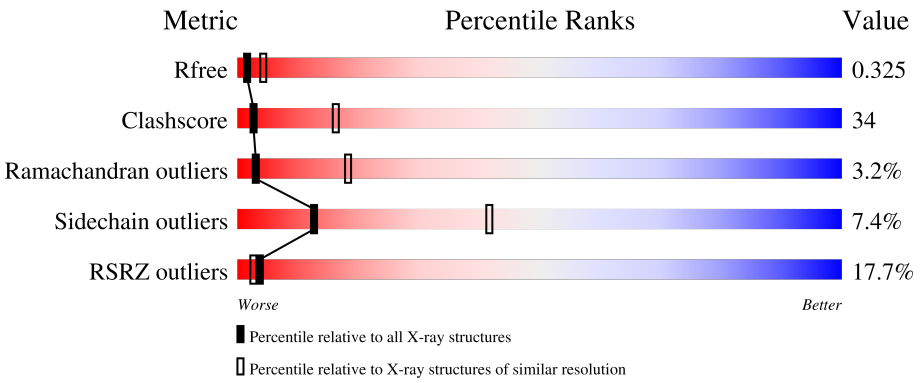
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 <=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	398	23% 47% 46% 6% •
1	B	398	13% 44% 47% 8% •
1	C	398	23% 55% 38% 7% •
1	D	398	12% 46% 45% 8% •

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
4	OXY	C	521	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12668 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.

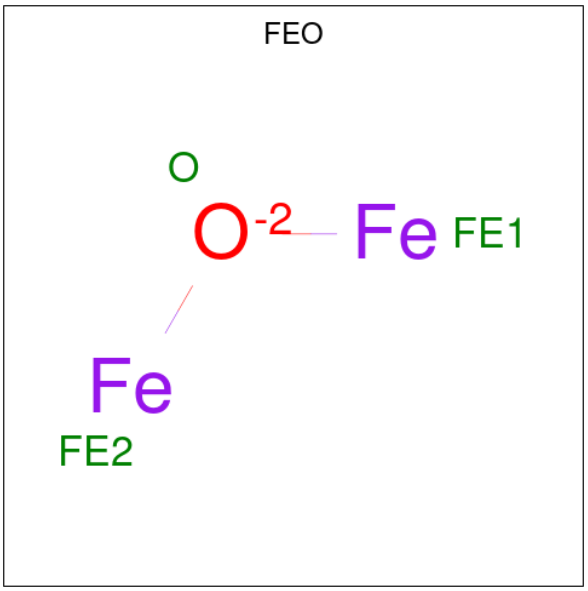
- Molecule 1 is a protein called Nitric oxide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	398	3115	2006	525	572	12	0	0	0
1	B	398	3115	2006	525	572	12	0	0	0
1	C	398	3115	2006	525	572	12	0	0	0
1	D	398	3115	2006	525	572	12	0	0	0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

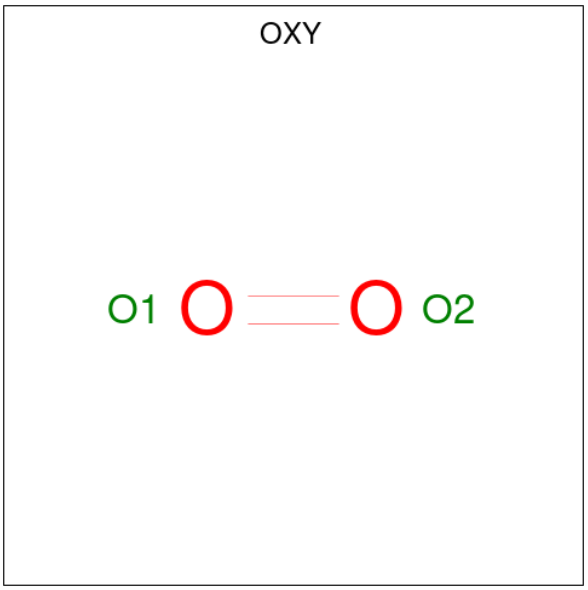
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0
2	B	1	1	1	0	0

- Molecule 3 is MU-OXO-DIIRON (CCD ID: FEO) (formula: Fe_2O).



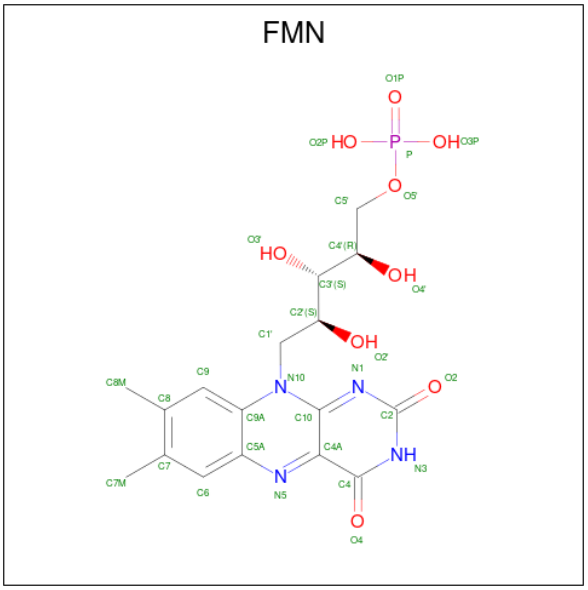
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	O		
3	A	1	3	2	1	0	0
3	B	1	3	2	1	0	0
3	C	1	3	2	1	0	0
3	D	1	3	2	1	0	0

- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	1	2	2	0	0
			Total	O		
4	B	1	2	2	0	0
			Total	O		
4	C	1	2	2	0	0
			Total	O		
4	D	1	2	2	0	0

- Molecule 5 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	31	17	4	9	1	0	0
			Total	C	N	O	P		
5	B	1	31	17	4	9	1	0	0
			Total	C	N	O	P		
5	C	1	31	17	4	9	1	0	0
			Total	C	N	O	P		
5	D	1	31	17	4	9	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	15	15	15	0	0
			Total	O		
6	B	14	14	14	0	0

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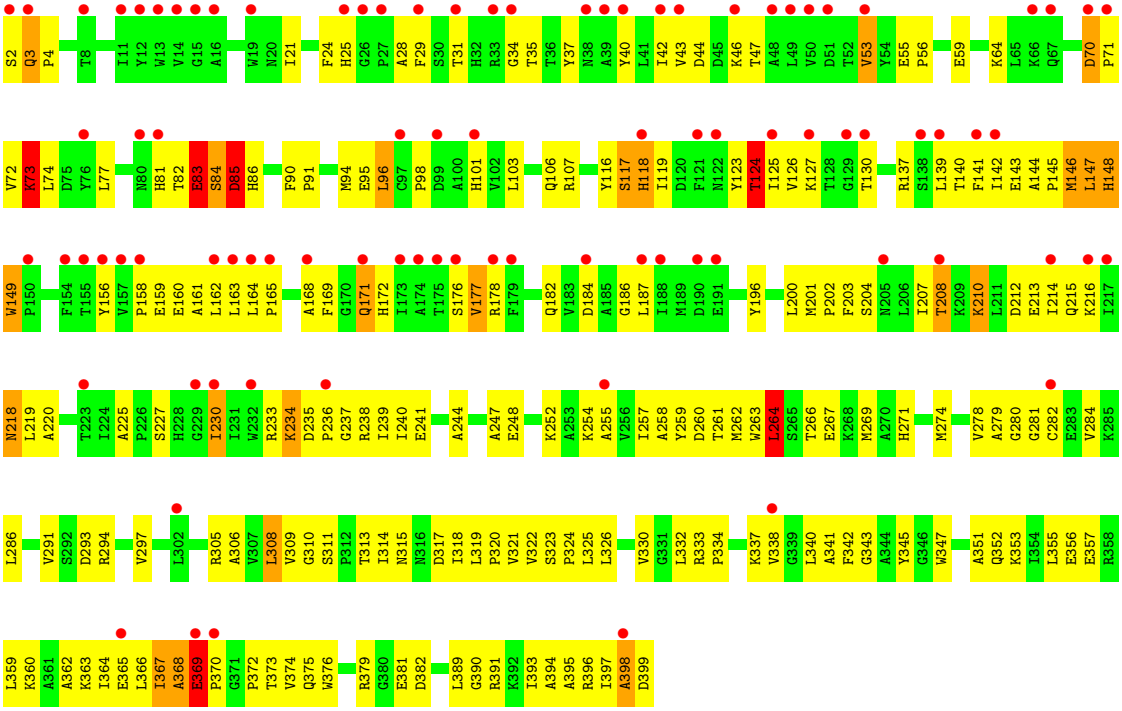
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	C	16	16	16	0	0
			Total	O		
6	D	16	16	16	0	0

3 Residue-property plots (i)

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.

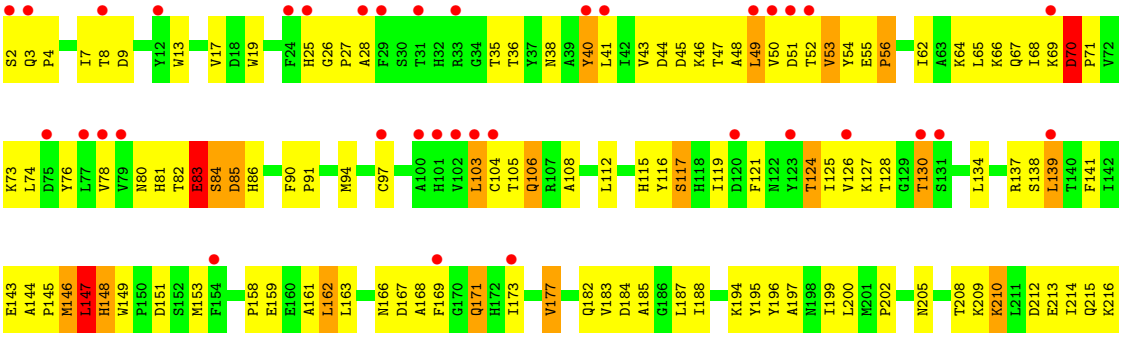
- Molecule 1: Nitric oxide reductase

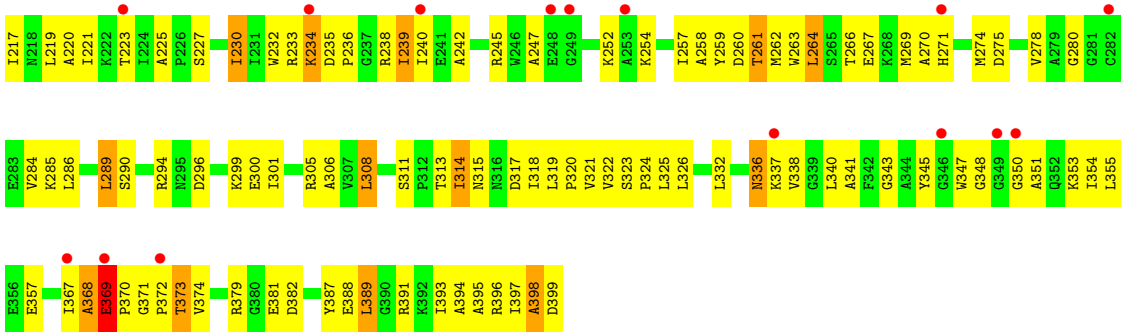
Chain A:



- Molecule 1: Nitric oxide reductase

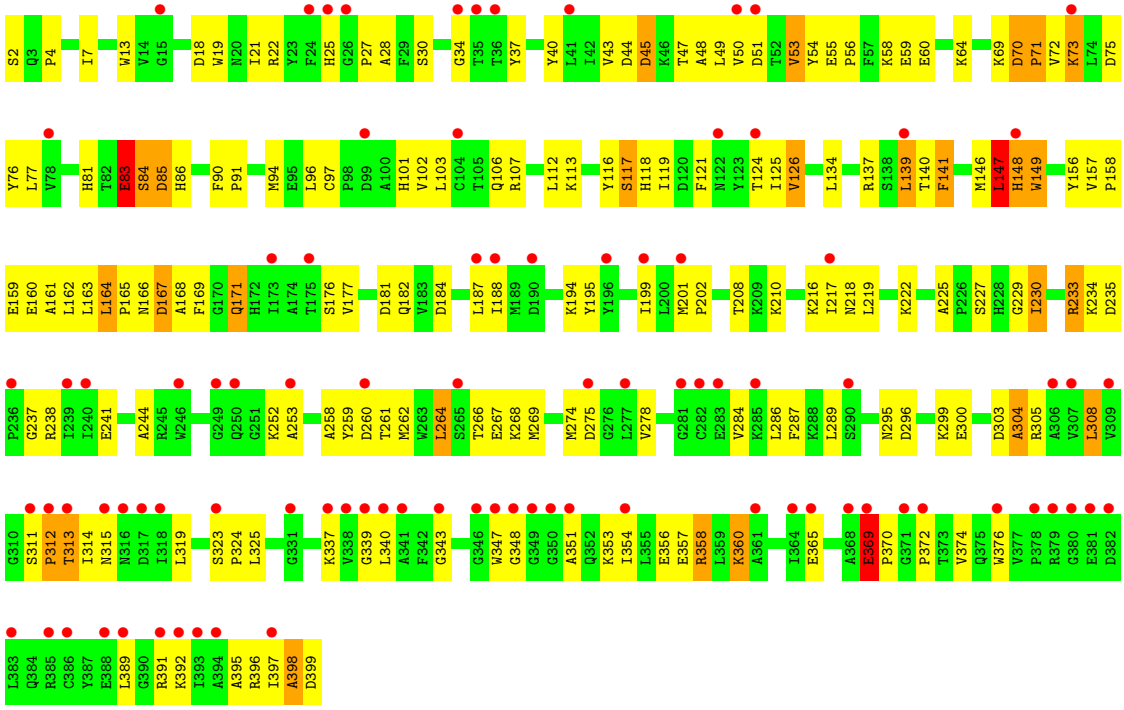
Chain B:





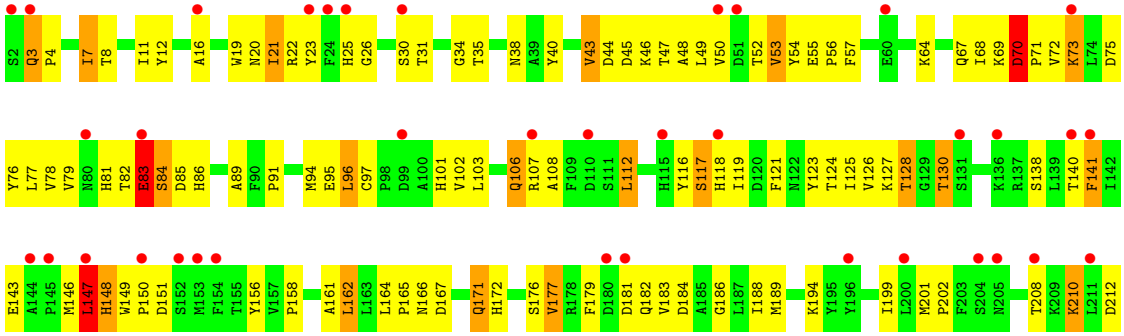
- Molecule 1: Nitric oxide reductase

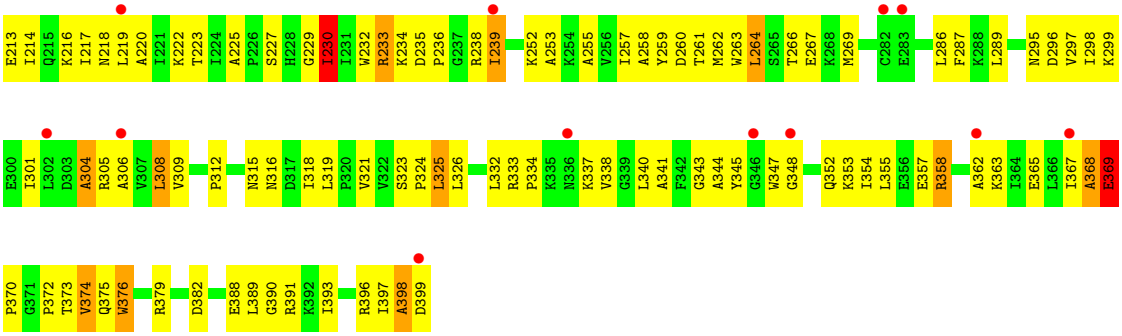
Chain C:



- Molecule 1: Nitric oxide reductase

Chain D:




E213 I214 Q215 K216 I217 N218 L219 A220 I221 K222 T223 I224 A225 P226 S227 H228 G229 I230 I231 W232 R233 K234 D235 P236 G237 R238 I239
K252 A253 K254 A255 V256 I257 A258 Y259 D260 T261 M262 W263 L264 S265 T266 E267 K268 M269
C282 E283
L286 F287 K288 L289
N295 D296 V297 I298 K299
E300 I301 L302 D303 A304 R305 A306 V307 L308 V309
P312
N315 N316 D317 I318 L319 P320 V321 V322 S323 P324 L325 L326
L332 R333 P334 K335 M336 K337 V338 G339 L340 A341 F342 G343 A344 Y345 G346 W347 G348
Q352 K353 I354 L355 E356 E357 R358
A362 K363 I364 E365 L366 I367 A368 E369
P370 G371 P372 T373 V374 Q375 W376
R379
D382
E388 L389 G390 R391 K392 I393
R396 I397 A398 D399

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	159.67Å 159.67Å 276.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.71 – 3.00 49.71 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.71-3.00) 99.2 (49.71-3.01)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 2.99Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.217 , 0.260 0.307 , 0.325	Depositor DCC
R_{free} test set	3604 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	81.2	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 59.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	12668	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FEO, ZN, OXY, FMN

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	0.43	0/3189	0.97	11/4335 (0.3%)
1	B	0.42	0/3189	0.99	17/4335 (0.4%)
1	C	0.44	0/3189	1.04	26/4335 (0.6%)
1	D	0.46	0/3189	1.07	25/4335 (0.6%)
All	All	0.44	0/12756	1.02	79/17340 (0.5%)

There are no bond length outliers.

