



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:14 AM UTC

PDB ID : 4C8R / pdb_00004c8r
Title : Human gamma-butyrobetaine dioxygenase (BBOX1) in complex with Ni(II) and N-(3-hydroxypicolinoyl)-S-(pyridin-2-ylmethyl)-L-cysteine (AR692B)
Authors : Chowdhury, R.; Rydzik, A.M.; Kochan, G.T.; McDonough, M.A.; Schofield, C.J.
Deposited on : 2013-10-01
Resolution : 2.82 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	:	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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

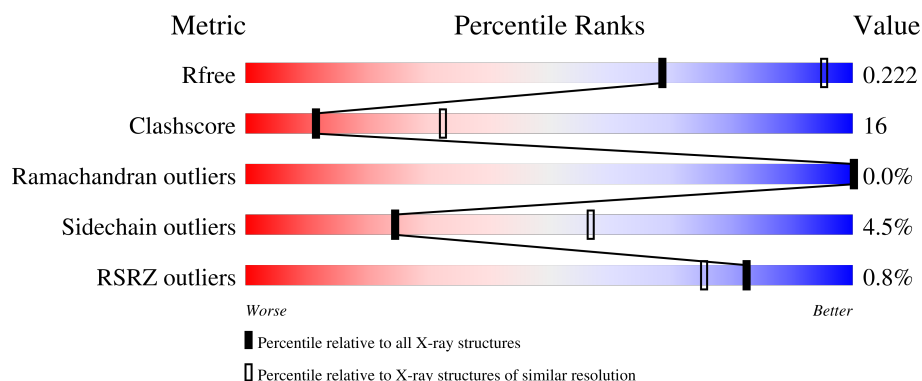
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	388	% 67% 29% ..
1	B	388	67% 29% ..
1	C	388	% 65% 31% ..
1	D	388	2% 62% 33% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	388	% 62% 34% ..
1	F	388	59% 38% ..

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	6YT	A	601	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19352 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 GAMMA-BUTYROBETAINE DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3116	1995	533	573	15			
1	B	384	Total	C	N	O	S	0	0	0
			3130	2006	535	574	15			
1	C	384	Total	C	N	O	S	0	0	0
			3117	1997	530	576	14			
1	D	384	Total	C	N	O	S	0	0	0
			3109	1995	535	565	14			
1	E	384	Total	C	N	O	S	0	0	0
			3097	1986	532	565	14			
1	F	384	Total	C	N	O	S	0	0	0
			3109	1997	531	567	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP O75936
B	0	SER	-	expression tag	UNP O75936
C	0	SER	-	expression tag	UNP O75936
D	0	SER	-	expression tag	UNP O75936
E	0	SER	-	expression tag	UNP O75936
F	0	SER	-	expression tag	UNP O75936

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

Continued on next page...

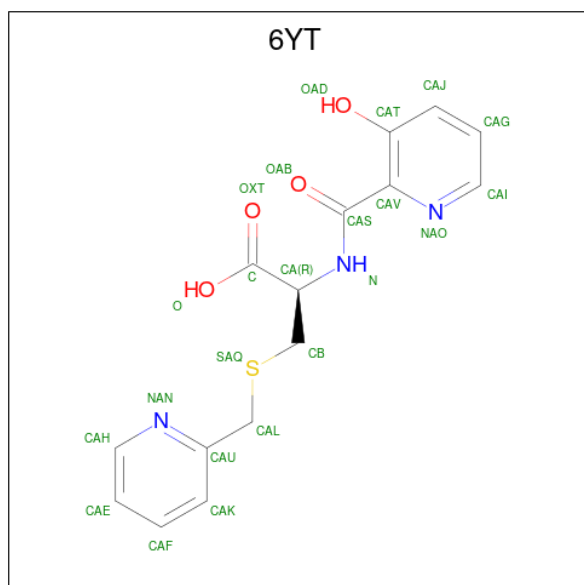
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Ni	0	0
			1	1		
2	E	1	Total	Ni	0	0
			1	1		
2	F	1	Total	Ni	0	0
			1	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

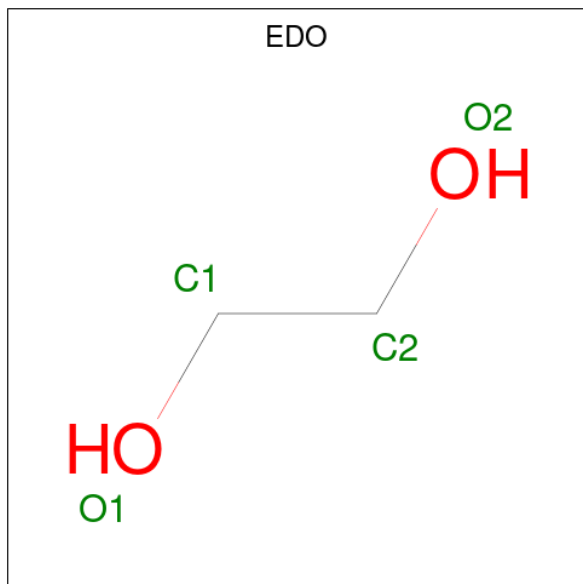
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is N-(3-hydroxypicolinoyl)-S-(pyridin-2-ylmethyl)-L-cysteine (CCD ID: 6YT) (formula: C₁₅H₁₅N₃O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			23	15	3	4	1		
4	B	1	Total	C	N	O	S	0	0
			23	15	3	4	1		
4	C	1	Total	C	N	O	S	0	0
			23	15	3	4	1		
4	D	1	Total	C	N	O	S	0	0
			23	15	3	4	1		
4	E	1	Total	C	N	O	S	0	0
			23	15	3	4	1		
4	F	1	Total	C	N	O	S	0	0
			23	15	3	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0

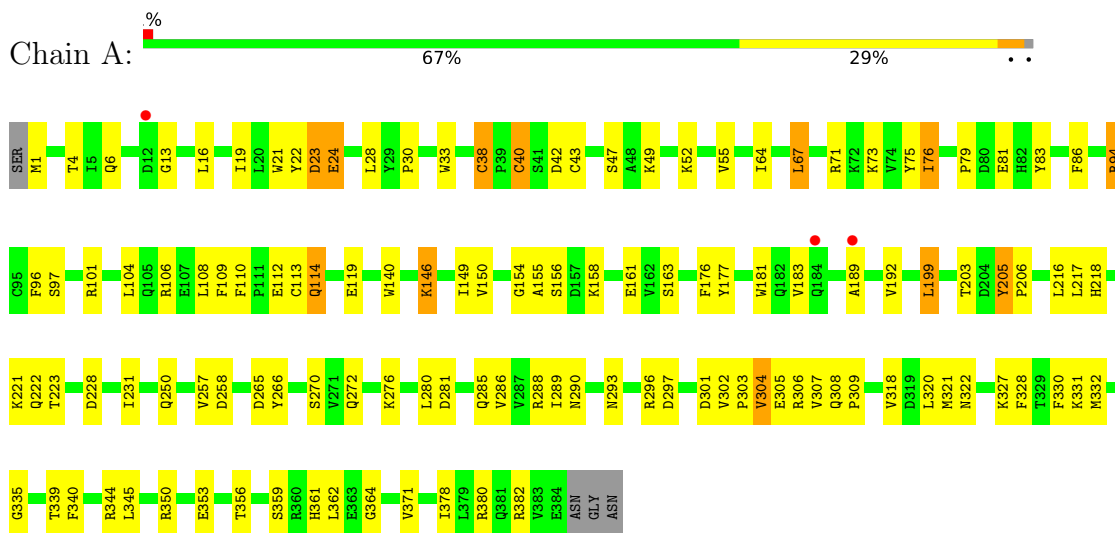
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	106	Total O 106 106	0	0
6	B	95	Total O 95 95	0	0
6	C	90	Total O 90 90	0	0
6	D	60	Total O 60 60	0	0
6	E	52	Total O 52 52	0	0
6	F	65	Total O 65 65	0	0

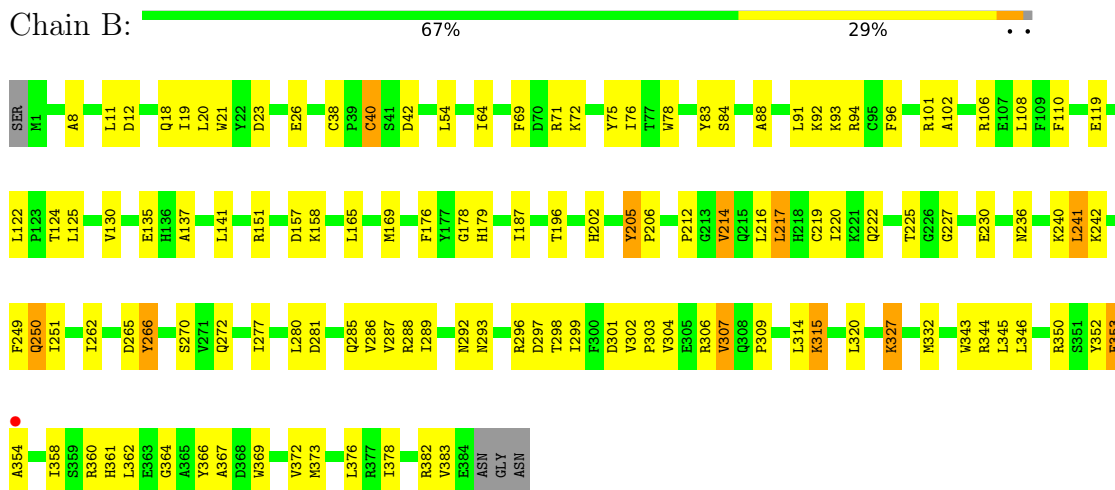
3 Residue-property plots

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: GAMMA-BUTYROBETAINE DIOXYGENASE