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	3	GLN	N-CA-C	11.14	126.34	110.40
1	C	147	LEU	N-CA-C	-9.02	96.09	109.62
1	C	83	GLU	N-CA-C	8.71	121.56	111.11
1	C	199	ILE	N-CA-C	8.39	119.17	112.12
1	D	85	ASP	N-CA-C	-7.78	103.79	113.20
1	D	3	GLN	CA-C-N	7.65	127.60	120.03
1	D	3	GLN	C-N-CA	7.65	127.60	120.03
1	C	85	ASP	N-CA-C	-7.60	104.14	113.19
1	A	85	ASP	N-CA-C	-7.51	103.99	113.01
1	B	97	CYS	CA-C-N	7.44	126.97	119.24
1	B	97	CYS	C-N-CA	7.44	126.97	119.24
1	D	147	LEU	N-CA-C	-7.20	97.95	109.39
1	B	19	TRP	N-CA-C	7.16	119.08	111.28
1	B	369	GLU	CA-C-N	-7.05	111.02	119.84
1	B	369	GLU	C-N-CA	-7.05	111.02	119.84
1	B	70	ASP	CA-C-N	-7.00	112.22	120.13
1	B	70	ASP	C-N-CA	-7.00	112.22	120.13
1	B	147	LEU	N-CA-C	-6.68	98.77	109.39
1	D	70	ASP	CA-C-N	-6.63	112.83	119.99
1	D	70	ASP	C-N-CA	-6.63	112.83	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	7	ILE	N-CA-C	-6.59	103.06	112.35
1	D	369	GLU	CA-C-N	-6.45	111.78	119.84
1	D	369	GLU	C-N-CA	-6.45	111.78	119.84
1	D	264	LEU	N-CA-C	6.43	123.28	113.51
1	A	3	GLN	N-CA-C	6.36	118.68	109.84
1	D	45	ASP	N-CA-C	-6.15	104.34	112.34
1	D	176	SER	N-CA-C	-6.12	104.89	112.90
1	B	52	THR	CB-CA-C	-6.11	107.55	116.53
1	C	164	LEU	CA-C-N	6.08	126.60	120.04
1	C	164	LEU	C-N-CA	6.08	126.60	120.04
1	C	312	PRO	N-CA-C	-6.07	100.62	110.40
1	D	390	GLY	N-CA-C	-6.06	105.25	113.37
1	A	70	ASP	CA-C-N	-6.06	112.27	119.84
1	A	70	ASP	C-N-CA	-6.06	112.27	119.84
1	D	199	ILE	N-CA-C	6.00	117.16	112.12
1	C	229	GLY	N-CA-C	5.93	123.05	112.02
1	A	369	GLU	CA-C-N	-5.93	112.43	119.84
1	A	369	GLU	C-N-CA	-5.93	112.43	119.84
1	C	176	SER	N-CA-C	-5.91	104.42	111.69
1	D	141	PHE	N-CA-C	5.84	118.92	109.40
1	A	264	LEU	N-CA-C	5.80	123.15	110.80
1	D	179	PHE	N-CA-C	5.73	118.89	109.72
1	C	13	TRP	N-CA-C	-5.72	100.50	109.25
1	D	83	GLU	N-CA-C	5.69	120.76	111.37
1	C	339	GLY	N-CA-C	5.66	119.56	111.12
1	C	369	GLU	CA-C-N	-5.64	112.79	119.84
1	C	369	GLU	C-N-CA	-5.64	112.79	119.84
1	A	178	ARG	N-CA-C	5.60	120.76	113.88
1	C	157	VAL	CA-C-N	5.57	125.67	119.32
1	C	157	VAL	C-N-CA	5.57	125.67	119.32
1	C	97	CYS	CA-C-N	5.55	125.38	119.28
1	C	97	CYS	C-N-CA	5.55	125.38	119.28
1	C	141	PHE	N-CA-C	5.49	118.67	109.95
1	C	45	ASP	N-CA-C	-5.44	104.78	111.75
1	C	304	ALA	N-CA-C	5.40	117.69	110.35
1	D	264	LEU	N-CA-CB	-5.34	108.76	114.10
1	C	149	TRP	CA-C-N	5.34	124.67	118.85
1	C	149	TRP	C-N-CA	5.34	124.67	118.85
1	C	19	TRP	N-CA-C	5.26	117.02	111.28
1	B	289	LEU	N-CA-C	5.26	120.05	111.37
1	B	240	ILE	N-CA-C	-5.25	105.38	110.42
1	D	230	ILE	N-CA-C	5.25	118.08	109.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	304	ALA	N-CA-C	5.25	117.65	110.24
1	D	43	VAL	N-CA-C	5.25	115.14	107.37
1	B	264	LEU	N-CA-C	5.24	121.51	113.28
1	D	229	GLY	N-CA-C	5.21	121.29	112.22
1	B	7	ILE	N-CA-C	-5.17	105.37	111.00
1	A	149	TRP	CA-C-N	5.16	124.61	119.24
1	A	149	TRP	C-N-CA	5.16	124.61	119.24
1	A	390	GLY	N-CA-C	-5.12	106.21	112.77
1	B	52	THR	CA-C-O	5.10	121.54	118.33
1	B	52	THR	N-CA-C	5.10	113.65	108.75
1	B	40	TYR	N-CA-C	5.09	117.20	108.90
1	C	167	ASP	N-CA-C	5.08	117.21	111.11
1	C	75	ASP	N-CA-C	-5.07	107.23	113.41
1	D	19	TRP	N-CA-C	5.04	116.86	111.36
1	B	85	ASP	N-CA-C	-5.04	106.83	112.87
1	D	235	ASP	N-CA-C	5.03	116.01	108.76
1	C	264	LEU	N-CA-C	5.03	121.50	110.80

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	3115	0	3130	231	1
1	B	3115	0	3131	239	0
1	C	3115	0	3131	169	1
1	D	3115	0	3131	233	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	1	0
3	C	3	0	0	0	0
3	D	3	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	2	0	0	0	0
4	D	2	0	0	1	0
5	A	31	0	19	1	0
5	B	31	0	19	1	0
5	C	31	0	19	0	0
5	D	31	0	19	1	0
6	A	15	0	0	0	0
6	B	14	0	0	3	1
6	C	16	0	0	2	0
6	D	16	0	0	3	1
All	All	12668	0	12599	850	2

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 34.