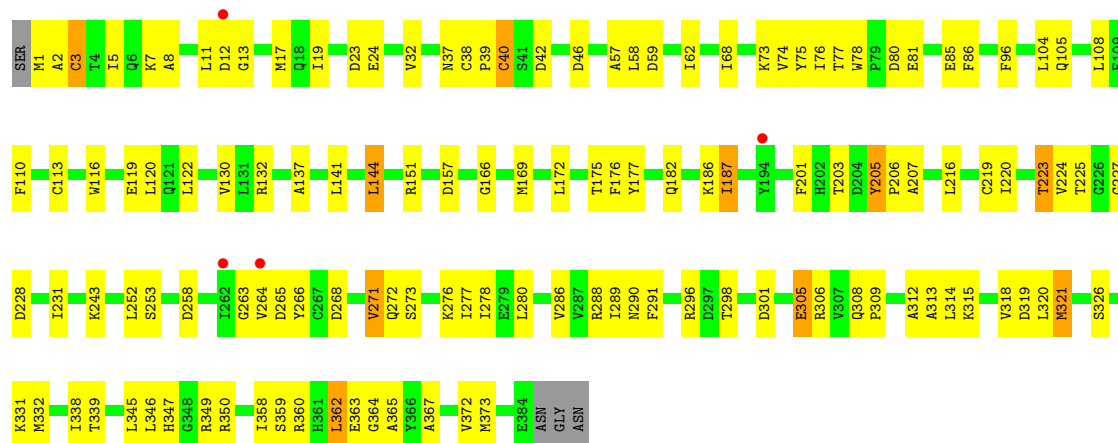


• Molecule 1: GAMMA-BUTYROBETAINE DIOXYGENASE

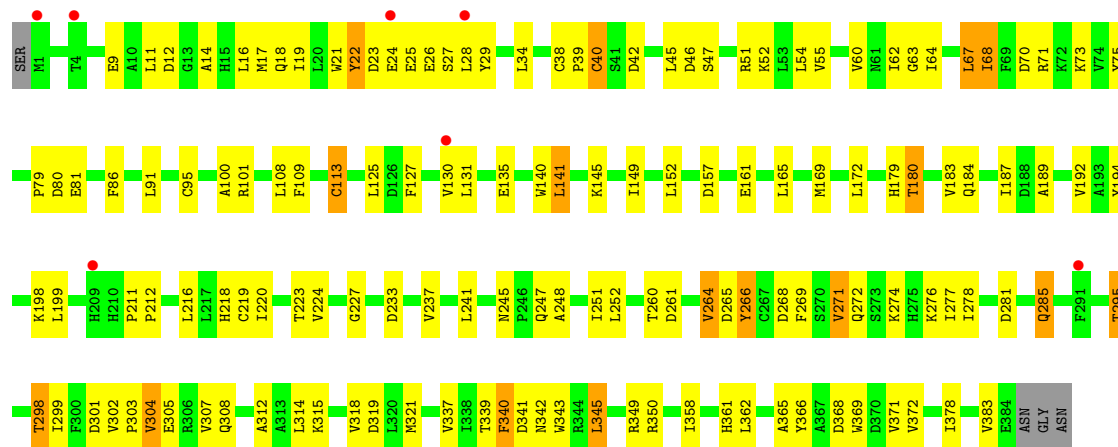


• Molecule 1: GAMMA-BUTYROBETAINE DIOXYGENASE

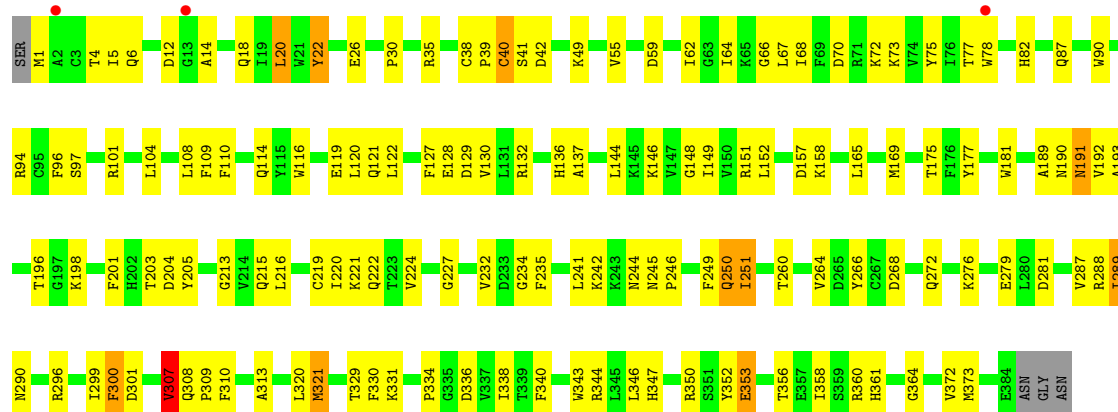




• Molecule 1: GAMMA-BUTYROBETAIN DIOXYGENASE

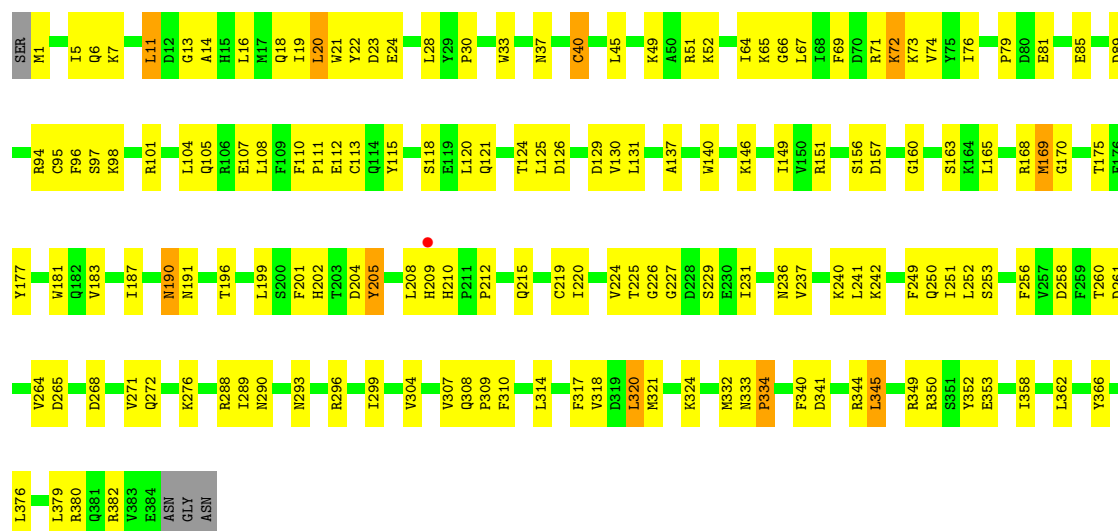


• Molecule 1: GAMMA-BUTYROBETAIN DIOXYGENASE



• Molecule 1: GAMMA-BUTYROBETAIN DIOXYGENASE

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	195.74Å 91.66Å 167.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.42 – 2.82 48.42 – 2.82	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.42-2.82) 96.9 (48.42-2.82)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.81Å)	Xtrriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.215 , 0.244 0.221 , 0.222	Depositor DCC
R_{free} test set	3577 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	58.8	Xtrriage
Anisotropy	0.233	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19352	wwPDB-VP
Average B, all atoms (Å ²)	62.0	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 33.22 % 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 8.2781e-04. 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: EDO, ZN, 6YT, NI

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	0.53	0/3193	0.98	16/4323 (0.4%)
1	B	0.54	0/3208	0.97	8/4341 (0.2%)
1	C	0.53	0/3195	0.92	11/4327 (0.3%)
1	D	0.52	0/3187	0.96	14/4315 (0.3%)
1	E	0.48	0/3175	0.89	9/4302 (0.2%)
1	F	0.51	0/3187	0.94	8/4315 (0.2%)
All	All	0.52	0/19145	0.94	66/25923 (0.3%)

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	23	ASP	N-CA-C	11.07	123.42	111.36
1	B	266	TYR	N-CA-C	-9.80	101.33	113.28
1	D	266	TYR	N-CA-C	-9.25	101.27	111.36
1	A	189	ALA	N-CA-C	9.06	121.16	111.28
1	E	266	TYR	N-CA-C	-8.96	101.77	112.89
1	C	266	TYR	N-CA-C	-8.61	102.21	112.89
1	E	353	GLU	N-CA-C	8.54	121.44	109.15
1	B	71	ARG	N-CA-C	8.47	121.64	111.82
1	C	12	ASP	N-CA-C	7.65	120.58	111.02
1	A	340	PHE	N-CA-C	7.21	120.12	109.24
1	F	169	MET	N-CA-C	7.08	118.68	110.97
1	D	24	GLU	N-CA-C	7.05	120.23	108.73
1	A	307	VAL	N-CA-C	7.00	117.09	110.30
1	A	266	TYR	N-CA-C	-6.90	104.67	113.23
1	B	307	VAL	N-CA-C	6.88	116.97	110.30
1	A	13	GLY	N-CA-C	-6.75	105.48	114.25
1	E	276	LYS	N-CA-C	-6.55	98.53	109.07
1	C	13	GLY	N-CA-C	-6.33	106.58	115.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	CYS	N-CA-C	-6.24	104.24	112.72
1	B	353	GLU	N-CA-C	6.18	119.31	110.10
1	B	11	LEU	CB-CA-C	-6.17	109.48	116.63
1	D	307	VAL	N-CA-C	6.12	116.60	110.23
1	D	276	LYS	N-CA-C	-6.11	99.75	109.59
1	E	307	VAL	N-CA-C	6.10	116.76	110.36
1	F	210	HIS	CA-C-N	6.02	124.06	119.66
1	F	210	HIS	C-N-CA	6.02	124.06	119.66
1	D	298	THR	N-CA-C	-5.99	105.93	113.18
1	E	109	PHE	N-CA-C	5.98	120.71	113.17
1	F	204	ASP	N-CA-C	5.98	119.38	109.46
1	D	264	VAL	CB-CA-C	-5.97	102.36	110.42
1	B	354	ALA	CB-CA-C	-5.92	109.73	116.54
1	F	72	LYS	N-CA-C	5.89	119.69	111.56
1	A	297	ASP	N-CA-C	5.84	117.83	110.24
1	F	190	ASN	N-CA-C	-5.75	102.25	110.59
1	A	24	GLU	CB-CA-C	-5.67	98.40	110.76
1	E	245	ASN	CA-C-N	5.67	125.52	119.28
1	E	245	ASN	C-N-CA	5.67	125.52	119.28
1	D	340	PHE	N-CA-C	5.65	117.86	108.99
1	A	76	ILE	N-CA-C	5.64	116.60	108.48
1	D	271	VAL	N-CA-C	5.54	117.32	108.89
1	A	203	THR	N-CA-C	-5.53	101.57	110.14
1	C	271	VAL	N-CA-C	5.47	116.45	108.58
1	C	291	PHE	N-CA-C	5.47	117.53	108.13
1	F	112	GLU	N-CA-C	5.46	118.14	109.96
1	A	276	LYS	N-CA-C	-5.42	100.34	108.96
1	D	109	PHE	N-CA-C	5.41	119.98	113.17
1	A	146	LYS	N-CA-C	5.35	116.79	111.07
1	C	276	LYS	N-CA-C	-5.34	100.47	109.07
1	B	179	HIS	N-CA-C	-5.33	105.38	111.14
1	D	22	TYR	N-CA-C	-5.27	99.18	108.08
1	E	353	GLU	CB-CA-C	-5.26	102.67	110.67
1	E	41	SER	N-CA-C	5.23	117.72	111.71
1	B	327	LYS	N-CA-C	5.22	118.13	109.46
1	A	108	LEU	N-CA-C	5.21	118.10	111.69
1	C	46	ASP	N-CA-C	5.18	116.61	111.07
1	C	298	THR	N-CA-C	-5.13	107.03	113.28
1	D	211	PRO	CA-C-N	5.12	125.36	119.83
1	D	211	PRO	C-N-CA	5.12	125.36	119.83
1	D	22	TYR	CB-CA-C	-5.10	110.71	116.63
1	F	340	PHE	N-CA-C	5.09	116.55	108.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	76	ILE	N-CA-C	5.08	115.79	108.48
1	A	38	CYS	CA-C-N	5.07	124.68	119.56
1	A	38	CYS	C-N-CA	5.07	124.68	119.56
1	C	132	ARG	N-CA-C	5.04	119.56	113.41
1	A	94	ARG	N-CA-C	5.02	118.55	112.93
1	A	23	ASP	CB-CA-C	-5.01	102.09	110.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3116	0	3043	88	0
1	B	3130	0	3070	95	0
1	C	3117	0	3031	102	0
1	D	3109	0	3042	111	0
1	E	3097	0	3012	116	0
1	F	3109	0	3042	121	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	23	0	14	7	0
4	B	23	0	14	5	0
4	C	23	0	14	0	0
4	D	23	0	14	1	0
4	E	23	0	14	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	23	0	14	2	0
5	A	12	0	18	0	0
5	B	8	0	12	0	0
5	C	16	0	24	1	0
5	E	12	0	18	2	0
5	F	8	0	12	0	0
6	A	106	0	0	5	0
6	B	95	0	0	2	0
6	C	90	0	0	5	0
6	D	60	0	0	4	0
6	E	52	0	0	2	0
6	F	65	0	0	5	0
All	All	19352	0	18408	596	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 16.

All (596) 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:F:199:LEU:HD21	1:F:349:ARG:HB3	1.34	1.09
1:B:93:LYS:HE2	1:B:94:ARG:HH12	1.32	0.91
1:F:140:TRP:HH2	1:F:169:MET:HE2	1.36	0.89
1:B:219:CYS:HB2	1:B:332:MET:HE2	1.55	0.89
1:F:224:VAL:HG12	1:F:358:ILE:HA	1.56	0.85
1:B:93:LYS:HE2	1:B:94:ARG:NH1	1.92	0.85
1:F:175:THR:HG23	1:F:177:TYR:H	1.43	0.84
1:D:187:ILE:HG13	1:D:358:ILE:HB	1.60	0.83
1:A:228:ASP:HB2	1:A:350:ARG:HD3	1.58	0.83
1:F:199:LEU:CD2	1:F:349:ARG:HB3	2.09	0.83
1:E:59:ASP:HB3	1:E:62:ILE:HB	1.59	0.83
1:F:219:CYS:HB2	1:F:332:MET:HE2	1.61	0.82
1:E:264:VAL:HG22	1:E:268:ASP:HA	1.60	0.82
1:C:104:LEU:HD21	1:D:299:ILE:HD12	1.62	0.82
1:F:140:TRP:CH2	1:F:169:MET:HE2	2.14	0.82
1:E:353:GLU:O	1:E:356:THR:HG23	1.81	0.80
1:E:201:PHE:HB2	1:E:321:MET:HE3	1.63	0.79
1:B:38:CYS:SG	1:B:40:CYS:HB3	2.23	0.78
1:F:318:VAL:HA	1:F:321:MET:HE2	1.66	0.78
1:F:175:THR:HG22	6:F:2030:HOH:O	1.83	0.78
1:E:38:CYS:SG	1:E:40:CYS:HB3	2.21	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:HD21	4:A:601:6YT:HAL1	1.68	0.75
1:F:1:MET:O	1:F:22:TYR:HB2	1.86	0.75
1:B:369:TRP:O	1:B:373:MET:HB2	1.86	0.75
1:F:107:GLU:HG3	1:F:380:ARG:HH22	1.52	0.75
1:F:183:VAL:HG21	1:F:362:LEU:HD12	1.69	0.75
1:B:358:ILE:HG22	6:B:2073:HOH:O	1.86	0.75
1:C:105:GLN:NE2	1:D:274:LYS:HE2	2.01	0.74
1:F:5:ILE:HG12	1:F:19:ILE:HD11	1.69	0.73
1:B:217:LEU:HD21	4:B:601:6YT:HAL1	1.70	0.73
1:F:45:LEU:HD21	1:F:52:LYS:HE3	1.71	0.72
1:B:222:GLN:HG3	1:B:360:ARG:HB3	1.70	0.72
1:F:7:LYS:HB3	1:F:20:LEU:HD23	1.72	0.71
1:C:40:CYS:SG	1:C:42:ASP:HB2	2.31	0.71
1:C:223:THR:HG23	1:C:359:SER:HB2	1.72	0.71
1:A:217:LEU:HD22	4:A:601:6YT:CAK	2.20	0.71
1:F:72:LYS:O	1:F:73:LYS:HG3	1.90	0.71
1:A:217:LEU:HD22	4:A:601:6YT:HAK	1.74	0.70
1:B:75:TYR:HD1	1:B:83:TYR:HH	1.37	0.70
1:C:116:TRP:HH2	1:C:231:ILE:HG22	1.57	0.70
1:A:30:PRO:HG3	1:B:307:VAL:HG11	1.73	0.69
1:B:94:ARG:HG3	1:B:94:ARG:HH11	1.55	0.69
1:F:264:VAL:HG12	1:F:268:ASP:HA	1.74	0.69
1:E:4:THR:HG22	1:E:72:LYS:HD3	1.74	0.69
5:E:703:EDO:H11	1:F:209:HIS:NE2	2.08	0.69
1:D:16:LEU:HD12	1:D:28:LEU:HD23	1.75	0.69
1:F:227:GLY:HA2	1:F:350:ARG:O	1.93	0.68
1:E:129:ASP:HB3	1:E:136:HIS:ND1	2.08	0.68
1:F:67:LEU:HD13	1:F:76:ILE:HG12	1.76	0.68
1:B:344:ARG:HG2	1:B:345:LEU:HD12	1.74	0.68
1:C:175:THR:HG22	6:C:2048:HOH:O	1.94	0.68
1:A:75:TYR:HD2	1:A:83:TYR:HH	1.42	0.68
1:C:38:CYS:SG	1:C:40:CYS:HB3	2.35	0.67
1:F:67:LEU:HD11	1:F:74:VAL:HG13	1.75	0.67
1:C:228:ASP:OD1	1:C:331:LYS:HG2	1.95	0.67
1:E:157:ASP:O	1:E:220:ILE:HG23	1.93	0.67
1:A:23:ASP:O	1:A:24:GLU:HB2	1.94	0.67
1:A:97:SER:O	1:A:101:ARG:HG3	1.95	0.66
1:C:272:GLN:HG3	1:D:108:LEU:HD22	1.77	0.66
1:F:224:VAL:HG12	1:F:358:ILE:CA	2.26	0.66
1:D:264:VAL:O	1:D:264:VAL:HG23	1.96	0.65
1:A:318:VAL:HA	1:A:321:MET:HE3	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:LEU:HD22	1:D:272:GLN:HG3	1.77	0.65
1:A:94:ARG:HG3	1:A:94:ARG:HH11	1.61	0.65
1:A:280:LEU:HD23	1:A:286:VAL:HA	1.77	0.65
1:E:347:HIS:HD1	1:E:347:HIS:H	1.44	0.65
1:D:341:ASP:OD1	1:D:343:TRP:HB2	1.97	0.64
1:F:183:VAL:HG22	1:F:362:LEU:HB2	1.79	0.64
1:A:304:VAL:HG22	1:B:96:PHE:HB3	1.80	0.64
1:D:187:ILE:CG1	1:D:358:ILE:HB	2.27	0.64
1:E:175:THR:HG23	1:E:177:TYR:H	1.62	0.64
1:E:288:ARG:HG2	1:E:289:ILE:N	2.12	0.64
1:C:110:PHE:HD1	1:C:373:MET:HE1	1.61	0.64
1:F:256:PHE:CE2	1:F:276:LYS:HE3	2.33	0.64
1:E:14:ALA:HB1	1:E:64:ILE:H	1.64	0.63
1:F:40:CYS:HA	6:F:2004:HOH:O	1.99	0.63
1:C:288:ARG:HG2	1:C:289:ILE:N	2.14	0.63
1:C:253:SER:HB3	1:C:278:ILE:HG13	1.79	0.63
1:E:5:ILE:HD12	1:E:70:ASP:O	1.99	0.62
1:A:55:VAL:O	1:B:315:LYS:HE3	2.00	0.62
1:B:72:LYS:HE3	6:B:2019:HOH:O	1.98	0.62
1:F:212:PRO:HB3	1:F:366:TYR:HB3	1.81	0.62
1:A:301:ASP:OD1	1:B:101:ARG:HB3	1.99	0.62
1:E:288:ARG:HG2	1:E:289:ILE:H	1.65	0.62
1:D:17:MET:HE3	1:D:19:ILE:HD11	1.82	0.62
1:D:140:TRP:CE3	1:D:141:LEU:HD13	2.35	0.61
1:A:21:TRP:HB2	1:A:23:ASP:OD1	2.00	0.61
1:C:308:GLN:HB3	1:C:309:PRO:HD3	1.83	0.61
1:C:219:CYS:HB2	1:C:332:MET:HE2	1.83	0.61
1:C:306:ARG:O	1:C:309:PRO:HD2	2.01	0.61
1:E:12:ASP:C	1:E:14:ALA:H	2.09	0.61
1:E:149:ILE:HD11	1:E:338:ILE:HG23	1.83	0.61
1:E:201:PHE:CB	1:E:321:MET:HE3	2.31	0.61
1:B:75:TYR:HD1	1:B:83:TYR:OH	1.84	0.60
1:C:227:GLY:HA2	1:C:350:ARG:O	2.00	0.60
1:E:227:GLY:HA2	1:E:350:ARG:O	2.01	0.60
1:E:234:GLY:HA3	1:E:289:ILE:HD13	1.83	0.60
1:F:94:ARG:HG3	1:F:94:ARG:HH11	1.67	0.60
1:E:289:ILE:HG21	1:E:346:LEU:HD11	1.84	0.60
1:D:219:CYS:HA	1:D:362:LEU:HD22	1.83	0.60
1:B:122:LEU:HD23	1:B:151:ARG:CZ	2.31	0.60
1:E:104:LEU:HD21	1:F:299:ILE:HG21	1.84	0.60
1:F:225:THR:O	1:F:353:GLU:HG2	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:PRO:HB3	1:B:366:TYR:HB3	1.83	0.59
1:F:67:LEU:HD13	1:F:76:ILE:CG1	2.32	0.59
1:B:236:ASN:HD21	1:B:240:LYS:NZ	2.00	0.59
1:E:49:LYS:HD2	1:F:260:THR:HG21	1.83	0.59
1:E:308:GLN:HB3	1:E:309:PRO:HD3	1.85	0.59
1:D:21:TRP:O	1:D:22:TYR:HB3	2.01	0.59
1:B:135:GLU:OE2	1:B:383:VAL:HG13	2.03	0.59
1:E:191:ASN:ND2	1:E:193:ALA:H	2.00	0.59
1:A:304:VAL:HG22	1:B:96:PHE:CB	2.33	0.58
1:B:262:ILE:HD12	1:B:262:ILE:C	2.28	0.58
1:D:227:GLY:HA2	1:D:350:ARG:O	2.03	0.58
1:C:122:LEU:HD23	1:C:151:ARG:CZ	2.34	0.58
1:C:224:VAL:HG12	1:C:358:ILE:HA	1.84	0.58
1:D:172:LEU:HD12	1:D:179:HIS:CE1	2.38	0.58
1:C:96:PHE:HB3	1:D:304:VAL:HG22	1.86	0.58
1:D:80:ASP:O	1:D:81:GLU:HB2	2.03	0.58
1:B:214:VAL:HG22	1:B:367:ALA:HB3	1.85	0.58
1:D:67:LEU:HD12	1:D:68:ILE:N	2.18	0.58
1:D:68:ILE:HA	6:D:2009:HOH:O	2.02	0.58
1:C:130:VAL:HG13	1:C:137:ALA:HA	1.86	0.58
1:F:318:VAL:HA	1:F:321:MET:CE	2.33	0.58
1:C:288:ARG:HD2	1:C:290:ASN:HD21	1.69	0.57
1:F:258:ASP:HB3	6:F:2047:HOH:O	2.04	0.57
1:F:187:ILE:HD12	1:F:358:ILE:HD11	1.86	0.57
1:C:216:LEU:O	1:C:364:GLY:HA2	2.05	0.57
1:D:302:VAL:HG23	1:D:303:PRO:HD2	1.87	0.57
1:B:169:MET:HE1	1:B:216:LEU:HD11	1.85	0.57
1:C:8:ALA:HA	1:C:19:ILE:HG22	1.86	0.57
1:D:14:ALA:HB1	1:D:64:ILE:HB	1.86	0.57
1:E:301:ASP:HA	1:F:101:ARG:HD2	1.86	0.57
1:F:21:TRP:O	1:F:24:GLU:N	2.38	0.57
1:C:176:PHE:HB2	1:C:205:TYR:OH	2.05	0.57
1:F:196:THR:HG21	1:F:352:TYR:HD2	1.68	0.57
1:A:64:ILE:HG23	1:A:76:ILE:HG23	1.86	0.57
1:A:353:GLU:HB3	1:A:356:THR:HG21	1.87	0.57
1:F:7:LYS:HA	1:F:69:PHE:CZ	2.40	0.57
1:B:303:PRO:HG2	1:B:306:ARG:HG3	1.86	0.56
1:D:277:ILE:HD13	1:D:314:LEU:HD13	1.87	0.56
1:A:223:THR:HB	1:A:359:SER:HB3	1.87	0.56
1:D:68:ILE:HG13	1:D:75:TYR:HB2	1.87	0.56
1:F:6:GLN:OE1	1:F:20:LEU:HD11	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:VAL:HG21	1:D:55:VAL:HG11	1.87	0.56
1:A:38:CYS:SG	1:A:40:CYS:HB3	2.45	0.56
1:D:180:THR:HG22	1:D:365:ALA:HB2	1.86	0.56