All (850) 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)
1:D:306:ALA:HB2	1:D:397:ILE:HD11	1.23	1.16
1:B:314:ILE:HD11	1:B:319:LEU:HA	1.15	1.09
1:D:261:THR:HG22	1:D:266:THR:HB	1.38	1.03
1:D:70:ASP:HB3	1:D:71:PRO:HD3	1.39	1.00
1:A:305:ARG:HH12	1:A:399:ASP:HB2	1.25	0.98
1:B:234:LYS:HE3	1:B:234:LYS:HA	1.43	0.98
1:D:127:LYS:O	1:D:130:THR:HG23	1.67	0.95
1:D:81:HIS:NE2	1:D:83:GLU:HG3	1.81	0.95
1:B:381:GLU:CD	1:B:381:GLU:H	1.76	0.94
1:B:104:CYS:HA	1:B:153:MET:HE1	1.51	0.92
1:A:369:GLU:HB3	1:A:370:PRO:HD3	1.48	0.92
1:A:314:ILE:HD13	1:A:319:LEU:HD12	1.48	0.92
1:A:261:THR:HG22	1:A:266:THR:HB	1.52	0.90
1:C:305:ARG:HH12	1:C:399:ASP:HB2	1.33	0.90
1:C:70:ASP:HB3	1:C:71:PRO:HD3	1.50	0.90
1:A:314:ILE:HD11	1:A:320:PRO:HD3	1.53	0.89
1:B:70:ASP:HB3	1:B:71:PRO:HD3	1.54	0.88
1:C:262:MET:HE2	1:D:25:HIS:HB3	1.56	0.87
1:A:171:GLN:HE22	1:A:230:ILE:H	1.14	0.87
1:B:105:THR:HG23	1:B:153:MET:HE2	1.56	0.87
1:C:369:GLU:HB3	1:C:370:PRO:HD3	1.54	0.87
1:B:47:THR:HG21	1:B:69:LYS:NZ	1.90	0.85
1:C:269:MET:HE1	1:C:343:GLY:C	2.01	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:GLU:HB3	1:D:370:PRO:HD3	1.56	0.85
1:B:171:GLN:HE22	1:B:230:ILE:H	1.25	0.84
1:D:35:THR:HG21	1:D:172:HIS:ND1	1.92	0.83
1:A:338:VAL:HG11	1:A:367:ILE:HD13	1.61	0.81
1:C:47:THR:HG21	1:C:73:LYS:HD3	1.59	0.81
1:D:55:GLU:HB3	1:D:56:PRO:HD3	1.62	0.81
1:A:81:HIS:NE2	1:A:83:GLU:HG3	1.95	0.81
1:A:70:ASP:HB3	1:A:71:PRO:HD3	1.62	0.81
1:B:305:ARG:HB2	1:B:397:ILE:HG23	1.64	0.80
1:B:55:GLU:HB3	1:B:56:PRO:HD3	1.64	0.80
1:B:314:ILE:HD11	1:B:319:LEU:CA	2.08	0.80
1:C:4:PRO:HB3	1:C:64:LYS:HG2	1.64	0.79
1:D:306:ALA:CB	1:D:397:ILE:HD11	2.09	0.79
1:A:261:THR:CG2	1:A:266:THR:HB	2.13	0.79
1:C:69:LYS:HG2	1:C:73:LYS:HE3	1.65	0.79
1:A:77:LEU:HD13	1:A:94:MET:HE1	1.62	0.79
1:A:274:MET:HG3	1:A:284:VAL:HG11	1.64	0.79
1:A:333:ARG:HD2	1:A:363:LYS:HD2	1.65	0.78
1:B:81:HIS:HE1	1:B:149:TRP:HB2	1.49	0.78
3:D:530:FEO:O	4:D:531:OXY:O1	1.99	0.78
1:B:372:PRO:HG3	1:B:389:LEU:CD1	2.13	0.78
1:B:274:MET:O	1:B:278:VAL:HG23	1.83	0.77
1:B:274:MET:HG3	1:B:284:VAL:HG11	1.65	0.77
1:D:269:MET:HE1	1:D:343:GLY:O	1.85	0.77
1:C:107:ARG:HG3	1:C:107:ARG:HH11	1.49	0.76
1:D:305:ARG:HD2	1:D:397:ILE:HG23	1.67	0.76
1:A:314:ILE:HD11	1:A:319:LEU:HA	1.66	0.76
1:D:128:THR:HB	1:D:143:GLU:H	1.51	0.76
1:B:369:GLU:HB3	1:B:370:PRO:HD3	1.67	0.75
1:C:177:VAL:HG11	1:C:182:GLN:HB2	1.68	0.75
1:C:356:GLU:O	1:C:360:LYS:HD3	1.86	0.75
1:D:305:ARG:HH12	1:D:399:ASP:HB2	1.51	0.75
1:B:194:LYS:HB2	1:B:299:LYS:HD3	1.69	0.75
1:A:81:HIS:HE1	1:A:149:TRP:HB2	1.53	0.74
1:A:237:GLY:O	1:A:241:GLU:HG3	1.88	0.74
1:D:91:PRO:HB3	1:D:119:ILE:HD11	1.69	0.74
1:A:313:THR:HG22	1:A:351:ALA:CB	2.18	0.73
1:B:47:THR:HG21	1:B:69:LYS:HZ3	1.50	0.73
1:C:25:HIS:HB3	1:D:262:MET:HE2	1.70	0.73
1:D:181:ASP:OD1	1:D:233:ARG:HD2	1.88	0.73
1:D:171:GLN:HE22	1:D:230:ILE:H	1.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:HIS:CE1	1:C:227:SER:HB2	2.23	0.73
1:A:305:ARG:NH1	1:A:399:ASP:HB2	2.02	0.72
1:C:305:ARG:NH1	1:C:399:ASP:HB2	2.04	0.72
1:B:70:ASP:CB	1:B:71:PRO:HD3	2.18	0.72
1:D:372:PRO:HG3	1:D:389:LEU:CD1	2.19	0.72
1:A:81:HIS:CE1	1:A:149:TRP:HB2	2.24	0.72
1:C:274:MET:O	1:C:278:VAL:HG23	1.90	0.72
1:A:323:SER:HB2	1:A:324:PRO:HD3	1.72	0.71
1:B:43:VAL:HA	1:B:47:THR:HG22	1.72	0.71
1:D:261:THR:CG2	1:D:266:THR:HB	2.18	0.71
1:D:369:GLU:HB3	1:D:370:PRO:CD	2.20	0.71
1:D:162:LEU:CD1	1:D:164:LEU:HD21	2.20	0.71
1:A:369:GLU:HB3	1:A:370:PRO:CD	2.20	0.71
1:C:369:GLU:HB3	1:C:370:PRO:CD	2.20	0.71
1:C:391:ARG:HG3	1:C:391:ARG:HH11	1.56	0.71
1:D:70:ASP:HB3	1:D:71:PRO:CD	2.18	0.70
1:B:2:SER:HB2	6:B:628:HOH:O	1.91	0.70
1:B:239:ILE:H	1:B:239:ILE:HD12	1.57	0.70
1:C:70:ASP:O	1:C:71:PRO:C	2.34	0.70
1:A:313:THR:HG22	1:A:351:ALA:HB3	1.74	0.69
1:B:232:TRP:CE2	1:B:239:ILE:HG12	2.27	0.69
1:D:162:LEU:HD11	1:D:164:LEU:HD21	1.73	0.69
1:A:367:ILE:HD11	1:A:396:ARG:HD3	1.74	0.69
1:B:128:THR:HB	1:B:143:GLU:H	1.57	0.69
1:C:21:ILE:HG23	1:C:34:GLY:HA2	1.74	0.69
1:D:70:ASP:CB	1:D:71:PRO:HD3	2.18	0.69
1:A:234:LYS:HE3	1:A:234:LYS:HA	1.73	0.69
1:A:294:ARG:HH11	1:A:294:ARG:HB3	1.56	0.69
1:D:257:ILE:HG12	1:D:308:LEU:HG	1.74	0.69
1:A:294:ARG:HB3	1:A:294:ARG:NH1	2.07	0.69
1:A:117:SER:C	1:A:119:ILE:H	2.00	0.69
1:A:118:HIS:ND1	6:D:670:HOH:O	2.25	0.69
1:A:214:ILE:HG23	1:A:219:LEU:HD12	1.73	0.69
1:A:117:SER:O	1:A:119:ILE:N	2.26	0.68
1:C:398:ALA:O	1:C:399:ASP:HB3	1.93	0.68
1:D:171:GLN:HE22	1:D:230:ILE:N	1.92	0.68
1:C:177:VAL:CG1	1:C:182:GLN:HB2	2.23	0.68
1:A:262:MET:HE3	1:B:25:HIS:HB3	1.74	0.68
1:A:340:LEU:HD11	1:A:372:PRO:HD3	1.75	0.68
1:D:369:GLU:CB	1:D:370:PRO:HD3	2.24	0.68
1:C:25:HIS:HB3	1:D:262:MET:CE	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ASP:O	1:C:72:VAL:N	2.26	0.68
1:C:296:ASP:OD2	6:C:655:HOH:O	2.12	0.68
1:B:126:VAL:HG13	1:B:130:THR:OG1	1.94	0.68
1:B:4:PRO:HG2	1:B:67:GLN:HB3	1.76	0.67
1:C:117:SER:C	1:C:119:ILE:H	2.02	0.67
1:C:124:THR:HG23	1:C:124:THR:O	1.92	0.67
1:B:294:ARG:NH1	1:B:294:ARG:HB3	2.09	0.67
1:C:357:GLU:HG3	1:C:358:ARG:N	2.08	0.67
1:D:312:PRO:HD2	1:D:319:LEU:HD22	1.76	0.67
1:B:81:HIS:NE2	1:B:83:GLU:HG3	2.08	0.67
1:C:323:SER:HB2	1:C:324:PRO:HD3	1.75	0.67
1:C:70:ASP:HB3	1:C:71:PRO:CD	2.20	0.66
1:A:369:GLU:CB	1:A:370:PRO:HD3	2.23	0.66
1:C:347:TRP:CD1	1:C:348:GLY:H	2.14	0.66
1:A:21:ILE:HG23	1:A:34:GLY:HA2	1.77	0.66
1:A:55:GLU:HB3	1:A:56:PRO:HD3	1.78	0.66
1:C:43:VAL:HA	1:C:47:THR:HG22	1.78	0.66
1:A:306:ALA:HB2	1:A:397:ILE:HD11	1.78	0.66
1:A:333:ARG:HD2	1:A:363:LYS:CD	2.26	0.66
1:A:333:ARG:NH1	1:A:363:LYS:HE3	2.11	0.66
1:D:252:LYS:O	1:D:305:ARG:HG3	1.96	0.66
1:D:81:HIS:HE1	1:D:149:TRP:HB2	1.61	0.65
1:A:313:THR:HG22	1:A:351:ALA:H	1.62	0.65
1:A:338:VAL:CG1	1:A:367:ILE:HD13	2.27	0.65
1:B:369:GLU:CB	1:B:370:PRO:HD3	2.25	0.65
1:D:269:MET:HE1	1:D:343:GLY:C	2.21	0.65
1:D:318:ILE:HG22	1:D:319:LEU:N	2.12	0.65
1:D:333:ARG:HD2	1:D:363:LYS:HD3	1.77	0.65
1:B:40:TYR:CZ	1:B:225:ALA:HB1	2.32	0.65
1:B:296:ASP:OD2	6:B:629:HOH:O	2.13	0.64
1:D:83:GLU:O	1:D:84:SER:CB	2.45	0.64
1:A:43:VAL:HA	1:A:47:THR:HG22	1.79	0.64
1:A:294:ARG:NH1	1:A:294:ARG:CB	2.60	0.64
1:A:398:ALA:O	1:A:399:ASP:HB3	1.98	0.64
1:B:258:ALA:HB1	1:B:289:LEU:HD21	1.80	0.64
1:C:369:GLU:CB	1:C:370:PRO:HD3	2.26	0.64
1:A:25:HIS:HB3	1:B:262:MET:CE	2.27	0.64
1:A:35:THR:HG21	1:A:172:HIS:ND1	2.12	0.64
1:B:269:MET:HE2	1:B:374:VAL:HB	1.81	0.63
1:D:30:SER:H	1:D:295:ASN:ND2	1.96	0.63
1:C:40:TYR:CZ	1:C:225:ALA:HB1	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:THR:HG22	1:B:9:ASP:N	2.13	0.63
1:C:181:ASP:OD1	1:C:233:ARG:HD2	1.98	0.63
1:B:177:VAL:HG11	1:B:182:GLN:HB2	1.79	0.63
1:A:117:SER:C	1:A:119:ILE:N	2.56	0.63
1:D:128:THR:HG22	1:D:143:GLU:OE1	1.98	0.63
1:A:35:THR:HG22	1:A:172:HIS:HB3	1.80	0.63
1:C:171:GLN:HE22	1:C:230:ILE:N	1.97	0.63
1:A:162:LEU:HD21	1:A:164:LEU:HD21	1.81	0.62
1:B:242:ALA:HA	1:B:245:ARG:NH1	2.14	0.62
1:A:90:PHE:CE1	1:A:94:MET:HE3	2.34	0.62
1:A:126:VAL:HG11	1:A:141:PHE:CD1	2.34	0.62
1:A:274:MET:O	1:A:278:VAL:HG23	1.98	0.62
1:B:313:THR:HG22	1:B:351:ALA:HB3	1.80	0.62
1:B:372:PRO:HG3	1:B:389:LEU:HD13	1.81	0.62
1:B:381:GLU:CD	1:B:381:GLU:N	2.54	0.62
1:B:306:ALA:HA	1:B:338:VAL:O	1.99	0.62
1:D:47:THR:HG21	1:D:73:LYS:HD3	1.82	0.62
1:B:173:ILE:CD1	1:B:188:ILE:HD12	2.29	0.62
1:B:261:THR:HG21	1:B:267:GLU:HB2	1.80	0.62
1:B:2:SER:N	6:B:628:HOH:O	2.32	0.61
1:C:171:GLN:HE22	1:C:230:ILE:H	1.46	0.61
1:C:252:LYS:O	1:C:305:ARG:HG3	2.00	0.61
1:C:47:THR:CG2	1:C:73:LYS:HD3	2.28	0.61
1:C:103:LEU:HD22	1:C:124:THR:CG2	2.29	0.61
1:D:127:LYS:H	1:D:130:THR:HG21	1.65	0.61
1:D:397:ILE:O	1:D:397:ILE:HG22	2.00	0.61
1:A:326:LEU:HD11	1:A:355:LEU:HD23	1.82	0.61
1:B:347:TRP:CD1	1:B:348:GLY:H	2.19	0.61
1:B:369:GLU:HB3	1:B:370:PRO:CD	2.30	0.61
1:D:318:ILE:HD11	1:D:354:ILE:HB	1.82	0.61
1:A:72:VAL:HG21	1:A:96:LEU:HD11	1.81	0.61
1:A:140:THR:HG23	1:A:156:TYR:HB3	1.83	0.61
1:B:313:THR:HG22	1:B:351:ALA:CB	2.31	0.61
1:B:354:ILE:O	1:B:357:GLU:HG2	1.99	0.61
1:D:127:LYS:H	1:D:130:THR:CG2	2.14	0.61
1:A:184:ASP:CG	1:A:187:LEU:HD13	2.26	0.60
1:C:258:ALA:HB1	1:C:289:LEU:HD21	1.83	0.60
1:B:294:ARG:HB3	1:B:294:ARG:HH11	1.65	0.60
1:B:369:GLU:CG	1:B:370:PRO:HD3	2.31	0.60
1:D:166:ASN:ND2	1:D:167:ASP:H	1.99	0.60
1:A:291:VAL:HG12	1:A:291:VAL:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:LYS:HE3	1:B:300:GLU:OE1	2.01	0.60
1:A:40:TYR:CZ	1:A:225:ALA:HB1	2.36	0.60
1:B:318:ILE:CG2	1:B:319:LEU:N	2.64	0.60
1:C:305:ARG:HD2	1:C:397:ILE:HG23	1.83	0.60
1:C:83:GLU:O	1:C:84:SER:HB2	2.01	0.60
1:B:353:LYS:HG3	1:B:354:ILE:N	2.16	0.60
1:D:7:ILE:HD11	1:D:40:TYR:CE1	2.37	0.60
1:C:106:GLN:NE2	1:C:125:ILE:HG12	2.16	0.60
1:C:259:TYR:CD1	1:C:260:ASP:N	2.70	0.60
1:B:379:ARG:HB3	1:B:381:GLU:OE1	2.01	0.59
1:B:83:GLU:O	1:B:84:SER:HB2	2.02	0.59
1:C:83:GLU:O	1:C:84:SER:CB	2.49	0.59
1:D:140:THR:HG23	1:D:156:TYR:HB3	1.84	0.59
1:A:2:SER:O	1:A:64:LYS:HE3	2.02	0.59
1:C:264:LEU:O	1:C:268:LYS:HG2	2.03	0.59
1:A:381:GLU:OE1	1:A:381:GLU:N	2.31	0.59
1:D:72:VAL:HB	1:D:96:LEU:HD11	1.83	0.59
1:D:357:GLU:HG3	1:D:358:ARG:N	2.18	0.59
1:B:2:SER:O	1:B:64:LYS:HG2	2.03	0.59
1:A:81:HIS:HE1	1:A:149:TRP:CB	2.15	0.59
1:C:126:VAL:HG21	1:C:141:PHE:CE2	2.37	0.59
1:D:81:HIS:CE1	1:D:149:TRP:HB2	2.36	0.59
1:B:171:GLN:HE22	1:B:230:ILE:N	1.95	0.59
1:A:163:LEU:HG	1:A:165:PRO:HD3	1.83	0.58
1:B:117:SER:C	1:B:119:ILE:H	2.10	0.58
1:B:128:THR:H	1:B:143:GLU:HG3	1.68	0.58
1:B:13:TRP:CZ3	1:B:64:LYS:HE2	2.39	0.58
1:A:372:PRO:HG3	1:A:389:LEU:CD1	2.33	0.58
1:A:291:VAL:O	1:A:291:VAL:CG1	2.50	0.58
1:A:73:LYS:HE2	1:A:73:LYS:HA	1.85	0.58
1:D:269:MET:HE2	1:D:374:VAL:HB	1.85	0.58
1:D:298:ILE:HD13	1:D:332:LEU:CD1	2.33	0.58
1:A:313:THR:CG2	1:A:351:ALA:H	2.16	0.58
1:B:314:ILE:CD1	1:B:319:LEU:HD12	2.34	0.58
1:B:177:VAL:CG1	1:B:182:GLN:HB2	2.33	0.58
1:B:367:ILE:HG21	1:B:393:ILE:HG12	1.85	0.58
1:C:323:SER:HB3	1:D:323:SER:HB3	1.86	0.58
1:C:353:LYS:HG3	1:C:354:ILE:N	2.17	0.58
1:C:55:GLU:HB3	1:C:56:PRO:HD3	1.84	0.58
1:D:86:HIS:CE1	1:D:227:SER:HB2	2.39	0.58
1:A:177:VAL:HG21	1:A:182:GLN:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:LEU:N	1:D:308:LEU:HD23	2.18	0.58
1:C:37:TYR:HB2	1:C:53:VAL:HG22	1.85	0.58
1:D:345:TYR:HE2	1:D:373:THR:HG22	1.68	0.58
1:B:232:TRP:CD2	1:B:239:ILE:HG12	2.39	0.57
1:D:107:ARG:HD2	1:D:150:PRO:HB3	1.85	0.57
1:A:72:VAL:CG1	1:A:74:LEU:HD13	2.35	0.57
1:A:365:GLU:OE1	1:A:396:ARG:NH2	2.37	0.57
1:B:350:GLY:O	1:B:353:LYS:HG2	2.04	0.57
1:D:372:PRO:HG3	1:D:389:LEU:HD12	1.85	0.57
1:A:126:VAL:HG13	1:A:130:THR:OG1	2.05	0.57
1:B:81:HIS:CE1	1:B:149:TRP:HB2	2.36	0.57
1:B:372:PRO:CG	1:B:389:LEU:HD13	2.34	0.57
1:B:393:ILE:HG22	1:B:397:ILE:HD11	1.87	0.57
1:C:117:SER:C	1:C:119:ILE:N	2.62	0.57
1:C:216:LYS:C	1:C:218:ASN:H	2.10	0.57
1:B:70:ASP:HB3	1:B:71:PRO:CD	2.30	0.57
1:C:27:PRO:HB2	1:D:321:VAL:HG21	1.87	0.57
1:C:102:VAL:HG21	1:C:121:PHE:CD2	2.40	0.57
1:D:261:THR:HG21	1:D:267:GLU:N	2.19	0.57
1:A:25:HIS:HE1	1:A:83:GLU:OE2	1.88	0.57
1:B:86:HIS:CE1	1:B:227:SER:HB2	2.40	0.57
1:B:144:ALA:N	1:B:145:PRO:HD3	2.19	0.57
1:B:314:ILE:CD1	1:B:319:LEU:HA	2.10	0.57
1:C:252:LYS:HG3	1:C:303:ASP:OD1	2.05	0.57
1:D:345:TYR:HA	5:D:704:FMN:O2'	2.05	0.57
3:B:510:FEO:O	4:B:511:OXY:O1	2.23	0.56
1:A:368:ALA:O	1:A:369:GLU:C	2.46	0.56
1:B:82:THR:HG22	1:B:112:LEU:HD13	1.87	0.56
1:D:259:TYR:CD1	1:D:260:ASP:N	2.73	0.56
1:A:25:HIS:HB3	1:B:262:MET:HE3	1.88	0.56
1:A:98:PRO:HB3	1:D:391:ARG:NH2	2.19	0.56
1:A:103:LEU:HD23	1:A:124:THR:HG23	1.87	0.56
1:A:139:LEU:HD13	1:A:141:PHE:CZ	2.40	0.56
1:A:254:LYS:HG2	1:A:255:ALA:N	2.18	0.56
1:B:234:LYS:HE3	1:B:234:LYS:CA	2.27	0.56
1:C:305:ARG:HH12	1:C:399:ASP:CB	2.11	0.56
1:D:213:GLU:HA	1:D:216:LYS:HD2	1.87	0.56
1:B:128:THR:N	1:B:143:GLU:HG3	2.20	0.56
1:B:305:ARG:HB2	1:B:397:ILE:CG2	2.35	0.56
1:D:396:ARG:C	1:D:398:ALA:H	2.13	0.56
1:A:391:ARG:HG3	1:A:391:ARG:HH11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:GLU:O	1:D:391:ARG:HB3	2.06	0.56
1:B:234:LYS:HA	1:B:234:LYS:CE	2.27	0.56
1:B:350:GLY:O	1:B:354:ILE:HG13	2.06	0.56
1:D:398:ALA:O	1:D:399:ASP:HB3	2.06	0.56
1:D:117:SER:C	1:D:119:ILE:H	2.13	0.56
1:D:367:ILE:HG21	1:D:393:ILE:HG12	1.87	0.56
1:A:393:ILE:HG22	1:A:397:ILE:HD11	1.88	0.56
1:C:181:ASP:HB3	1:C:234:LYS:HE3	1.89	0.56
1:C:107:ARG:HG3	1:C:107:ARG:NH1	2.21	0.55
1:A:359:LEU:HD23	1:A:364:ILE:HD12	1.88	0.55
1:B:126:VAL:HG11	1:B:141:PHE:CG	2.41	0.55