1:E:169:MET:HE2	1:E:372:VAL:HG22	1.87	0.56
1:E:127:PHE:CE1	1:E:165:LEU:HD13	2.41	0.56
1:A:30:PRO:HG2	1:A:33:TRP:HB3	1.87	0.56
1:D:140:TRP:CH2	1:D:165:LEU:HD22	2.41	0.56
1:E:307:VAL:HG11	1:F:30:PRO:HG2	1.87	0.56
1:E:191:ASN:HD22	1:E:193:ALA:H	1.52	0.56
1:F:64:ILE:HG23	1:F:76:ILE:HG23	1.88	0.56
1:C:104:LEU:CD2	1:D:299:ILE:HD12	2.35	0.56
1:E:68:ILE:HG13	1:E:75:TYR:HD2	1.69	0.56
1:E:127:PHE:HE1	1:E:165:LEU:HD13	1.70	0.55
1:D:315:LYS:HE2	1:D:319:ASP:OD2	2.05	0.55
1:F:157:ASP:O	1:F:220:ILE:HG23	2.05	0.55
1:A:43:CYS:O	1:A:52:LYS:HG2	2.06	0.55
1:B:94:ARG:NH1	1:B:94:ARG:HG3	2.22	0.55
1:A:30:PRO:HG2	1:A:33:TRP:CB	2.36	0.55
1:C:32:VAL:HG12	6:C:2001:HOH:O	2.06	0.55
1:C:201:PHE:CB	1:C:321:MET:HE3	2.36	0.55
1:E:122:LEU:HD23	1:E:151:ARG:CZ	2.37	0.55
1:B:157:ASP:O	1:B:158:LYS:HD3	2.06	0.55
1:C:141:LEU:HD22	1:C:372:VAL:HG13	1.89	0.55
1:E:78:TRP:HD1	1:E:82:HIS:HB3	1.71	0.55
1:B:206:PRO:HG2	1:B:292:ASN:HB2	1.88	0.55
1:C:301:ASP:HA	1:D:101:ARG:HD2	1.89	0.55
1:B:54:LEU:N	1:B:54:LEU:HD12	2.22	0.54
1:A:288:ARG:HG2	1:A:289:ILE:N	2.22	0.54
1:A:371:VAL:HG13	6:A:2047:HOH:O	2.08	0.54
1:D:345:LEU:HD23	1:D:345:LEU:N	2.22	0.54
1:A:4:THR:HG23	1:A:71:ARG:HB3	1.89	0.54
1:C:5:ILE:HD13	1:C:74:VAL:HG23	1.90	0.54
1:A:23:ASP:O	1:A:24:GLU:CB	2.56	0.54
1:D:12:ASP:C	1:D:14:ALA:H	2.15	0.54
1:A:281:ASP:OD2	1:A:285:GLN:HB2	2.07	0.54
1:A:106:ARG:NH1	6:A:2031:HOH:O	2.40	0.54
1:A:302:VAL:HG22	1:A:306:ARG:HB2	1.90	0.54
1:A:75:TYR:HD2	1:A:83:TYR:OH	1.90	0.54
1:A:101:ARG:HD2	1:B:301:ASP:HA	1.89	0.54
1:D:70:ASP:OD1	1:D:73:LYS:HB2	2.07	0.53
1:E:130:VAL:HG13	1:E:137:ALA:HA	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:HD21	1:A:28:LEU:HD13	1.90	0.53
1:F:177:TYR:HD1	1:F:265:ASP:OD2	1.91	0.53
1:C:1:MET:O	1:C:2:ALA:HB3	2.08	0.53
1:A:270:SER:HB2	1:B:378:ILE:HD11	1.89	0.53
1:B:281:ASP:HB3	1:B:287:VAL:HG11	1.90	0.53
1:C:360:ARG:HG2	1:C:362:LEU:HD13	1.90	0.53
1:E:1:MET:H2	1:E:22:TYR:HB3	1.74	0.53
1:F:107:GLU:CG	1:F:380:ARG:HH22	2.21	0.53
1:A:205:TYR:N	1:A:206:PRO:HD3	2.24	0.53
1:B:205:TYR:N	1:B:206:PRO:HD3	2.24	0.53
1:B:236:ASN:HD21	1:B:240:LYS:HZ3	1.55	0.53
1:D:157:ASP:C	1:D:220:ILE:HG23	2.34	0.53
1:D:305:GLU:CD	1:D:305:GLU:H	2.17	0.53
1:A:221:LYS:HE3	1:A:222:GLN:N	2.22	0.53
1:D:247:GLN:O	1:D:251:ILE:HG13	2.09	0.53
1:D:345:LEU:HD23	1:D:345:LEU:H	1.73	0.53
5:E:703:EDO:C1	1:F:209:HIS:NE2	2.71	0.53
1:A:104:LEU:HD21	1:B:299:ILE:HD13	1.91	0.52
1:A:199:LEU:HD13	4:A:601:6YT:HA	1.90	0.52
1:B:281:ASP:OD2	1:B:285:GLN:HB2	2.09	0.52
1:E:144:LEU:O	1:E:148:GLY:HA2	2.09	0.52
1:E:260:THR:HG21	1:F:49:LYS:HE3	1.90	0.52
1:A:288:ARG:HD3	1:A:290:ASN:OD1	2.09	0.52
1:A:380:ARG:CZ	1:A:380:ARG:HB3	2.38	0.52
1:C:268:ASP:OD2	1:D:378:ILE:HD13	2.09	0.52
1:E:251:ILE:HD13	1:E:310:PHE:HA	1.91	0.52
1:A:176:PHE:O	1:A:265:ASP:HB3	2.09	0.52
1:F:205:TYR:CD1	1:F:208:LEU:HG	2.44	0.52
1:A:104:LEU:HD21	1:B:299:ILE:CD1	2.39	0.52
1:A:183:VAL:O	1:A:361:HIS:HA	2.10	0.52
1:E:67:LEU:C	1:E:67:LEU:HD23	2.34	0.52
1:B:20:LEU:HG	1:B:26:GLU:HG2	1.92	0.52
1:D:140:TRP:CH2	1:D:169:MET:HE3	2.45	0.52
1:A:43:CYS:C	1:A:52:LYS:HG2	2.35	0.52
1:D:187:ILE:HD12	1:D:187:ILE:O	2.10	0.52
1:D:264:VAL:HG12	1:D:268:ASP:HA	1.91	0.52
1:C:264:VAL:HG22	1:C:268:ASP:HB3	1.92	0.52
4:B:601:6YT:OAD	4:B:601:6YT:N	2.42	0.51
1:F:288:ARG:HG2	1:F:289:ILE:N	2.23	0.51
1:C:122:LEU:HD23	1:C:151:ARG:NH1	2.25	0.51
1:C:175:THR:HG23	1:C:177:TYR:H	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:LEU:HD23	1:F:199:LEU:H	1.75	0.51
1:B:361:HIS:O	1:B:362:LEU:HD23	2.11	0.51
1:E:1:MET:N	1:E:22:TYR:HB3	2.25	0.51
1:E:264:VAL:HG22	1:E:268:ASP:CA	2.37	0.51
1:A:79:PRO:C	1:A:81:GLU:H	2.18	0.51
1:D:318:VAL:HA	1:D:321:MET:HE2	1.91	0.51
1:E:144:LEU:O	1:E:144:LEU:HD23	2.10	0.51
1:B:217:LEU:HD22	4:B:601:6YT:CAK	2.40	0.51
1:C:96:PHE:CB	1:D:304:VAL:HG22	2.41	0.51
1:C:296:ARG:HB3	1:D:51:ARG:HH12	1.75	0.51
1:E:96:PHE:CB	1:F:304:VAL:HG22	2.40	0.51
1:B:178:GLY:HA2	1:B:266:TYR:CD2	2.46	0.51
1:F:131:LEU:HA	1:F:168:ARG:HD3	1.92	0.51
1:D:16:LEU:N	1:D:16:LEU:HD23	2.25	0.51
1:D:73:LYS:HD3	1:D:75:TYR:OH	2.11	0.51
1:D:302:VAL:CG2	1:D:303:PRO:HD2	2.41	0.51
1:E:191:ASN:HD22	1:E:192:VAL:N	2.09	0.51
1:D:79:PRO:C	1:D:81:GLU:H	2.19	0.51
1:A:155:ALA:HB3	1:A:335:GLY:O	2.11	0.50
1:D:199:LEU:HB2	1:D:349:ARG:HB3	1.92	0.50
1:F:237:VAL:HG13	1:F:320:LEU:HD13	1.93	0.50
1:B:187:ILE:HB	1:B:358:ILE:HG12	1.93	0.50
1:B:219:CYS:HA	1:B:362:LEU:HD22	1.92	0.50
1:E:55:VAL:HG23	6:E:2006:HOH:O	2.11	0.50
1:E:96:PHE:HB2	1:F:304:VAL:HG22	1.93	0.50
1:D:127:PHE:O	1:D:130:VAL:HG22	2.11	0.50
1:E:307:VAL:O	1:E:310:PHE:HB3	2.12	0.50
1:F:6:GLN:HB2	1:F:22:TYR:CD1	2.47	0.50
4:A:601:6YT:N	4:A:601:6YT:OAD	2.42	0.50
1:C:280:LEU:HD23	1:C:286:VAL:HA	1.92	0.50
1:D:260:THR:HB	1:D:272:GLN:NE2	2.27	0.50
1:E:67:LEU:HD23	1:E:68:ILE:N	2.27	0.50
1:C:264:VAL:HG22	1:C:268:ASP:CB	2.42	0.50
1:F:242:LYS:HD2	1:F:249:PHE:CE2	2.47	0.50
1:B:227:GLY:HA3	1:B:352:TYR:CE1	2.47	0.50
1:A:217:LEU:CD2	4:A:601:6YT:HAL1	2.41	0.49
1:E:114:GLN:HG3	1:E:146:LYS:HE2	1.94	0.49
1:F:160:GLY:O	1:F:163:SER:HB2	2.12	0.49
1:F:314:LEU:O	1:F:318:VAL:HG23	2.12	0.49
1:A:16:LEU:HD12	1:A:30:PRO:HA	1.94	0.49
1:B:64:ILE:HG23	1:B:76:ILE:HG23	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ILE:HD12	1:B:358:ILE:HD11	1.93	0.49
1:C:8:ALA:CB	1:C:19:ILE:HG22	2.42	0.49
1:B:302:VAL:CG2	1:B:303:PRO:HD2	2.42	0.49
1:C:187:ILE:HG13	1:C:358:ILE:HB	1.94	0.49
1:E:14:ALA:HB1	1:E:64:ILE:N	2.27	0.49
1:E:94:ARG:HG3	1:E:94:ARG:HH11	1.77	0.49
1:E:279:GLU:O	1:E:287:VAL:HG22	2.12	0.49
1:C:186:LYS:HA	1:C:358:ILE:O	2.13	0.49
1:B:93:LYS:CE	1:B:94:ARG:HH12	2.16	0.49
1:D:261:ASP:HB3	1:D:271:VAL:HG22	1.95	0.49
1:D:11:LEU:HD12	1:D:16:LEU:HD11	1.94	0.49
1:D:216:LEU:N	1:D:216:LEU:HD12	2.28	0.49
1:B:262:ILE:HD12	1:B:262:ILE:O	2.13	0.49
1:D:281:ASP:OD1	1:D:285:GLN:N	2.45	0.49
1:E:108:LEU:HD22	1:F:272:GLN:HG3	1.94	0.49
1:B:217:LEU:CD2	4:B:601:6YT:HAL1	2.42	0.49
1:E:353:GLU:O	1:E:356:THR:CG2	2.58	0.49
1:F:23:ASP:O	1:F:24:GLU:CB	2.59	0.48
1:B:21:TRP:CE2	1:B:92:LYS:HD3	2.48	0.48
1:C:252:LEU:HD22	1:C:277:ILE:HD12	1.94	0.48
1:C:347:HIS:ND1	1:C:347:HIS:N	2.61	0.48
1:F:253:SER:O	1:F:276:LYS:HD3	2.13	0.48
1:D:145:LYS:HG2	1:D:369:TRP:CZ3	2.48	0.48
1:D:312:ALA:O	1:D:315:LYS:HB3	2.12	0.48
1:C:3:CYS:SG	1:C:3:CYS:O	2.70	0.48
1:A:380:ARG:HG2	1:A:380:ARG:HH11	1.78	0.48
1:E:220:ILE:HG21	1:E:361:HIS:HD2	1.77	0.48
1:F:115:TYR:HB3	1:F:236:ASN:HB2	1.96	0.48
1:F:288:ARG:HD3	1:F:290:ASN:OD1	2.14	0.48