1:B:294:ARG:NH1	1:B:294:ARG:CB	2.69	0.55
1:C:313:THR:HB	1:C:351:ALA:HB2	1.88	0.55
1:A:158:PRO:HG2	1:A:159:GLU:OE2	2.06	0.55
1:B:138:SER:H	1:B:159:GLU:CD	2.15	0.55
1:A:144:ALA:N	1:A:145:PRO:HD3	2.22	0.55
1:C:126:VAL:HG21	1:C:141:PHE:CD2	2.41	0.55
1:A:261:THR:HG21	1:A:267:GLU:N	2.21	0.55
1:D:340:LEU:HD11	1:D:372:PRO:HD3	1.89	0.55
1:D:261:THR:HG21	1:D:267:GLU:H	1.70	0.55
1:B:137:ARG:HA	1:B:159:GLU:HG2	1.89	0.54
1:A:83:GLU:O	1:A:84:SER:HB2	2.07	0.54
1:B:379:ARG:HB2	1:B:382:ASP:OD2	2.07	0.54
1:C:269:MET:HE1	1:C:343:GLY:O	2.07	0.54
1:D:47:THR:OG1	1:D:73:LYS:HD3	2.07	0.54
1:A:305:ARG:HD2	1:A:397:ILE:HG23	1.89	0.54
1:D:323:SER:HB2	1:D:324:PRO:HD3	1.88	0.54
1:B:314:ILE:HD12	1:B:320:PRO:HD3	1.89	0.54
1:C:148:HIS:HD2	1:C:167:ASP:OD2	1.90	0.54
1:D:126:VAL:HG11	1:D:141:PHE:CD2	2.42	0.54
1:D:391:ARG:HG3	1:D:391:ARG:HH11	1.72	0.54
1:B:389:LEU:O	1:B:393:ILE:HG13	2.08	0.54
1:D:3:GLN:OE1	1:D:67:GLN:HG2	2.08	0.54
1:D:50:VAL:HG21	1:D:164:LEU:HD12	1.90	0.54
1:D:83:GLU:O	1:D:84:SER:HB2	2.08	0.54
1:A:314:ILE:HD11	1:A:320:PRO:CD	2.34	0.54
1:B:162:LEU:HD23	1:B:163:LEU:N	2.22	0.54
1:B:166:ASN:ND2	1:B:167:ASP:H	2.06	0.54
1:B:213:GLU:HA	1:B:216:LYS:HD2	1.90	0.54
1:B:368:ALA:O	1:B:369:GLU:C	2.50	0.54
1:A:210:LYS:HE3	1:A:210:LYS:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ASP:O	1:B:216:LYS:HG3	2.08	0.54
1:B:367:ILE:HD13	1:B:396:ARG:HD2	1.89	0.54
1:D:166:ASN:HD22	1:D:167:ASP:H	1.55	0.54
1:A:70:ASP:O	1:A:72:VAL:N	2.41	0.54
1:B:236:PRO:O	1:B:239:ILE:HD12	2.07	0.54
1:C:372:PRO:HG3	1:C:389:LEU:HD12	1.89	0.54
1:D:326:LEU:HD11	1:D:355:LEU:HD23	1.90	0.54
1:A:305:ARG:HB2	1:A:397:ILE:HG23	1.89	0.53
1:A:257:ILE:HG12	1:A:308:LEU:HG	1.89	0.53
1:B:323:SER:HB2	1:B:324:PRO:HD3	1.90	0.53
1:D:287:PHE:CG	1:D:297:VAL:HG22	2.43	0.53
1:A:244:ALA:O	1:A:248:GLU:HG3	2.09	0.53
1:C:194:LYS:HB2	1:C:299:LYS:HD3	1.90	0.53
1:D:117:SER:O	1:D:119:ILE:N	2.42	0.53
1:D:212:ASP:O	1:D:216:LYS:HG3	2.08	0.53
1:A:271:HIS:HD1	1:A:274:MET:CE	2.21	0.53
1:B:104:CYS:CA	1:B:153:MET:HE1	2.33	0.53
1:B:139:LEU:HD12	1:B:139:LEU:O	2.09	0.53
1:C:158:PRO:HG2	1:C:159:GLU:OE2	2.08	0.53
1:D:233:ARG:HG2	1:D:234:LYS:N	2.23	0.53
1:A:118:HIS:HD1	1:D:388:GLU:CD	2.17	0.53
1:C:18:ASP:O	1:C:21:ILE:HG22	2.08	0.53
1:D:44:ASP:C	1:D:46:LYS:N	2.64	0.53
1:A:123:TYR:C	1:A:124:THR:HG22	2.34	0.53
1:B:173:ILE:HD12	1:B:188:ILE:CD1	2.38	0.53
1:D:345:TYR:HE2	1:D:373:THR:CG2	2.22	0.53
1:A:83:GLU:O	1:A:84:SER:CB	2.56	0.53
1:C:237:GLY:O	1:C:241:GLU:HG3	2.09	0.53
1:A:321:VAL:HG21	1:B:27:PRO:HG2	1.89	0.53
1:D:101:HIS:HE2	1:D:123:TYR:C	2.17	0.53
1:A:146:MET:HE1	1:B:347:TRP:CZ2	2.43	0.53
1:D:369:GLU:CB	1:D:370:PRO:CD	2.86	0.53
1:A:35:THR:HG22	1:A:172:HIS:CB	2.38	0.52
1:A:37:TYR:HB2	1:A:53:VAL:HG22	1.91	0.52
1:B:305:ARG:CB	1:B:397:ILE:HG23	2.36	0.52
1:B:367:ILE:O	1:B:367:ILE:HG13	2.09	0.52
1:B:242:ALA:HA	1:B:245:ARG:HH12	1.74	0.52
1:B:269:MET:CE	1:B:374:VAL:HB	2.39	0.52
1:C:166:ASN:ND2	1:C:167:ASP:H	2.08	0.52
1:B:17:VAL:HG13	1:B:36:THR:HG22	1.90	0.52
1:C:391:ARG:HG3	1:C:391:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ARG:HD2	1:A:397:ILE:CG2	2.39	0.52
1:C:216:LYS:C	1:C:218:ASN:N	2.67	0.52
1:C:369:GLU:CB	1:C:370:PRO:CD	2.87	0.52
1:B:326:LEU:HD11	1:B:355:LEU:HD23	1.90	0.52
1:A:21:ILE:CG2	1:A:34:GLY:HA2	2.40	0.52
1:B:263:TRP:O	1:B:264:LEU:HB2	2.09	0.52
1:D:108:ALA:HB2	1:D:151:ASP:HB2	1.91	0.52
1:D:43:VAL:HA	1:D:47:THR:HG22	1.92	0.52
1:D:183:VAL:HG12	1:D:184:ASP:N	2.24	0.52
1:D:362:ALA:O	1:D:363:LYS:HB2	2.09	0.52
1:A:213:GLU:HA	1:A:216:LYS:HD2	1.92	0.52
1:C:395:ALA:O	1:C:398:ALA:HB2	2.10	0.52
1:D:217:ILE:HG13	1:D:219:LEU:HG	1.92	0.52
1:A:314:ILE:CD1	1:A:319:LEU:HD12	2.31	0.52
1:A:375:GLN:O	1:A:376:TRP:HB2	2.08	0.52
1:B:46:LYS:O	1:B:134:LEU:HB3	2.08	0.52
1:B:53:VAL:CG1	1:B:54:TYR:N	2.73	0.52
1:B:185:ALA:C	1:B:238:ARG:HH22	2.17	0.52
1:C:140:THR:HG23	1:C:156:TYR:HB3	1.92	0.52
1:D:69:LYS:HG2	1:D:73:LYS:HE3	1.91	0.52
1:B:173:ILE:HD12	1:B:188:ILE:HD12	1.91	0.51
1:A:269:MET:HE1	1:A:343:GLY:C	2.36	0.51
1:C:30:SER:H	1:C:295:ASN:ND2	2.08	0.51
1:C:262:MET:CE	1:D:25:HIS:HB3	2.33	0.51
1:D:4:PRO:HG3	1:D:64:LYS:HB3	1.92	0.51
1:D:103:LEU:HD23	1:D:124:THR:CG2	2.40	0.51
1:D:162:LEU:HD13	1:D:164:LEU:HD21	1.92	0.51
1:A:314:ILE:O	1:A:315:ASN:C	2.52	0.51
1:A:161:ALA:HB1	1:A:220:ALA:O	2.10	0.51
1:B:314:ILE:CD1	1:B:320:PRO:HD3	2.40	0.51
1:D:47:THR:HG21	1:D:73:LYS:NZ	2.26	0.51
1:D:161:ALA:HB1	1:D:220:ALA:O	2.11	0.51
1:D:263:TRP:O	1:D:264:LEU:HB2	2.10	0.51
1:D:379:ARG:HG3	1:D:382:ASP:OD2	2.10	0.51
1:A:72:VAL:HG12	1:A:74:LEU:HD13	1.93	0.51
1:D:253:ALA:HA	1:D:397:ILE:HG22	1.93	0.51
1:C:372:PRO:HG3	1:C:389:LEU:CD1	2.41	0.51
1:D:21:ILE:HG23	1:D:34:GLY:HA2	1.91	0.51
1:D:255:ALA:HB2	1:D:306:ALA:HB3	1.92	0.51
1:A:162:LEU:HD21	1:A:164:LEU:CD2	2.40	0.51
1:B:82:THR:O	1:B:84:SER:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:HIS:CE1	1:C:149:TRP:HB2	2.45	0.51
1:C:365:GLU:CD	1:C:396:ARG:HH22	2.19	0.51
1:D:127:LYS:O	1:D:130:THR:CG2	2.49	0.51
1:A:31:THR:HG22	1:A:172:HIS:HB3	1.92	0.51
1:A:90:PHE:CZ	1:A:94:MET:HE3	2.46	0.51
1:D:35:THR:HG22	1:D:172:HIS:HB3	1.92	0.51
1:D:43:VAL:HG13	1:D:47:THR:CG2	2.41	0.51
1:D:345:TYR:CE2	1:D:373:THR:CG2	2.94	0.51
1:A:236:PRO:O	1:A:240:ILE:HG13	2.11	0.51
1:B:83:GLU:HA	1:B:149:TRP:CZ3	2.46	0.51
1:B:161:ALA:HB1	1:B:220:ALA:O	2.11	0.51
1:B:271:HIS:NE2	1:B:275:ASP:OD2	2.44	0.51
1:C:163:LEU:HG	1:C:165:PRO:HG3	1.92	0.51
1:A:356:GLU:O	1:A:360:LYS:HD3	2.11	0.50
1:D:123:TYR:CE1	1:D:125:ILE:HD13	2.46	0.50
1:D:38:ASN:HB2	1:D:227:SER:HA	1.92	0.50
1:D:47:THR:CG2	1:D:73:LYS:HD3	2.42	0.50
1:A:294:ARG:CZ	1:A:294:ARG:HB2	2.41	0.50
1:A:362:ALA:O	1:A:363:LYS:HB2	2.11	0.50
1:B:391:ARG:HG3	1:B:391:ARG:HH11	1.76	0.50
1:B:393:ILE:O	1:B:397:ILE:HG13	2.12	0.50
1:D:214:ILE:HG23	1:D:219:LEU:HD12	1.91	0.50
1:B:214:ILE:HG21	1:B:221:ILE:HD11	1.92	0.50
1:C:76:TYR:CD1	1:C:101:HIS:HB3	2.47	0.50
1:C:81:HIS:HE1	1:C:149:TRP:HB2	1.76	0.50
1:D:117:SER:C	1:D:119:ILE:N	2.63	0.50
1:A:31:THR:HG21	1:A:35:THR:CG2	2.42	0.50
1:A:118:HIS:ND1	1:D:388:GLU:OE2	2.45	0.50
1:A:235:ASP:CG	1:A:238:ARG:HG2	2.36	0.50
1:C:117:SER:O	1:C:119:ILE:N	2.44	0.50
1:D:177:VAL:CG1	1:D:182:GLN:HB2	2.42	0.50
1:A:147:LEU:O	1:A:148:HIS:HB3	2.11	0.50
1:B:83:GLU:O	1:B:84:SER:CB	2.59	0.50
1:C:84:SER:C	1:C:86:HIS:H	2.18	0.50
1:C:168:ALA:O	1:C:169:PHE:HB2	2.12	0.50
1:D:16:ALA:HB1	1:D:57:PHE:CD1	2.47	0.50
1:B:50:VAL:HA	1:B:78:VAL:HB	1.94	0.50
1:C:124:THR:O	1:C:124:THR:CG2	2.60	0.50
1:C:156:TYR:CZ	1:C:219:LEU:HD22	2.47	0.50
1:C:266:THR:HA	1:C:269:MET:HE3	1.94	0.50
1:B:168:ALA:O	1:B:169:PHE:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ALA:CB	1:B:299:LYS:HA	2.42	0.50
1:D:148:HIS:HD2	1:D:167:ASP:OD2	1.94	0.50
1:D:162:LEU:HD23	1:D:223:THR:OG1	2.12	0.50
1:D:171:GLN:NE2	1:D:230:ILE:H	2.09	0.50
1:A:139:LEU:O	1:A:139:LEU:HD12	2.12	0.50
1:B:235:ASP:OD1	1:B:238:ARG:HB2	2.12	0.50
1:B:369:GLU:HG3	1:B:370:PRO:HD3	1.94	0.50
1:C:94:MET:HE2	1:C:121:PHE:HB3	1.94	0.49
1:C:235:ASP:CG	1:C:238:ARG:HG2	2.37	0.49
1:C:314:ILE:HG12	1:C:315:ASN:ND2	2.27	0.49
1:B:159:GLU:CD	1:B:159:GLU:H	2.21	0.49
1:D:107:ARG:HD2	1:D:150:PRO:CB	2.42	0.49
1:A:263:TRP:O	1:A:264:LEU:HB2	2.11	0.49
1:B:158:PRO:HG2	1:B:159:GLU:OE2	2.10	0.49
1:C:163:LEU:O	1:C:165:PRO:HD3	2.12	0.49
1:A:314:ILE:CD1	1:A:319:LEU:HA	2.40	0.49
1:B:83:GLU:HA	1:B:149:TRP:CH2	2.48	0.49
1:B:257:ILE:HG12	1:B:308:LEU:HG	1.94	0.49
1:A:44:ASP:C	1:A:46:LYS:N	2.70	0.49
1:A:116:TYR:C	1:A:117:SER:O	2.52	0.49
1:A:308:LEU:HD23	1:A:308:LEU:N	2.28	0.49
1:D:69:LYS:O	1:D:70:ASP:C	2.56	0.49
1:D:177:VAL:HG11	1:D:182:GLN:HB2	1.94	0.49
1:B:318:ILE:HG23	1:B:319:LEU:N	2.27	0.49
1:B:369:GLU:CB	1:B:370:PRO:CD	2.87	0.49
1:C:94:MET:HE2	1:C:121:PHE:CB	2.42	0.49
1:D:20:ASN:HA	1:D:22:ARG:HH12	1.77	0.49
1:A:235:ASP:OD1	1:A:238:ARG:HG2	2.12	0.49
1:C:81:HIS:CD2	1:C:83:GLU:HB2	2.48	0.49
1:D:91:PRO:HB3	1:D:119:ILE:CD1	2.40	0.49
1:D:365:GLU:CD	1:D:396:ARG:HH12	2.20	0.49
1:B:49:LEU:HD12	1:B:74:LEU:HD21	1.94	0.49
1:D:23:TYR:HB3	1:D:26:GLY:O	2.13	0.49
1:D:325:LEU:HD22	1:D:325:LEU:O	2.13	0.49
1:B:94:MET:HE2	1:B:121:PHE:HB3	1.95	0.48
1:C:83:GLU:HB3	1:C:85:ASP:OD1	2.12	0.48
1:D:146:MET:C	1:D:148:HIS:N	2.69	0.48
1:D:318:ILE:CG2	1:D:319:LEU:N	2.76	0.48
1:A:341:ALA:C	1:A:352:GLN:HE22	2.19	0.48
1:D:372:PRO:CG	1:D:389:LEU:CD1	2.91	0.48
1:A:162:LEU:HD23	1:A:163:LEU:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ARG:HG2	1:B:396:ARG:HH11	1.78	0.48
1:C:253:ALA:HA	1:C:397:ILE:HG22	1.95	0.48
1:C:312:PRO:HD2	1:C:319:LEU:HD22	1.94	0.48
1:D:146:MET:C	1:D:148:HIS:H	2.21	0.48
1:B:177:VAL:HG13	1:B:182:GLN:OE1	2.13	0.48
1:B:217:ILE:HG22	1:B:217:ILE:O	2.12	0.48
1:D:253:ALA:HA	1:D:397:ILE:CG2	2.43	0.48
1:D:305:ARG:CD	1:D:397:ILE:HG23	2.39	0.48
1:A:106:GLN:OE1	1:A:125:ILE:HG12	2.13	0.48
1:A:212:ASP:O	1:A:215:GLN:HB3	2.13	0.48
1:A:372:PRO:HG3	1:A:389:LEU:HD12	1.95	0.48
1:C:90:PHE:HB3	1:C:91:PRO:CD	2.44	0.48
1:B:379:ARG:O	1:B:382:ASP:HB2	2.13	0.48
1:D:50:VAL:HA	1:D:78:VAL:HB	1.96	0.48
1:A:86:HIS:CE1	1:A:227:SER:HB2	2.48	0.48
1:A:125:ILE:HG22	1:A:127:LYS:HZ2	1.79	0.48
1:B:4:PRO:HD3	1:B:67:GLN:HG2	1.94	0.48
1:B:194:LYS:CB	1:B:299:LYS:HD3	2.39	0.48
1:B:395:ALA:O	1:B:398:ALA:HB2	2.13	0.48
1:B:314:ILE:HD13	1:B:319:LEU:HD12	1.95	0.48
1:D:156:TYR:CE2	1:D:219:LEU:HD22	2.49	0.48
1:A:294:ARG:HD2	1:A:324:PRO:HB2	1.96	0.48
1:B:70:ASP:CG	1:B:71:PRO:HD3	2.38	0.48
1:C:84:SER:C	1:C:86:HIS:N	2.71	0.48
1:A:116:TYR:O	1:A:117:SER:C	2.56	0.47
1:A:171:GLN:HE22	1:A:230:ILE:N	1.97	0.47
1:B:127:LYS:O	1:B:130:THR:HG23	2.14	0.47
1:B:147:LEU:O	1:B:148:HIS:HB3	2.13	0.47
1:C:177:VAL:HG11	1:C:182:GLN:CB	2.39	0.47
1:D:305:ARG:NH1	1:D:399:ASP:HB2	2.22	0.47
1:D:236:PRO:O	1:D:239:ILE:HD12	2.13	0.47
1:A:238:ARG:HD3	1:A:241:GLU:OE1	2.14	0.47
1:A:353:LYS:O	1:A:357:GLU:HB2	2.15	0.47
1:A:83:GLU:HA	1:A:149:TRP:CZ3	2.50	0.47
1:A:379:ARG:H	1:A:382:ASP:HB2	1.80	0.47
1:C:81:HIS:HE1	1:C:149:TRP:CG	2.33	0.47
1:C:304:ALA:O	1:C:337:LYS:HE3	2.15	0.47
1:D:50:VAL:HG21	1:D:164:LEU:CD1	2.44	0.47
1:D:81:HIS:HE1	1:D:149:TRP:CB	2.27	0.47
1:D:116:TYR:O	1:D:117:SER:C	2.58	0.47
1:A:118:HIS:CE1	6:D:670:HOH:O	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:VAL:HG21	1:B:27:PRO:CG	2.44	0.47
1:A:393:ILE:HG22	1:A:397:ILE:CD1	2.45	0.47
1:C:146:MET:C	1:C:148:HIS:N	2.73	0.47
1:D:333:ARG:NH1	1:D:333:ARG:HG3	2.29	0.47
1:A:252:LYS:O	1:A:305:ARG:HG3	2.15	0.47
1:C:134:LEU:HD11	1:C:139:LEU:HD23	1.96	0.47
1:B:8:THR:HG22	1:B:9:ASP:H	1.77	0.47
1:B:54:TYR:CD2	1:B:56:PRO:HD2	2.50	0.47
1:B:167:ASP:O	1:B:195:TYR:HE2	1.97	0.47
1:C:156:TYR:CE2	1:C:158:PRO:HA	2.49	0.47
1:C:171:GLN:NE2	1:C:230:ILE:H	2.12	0.47
1:B:117:SER:C	1:B:119:ILE:N	2.69	0.47
1:C:217:ILE:HG22	1:C:217:ILE:O	2.15	0.47
1:D:40:TYR:CZ	1:D:225:ALA:HB1	2.50	0.47
1:A:234:LYS:HA	1:A:234:LYS:CE	2.44	0.47
1:B:83:GLU:HB3	1:B:85:ASP:OD1	2.15	0.47
1:B:116:TYR:O	1:B:117:SER:O	2.31	0.47
1:A:70:ASP:HB3	1:A:71:PRO:CD	2.37	0.46
1:A:159:GLU:CD	1:A:159:GLU:H	2.24	0.46
1:A:345:TYR:CD1	1:A:345:TYR:C	2.93	0.46
1:C:365:GLU:OE1	1:C:396:ARG:NH2	2.47	0.46
1:A:165:PRO:HG3	1:A:169:PHE:HD2	1.80	0.46
1:A:262:MET:CE	1:B:25:HIS:HB3	2.42	0.46
1:A:70:ASP:O	1:A:71:PRO:C	2.57	0.46
1:A:294:ARG:CB	1:A:294:ARG:CZ	2.93	0.46
1:D:69:LYS:HZ3	1:D:71:PRO:HD2	1.80	0.46
1:D:106:GLN:NE2	1:D:125:ILE:HG12	2.29	0.46
1:A:59:GLU:CD	1:A:59:GLU:H	2.23	0.46
1:A:168:ALA:O	1:A:169:PHE:HB2	2.16	0.46
1:B:267:GLU:O	1:B:270:ALA:HB3	2.16	0.46
1:D:124:THR:HG23	1:D:124:THR:O	2.15	0.46
1:D:369:GLU:CG	1:D:370:PRO:HD3	2.45	0.46
1:A:356:GLU:HG2	1:A:366:LEU:HD13	1.98	0.46
1:B:44:ASP:O	1:B:45:ASP:C	2.59	0.46
1:C:171:GLN:NE2	1:C:188:ILE:HD11	2.30	0.46
1:A:73:LYS:HE2	1:A:73:LYS:CA	2.45	0.46
1:C:253:ALA:HA	1:C:397:ILE:CG2	2.45	0.46
1:D:46:LYS:HA	1:D:75:ASP:OD2	2.15	0.46
1:A:42:ILE:O	1:A:47:THR:HA	2.15	0.46
1:A:148:HIS:O	1:A:149:TRP:HD1	1.99	0.46
1:C:156:TYR:CE2	1:C:219:LEU:HD22	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:SER:C	1:D:86:HIS:H	2.21	0.46
1:D:184:ASP:O	1:D:188:ILE:HG22	2.15	0.46
1:D:76:TYR:CD1	1:D:101:HIS:HB3	2.50	0.46
1:B:94:MET:HE2	1:B:121:PHE:CB	2.47	0.45
1:B:280:GLY:HA3	1:B:394:ALA:CB	2.46	0.45
1:B:80:ASN:HA	1:B:153:MET:HG2	1.98	0.45
1:B:90:PHE:N	1:B:91:PRO:HD2	2.31	0.45
1:C:58:LYS:HE3	1:C:59:GLU:OE2	2.16	0.45
1:D:116:TYR:C	1:D:117:SER:O	2.57	0.45
1:D:318:ILE:HG22	1:D:319:LEU:H	1.81	0.45
1:A:91:PRO:HB3	1:A:119:ILE:HD11	1.97	0.45
1:A:147:LEU:HA	1:A:147:LEU:HD12	1.45	0.45
1:A:204:SER:O	1:A:207:ILE:HB	2.16	0.45
1:A:294:ARG:HH11	1:A:294:ARG:CB	2.25	0.45
1:D:82:THR:CG2	1:D:112:LEU:HD13	2.46	0.45
1:D:376:TRP:HA	1:D:376:TRP:CE3	2.51	0.45
1:A:84:SER:C	1:A:86:HIS:H	2.25	0.45
1:A:305:ARG:CB	1:A:397:ILE:HG23	2.46	0.45
1:B:68:ILE:O	1:B:69:LYS:HG3	2.15	0.45
1:B:294:ARG:HD2	1:B:324:PRO:HB2	1.98	0.45
1:A:381:GLU:H	1:A:381:GLU:CD	2.23	0.45
1:B:127:LYS:H	1:B:130:THR:HG21	1.80	0.45
1:C:44:ASP:H	1:C:47:THR:HG22	1.81	0.45
1:C:69:LYS:CG	1:C:73:LYS:HE3	2.42	0.45
1:C:347:TRP:CG	1:C:348:GLY:H	2.33	0.45
1:C:372:PRO:CG	1:C:389:LEU:HD12	2.46	0.45
1:D:8:THR:CG2	1:D:11:ILE:HD12	2.47	0.45
1:D:79:VAL:HG12	1:D:79:VAL:O	2.15	0.45
1:D:210:LYS:HE3	1:D:210:LYS:HA	1.98	0.45
1:A:261:THR:HG21	1:A:267:GLU:H	1.82	0.45
1:A:395:ALA:O	1:A:398:ALA:HB2	2.17	0.45
1:B:4:PRO:CD	1:B:67:GLN:HG2	2.47	0.45
1:D:140:THR:HG22	1:D:158:PRO:HD3	1.99	0.45
1:A:143:GLU:C	1:A:145:PRO:HD3	2.41	0.45
1:A:201:MET:N	1:A:202:PRO:HD2	2.32	0.45
1:A:333:ARG:HH11	1:A:363:LYS:NZ	2.14	0.45
1:A:391:ARG:HG3	1:A:391:ARG:NH1	2.30	0.45
1:B:62:ILE:CG2	1:B:66:LYS:HE3	2.47	0.45
1:C:166:ASN:HA	1:C:227:SER:HB3	1.98	0.45
1:A:77:LEU:HD13	1:A:94:MET:CE	2.40	0.45
1:A:98:PRO:HB3	1:D:391:ARG:CZ	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:THR:CG2	1:B:9:ASP:N	2.78	0.45
1:B:41:LEU:HD22	1:B:65:LEU:CD2	2.47	0.45
1:C:347:TRP:CD1	1:C:348:GLY:N	2.83	0.45
1:D:147:LEU:HA	1:D:147:LEU:HD12	1.42	0.45
1:D:367:ILE:HG21	1:D:393:ILE:CG1	2.47	0.45
1:B:127:LYS:H	1:B:130:THR:CG2	2.30	0.45
1:D:95:GLU:OE1	1:D:95:GLU:HA	2.17	0.45
1:D:102:VAL:HG21	1:D:121:PHE:CD2	2.52	0.45
1:A:310:GLY:HA2	1:A:342:PHE:O	2.17	0.45
1:B:38:ASN:HB2	1:B:227:SER:HA	1.99	0.45
1:B:261:THR:HB	1:B:266:THR:HB	1.98	0.45
1:B:318:ILE:HG23	1:B:319:LEU:H	1.81	0.45
1:B:353:LYS:CG	1:B:354:ILE:N	2.79	0.45
1:C:165:PRO:O	1:C:166:ASN:HB3	2.17	0.45
1:D:48:ALA:HB2	1:D:76:TYR:HB2	1.99	0.45
1:D:53:VAL:CG1	1:D:54:TYR:N	2.79	0.45
1:B:208:THR:HG23	1:B:247:ALA:HB1	1.99	0.44
1:B:269:MET:HE1	1:B:343:GLY:C	2.42	0.44
1:B:290:SER:HB3	1:B:321:VAL:HG11	1.99	0.44
1:B:347:TRP:CD1	1:B:348:GLY:N	2.85	0.44
1:C:48:ALA:HB2	1:C:76:TYR:HB2	1.99	0.44
1:C:308:LEU:N	1:C:308:LEU:HD23	2.32	0.44
1:D:258:ALA:HB1	1:D:289:LEU:HD21	1.98	0.44
1:A:293:ASP:O	1:A:297:VAL:HG23	2.18	0.44
1:D:12:TYR:CE2	1:D:68:ILE:HD12	2.52	0.44
1:A:208:THR:HG23	1:A:247:ALA:HB3	1.98	0.44
1:B:80:ASN:HA	1:B:153:MET:HE3	2.00	0.44
1:C:69:LYS:HG2	1:C:73:LYS:CE	2.43	0.44
1:D:236:PRO:HA	1:D:239:ILE:HD11	2.00	0.44
1:D:353:LYS:HG3	1:D:354:ILE:N	2.32	0.44
1:B:41:LEU:HD22	1:B:65:LEU:HD23	1.99	0.44
1:B:105:THR:HG23	1:B:153:MET:CE	2.39	0.44
1:C:161:ALA:HB3	1:C:222:LYS:HB2	1.99	0.44
1:C:287:PHE:HZ	1:C:300:GLU:HG3	1.83	0.44
1:D:35:THR:CG2	1:D:172:HIS:HB3	2.46	0.44
1:D:94:MET:HE2	1:D:121:PHE:CB	2.47	0.44
1:D:397:ILE:O	1:D:398:ALA:C	2.60	0.44
1:A:333:ARG:NH1	1:A:363:LYS:CE	2.81	0.44
1:A:374:VAL:CG1	1:A:375:GLN:N	2.80	0.44
1:B:35:THR:OG1	1:B:36:THR:N	2.51	0.44
1:B:205:ASN:O	1:B:209:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:GLU:HG3	1:B:370:PRO:CD	2.47	0.44
1:D:201:MET:N	1:D:202:PRO:HD2	2.33	0.44
1:A:126:VAL:CG1	1:A:127:LYS:N	2.81	0.44
1:A:184:ASP:OD1	1:A:186:GLY:N	2.51	0.44
1:A:305:ARG:HB2	1:A:397:ILE:CG2	2.48	0.44
1:B:139:LEU:HD13	1:B:141:PHE:CZ	2.52	0.44
1:B:210:LYS:HB2	1:B:210:LYS:NZ	2.33	0.44
1:D:52:THR:HB	1:D:89:ALA:HB3	2.00	0.44
1:D:255:ALA:CB	1:D:306:ALA:HB3	2.47	0.44
1:A:116:TYR:O	1:A:117:SER:O	2.35	0.44
1:A:234:LYS:HE3	1:A:234:LYS:CA	2.45	0.44
1:B:294:ARG:CB	1:B:294:ARG:CZ	2.95	0.44
1:C:103:LEU:CD2	1:C:124:THR:HG22	2.47	0.44
1:C:398:ALA:O	1:C:399:ASP:CB	2.62	0.44
1:D:35:THR:HG22	1:D:172:HIS:C	2.43	0.44
1:A:81:HIS:NE2	1:A:83:GLU:CG	2.74	0.44
1:B:212:ASP:HB3	1:B:216:LYS:HE3	2.00	0.44
1:B:260:ASP:HB3	1:B:319:LEU:HD23	2.00	0.44
1:B:301:ILE:O	1:B:337:LYS:HE3	2.18	0.44
1:B:318:ILE:HD11	1:B:355:LEU:HG	2.00	0.44
1:D:94:MET:HE2	1:D:121:PHE:HB2	1.99	0.44
1:D:216:LYS:C	1:D:218:ASN:H	2.25	0.44
1:D:333:ARG:HG3	1:D:333:ARG:HH11	1.82	0.44
1:B:106:GLN:HG2	1:B:125:ILE:HG21	1.99	0.44
1:B:127:LYS:HG2	1:B:143:GLU:OE1	2.18	0.44
1:B:336:ASN:O	1:B:337:LYS:HG2	2.18	0.44
1:C:107:ARG:NH1	1:C:107:ARG:CG	2.80	0.44
1:A:29:PHE:C	1:A:29:PHE:CD2	2.97	0.43
1:A:35:THR:HG21	1:A:172:HIS:HD1	1.79	0.43
1:A:280:GLY:HA3	1:A:394:ALA:HB1	1.99	0.43
1:B:184:ASP:HB3	1:B:187:LEU:HB2	2.01	0.43
1:B:199:ILE:HG22	1:B:200:LEU:HD23	2.00	0.43
1:B:311:SER:HB2	1:B:322:VAL:HG21	2.00	0.43
1:D:123:TYR:C	1:D:123:TYR:CD1	2.96	0.43
1:C:2:SER:N	1:C:60:GLU:OE2	2.51	0.43
1:C:274:MET:HG3	1:C:284:VAL:HG11	1.99	0.43
1:D:269:MET:CE	1:D:374:VAL:HB	2.47	0.43
1:D:315:ASN:O	1:D:316:ASN:HB2	2.17	0.43
1:A:82:THR:O	1:A:83:GLU:C	2.61	0.43
1:A:203:PHE:O	1:A:207:ILE:HG12	2.17	0.43
1:A:280:GLY:HA3	1:A:394:ALA:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:SER:HB3	1:B:323:SER:HB3	1.99	0.43
1:B:269:MET:HE1	1:B:343:GLY:O	2.18	0.43
1:C:113:LYS:HE2	1:C:113:LYS:HB3	1.85	0.43
1:D:16:ALA:HB1	1:D:57:PHE:HD1	1.83	0.43
1:D:35:THR:HG22	1:D:172:HIS:CB	2.48	0.43
1:D:54:TYR:O	1:D:55:GLU:C	2.61	0.43
1:D:81:HIS:HE1	1:D:149:TRP:CG	2.35	0.43
1:D:389:LEU:O	1:D:393:ILE:HG13	2.18	0.43
1:A:126:VAL:HG11	1:A:141:PHE:CG	2.54	0.43
1:A:333:ARG:CZ	1:A:363:LYS:HE3	2.49	0.43
1:C:181:ASP:CB	1:C:234:LYS:HE3	2.49	0.43
1:D:106:GLN:HE21	1:D:125:ILE:HG12	1.83	0.43
1:D:194:LYS:HB2	1:D:299:LYS:HD3	2.01	0.43
1:B:280:GLY:HA3	1:B:394:ALA:HB1	1.99	0.43
1:C:7:ILE:HD11	1:C:40:TYR:CE1	2.54	0.43
1:C:261:THR:HG21	1:C:267:GLU:HB2	2.01	0.43
1:C:308:LEU:HD13	1:C:340:LEU:HD23	2.00	0.43
1:A:90:PHE:HB3	1:A:91:PRO:CD	2.48	0.43
1:A:137:ARG:HA	1:A:159:GLU:HG2	2.00	0.43
1:A:326:LEU:O	1:A:330:VAL:HG23	2.18	0.43
1:C:44:ASP:O	1:C:45:ASP:C	2.61	0.43
1:C:50:VAL:HG21	1:C:164:LEU:CD1	2.49	0.43
1:C:126:VAL:HG11	1:C:141:PHE:CD2	2.54	0.43
1:C:171:GLN:HE21	1:C:188:ILE:HD11	1.84	0.43
1:D:375:GLN:O	1:D:376:TRP:HB2	2.18	0.43
1:A:24:PHE:HZ	1:A:85:ASP:CG	2.27	0.43
1:C:147:LEU:HD12	1:C:147:LEU:HA	1.52	0.43
1:A:200:LEU:C	1:A:202:PRO:HD2	2.44	0.43
1:A:311:SER:HB2	1:A:322:VAL:HG21	2.01	0.43
1:C:116:TYR:C	1:C:117:SER:O	2.58	0.43
1:D:318:ILE:HD13	1:D:355:LEU:HD23	2.00	0.43
1:A:84:SER:C	1:A:86:HIS:N	2.74	0.43
1:A:177:VAL:HG22	1:A:182:GLN:CD	2.44	0.43
1:B:49:LEU:HD22	1:B:51:ASP:O	2.18	0.43
1:B:306:ALA:HB2	1:B:397:ILE:HD11	2.01	0.43
1:B:367:ILE:CD1	1:B:396:ARG:HD2	2.49	0.43
1:C:53:VAL:HG13	1:C:54:TYR:N	2.34	0.43
1:C:389:LEU:HD23	1:C:389:LEU:HA	1.86	0.43
1:D:138:SER:O	1:D:158:PRO:HD2	2.19	0.43
1:C:25:HIS:CB	1:D:262:MET:HE2	2.45	0.43
1:D:354:ILE:HA	1:D:357:GLU:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:VAL:HG13	1:D:47:THR:HG22	2.00	0.42
1:A:202:PRO:HB3	1:A:332:LEU:O	2.19	0.42
1:D:398:ALA:O	1:D:399:ASP:CB	2.67	0.42
1:A:305:ARG:HH12	1:A:399:ASP:CB	2.13	0.42
1:B:116:TYR:C	1:B:117:SER:O	2.62	0.42
1:B:314:ILE:O	1:B:315:ASN:C	2.62	0.42
1:D:53:VAL:HG13	1:D:54:TYR:N	2.34	0.42
1:A:317:ASP:OD1	1:A:318:ILE:N	2.46	0.42
1:B:274:MET:HG3	1:B:284:VAL:CG1	2.43	0.42
1:C:91:PRO:HB3	1:C:119:ILE:HD11	2.00	0.42
1:D:184:ASP:OD1	1:D:186:GLY:N	2.53	0.42
1:D:347:TRP:CD1	1:D:348:GLY:H	2.38	0.42
1:B:70:ASP:CB	1:B:71:PRO:CD	2.86	0.42
1:B:387:TYR:C	1:B:387:TYR:CD2	2.97	0.42
1:C:47:THR:HG21	1:C:73:LYS:CD	2.40	0.42
1:C:146:MET:C	1:C:148:HIS:H	2.27	0.42
1:C:312:PRO:CD	1:C:319:LEU:HD22	2.49	0.42
1:C:397:ILE:O	1:C:398:ALA:C	2.63	0.42
1:D:31:THR:HG23	1:D:31:THR:O	2.19	0.42
1:A:208:THR:HG23	1:A:247:ALA:CB	2.50	0.42
1:A:351:ALA:O	1:A:355:LEU:HG	2.20	0.42
1:A:367:ILE:O	1:A:367:ILE:HG23	2.19	0.42
1:B:317:ASP:HA	1:B:354:ILE:CD1	2.49	0.42
1:A:258:ALA:O	1:A:309:VAL:HA	2.20	0.42
1:A:259:TYR:CD1	1:A:260:ASP:N	2.88	0.42
1:A:279:ALA:C	1:A:281:GLY:H	2.27	0.42
1:B:147:LEU:O	1:B:148:HIS:CB	2.67	0.42
1:B:345:TYR:HE2	1:B:373:THR:OG1	2.03	0.42
1:C:391:ARG:NH1	1:C:391:ARG:CG	2.82	0.42
1:B:305:ARG:HD2	1:B:397:ILE:CG2	2.50	0.42
1:D:189:MET:HB2	1:D:238:ARG:NH2	2.34	0.42
1:D:258:ALA:O	1:D:309:VAL:HA	2.20	0.42
1:D:260:ASP:O	1:D:312:PRO:HD3	2.19	0.42
1:D:396:ARG:C	1:D:398:ALA:N	2.73	0.42
1:A:376:TRP:CD2	1:B:115:HIS:HE1	2.38	0.42
1:D:96:LEU:HD13	1:D:97:CYS:SG	2.60	0.42
1:B:54:TYR:O	1:B:55:GLU:C	2.62	0.41
1:B:294:ARG:CZ	1:B:294:ARG:HB2	2.50	0.41
1:B:317:ASP:HA	1:B:354:ILE:HD11	2.02	0.41
1:B:398:ALA:O	1:B:399:ASP:CB	2.67	0.41
1:C:201:MET:N	1:C:202:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:THR:HG22	1:D:172:HIS:CA	2.50	0.41
1:B:202:PRO:HB3	1:B:332:LEU:O	2.20	0.41
1:C:103:LEU:CD2	1:C:124:THR:CG2	2.97	0.41
1:C:195:TYR:CE2	6:C:640:HOH:O	2.74	0.41
1:D:53:VAL:CG1	1:D:57:PHE:HB2	2.50	0.41
1:D:301:ILE:O	1:D:337:LYS:HE3	2.19	0.41
1:A:25:HIS:HB3	1:B:262:MET:HE2	2.02	0.41
1:A:81:HIS:HE1	1:A:149:TRP:CG	2.38	0.41
1:A:306:ALA:HA	1:A:338:VAL:O	2.20	0.41
1:B:259:TYR:CD1	1:B:260:ASP:N	2.89	0.41
1:B:308:LEU:N	1:B:308:LEU:HD23	2.35	0.41
1:B:345:TYR:HA	5:B:702:FMN:O2'	2.20	0.41
1:B:369:GLU:O	1:B:371:GLY:N	2.53	0.41
1:C:357:GLU:CG	1:C:358:ARG:N	2.80	0.41
1:D:232:TRP:CE2	1:D:239:ILE:HG12	2.55	0.41
1:D:344:ALA:HA	1:D:374:VAL:O	2.19	0.41
1:A:81:HIS:NE2	1:A:148:HIS:CD2	2.89	0.41
1:A:171:GLN:NE2	1:A:230:ILE:H	1.96	0.41
1:A:196:TYR:CD2	1:A:196:TYR:C	2.98	0.41
1:B:76:TYR:CD1	1:B:103:LEU:HD21	2.56	0.41
1:B:117:SER:O	1:B:119:ILE:N	2.53	0.41
1:B:236:PRO:HA	1:B:239:ILE:HD11	2.03	0.41
1:C:125:ILE:HD12	1:C:125:ILE:N	2.35	0.41
1:D:7:ILE:HD11	1:D:40:TYR:HE1	1.83	0.41
1:D:35:THR:HG21	1:D:172:HIS:CG	2.53	0.41
1:D:161:ALA:HB3	1:D:222:LYS:HB2	2.03	0.41
1:D:296:ASP:OD2	6:D:672:HOH:O	2.21	0.41
1:D:357:GLU:CG	1:D:358:ARG:N	2.83	0.41
1:D:368:ALA:O	1:D:369:GLU:C	2.64	0.41
1:B:212:ASP:O	1:B:215:GLN:HB3	2.20	0.41
1:C:54:TYR:CG	1:C:56:PRO:HD2	2.55	0.41
1:C:73:LYS:H	1:C:73:LYS:HG2	1.47	0.41
1:D:338:VAL:HG11	1:D:367:ILE:HD13	2.03	0.41
1:A:3:GLN:HA	1:A:4:PRO:HD3	1.84	0.41
1:A:334:PRO:HB2	1:A:337:LYS:HG3	2.03	0.41
1:B:3:GLN:HA	1:B:4:PRO:HD3	1.92	0.41
1:B:144:ALA:N	1:B:145:PRO:CD	2.83	0.41
1:C:323:SER:HB3	1:D:323:SER:CB	2.49	0.41
1:D:70:ASP:CB	1:D:71:PRO:CD	2.88	0.41
1:D:103:LEU:CD2	1:D:124:THR:HG21	2.51	0.41
1:D:304:ALA:O	1:D:337:LYS:HE3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PRO:HB3	1:A:119:ILE:CD1	2.51	0.41
1:A:262:MET:HA	1:B:26:GLY:HA3	2.03	0.41
1:A:263:TRP:O	1:A:264:LEU:CB	2.69	0.41
1:B:196:TYR:CD2	1:B:196:TYR:C	2.99	0.41
1:C:372:PRO:CG	1:C:389:LEU:CD1	2.98	0.41
1:D:263:TRP:O	1:D:264:LEU:CB	2.69	0.41
1:A:369:GLU:CB	1:A:370:PRO:CD	2.88	0.41
1:A:398:ALA:O	1:A:399:ASP:CB	2.69	0.41
1:D:305:ARG:HD2	1:D:397:ILE:CG2	2.43	0.41
1:A:90:PHE:N	1:A:91:PRO:HD2	2.36	0.41
1:B:41:LEU:HD12	1:B:48:ALA:O	2.21	0.41
1:B:252:LYS:O	1:B:254:LYS:N	2.49	0.41
1:B:340:LEU:HG	1:B:341:ALA:N	2.35	0.41
1:B:388:GLU:O	1:B:391:ARG:HB3	2.21	0.41
1:C:134:LEU:HB2	1:C:137:ARG:O	2.21	0.41
1:D:165:PRO:O	1:D:166:ASN:HB3	2.21	0.41
1:D:333:ARG:O	1:D:334:PRO:C	2.64	0.41
1:A:216:LYS:C	1:A:218:ASN:N	2.77	0.41
1:B:146:MET:C	1:B:148:HIS:N	2.79	0.40
1:B:210:LYS:O	1:B:214:ILE:HG13	2.20	0.40
1:C:126:VAL:HG11	1:C:141:PHE:CG	2.56	0.40
1:C:184:ASP:HB3	1:C:187:LEU:HB2	2.03	0.40
1:C:241:GLU:O	1:C:244:ALA:HB3	2.20	0.40
1:A:142:ILE:HD11	1:A:219:LEU:HD11	2.03	0.40
1:B:108:ALA:CA	1:B:151:ASP:HB2	2.52	0.40
1:B:274:MET:HE2	1:B:274:MET:HB3	1.78	0.40
1:C:22:ARG:HD3	1:C:22:ARG:HA	1.83	0.40
1:C:311:SER:O	1:C:343:GLY:HA3	2.22	0.40
1:D:147:LEU:O	1:D:148:HIS:HB3	2.22	0.40
1:D:341:ALA:C	1:D:352:GLN:HE22	2.29	0.40
1:A:95:GLU:OE2	1:A:95:GLU:C	2.65	0.40
1:A:160:GLU:O	1:A:161:ALA:HB3	2.22	0.40
1:A:318:ILE:HD11	1:A:355:LEU:HD21	2.04	0.40
1:B:53:VAL:HG12	1:B:54:TYR:O	2.22	0.40
1:B:143:GLU:C	1:B:145:PRO:HD3	2.47	0.40
1:C:4:PRO:CB	1:C:64:LYS:HG2	2.42	0.40
1:C:47:THR:OG1	1:C:73:LYS:HD3	2.21	0.40
1:C:324:PRO:HD3	1:D:324:PRO:HG3	2.02	0.40
1:B:80:ASN:HB3	1:B:153:MET:O	2.21	0.40
1:C:140:THR:HG22	1:C:158:PRO:HD3	2.02	0.40
1:C:392:LYS:O	1:C:395:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:THR:HG22	1:D:11:ILE:HB	2.02	0.40
1:A:40:TYR:CD2	1:A:164:LEU:HD22	2.56	0.40
1:A:261:THR:HB	5:A:701:FMN:O1P	2.21	0.40
1:B:183:VAL:HG12	1:B:184:ASP:N	2.36	0.40
1:D:44:ASP:C	1:D:46:LYS:H	2.30	0.40
1:D:181:ASP:HB3	1:D:234:LYS:CG	2.51	0.40
1:D:298:ILE:HD13	1:D:332:LEU:HD11	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:SER:OG	1:C:275:ASP:OD2[5_653]	1.73	0.47
6:B:628:HOH:O	6:D:675:HOH:O[5_653]	1.92	0.28