1:F:293:ASN:OD1	1:F:296:ARG:NH2	2.47	0.48
1:A:199:LEU:CD1	4:A:601:6YT:HA	2.43	0.48
1:B:230:GLU:OE2	1:B:350:ARG:HD3	2.13	0.48
1:E:244:ASN:C	1:E:246:PRO:HD3	2.39	0.48
1:E:251:ILE:HD11	1:E:313:ALA:HB3	1.96	0.48
1:A:217:LEU:HD23	1:A:332:MET:HE1	1.94	0.48
1:B:262:ILE:HG22	1:B:270:SER:HA	1.96	0.48
1:B:288:ARG:HG3	1:B:343:TRP:CG	2.48	0.48
1:E:222:GLN:H	1:E:334:PRO:HG3	1.79	0.48
4:D:601:6YT:OAD	4:D:601:6YT:N	2.42	0.48
1:A:308:GLN:HB3	1:A:309:PRO:HD3	1.96	0.47
1:F:72:LYS:O	1:F:73:LYS:CG	2.61	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ASP:OD1	1:C:265:ASP:C	2.56	0.47
1:D:127:PHE:CZ	1:D:161:GLU:HG3	2.50	0.47
1:E:235:PHE:CD2	1:E:344:ARG:HD2	2.49	0.47
1:B:358:ILE:O	1:B:358:ILE:HG13	2.15	0.47
1:C:116:TRP:CG	1:C:120:LEU:HD13	2.48	0.47
1:A:47:SER:HA	6:A:2014:HOH:O	2.14	0.47
1:A:322:ASN:O	1:A:327:LYS:NZ	2.47	0.47
1:A:378:ILE:O	1:A:382:ARG:HG3	2.14	0.47
1:C:166:GLY:HA2	1:C:169:MET:HE2	1.95	0.47
1:C:312:ALA:HA	1:D:60:VAL:HG11	1.95	0.47
1:F:73:LYS:HZ1	1:F:85:GLU:HB3	1.78	0.47
1:B:176:PHE:HB2	1:B:205:TYR:OH	2.15	0.47
1:E:251:ILE:CD1	1:E:310:PHE:HA	2.44	0.47
1:A:101:ARG:HB3	1:B:301:ASP:OD1	2.13	0.47
1:B:21:TRP:HB2	1:B:23:ASP:OD1	2.15	0.47
1:B:40:CYS:SG	1:B:42:ASP:HB2	2.55	0.47
1:C:201:PHE:HB2	1:C:321:MET:HE3	1.96	0.47
1:E:40:CYS:SG	1:E:42:ASP:N	2.87	0.47
1:E:73:LYS:NZ	1:E:73:LYS:HB3	2.30	0.47
1:E:213:GLY:HA2	1:E:343:TRP:NE1	2.30	0.47
1:F:241:LEU:HD21	1:F:252:LEU:HD12	1.96	0.47
1:A:94:ARG:HG3	1:A:94:ARG:NH1	2.29	0.47
1:B:176:PHE:O	1:B:265:ASP:HB3	2.15	0.47
1:D:113:CYS:HB3	6:D:2017:HOH:O	2.15	0.47
1:E:97:SER:O	1:E:101:ARG:HG3	2.14	0.47
1:F:72:LYS:C	1:F:73:LYS:HG3	2.39	0.47
1:F:251:ILE:HG21	1:F:310:PHE:HA	1.96	0.47
1:B:72:LYS:HA	1:B:88:ALA:HB2	1.97	0.47
1:D:52:LYS:O	1:D:54:LEU:HD12	2.15	0.47
1:D:274:LYS:NZ	1:D:301:ASP:HB3	2.30	0.47
1:E:215:GLN:NE2	1:E:340:PHE:HZ	2.13	0.47
1:E:279:GLU:HG3	1:E:290:ASN:ND2	2.29	0.47
1:B:196:THR:HG21	1:B:352:TYR:HB2	1.97	0.47
1:E:191:ASN:HD22	1:E:191:ASN:C	2.23	0.47
1:C:7:LYS:O	1:C:19:ILE:HA	2.15	0.47
1:F:21:TRP:C	1:F:24:GLU:H	2.22	0.47
1:F:130:VAL:HG13	1:F:137:ALA:HA	1.97	0.47
1:C:110:PHE:CD1	1:C:373:MET:HE1	2.47	0.46
1:E:94:ARG:HG2	1:F:299:ILE:HG22	1.97	0.46
1:A:302:VAL:HG23	1:A:303:PRO:HD2	1.97	0.46
1:E:260:THR:HB	1:E:272:GLN:NE2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:ARG:HG3	1:F:71:ARG:HH11	1.79	0.46
1:F:181:TRP:HZ2	1:F:215:GLN:HE21	1.63	0.46
1:C:5:ILE:CD1	1:C:74:VAL:HG23	2.46	0.46
1:C:57:ALA:HB1	5:C:704:EDO:H21	1.97	0.46
1:F:94:ARG:HG3	1:F:94:ARG:NH1	2.29	0.46
1:F:113:CYS:HA	1:F:146:LYS:HG3	1.98	0.46
1:F:118:SER:HB3	1:F:324:LYS:O	2.15	0.46
1:D:21:TRP:HE1	1:D:27:SER:CB	2.28	0.46
1:D:368:ASP:O	1:D:371:VAL:HG22	2.14	0.46
1:E:299:ILE:HG12	1:F:104:LEU:HD21	1.98	0.46
1:A:181:TRP:CZ2	1:A:364:GLY:HA3	2.50	0.46
1:F:11:LEU:HD23	1:F:18:GLN:HB3	1.98	0.46
1:B:130:VAL:HG13	1:B:137:ALA:HA	1.98	0.46
1:A:176:PHE:HB2	1:A:205:TYR:OH	2.16	0.46
1:C:315:LYS:NZ	1:C:319:ASP:OD2	2.46	0.46
1:D:45:LEU:HB2	1:D:52:LYS:HD2	1.96	0.46
1:D:71:ARG:HG3	1:D:71:ARG:HH11	1.80	0.46
1:B:18:GLN:HE21	1:B:26:GLU:HB3	1.81	0.46
1:C:207:ALA:O	1:C:273:SER:HB2	2.16	0.46
1:C:268:ASP:HB2	6:C:2073:HOH:O	2.15	0.46
1:A:177:TYR:HD1	1:A:265:ASP:OD2	1.99	0.46
1:C:201:PHE:HB3	1:C:321:MET:HE3	1.97	0.46
1:E:216:LEU:O	1:E:364:GLY:HA2	2.15	0.46
1:E:272:GLN:HG3	1:F:108:LEU:HD22	1.98	0.46
1:F:33:TRP:NE1	1:F:37:ASN:ND2	2.64	0.46
1:C:17:MET:HE3	1:C:19:ILE:HG21	1.98	0.45
1:C:264:VAL:HG22	1:C:268:ASP:HA	1.98	0.45
1:A:104:LEU:HD12	1:A:104:LEU:O	2.17	0.45
1:D:62:ILE:HG12	1:D:63:GLY:N	2.32	0.45
1:D:340:PHE:HE2	6:D:2060:HOH:O	1.98	0.45
1:E:241:LEU:HG	1:E:249:PHE:HB2	1.99	0.45
1:F:120:LEU:HD12	1:F:121:GLN:H	1.82	0.45
1:F:219:CYS:HA	1:F:362:LEU:HD23	1.99	0.45
1:C:1:MET:C	1:C:3:CYS:H	2.24	0.45
1:E:30:PRO:HG2	1:F:307:VAL:HB	1.98	0.45
1:E:232:VAL:HG12	1:E:346:LEU:HB2	1.98	0.45
1:F:229:SER:OG	4:F:601:6YT:HAH	2.16	0.45
1:B:225:THR:HG21	1:B:353:GLU:OE1	2.17	0.45
1:C:59:ASP:HB3	1:C:62:ILE:HB	1.97	0.45
1:C:73:LYS:HD2	1:C:75:TYR:CE2	2.51	0.45
1:F:261:ASP:O	1:F:271:VAL:HG22	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:ASP:HB3	1:F:129:ASP:OD2	2.17	0.45
1:C:172:LEU:HD22	1:C:365:ALA:HB1	1.98	0.45
1:D:34:LEU:HD22	1:D:86:PHE:CE2	2.52	0.45
1:D:135:GLU:OE2	1:D:383:VAL:HG13	2.17	0.45
1:D:224:VAL:HG12	1:D:358:ILE:HA	1.98	0.45
1:D:233:ASP:O	1:D:237:VAL:HG23	2.17	0.45
1:B:102:ALA:O	1:B:106:ARG:HG3	2.17	0.45
1:C:205:TYR:N	1:C:206:PRO:HD3	2.32	0.45
1:C:332:MET:HE2	1:C:332:MET:HB3	1.88	0.45
1:E:232:VAL:CG1	1:E:346:LEU:HB2	2.47	0.45
1:F:110:PHE:N	1:F:111:PRO:HD3	2.32	0.45
1:F:131:LEU:HD21	1:F:165:LEU:HD23	1.98	0.45
1:C:105:GLN:HE22	1:D:274:LYS:HE2	1.76	0.44
1:E:12:ASP:C	1:E:14:ALA:N	2.75	0.44
1:E:347:HIS:ND1	1:E:347:HIS:N	2.65	0.44
1:F:149:ILE:HD13	1:F:231:ILE:CD1	2.47	0.44
1:A:23:ASP:OD1	1:A:23:ASP:C	2.59	0.44
1:E:242:LYS:O	1:E:246:PRO:HG3	2.17	0.44
1:E:288:ARG:HG3	1:E:343:TRP:HB3	1.98	0.44
1:A:328:PHE:CE2	1:A:330:PHE:HB3	2.53	0.44
1:C:23:ASP:O	1:C:24:GLU:HB2	2.17	0.44
1:B:302:VAL:HG22	1:B:303:PRO:HD2	1.99	0.44
1:E:272:GLN:NE2	6:E:2037:HOH:O	2.50	0.44
1:C:39:PRO:HD3	1:C:86:PHE:CE1	2.53	0.44
1:D:21:TRP:O	1:D:22:TYR:CB	2.64	0.44
1:D:25:GLU:O	1:D:26:GLU:CG	2.66	0.44
1:D:165:LEU:HD23	1:D:165:LEU:HA	1.89	0.44
1:D:245:ASN:HB3	1:D:248:ALA:HB3	2.00	0.44
1:B:378:ILE:O	1:B:382:ARG:HG3	2.18	0.44
1:C:288:ARG:HG2	1:C:289:ILE:H	1.82	0.44
1:D:261:ASP:HB3	1:D:271:VAL:CG2	2.47	0.44
1:A:49:LYS:HB3	1:A:49:LYS:HE2	1.76	0.44
1:D:9:GLU:OE2	1:D:18:GLN:HB3	2.17	0.44
1:D:125:LEU:O	1:D:152:LEU:HA	2.18	0.44
1:A:67:LEU:HD12	1:A:67:LEU:C	2.43	0.44
1:B:216:LEU:O	1:B:364:GLY:HA2	2.18	0.44
1:B:280:LEU:HD23	1:B:286:VAL:HA	1.99	0.44
1:C:116:TRP:CH2	1:C:231:ILE:HG22	2.46	0.44
1:D:25:GLU:O	1:D:26:GLU:HG3	2.18	0.44
1:D:265:ASP:HB3	1:D:266:TYR:H	1.73	0.44
1:F:98:LYS:HA	1:F:98:LYS:HD2	1.74	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:THR:O	1:F:125:LEU:HG	2.18	0.44
1:F:124:THR:HG22	1:F:125:LEU:N	2.32	0.44
1:F:199:LEU:HD23	1:F:199:LEU:N	2.33	0.44
1:B:202:HIS:O	1:B:346:LEU:HA	2.18	0.43
1:B:219:CYS:HB2	1:B:332:MET:CE	2.35	0.43
1:C:77:THR:HG22	1:C:78:TRP:N	2.33	0.43
1:D:70:ASP:OD1	1:D:73:LYS:N	2.50	0.43
1:F:16:LEU:HD21	1:F:28:LEU:HD13	2.00	0.43
1:A:73:LYS:HG3	1:A:86:PHE:O	2.19	0.43
1:A:344:ARG:HG2	1:A:345:LEU:HD23	1.99	0.43
1:A:362:LEU:N	1:A:362:LEU:HD12	2.34	0.43
1:E:203:THR:HG21	1:E:289:ILE:O	2.17	0.43
1:E:329:THR:HG22	1:E:330:PHE:N	2.34	0.43
1:C:37:ASN:OD1	1:D:298:THR:HG22	2.18	0.43
1:C:157:ASP:O	1:C:220:ILE:HG23	2.18	0.43
1:D:218:HIS:HB2	1:D:337:VAL:HG22	2.00	0.43
1:E:6:GLN:HB3	1:E:20:LEU:O	2.18	0.43
1:E:110:PHE:HD1	1:E:373:MET:HE1	1.84	0.43
1:B:241:LEU:HD23	1:B:320:LEU:HD22	2.01	0.43
1:B:277:ILE:HD13	1:B:314:LEU:HD13	2.00	0.43
1:C:288:ARG:HD2	1:C:290:ASN:ND2	2.31	0.43
1:E:18:GLN:NE2	1:E:26:GLU:CG	2.81	0.43
1:E:221:LYS:O	1:E:360:ARG:HA	2.18	0.43
1:F:124:THR:HA	1:F:151:ARG:O	2.19	0.43
1:B:306:ARG:O	1:B:309:PRO:HG2	2.19	0.43
1:E:68:ILE:HG13	1:E:75:TYR:CD2	2.52	0.43
1:E:152:LEU:O	1:E:336:ASP:HA	2.18	0.43
1:E:158:LYS:HD2	1:E:158:LYS:N	2.33	0.43
1:A:156:SER:OG	1:A:158:LYS:HG2	2.19	0.43
1:A:308:GLN:N	1:A:309:PRO:CD	2.82	0.43
1:B:293:ASN:OD1	1:B:296:ARG:NH2	2.47	0.43
1:C:313:ALA:O	1:C:314:LEU:C	2.60	0.43
1:C:332:MET:HE3	1:C:338:ILE:HG12	2.00	0.43
1:D:62:ILE:HG12	1:D:63:GLY:H	1.83	0.43
1:E:87:GLN:HB2	1:E:90:TRP:HB2	2.00	0.43
1:F:126:ASP:HB3	1:F:129:ASP:HB2	1.99	0.43
1:A:109:PHE:O	1:A:110:PHE:C	2.61	0.43
1:D:79:PRO:C	1:D:81:GLU:N	2.76	0.43
1:F:345:LEU:HD23	1:F:345:LEU:N	2.34	0.43
1:D:38:CYS:SG	1:D:40:CYS:HB3	2.58	0.43
1:E:181:TRP:CH2	1:E:364:GLY:HA3	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLN:HG2	1:A:146:LYS:HE2	2.01	0.43
1:E:196:THR:HG21	1:E:352:TYR:HD2	1.83	0.43
1:A:154:GLY:HA3	6:A:2037:HOH:O	2.19	0.42
1:B:110:PHE:N	1:B:110:PHE:CD1	2.87	0.42
1:B:250:GLN:HG3	1:B:251:ILE:N	2.33	0.42
1:C:305:GLU:CD	1:C:305:GLU:H	2.27	0.42
1:E:116:TRP:CE3	1:E:120:LEU:HD22	2.54	0.42
1:A:286:VAL:HG23	6:A:2085:HOH:O	2.20	0.42
1:A:293:ASN:OD1	1:A:296:ARG:NH2	2.50	0.42
1:B:141:LEU:HD22	1:B:372:VAL:HG13	2.01	0.42
1:C:203:THR:HG23	1:C:346:LEU:HG	2.01	0.42
1:C:263:GLY:C	1:C:264:VAL:HG23	2.43	0.42
1:E:213:GLY:HA2	1:E:343:TRP:CD1	2.53	0.42
1:B:165:LEU:O	1:B:169:MET:HG3	2.19	0.42
1:C:11:LEU:HD12	1:C:11:LEU:O	2.19	0.42
1:C:17:MET:HE3	1:C:19:ILE:CG2	2.49	0.42
1:C:119:GLU:HA	1:E:331:LYS:HD2	2.02	0.42
1:E:66:GLY:HA3	1:E:77:THR:OG1	2.19	0.42
1:E:189:ALA:O	1:E:190:ASN:HB2	2.18	0.42
1:E:288:ARG:HG3	1:E:343:TRP:CB	2.49	0.42
1:F:110:PHE:CE2	1:F:380:ARG:HD3	2.54	0.42
1:B:373:MET:HE3	1:B:376:LEU:HD23	2.01	0.42
1:D:12:ASP:C	1:D:14:ALA:N	2.77	0.42
1:F:382:ARG:HG2	6:F:2064:HOH:O	2.18	0.42
1:C:105:GLN:HB3	6:C:2026:HOH:O	2.19	0.42
1:C:216:LEU:CD2	1:C:339:THR:HG22	2.50	0.42
1:D:212:PRO:HB3	1:D:366:TYR:HB3	2.02	0.42
1:D:342:ASN:CG	1:D:342:ASN:O	2.62	0.42
1:F:308:GLN:CB	1:F:309:PRO:HD3	2.49	0.42
1:A:149:ILE:HD13	1:A:231:ILE:HD13	2.02	0.42
1:C:278:ILE:HG13	1:C:278:ILE:O	2.19	0.42
1:D:140:TRP:CZ2	1:D:169:MET:HE3	2.55	0.42
1:F:65:LYS:HG3	1:F:66:GLY:N	2.34	0.42
1:A:6:GLN:HG3	1:A:22:TYR:CZ	2.55	0.42
1:C:80:ASP:O	1:C:81:GLU:HB3	2.19	0.42
1:D:252:LEU:HB2	1:D:278:ILE:HD12	2.01	0.42
1:F:358:ILE:HG13	1:F:358:ILE:O	2.20	0.42
1:A:272:GLN:HG2	1:B:108:LEU:HD22	2.02	0.42
1:D:165:LEU:HD13	1:D:216:LEU:HD23	2.02	0.42
1:F:130:VAL:O	1:F:168:ARG:NE	2.51	0.42
1:B:124:THR:O	1:B:125:LEU:HG	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:CYS:HA	1:D:362:LEU:CD2	2.47	0.42
1:D:269:PHE:CD1	1:D:269:PHE:C	2.98	0.42
1:E:165:LEU:HD23	1:E:216:LEU:HD22	2.01	0.42
1:F:95:CYS:SG	1:F:97:SER:HB3	2.60	0.42
1:F:264:VAL:HG12	1:F:268:ASP:CA	2.46	0.42
1:B:196:THR:HG21	1:B:352:TYR:HD2	1.84	0.42
1:B:242:LYS:HB3	1:B:249:PHE:CG	2.55	0.42
1:D:21:TRP:HE1	1:D:27:SER:HB2	1.85	0.42
1:D:184:GLN:HG2	1:D:361:HIS:CD2	2.55	0.42
1:E:38:CYS:HA	1:E:39:PRO:HD3	1.85	0.42
1:E:78:TRP:CD1	1:E:82:HIS:HB3	2.54	0.42
1:A:302:VAL:CG2	1:A:303:PRO:HD2	2.50	0.41
1:F:79:PRO:C	1:F:81:GLU:H	2.27	0.41
1:F:190:ASN:O	1:F:191:ASN:HB2	2.20	0.41
1:A:155:ALA:N	1:A:335:GLY:O	2.53	0.41
1:C:8:ALA:CA	1:C:19:ILE:HG22	2.49	0.41
1:D:17:MET:O	1:D:28:LEU:HA	2.20	0.41
1:E:260:THR:OG1	1:E:272:GLN:NE2	2.53	0.41
1:E:281:ASP:C	1:E:281:ASP:OD1	2.62	0.41
1:F:20:LEU:HD12	1:F:21:TRP:O	2.20	0.41
1:A:140:TRP:HD1	1:A:150:VAL:HG11	1.86	0.41
1:C:219:CYS:HB2	1:C:332:MET:CE	2.50	0.41
1:E:175:THR:C	1:E:177:TYR:H	2.28	0.41
1:F:13:GLY:O	1:F:14:ALA:HB3	2.20	0.41
1:A:161:GLU:HG3	1:A:218:HIS:CE1	2.55	0.41
1:B:8:ALA:HB3	1:B:69:PHE:CD1	2.55	0.41
1:D:183:VAL:HG13	1:D:183:VAL:O	2.19	0.41
1:E:73:LYS:HB3	1:E:73:LYS:HZ3	1.85	0.41
1:E:250:GLN:HG3	1:E:251:ILE:N	2.35	0.41
1:F:252:LEU:CD1	1:F:317:PHE:HB2	2.51	0.41
1:F:333:ASN:O	1:F:334:PRO:C	2.63	0.41
1:E:35:ARG:HA	1:E:35:ARG:HD2	1.85	0.41
1:E:296:ARG:O	1:F:51:ARG:NH2	2.54	0.41
1:F:156:SER:HB2	6:F:2025:HOH:O	2.20	0.41
1:F:308:GLN:HB3	1:F:309:PRO:HD3	2.01	0.41
1:B:288:ARG:HG2	1:B:289:ILE:N	2.36	0.41
1:C:104:LEU:HD21	1:D:299:ILE:CD1	2.42	0.41
1:C:144:LEU:HD22	1:C:144:LEU:O	2.20	0.41
1:E:198:LYS:HE3	1:E:198:LYS:HB2	1.85	0.41
1:C:113:CYS:HB3	6:C:2029:HOH:O	2.21	0.41
1:D:218:HIS:HD2	6:D:2029:HOH:O	2.04	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:LEU:HD12	1:D:245:ASN:HB2	2.03	0.41
1:D:264:VAL:O	1:D:264:VAL:CG2	2.67	0.41
1:A:216:LEU:HD22	1:A:339:THR:HG22	2.03	0.41
1:C:73:LYS:HD3	1:C:85:GLU:OE1	2.20	0.41
1:C:207:ALA:HB1	1:C:271:VAL:HG23	2.03	0.41
1:D:260:THR:O	1:D:295:THR:HG22	2.21	0.41
1:B:202:HIS:CE1	4:B:601:6YT:OAB	2.74	0.41
1:B:297:ASP:OD1	1:B:298:THR:N	2.54	0.41
1:C:58:LEU:HD12	1:C:59:ASP:N	2.35	0.41
1:C:68:ILE:CG1	1:C:75:TYR:HB2	2.51	0.41
1:C:169:MET:HE1	1:C:367:ALA:HB2	2.03	0.41
1:D:95:CYS:HB3	1:D:100:ALA:CB	2.51	0.41
1:D:149:ILE:HA	1:D:339:THR:O	2.21	0.41
1:D:187:ILE:HD13	1:D:194:TYR:CE1	2.56	0.41
1:E:18:GLN:NE2	1:E:26:GLU:HB2	2.35	0.41
1:E:244:ASN:O	1:E:246:PRO:HD3	2.20	0.41
1:F:201:PHE:O	1:F:202:HIS:HB3	2.20	0.41
4:F:601:6YT:OAD	4:F:601:6YT:N	2.52	0.41
1:E:224:VAL:HG12	1:E:358:ILE:HA	2.03	0.41
1:C:278:ILE:HG22	1:C:289:ILE:HD12	2.03	0.40
1:D:14:ALA:HB1	1:D:64:ILE:H	1.86	0.40
1:D:29:TYR:CE1	1:D:91:LEU:HD22	2.56	0.40
1:E:300:PHE:HB3	1:F:96:PHE:HE1	1.85	0.40
1:F:226:GLY:HA3	1:F:353:GLU:OE2	2.20	0.40
1:B:272:GLN:HE21	1:B:272:GLN:HB3	1.68	0.40
1:F:240:LYS:HB3	1:F:320:LEU:HD11	2.03	0.40
1:A:30:PRO:HD2	1:A:96:PHE:CE2	2.56	0.40
1:A:181:TRP:CE2	1:A:364:GLY:HA3	2.57	0.40
1:A:353:GLU:HB3	1:A:356:THR:CG2	2.50	0.40
1:B:19:ILE:CD1	1:B:91:LEU:HD13	2.52	0.40
1:B:157:ASP:C	1:B:220:ILE:HG23	2.46	0.40
1:C:38:CYS:HA	1:C:39:PRO:HD3	1.88	0.40
1:D:189:ALA:CB	1:D:192:VAL:HG22	2.51	0.40
1:E:128:GLU:O	1:E:132:ARG:HG2	2.21	0.40
1:F:101:ARG:O	1:F:105:GLN:HG2	2.21	0.40
1:F:187:ILE:HB	1:F:358:ILE:CG1	2.52	0.40
1:A:112:GLU:HG2	1:A:113:CYS:N	2.35	0.40
1:B:361:HIS:C	1:B:362:LEU:HD23	2.46	0.40
1:E:219:CYS:SG	1:E:222:GLN:HB2	2.61	0.40
1:F:341:ASP:HB3	1:F:344:ARG:HB3	2.02	0.40
1:B:78:TRP:HZ3	1:B:84:SER:HB3	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:CYS:HA	1:D:39:PRO:HD3	1.92	0.40