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	396/398 (100%)	347 (88%)	36 (9%)	13 (3%)	3 17
1	B	396/398 (100%)	337 (85%)	44 (11%)	15 (4%)	2 15
1	C	396/398 (100%)	348 (88%)	36 (9%)	12 (3%)	3 19
1	D	396/398 (100%)	350 (88%)	36 (9%)	10 (2%)	4 23
All	All	1584/1592 (100%)	1382 (87%)	152 (10%)	50 (3%)	3 18

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ALA
1	A	118	HIS

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Mol	Chain	Res	Type
1	A	124	THR
1	A	148	HIS
1	A	369	GLU
1	A	398	ALA
1	B	70	ASP
1	B	83	GLU
1	B	148	HIS
1	B	369	GLU
1	B	398	ALA
1	C	70	ASP
1	C	73	LYS
1	C	148	HIS
1	C	369	GLU
1	C	398	ALA
1	D	73	LYS
1	D	148	HIS
1	D	369	GLU
1	D	398	ALA
1	A	83	GLU
1	A	84	SER
1	B	84	SER
1	B	117	SER
1	B	124	THR
1	C	84	SER
1	D	70	ASP
1	D	84	SER
1	A	117	SER
1	A	368	ALA
1	B	146	MET
1	B	336	ASN
1	B	368	ALA
1	C	28	ALA
1	D	117	SER
1	D	368	ALA
1	A	73	LYS
1	A	347	TRP
1	B	28	ALA
1	B	130	THR
1	C	117	SER
1	C	376	TRP
1	D	118	HIS
1	A	264	LEU

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Mol	Chain	Res	Type
1	C	51	ASP
1	C	118	HIS
1	D	376	TRP
1	B	73	LYS
1	B	56	PRO
1	C	71	PRO

5.3.2 Protein sidechains (i)

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	329/329 (100%)	303 (92%)	26 (8%)	11	39
1	B	329/329 (100%)	304 (92%)	25 (8%)	12	41
1	C	329/329 (100%)	306 (93%)	23 (7%)	14	44
1	D	329/329 (100%)	305 (93%)	24 (7%)	13	42
All	All	1316/1316 (100%)	1218 (93%)	98 (7%)	13	42

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
1	A	73	LYS
1	A	83	GLU
1	A	85	ASP
1	A	96	LEU
1	A	101	HIS
1	A	107	ARG
1	A	124	THR
1	A	146	MET
1	A	147	LEU
1	A	171	GLN
1	A	176	SER
1	A	177	VAL
1	A	208	THR
1	A	210	LYS

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Mol	Chain	Res	Type
1	A	218	ASN
1	A	230	ILE
1	A	233	ARG
1	A	234	LYS
1	A	239	ILE
1	A	282	CYS
1	A	286	LEU
1	A	308	LEU
1	A	325	LEU
1	A	367	ILE
1	A	373	THR
1	B	49	LEU
1	B	53	VAL
1	B	83	GLU
1	B	103	LEU
1	B	106	GLN
1	B	124	THR
1	B	139	LEU
1	B	147	LEU
1	B	162	LEU
1	B	171	GLN
1	B	177	VAL
1	B	210	LYS
1	B	219	LEU
1	B	223	THR
1	B	230	ILE
1	B	233	ARG
1	B	234	LYS
1	B	239	ILE
1	B	261	THR
1	B	286	LEU
1	B	308	LEU
1	B	314	ILE
1	B	325	LEU
1	B	373	THR
1	B	389	LEU
1	C	49	LEU
1	C	53	VAL
1	C	77	LEU
1	C	83	GLU
1	C	96	LEU
1	C	112	LEU

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Mol	Chain	Res	Type
1	C	126	VAL
1	C	139	LEU
1	C	147	LEU
1	C	160	GLU
1	C	162	LEU
1	C	171	GLN
1	C	208	THR
1	C	210	LYS
1	C	230	ILE
1	C	233	ARG
1	C	286	LEU
1	C	308	LEU
1	C	313	THR
1	C	325	LEU
1	C	358	ARG
1	C	360	LYS
1	C	374	VAL
1	D	21	ILE
1	D	49	LEU
1	D	53	VAL
1	D	77	LEU
1	D	83	GLU
1	D	96	LEU
1	D	106	GLN
1	D	112	LEU
1	D	128	THR
1	D	130	THR
1	D	147	LEU
1	D	162	LEU
1	D	171	GLN
1	D	177	VAL
1	D	208	THR
1	D	210	LYS
1	D	230	ILE
1	D	233	ARG
1	D	239	ILE
1	D	286	LEU
1	D	308	LEU
1	D	325	LEU
1	D	358	ARG
1	D	374	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	67	GLN
1	A	80	ASN
1	A	101	HIS
1	A	148	HIS
1	A	166	ASN
1	A	171	GLN
1	A	205	ASN
1	A	218	ASN
1	A	352	GLN
1	A	375	GLN
1	B	115	HIS
1	B	166	ASN
1	B	171	GLN
1	B	295	ASN
1	B	352	GLN
1	B	375	GLN
1	B	384	GLN
1	C	3	GLN
1	C	25	HIS
1	C	80	ASN
1	C	81	HIS
1	C	101	HIS
1	C	106	GLN
1	C	115	HIS
1	C	166	ASN
1	C	171	GLN
1	C	205	ASN
1	C	218	ASN
1	C	295	ASN
1	C	315	ASN
1	C	375	GLN
1	C	384	GLN
1	D	25	HIS
1	D	81	HIS
1	D	106	GLN
1	D	122	ASN
1	D	166	ASN
1	D	171	GLN
1	D	250	GLN
1	D	271	HIS
1	D	295	ASN

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Mol	Chain	Res	Type
1	D	375	GLN
1	D	384	GLN

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 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	FEO	B	510	1,4	0,2,2	-	-	-		
4	OXY	D	531	3	1,1,1	0.20	0	-		
3	FEO	A	500	1	0,2,2	-	-	-		
4	OXY	A	501	-	1,1,1	0.27	0	-		
5	FMN	A	701	-	33,33,33	3.00	12 (36%)	48,50,50	2.47	17 (35%)
5	FMN	B	702	-	33,33,33	3.09	11 (33%)	48,50,50	2.45	16 (33%)
3	FEO	D	530	1,4	0,2,2	-	-	-		
4	OXY	C	521	-	1,1,1	0.29	0	-		
3	FEO	C	520	1	0,2,2	-	-	-		
5	FMN	D	704	-	33,33,33	3.01	12 (36%)	48,50,50	2.45	18 (37%)
5	FMN	C	703	-	33,33,33	3.00	11 (33%)	48,50,50	2.43	17 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	OXY	B	511	3	1,1,1	0.28	0	-		

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
5	FMN	C	703	-	-	0/18/18/18	0/3/3/3
5	FMN	A	701	-	-	2/18/18/18	0/3/3/3
5	FMN	B	702	-	-	0/18/18/18	0/3/3/3
5	FMN	D	704	-	-	0/18/18/18	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	702	FMN	C9A-C5A	7.82	1.53	1.41
5	C	703	FMN	C9-C9A	7.73	1.52	1.39
5	B	702	FMN	C9-C9A	7.68	1.52	1.39
5	A	701	FMN	C9-C9A	7.59	1.51	1.39
5	C	703	FMN	C9A-C5A	7.50	1.53	1.41
5	D	704	FMN	C9-C9A	7.37	1.51	1.39
5	D	704	FMN	C9A-C5A	7.27	1.52	1.41
5	A	701	FMN	C9A-C5A	7.20	1.52	1.41
5	B	702	FMN	C6-C7	6.83	1.48	1.39
5	D	704	FMN	C6-C7	6.68	1.48	1.39
5	C	703	FMN	C6-C7	6.33	1.48	1.39
5	A	701	FMN	C6-C7	6.24	1.48	1.39
5	B	702	FMN	C2-N3	5.37	1.50	1.39
5	D	704	FMN	C2-N3	5.34	1.50	1.39
5	C	703	FMN	C2-N3	5.25	1.50	1.39
5	A	701	FMN	C2-N3	5.16	1.50	1.39
5	B	702	FMN	C4A-C10	4.70	1.58	1.44
5	D	704	FMN	C4A-C10	4.53	1.57	1.44
5	A	701	FMN	C4A-C10	4.49	1.57	1.44
5	C	703	FMN	C4A-C10	4.45	1.57	1.44
5	A	701	FMN	C5'-C4'	4.25	1.57	1.51
5	D	704	FMN	C4-N3	4.13	1.46	1.38
5	C	703	FMN	C4-N3	4.06	1.46	1.38
5	B	702	FMN	C4-N3	4.01	1.46	1.38
5	A	701	FMN	C4-N3	3.93	1.46	1.38
5	C	703	FMN	C8-C7	3.68	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	704	FMN	C5'-C4'	3.68	1.56	1.51
5	D	704	FMN	C6-C5A	3.68	1.45	1.40
5	B	702	FMN	C6-C5A	3.63	1.45	1.40
5	B	702	FMN	C8-C7	3.58	1.49	1.40
5	B	702	FMN	C5A-N5	3.48	1.45	1.39
5	A	701	FMN	C8-C7	3.47	1.49	1.40
5	D	704	FMN	C8-C7	3.41	1.49	1.40
5	A	701	FMN	C6-C5A	3.41	1.45	1.40
5	C	703	FMN	C5A-N5	3.33	1.45	1.39
5	C	703	FMN	C6-C5A	3.30	1.45	1.40
5	B	702	FMN	C5'-C4'	3.10	1.56	1.51
5	D	704	FMN	C5A-N5	3.07	1.45	1.39
5	A	701	FMN	C5A-N5	2.94	1.44	1.39
5	C	703	FMN	C5'-C4'	2.82	1.55	1.51
5	B	702	FMN	O3'-C3'	2.25	1.48	1.43
5	C	703	FMN	O3'-C3'	2.21	1.48	1.43
5	D	704	FMN	C8M-C8	-2.19	1.46	1.51
5	A	701	FMN	C10-N10	2.06	1.41	1.37
5	D	704	FMN	O3'-C3'	2.04	1.48	1.43
5	A	701	FMN	C8M-C8	-2.01	1.47	1.51

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	704	FMN	C5A-C9A-N10	7.07	124.36	117.97
5	B	702	FMN	C5A-C9A-N10	6.84	124.15	117.97
5	A	701	FMN	C5A-C9A-N10	6.80	124.12	117.97
5	C	703	FMN	C5A-C9A-N10	6.55	123.89	117.97
5	C	703	FMN	C7M-C7-C6	-6.28	108.52	119.57
5	A	701	FMN	C7M-C7-C6	-6.23	108.60	119.57
5	B	702	FMN	C7M-C7-C6	-6.16	108.71	119.57
5	D	704	FMN	C7M-C7-C6	-6.11	108.81	119.57
5	C	703	FMN	C9A-C5A-N5	-5.48	116.64	122.45
5	D	704	FMN	C9A-C5A-N5	-5.40	116.73	122.45
5	B	702	FMN	C9A-C5A-N5	-5.38	116.74	122.45
5	A	701	FMN	C9A-C5A-N5	-5.33	116.80	122.45
5	A	701	FMN	C7M-C7-C8	5.20	131.39	120.76
5	C	703	FMN	C7M-C7-C8	5.17	131.31	120.76
5	B	702	FMN	C7M-C7-C8	5.04	131.04	120.76
5	D	704	FMN	C7M-C7-C8	5.03	131.02	120.76
5	A	701	FMN	O2-C2-N1	4.23	128.83	121.80
5	B	702	FMN	O2-C2-N1	4.14	128.68	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	704	FMN	C10-N1-C2	3.97	125.45	116.85
5	C	703	FMN	O2-C2-N1	3.97	128.39	121.80
5	C	703	FMN	C10-N1-C2	3.96	125.43	116.85
5	D	704	FMN	O2-C2-N1	3.93	128.33	121.80
5	B	702	FMN	C10-N1-C2	3.93	125.35	116.85
5	A	701	FMN	C10-N1-C2	3.88	125.25	116.85
5	D	704	FMN	C4A-C10-N10	3.29	121.20	116.48
5	C	703	FMN	C1'-N10-C9A	3.29	127.03	120.63
5	D	704	FMN	C9A-N10-C10	-3.29	115.74	120.75
5	A	701	FMN	C9A-N10-C10	-3.20	115.87	120.75
5	B	702	FMN	C4A-C10-N10	3.19	121.05	116.48
5	B	702	FMN	O4-C4-N3	-3.18	114.14	120.11
5	C	703	FMN	C4A-C10-N10	3.17	121.03	116.48
5	D	704	FMN	O4-C4-N3	-3.16	114.17	120.11
5	B	702	FMN	C9A-N10-C10	-3.13	115.97	120.75
5	B	702	FMN	C1'-N10-C9A	3.13	126.71	120.63
5	D	704	FMN	C1'-N10-C9A	3.12	126.69	120.63
5	A	701	FMN	O4-C4-N3	-3.10	114.29	120.11
5	C	703	FMN	O4-C4-N3	-3.07	114.33	120.11
5	B	702	FMN	C6-C5A-N5	3.03	123.47	118.44
5	D	704	FMN	C6-C5A-N5	3.01	123.44	118.44
5	C	703	FMN	C9A-N10-C10	-3.01	116.16	120.75
5	A	701	FMN	C4A-C10-N10	2.97	120.73	116.48
5	A	701	FMN	C4'-C3'-C2'	2.95	118.48	113.57
5	C	703	FMN	C6-C5A-N5	2.95	123.34	118.44
5	A	701	FMN	C1'-N10-C9A	2.94	126.34	120.63
5	A	701	FMN	O3'-C3'-C4'	-2.88	102.39	108.93
5	A	701	FMN	C4A-C10-N1	-2.85	117.61	124.59
5	A	701	FMN	C6-C5A-N5	2.82	123.13	118.44
5	B	702	FMN	O3'-C3'-C4'	-2.80	102.56	108.93
5	D	704	FMN	C4A-C10-N1	-2.76	117.81	124.59
5	B	702	FMN	C4A-C10-N1	-2.74	117.86	124.59
5	C	703	FMN	C4A-C10-N1	-2.72	117.93	124.59
5	A	701	FMN	O2-C2-N3	-2.58	113.64	118.58
5	C	703	FMN	O3'-C3'-C4'	-2.57	103.09	108.93
5	D	704	FMN	O3'-C3'-C4'	-2.53	103.18	108.93
5	B	702	FMN	C4'-C3'-C2'	2.44	117.63	113.57
5	B	702	FMN	O2-C2-N3	-2.39	113.99	118.58
5	D	704	FMN	C4'-C3'-C2'	2.35	117.48	113.57
5	D	704	FMN	C9-C9A-N10	-2.31	118.75	121.85
5	D	704	FMN	O2-C2-N3	-2.29	114.19	118.58
5	C	703	FMN	O2-C2-N3	-2.27	114.22	118.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	703	FMN	C4'-C3'-C2'	2.22	117.27	113.57
5	A	701	FMN	C5A-N5-C4A	2.20	121.65	118.09
5	C	703	FMN	C5A-N5-C4A	2.20	121.64	118.09
5	B	702	FMN	C9-C9A-N10	-2.11	119.02	121.85
5	D	704	FMN	C10-C4A-N5	-2.07	120.58	124.81
5	D	704	FMN	C5A-N5-C4A	2.05	121.40	118.09
5	C	703	FMN	C10-C4A-N5	-2.04	120.63	124.81
5	A	701	FMN	C4-C4A-C10	2.02	120.39	116.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	701	FMN	O4'-C4'-C5'-O5'
5	A	701	FMN	C3'-C4'-C5'-O5'

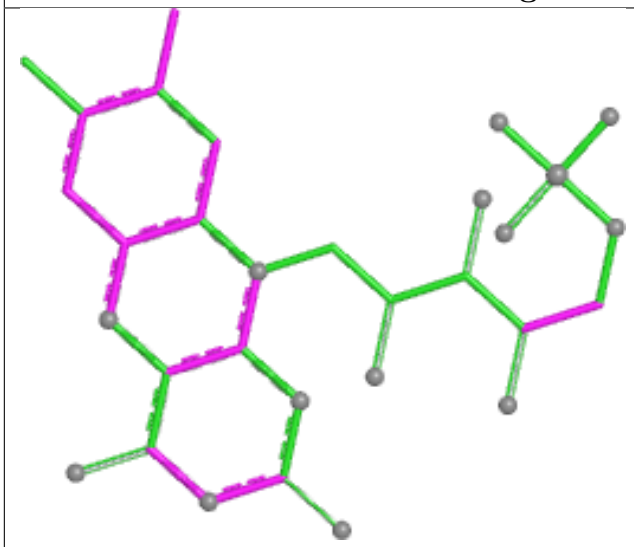
There are no ring outliers.