There are no symmetry-related clashes.

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	382/388 (98%)	353 (92%)	29 (8%)	0	100	100
1	B	382/388 (98%)	349 (91%)	33 (9%)	0	100	100
1	C	382/388 (98%)	341 (89%)	41 (11%)	0	100	100
1	D	382/388 (98%)	356 (93%)	26 (7%)	0	100	100
1	E	382/388 (98%)	349 (91%)	33 (9%)	0	100	100
1	F	382/388 (98%)	355 (93%)	26 (7%)	1 (0%)	36	64
All	All	2292/2328 (98%)	2103 (92%)	188 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	170	GLY

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	336/343 (98%)	318 (95%)	18 (5%)	20	50
1	B	339/343 (99%)	328 (97%)	11 (3%)	34	68
1	C	335/343 (98%)	318 (95%)	17 (5%)	21	52
1	D	333/343 (97%)	315 (95%)	18 (5%)	20	50
1	E	330/343 (96%)	315 (96%)	15 (4%)	24	57
1	F	333/343 (97%)	322 (97%)	11 (3%)	33	67
All	All	2006/2058 (98%)	1916 (96%)	90 (4%)	24	57

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	19	ILE
1	A	40	CYS
1	A	42	ASP
1	A	67	LEU
1	A	114	GLN
1	A	119	GLU
1	A	163	SER
1	A	192	VAL
1	A	199	LEU
1	A	205	TYR
1	A	250	GLN
1	A	257	VAL
1	A	258	ASP
1	A	304	VAL
1	A	305	GLU
1	A	320	LEU
1	A	331	LYS
1	B	12	ASP
1	B	40	CYS
1	B	119	GLU
1	B	205	TYR
1	B	214	VAL
1	B	217	LEU
1	B	241	LEU
1	B	250	GLN
1	B	304	VAL
1	B	315	LYS
1	B	327	LYS
1	C	40	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	144	LEU
1	C	182	GLN
1	C	187	ILE
1	C	205	TYR
1	C	223	THR
1	C	225	THR
1	C	243	LYS
1	C	258	ASP
1	C	305	GLU
1	C	320	LEU
1	C	321	MET
1	C	326	SER
1	C	345	LEU
1	C	349	ARG
1	C	362	LEU
1	C	363	GLU
1	D	40	CYS
1	D	42	ASP
1	D	46	ASP
1	D	47	SER
1	D	67	LEU
1	D	68	ILE
1	D	113	CYS
1	D	131	LEU
1	D	141	LEU
1	D	180	THR
1	D	198	LYS
1	D	223	THR
1	D	285	GLN
1	D	295	THR
1	D	304	VAL
1	D	308	GLN
1	D	345	LEU
1	D	372	VAL
1	E	20	LEU
1	E	22	TYR
1	E	40	CYS
1	E	119	GLU
1	E	121	GLN
1	E	191	ASN
1	E	204	ASP
1	E	205	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	250	GLN
1	E	251	ILE
1	E	289	ILE
1	E	300	PHE
1	E	307	VAL
1	E	320	LEU
1	E	321	MET
1	F	11	LEU
1	F	20	LEU
1	F	40	CYS
1	F	89	ASP
1	F	205	TYR
1	F	250	GLN
1	F	320	LEU
1	F	334	PRO
1	F	345	LEU
1	F	376	LEU
1	F	379	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	114	GLN
1	A	191	ASN
1	A	215	GLN
1	A	218	HIS
1	A	222	GLN
1	A	236	ASN
1	A	244	ASN
1	A	250	GLN
1	A	292	ASN
1	B	18	GLN
1	B	136	HIS
1	B	236	ASN
1	B	250	GLN
1	B	272	GLN
1	C	6	GLN
1	C	61	ASN
1	C	105	GLN
1	C	215	GLN
1	C	250	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	105	GLN
1	D	114	GLN
1	D	179	HIS
1	D	182	GLN
1	D	285	GLN
1	D	308	GLN
1	D	322	ASN
1	E	18	GLN
1	E	121	GLN
1	E	191	ASN
1	E	215	GLN
1	E	239	GLN
1	E	245	ASN
1	E	250	GLN
1	E	272	GLN
1	E	292	ASN
1	E	333	ASN
1	E	361	HIS
1	F	114	GLN
1	F	182	GLN
1	F	184	GLN
1	F	215	GLN
1	F	222	GLN
1	F	236	ASN
1	F	250	GLN
1	F	308	GLN
1	F	347	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 12 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
5	EDO	A	701	-	3,3,3	0.58	0	2,2,2	0.26	0
5	EDO	F	701	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	A	702	-	3,3,3	0.50	0	2,2,2	0.31	0
4	6YT	B	601	2	24,24,24	2.32	4 (16%)	27,31,31	1.37	4 (14%)
4	6YT	A	601	2	24,24,24	2.32	4 (16%)	27,31,31	1.37	4 (14%)
5	EDO	C	704	-	3,3,3	0.44	0	2,2,2	0.41	0
5	EDO	F	702	-	3,3,3	0.49	0	2,2,2	0.35	0
5	EDO	E	702	-	3,3,3	0.53	0	2,2,2	0.32	0
4	6YT	F	601	2	24,24,24	2.22	4 (16%)	27,31,31	1.32	6 (22%)
4	6YT	C	601	2	24,24,24	2.15	4 (16%)	27,31,31	1.10	1 (3%)
5	EDO	C	703	-	3,3,3	0.50	0	2,2,2	0.33	0
5	EDO	E	701	-	3,3,3	0.46	0	2,2,2	0.33	0
5	EDO	C	701	-	3,3,3	0.49	0	2,2,2	0.36	0
5	EDO	E	703	-	3,3,3	0.48	0	2,2,2	0.30	0
5	EDO	B	702	-	3,3,3	0.43	0	2,2,2	0.38	0
4	6YT	D	601	2	24,24,24	2.16	4 (16%)	27,31,31	1.20	4 (14%)
5	EDO	A	703	-	3,3,3	0.49	0	2,2,2	0.32	0
5	EDO	B	701	-	3,3,3	0.48	0	2,2,2	0.34	0
4	6YT	E	601	2	24,24,24	2.12	3 (12%)	27,31,31	1.24	5 (18%)
5	EDO	C	702	-	3,3,3	0.50	0	2,2,2	0.29	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	EDO	A	701	-	-	0/1/1/1	-
5	EDO	F	701	-	-	0/1/1/1	-
5	EDO	A	702	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	6YT	B	601	2	-	6/18/18/18	0/2/2/2
4	6YT	A	601	2	-	6/18/18/18	0/2/2/2
5	EDO	C	704	-	-	0/1/1/1	-
5	EDO	F	702	-	-	0/1/1/1	-
5	EDO	E	702	-	-	0/1/1/1	-
4	6YT	F	601	2	-	5/18/18/18	0/2/2/2
4	6YT	C	601	2	-	6/18/18/18	0/2/2/2
5	EDO	C	703	-	-	0/1/1/1	-
5	EDO	E	701	-	-	0/1/1/1	-
5	EDO	C	701	-	-	0/1/1/1	-
5	EDO	E	703	-	-	1/1/1/1	-
5	EDO	B	702	-	-	1/1/1/1	-
4	6YT	D	601	2	-	8/18/18/18	0/2/2/2
5	EDO	A	703	-	-	1/1/1/1	-
5	EDO	B	701	-	-	0/1/1/1	-
4	6YT	E	601	2	-	7/18/18/18	0/2/2/2
5	EDO	C	702	-	-	0/1/1/1	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	6YT	CAV-CAS	-8.34	1.38	1.50
4	A	601	6YT	CAV-CAS	-8.32	1.38	1.50
4	F	601	6YT	CAV-CAS	-8.06	1.39	1.50
4	D	601	6YT	CAV-CAS	-7.39	1.39	1.50
4	C	601	6YT	CAV-CAS	-7.27	1.40	1.50
4	E	601	6YT	CAV-CAS	-7.09	1.40	1.50
4	E	601	6YT	OAB-CAS	5.36	1.35	1.23
4	C	601	6YT	OAB-CAS	5.25	1.35	1.23
4	D	601	6YT	OAB-CAS	5.20	1.35	1.23
4	A	601	6YT	OAB-CAS	5.16	1.35	1.23
4	B	601	6YT	OAB-CAS	5.16	1.35	1.23
4	F	601	6YT	OAB-CAS	4.71	1.34	1.23
4	A	601	6YT	CAL-SAQ	-2.64	1.77	1.82
4	B	601	6YT	CAL-SAQ	-2.61	1.77	1.82
4	F	601	6YT	OAD-CAT	2.56	1.41	1.36
4	A	601	6YT	OAD-CAT	2.49	1.41	1.36
4	B	601	6YT	OAD-CAT	2.48	1.41	1.36
4	D	601	6YT	OAD-CAT	2.47	1.41	1.36
4	E	601	6YT	OAD-CAT	2.45	1.41	1.36
4	C	601	6YT	OAD-CAT	2.44	1.41	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	601	6YT	CAL-SAQ	-2.40	1.77	1.82
4	D	601	6YT	CAL-SAQ	-2.11	1.78	1.82
4	C	601	6YT	CAL-SAQ	-2.07	1.78	1.82