7 monomers are involved in 5 short contacts:

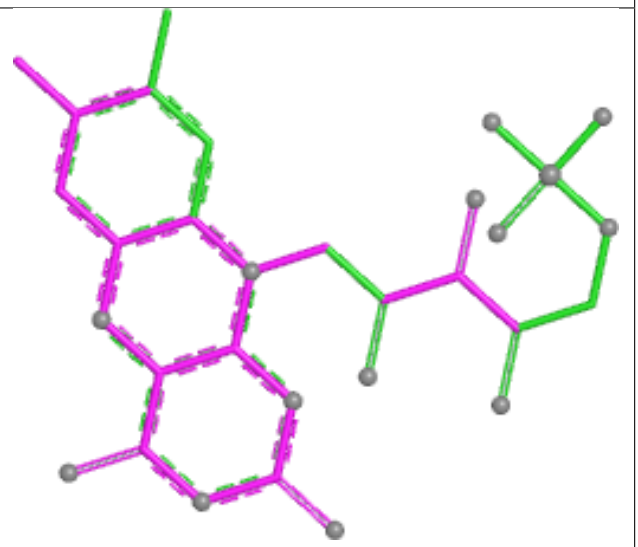
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	510	FEO	1	0
4	D	531	OXY	1	0
5	A	701	FMN	1	0
5	B	702	FMN	1	0
3	D	530	FEO	1	0
5	D	704	FMN	1	0
4	B	511	OXY	1	0

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 then 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.

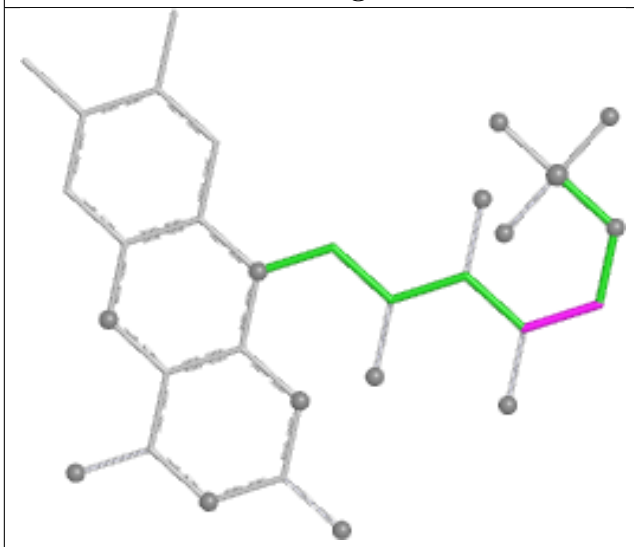
Ligand FMN A 701



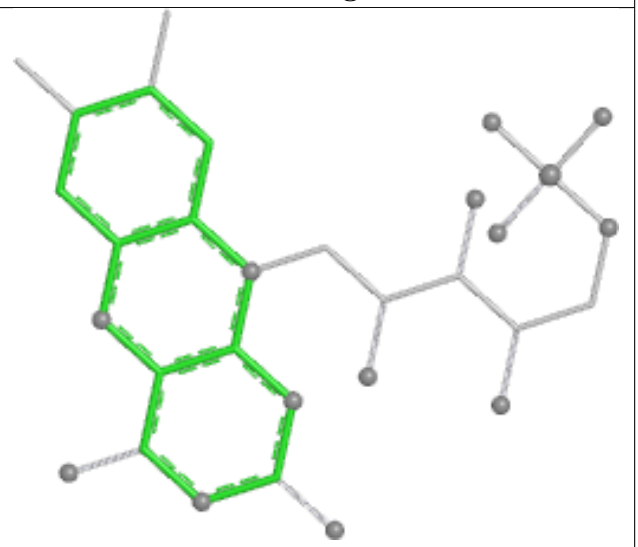
Bond lengths



Bond angles

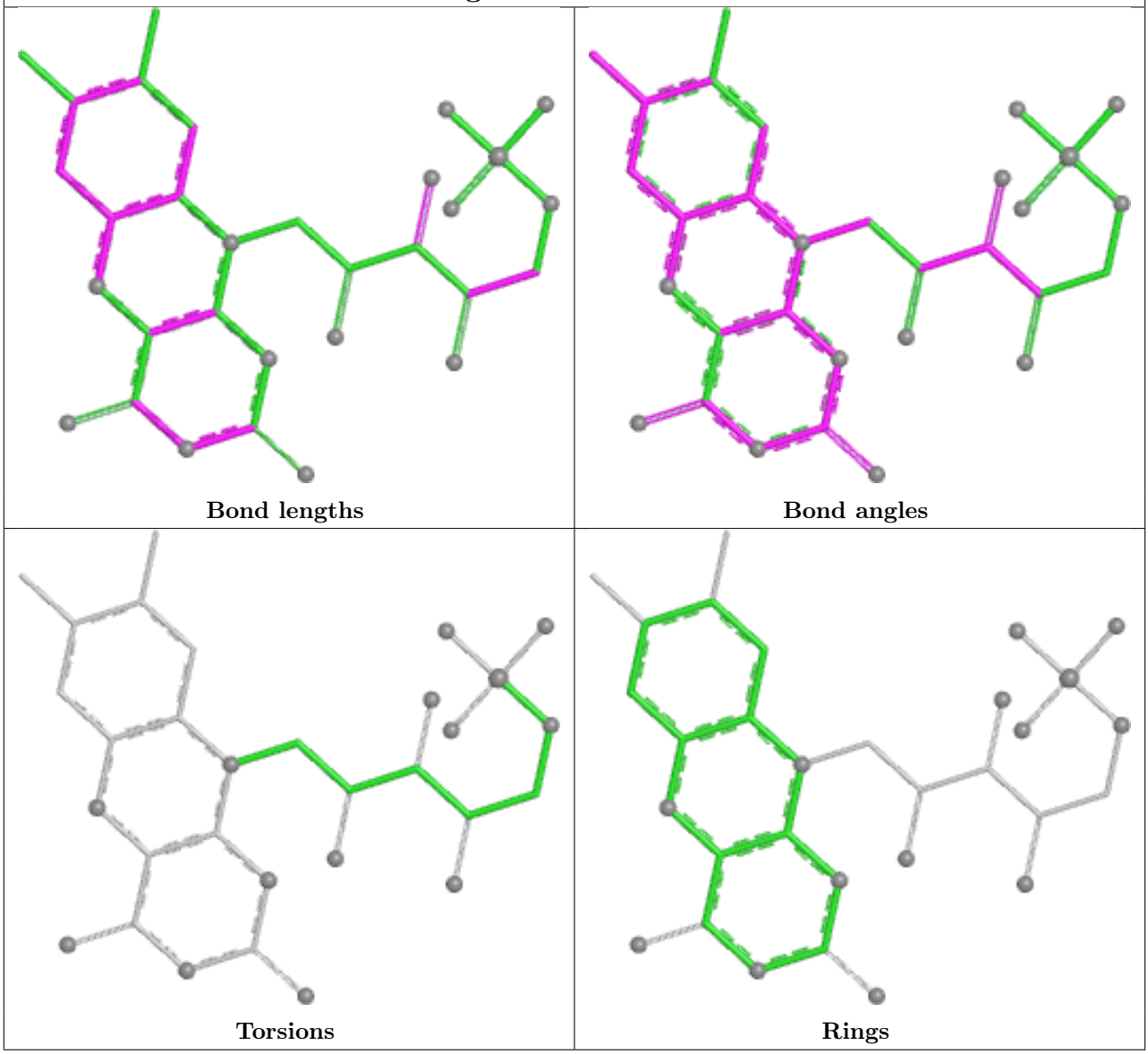


Torsions

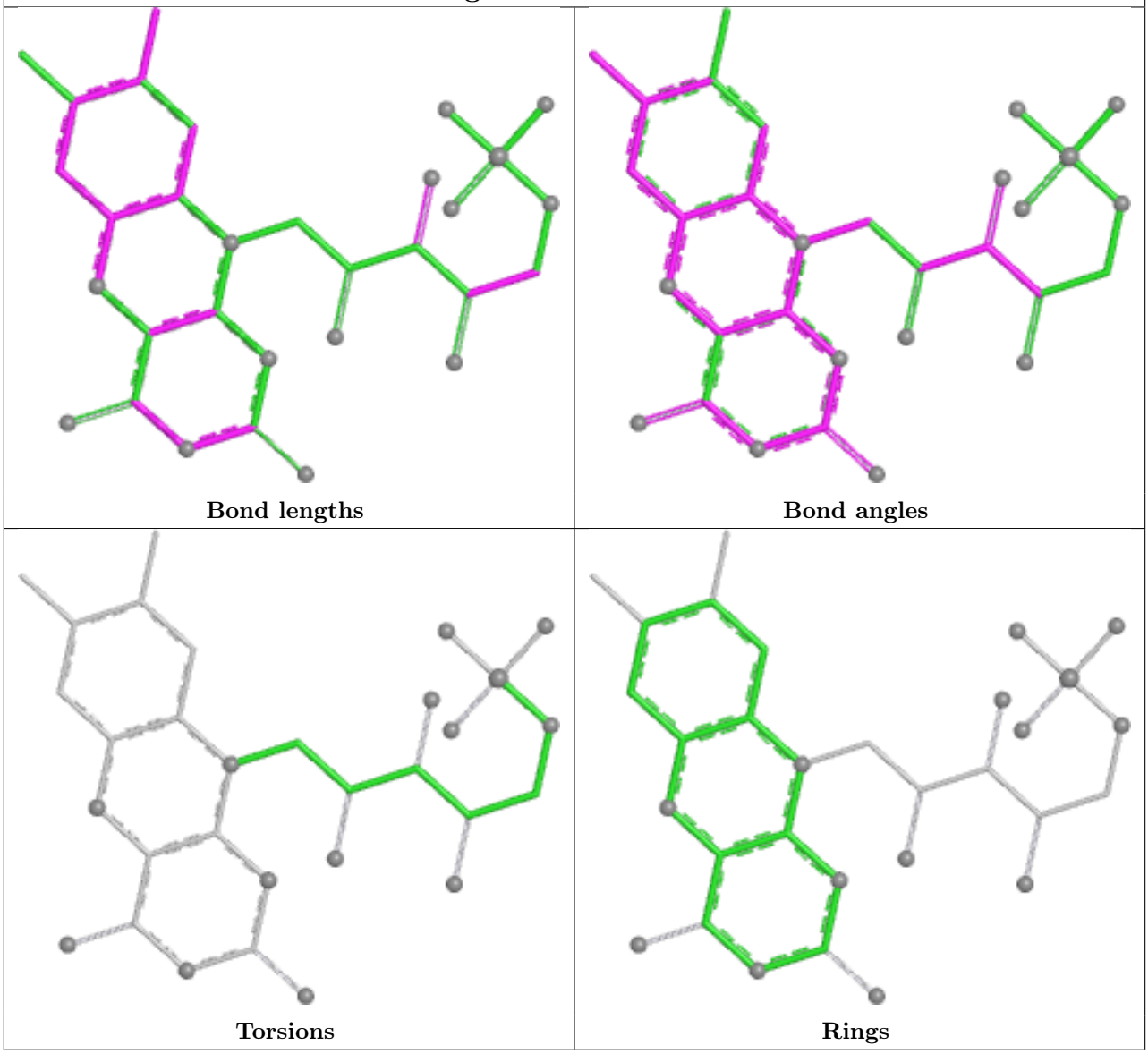


Rings

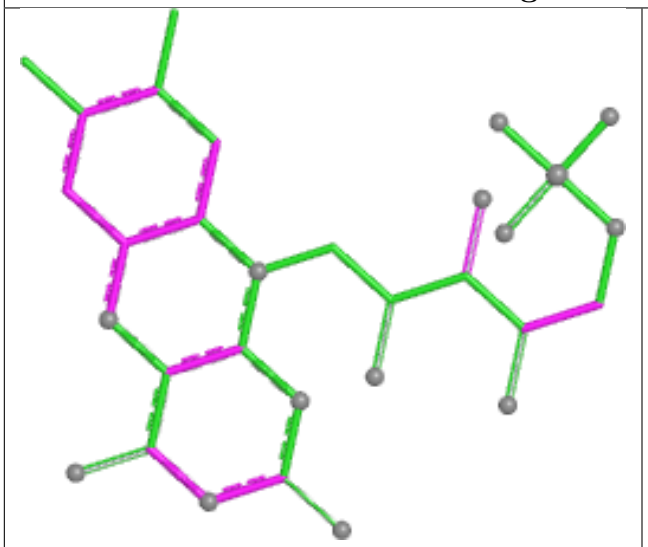
Ligand FMN B 702



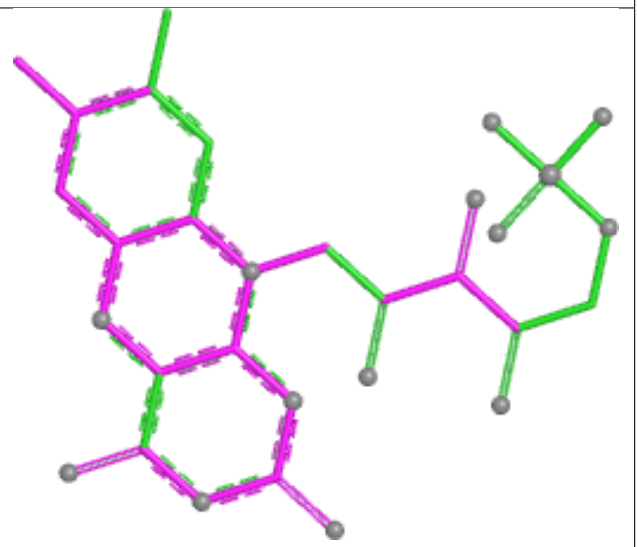
Ligand FMN D 704



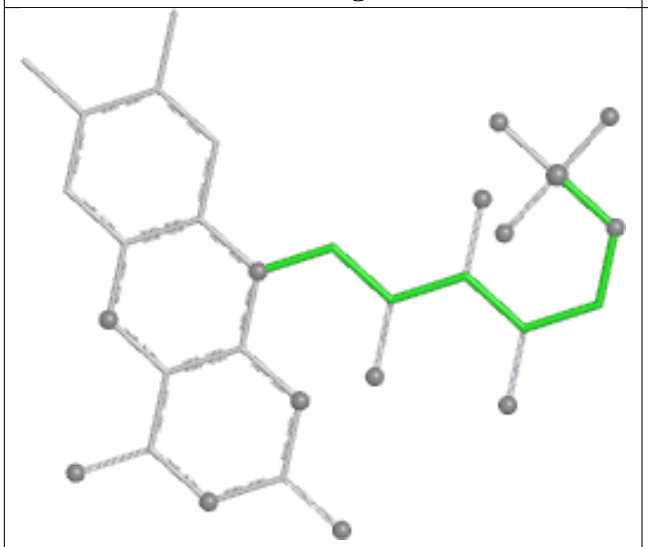
Ligand FMN C 703



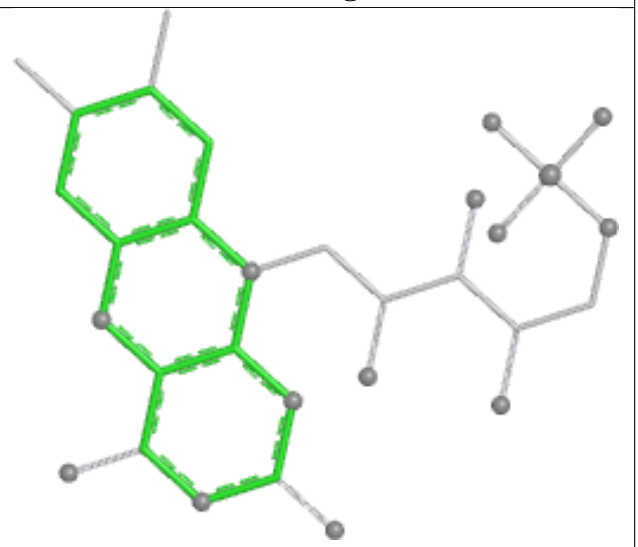
Bond lengths



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	398/398 (100%)	1.25	90 (22%)	2	1	20, 56, 82, 102	2 (0%)
1	B	398/398 (100%)	1.05	51 (12%)	7	5	24, 59, 93, 117	2 (0%)
1	C	398/398 (100%)	1.45	91 (22%)	2	1	9, 49, 74, 102	2 (0%)
1	D	398/398 (100%)	1.01	49 (12%)	8	5	11, 47, 76, 99	2 (0%)
All	All	1592/1592 (100%)	1.19	281 (17%)	4	2	9, 52, 84, 117	8 (0%)

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	ASP	14.4
1	D	51	ASP	12.4
1	C	51	ASP	12.2
1	A	51	ASP	10.1
1	C	50	VAL	10.0
1	B	50	VAL	10.0
1	A	50	VAL	8.5
1	D	50	VAL	7.9
1	D	136	LYS	5.9
1	D	25	HIS	5.7
1	D	2	SER	5.3
1	B	2	SER	5.2
1	B	77	LEU	5.1
1	A	25	HIS	5.1
1	C	26	GLY	4.6
1	D	362	ALA	4.4
1	D	99	ASP	4.4
1	A	175	THR	4.2
1	A	155	THR	4.1
1	A	229	GLY	4.1
1	C	250	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	339	GLY	4.0
1	C	307	VAL	4.0
1	C	318	ILE	4.0
1	D	24	PHE	4.0
1	C	372	PRO	4.0
1	C	25	HIS	4.0
1	C	283	GLU	4.0
1	A	80	ASN	3.9
1	A	42	ILE	3.9
1	A	130	THR	3.8
1	C	282	CYS	3.8
1	D	200	LEU	3.8
1	D	208	THR	3.8
1	A	12	TYR	3.7
1	A	369	GLU	3.7
1	C	382	ASP	3.7
1	C	386	CYS	3.7
1	A	187	LEU	3.7
1	B	25	HIS	3.7
1	A	188	ILE	3.6
1	B	240	ILE	3.6
1	C	393	ILE	3.6
1	A	15	GLY	3.6
1	A	43	VAL	3.6
1	C	340	LEU	3.6
1	A	171	GLN	3.6
1	B	282	CYS	3.5
1	C	389	LEU	3.5
1	B	349	GLY	3.5
1	C	275	ASP	3.5
1	C	317	ASP	3.5
1	B	24	PHE	3.4
1	C	383	LEU	3.4
1	D	145	PRO	3.4
1	C	346	GLY	3.4
1	C	371	GLY	3.3
1	A	48	ALA	3.3
1	A	33	ARG	3.3
1	C	354	ILE	3.3
1	A	236	PRO	3.3
1	B	49	LEU	3.3
1	B	78	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	232	TRP	3.3
1	C	246	TRP	3.2
1	C	24	PHE	3.2
1	C	316	ASN	3.2
1	D	336	ASN	3.2
1	A	282	CYS	3.2
1	C	348	GLY	3.2
1	A	40	TYR	3.2
1	C	351	ALA	3.2
1	A	217	ILE	3.2
1	A	8	THR	3.2
1	A	13	TRP	3.1
1	C	124	THR	3.1
1	C	281	GLY	3.1
1	A	14	VAL	3.1
1	C	361	ALA	3.1
1	A	2	SER	3.1
1	A	184	ASP	3.1
1	A	122	ASN	3.1
1	C	350	GLY	3.1
1	A	176	SER	3.1
1	A	214	ILE	3.1
1	A	11	ILE	3.0
1	D	196	TYR	3.0
1	B	28	ALA	3.0
1	C	139	LEU	3.0
1	A	157	VAL	3.0
1	A	19	TRP	3.0
1	D	131	SER	3.0
1	A	99	ASP	3.0
1	D	306	ALA	3.0
1	B	79	VAL	3.0
1	C	369	GLU	3.0
1	D	204	SER	3.0
1	A	138	SER	2.9
1	D	150	PRO	2.9
1	C	173	ILE	2.9
1	A	139	LEU	2.9
1	B	223	THR	2.9
1	B	131	SER	2.9
1	B	173	ILE	2.9
1	C	313	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	104	CYS	2.9
1	D	23	TYR	2.9
1	B	100	ALA	2.8
1	C	365	GLU	2.8
1	A	179	PHE	2.8
1	A	3	GLN	2.8
1	C	217	ILE	2.8
1	C	312	PRO	2.8
1	B	41	LEU	2.8
1	A	34	GLY	2.8
1	C	331	GLY	2.8
1	C	341	ALA	2.8
1	A	162	LEU	2.8
1	D	30	SER	2.8
1	A	125	ILE	2.7
1	C	201	MET	2.7
1	C	388	GLU	2.7
1	A	67	GLN	2.7
1	B	3	GLN	2.7
1	C	36	THR	2.7
1	C	323	SER	2.7
1	D	107	ARG	2.7
1	A	101	HIS	2.7
1	C	338	VAL	2.7
1	B	103	LEU	2.7
1	C	364	ILE	2.7
1	C	34	GLY	2.7
1	C	260	ASP	2.7
1	D	73	LYS	2.6
1	A	49	LEU	2.6
1	C	253	ALA	2.6
1	B	367	ILE	2.6
1	C	315	ASN	2.6
1	B	350	GLY	2.6
1	A	141	PHE	2.6
1	B	120	ASP	2.6
1	C	249	GLY	2.6
1	D	346	GLY	2.6
1	B	248	GLU	2.6
1	A	163	LEU	2.6
1	A	39	ALA	2.6
1	D	118	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	191	GLU	2.6
1	A	76	TYR	2.6
1	C	15	GLY	2.6
1	D	60	GLU	2.6
1	C	376	TRP	2.5
1	C	385	ARG	2.5
1	C	35	THR	2.5
1	C	380	GLY	2.5
1	A	365	GLU	2.5
1	A	398	ALA	2.5
1	D	399	ASP	2.5
1	B	12	TYR	2.5
1	C	122	ASN	2.5
1	C	239	ILE	2.5
1	D	180	ASP	2.5
1	D	367	ILE	2.5
1	B	31	THR	2.5
1	B	372	PRO	2.5
1	C	379	ARG	2.5
1	C	368	ALA	2.5
1	B	234	LYS	2.5
1	A	156	TYR	2.5
1	A	129	GLY	2.5
1	D	282	CYS	2.4
1	D	147	LEU	2.4
1	C	188	ILE	2.4
1	C	199	ILE	2.4
1	A	26	GLY	2.4
1	A	16	ALA	2.4
1	B	33	ARG	2.4
1	B	102	VAL	2.4
1	C	99	ASP	2.4
1	C	343	GLY	2.4
1	C	306	ALA	2.4
1	A	164	LEU	2.4
1	A	208	THR	2.4
1	C	394	ALA	2.4
1	B	337	LYS	2.4
1	C	236	PRO	2.4
1	A	223	THR	2.3
1	A	70	ASP	2.3
1	A	53	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	265	SER	2.3
1	C	392	LYS	2.3
1	A	168	ALA	2.3
1	A	174	ALA	2.3
1	B	253	ALA	2.3
1	D	144	ALA	2.3
1	B	40	TYR	2.3
1	D	219	LEU	2.3
1	C	78	VAL	2.3
1	A	216	LYS	2.3
1	A	165	PRO	2.3
1	A	230	ILE	2.3
1	D	348	GLY	2.3
1	A	118	HIS	2.3
1	C	148	HIS	2.3
1	D	153	MET	2.3
1	D	205	ASN	2.3
1	A	154	PHE	2.3
1	B	75	ASP	2.3
1	A	178	ARG	2.3
1	A	29	PHE	2.3
1	A	190	ASP	2.3
1	B	369	GLU	2.3
1	C	381	GLU	2.3
1	B	346	GLY	2.3
1	C	349	GLY	2.3
1	C	175	THR	2.3
1	C	311	SER	2.3
1	B	69	LYS	2.3
1	B	97	CYS	2.3
1	C	104	CYS	2.3
1	C	240	ILE	2.2
1	C	397	ILE	2.2
1	A	31	THR	2.2
1	B	123	TYR	2.2
1	A	97	CYS	2.2
1	C	309	VAL	2.2
1	A	66	LYS	2.2
1	D	80	ASN	2.2
1	B	101	HIS	2.2
1	C	187	LEU	2.2
1	D	302	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	29	PHE	2.2
1	C	391	ARG	2.2
1	B	139	LEU	2.2
1	D	211	LEU	2.2
1	A	71	PRO	2.2
1	A	150	PRO	2.2
1	D	110	ASP	2.2
1	B	130	THR	2.1
1	A	127	LYS	2.1
1	D	16	ALA	2.1
1	D	152	SER	2.1
1	B	249	GLY	2.1
1	B	169	PHE	2.1
1	D	140	THR	2.1
1	D	239	ILE	2.1
1	C	285	LYS	2.1
1	C	378	PRO	2.1
1	D	141	PHE	2.1
1	A	142	ILE	2.1
1	A	302	LEU	2.1
1	A	255	ALA	2.1
1	A	27	PRO	2.1
1	D	83	GLU	2.1
1	C	290	SER	2.1
1	A	205	ASN	2.1
1	A	338	VAL	2.1
1	A	46	LYS	2.1
1	A	81	HIS	2.1
1	C	277	LEU	2.1
1	C	196	TYR	2.1
1	B	154	PHE	2.1
1	C	337	LYS	2.1
1	B	271	HIS	2.1
1	C	347	TRP	2.1
1	D	115	HIS	2.1
1	A	121	PHE	2.1
1	A	370	PRO	2.1
1	D	154	PHE	2.1
1	B	126	VAL	2.0
1	C	73	LYS	2.0
1	A	38	ASN	2.0
1	A	173	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	8	THR	2.0
1	B	52	THR	2.0
1	C	190	ASP	2.0
1	D	181	ASP	2.0
1	A	158	PRO	2.0
1	D	3	GLN	2.0
1	D	283	GLU	2.0
1	C	41	LEU	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)

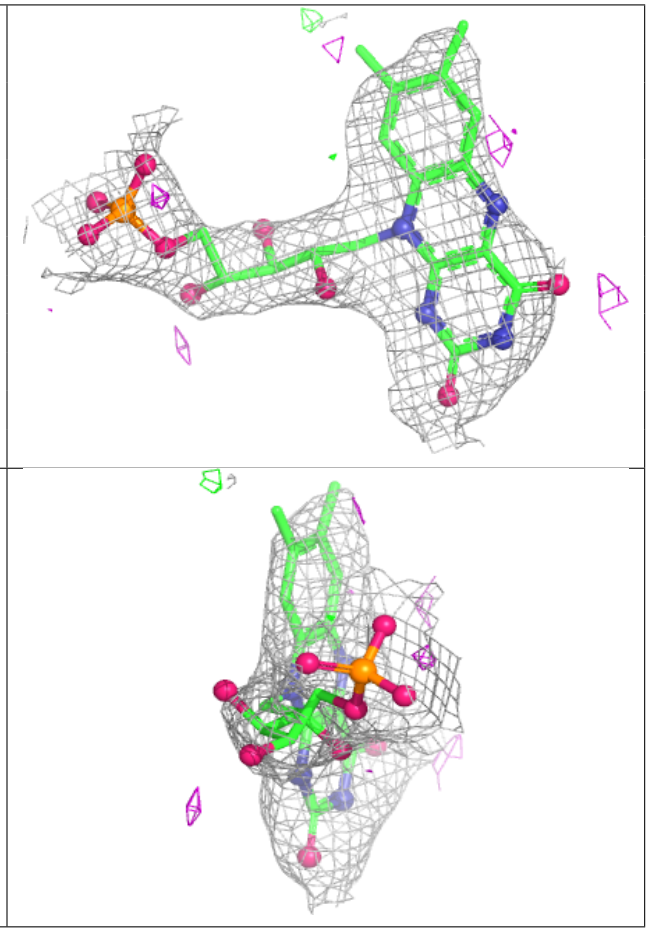
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	OXY	D	531	2/2	0.64	0.24	38,38,38,38	0
2	ZN	A	502	1/1	0.70	0.12	70,70,70,70	0
4	OXY	C	521	2/2	0.72	0.43	42,42,42,56	0
4	OXY	B	511	2/2	0.85	0.37	73,73,73,76	0
2	ZN	B	512	1/1	0.86	0.16	132,132,132,132	0
4	OXY	A	501	2/2	0.87	0.35	51,51,51,56	0
5	FMN	C	703	31/31	0.87	0.15	26,44,57,63	0
5	FMN	D	704	31/31	0.87	0.15	30,53,61,68	0
5	FMN	A	701	31/31	0.90	0.15	39,76,89,98	0
2	ZN	A	503	1/1	0.92	0.15	71,71,71,71	0
5	FMN	B	702	31/31	0.92	0.14	40,72,81,90	0
3	FEO	D	530	3/3	0.96	0.06	38,38,44,46	0
3	FEO	A	500	3/3	0.97	0.06	45,45,51,54	0
3	FEO	C	520	3/3	0.98	0.06	34,34,39,40	0
3	FEO	B	510	3/3	0.98	0.04	51,51,52,56	0

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.

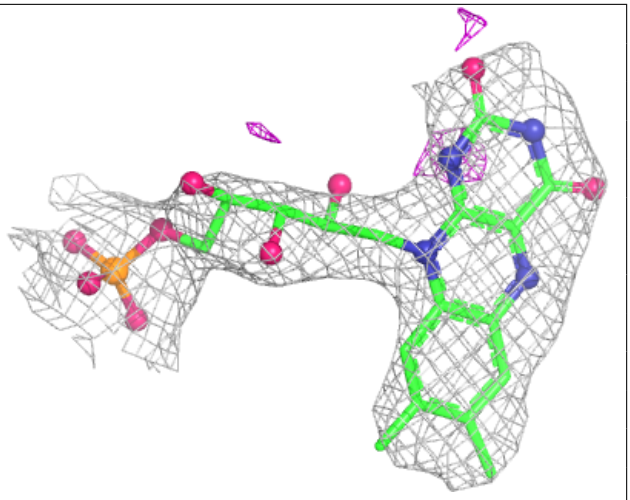
Electron density around FMN C 703:

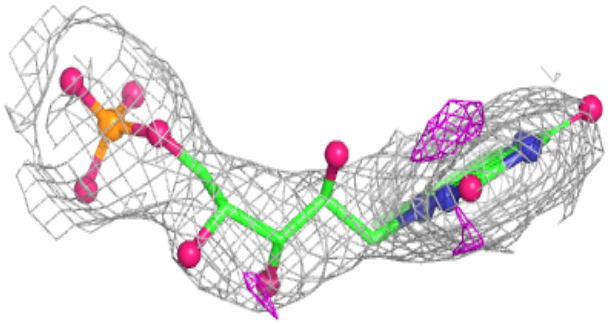
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

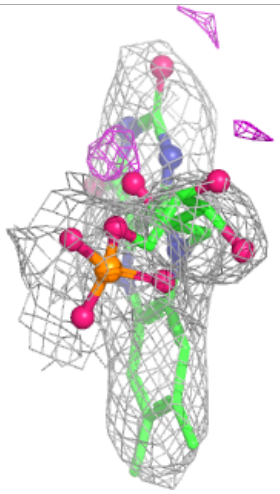


Electron density around FMN D 704:

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

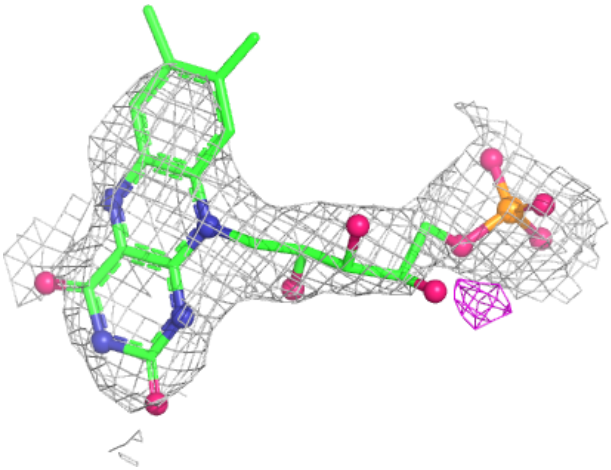


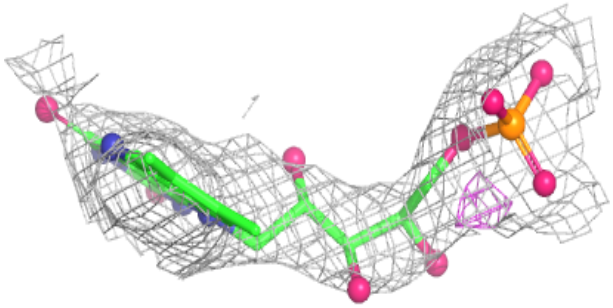


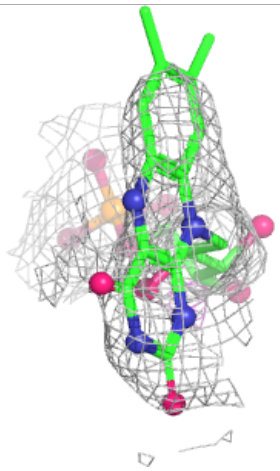


Electron density around FMN A 701:

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

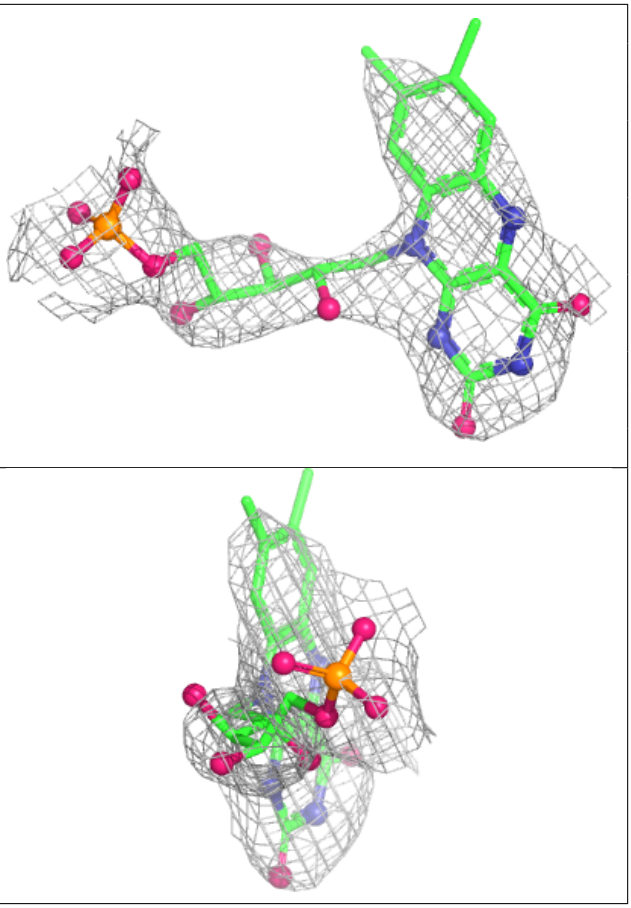






Electron density around FMN B 702:

$2mF_o$-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.