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	6YT	CAL-CAU-NAN	2.51	120.28	116.53
4	B	601	6YT	CAL-CAU-NAN	2.51	120.28	116.53
4	F	601	6YT	CAL-CAU-NAN	2.38	120.09	116.53
4	E	601	6YT	CAH-NAN-CAU	2.38	120.75	117.41
4	B	601	6YT	CAS-CAV-NAO	2.36	120.03	115.81
4	A	601	6YT	CAS-CAV-NAO	2.36	120.02	115.81
4	F	601	6YT	CB-SAQ-CAL	-2.29	96.47	101.24
4	B	601	6YT	CAG-CAI-NAO	-2.27	119.82	123.42
4	A	601	6YT	CAG-CAI-NAO	-2.25	119.86	123.42
4	E	601	6YT	CAG-CAI-NAO	-2.24	119.88	123.42
4	D	601	6YT	CAS-CAV-NAO	2.20	119.74	115.81
4	F	601	6YT	CAE-CAH-NAN	-2.19	119.95	123.42
4	F	601	6YT	CAH-NAN-CAU	2.18	120.47	117.41
4	E	601	6YT	CAI-NAO-CAV	2.17	121.03	116.80
4	D	601	6YT	CAG-CAI-NAO	-2.17	119.98	123.42
4	E	601	6YT	CAE-CAH-NAN	-2.16	120.00	123.42
4	E	601	6YT	CAK-CAU-NAN	-2.13	119.16	122.22
4	A	601	6YT	CAE-CAH-NAN	-2.12	120.06	123.42
4	B	601	6YT	CAE-CAH-NAN	-2.12	120.07	123.42
4	D	601	6YT	CAL-CAU-NAN	2.09	119.66	116.53
4	C	601	6YT	CAG-CAI-NAO	-2.07	120.14	123.42
4	F	601	6YT	OAB-CAS-CAV	-2.05	117.49	120.75
4	F	601	6YT	CAG-CAI-NAO	-2.04	120.19	123.42
4	D	601	6YT	CAE-CAH-NAN	-2.03	120.21	123.42

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	6YT	N-CAS-CAV-NAO
4	A	601	6YT	N-CAS-CAV-CAT
4	A	601	6YT	OAB-CAS-CAV-NAO
4	A	601	6YT	OAB-CAS-CAV-CAT
4	B	601	6YT	N-CAS-CAV-NAO
4	B	601	6YT	N-CAS-CAV-CAT

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	601	6YT	OAB-CAS-CAV-NAO
4	B	601	6YT	OAB-CAS-CAV-CAT
4	C	601	6YT	N-CAS-CAV-NAO
4	C	601	6YT	N-CAS-CAV-CAT
4	C	601	6YT	OAB-CAS-CAV-NAO
4	C	601	6YT	OAB-CAS-CAV-CAT
4	E	601	6YT	CAU-CAL-SAQ-CB
4	E	601	6YT	N-CAS-CAV-NAO
4	E	601	6YT	N-CAS-CAV-CAT
4	E	601	6YT	OAB-CAS-CAV-NAO
4	E	601	6YT	OAB-CAS-CAV-CAT
4	F	601	6YT	N-CAS-CAV-NAO
4	F	601	6YT	N-CAS-CAV-CAT
4	F	601	6YT	OAB-CAS-CAV-NAO
4	F	601	6YT	OAB-CAS-CAV-CAT
4	D	601	6YT	OAB-CAS-CAV-NAO
4	D	601	6YT	N-CAS-CAV-NAO
5	A	702	EDO	O1-C1-C2-O2
5	E	703	EDO	O1-C1-C2-O2
4	C	601	6YT	SAQ-CAL-CAU-NAN
4	E	601	6YT	SAQ-CAL-CAU-NAN
4	C	601	6YT	SAQ-CAL-CAU-CAK
4	E	601	6YT	SAQ-CAL-CAU-CAK
4	D	601	6YT	N-CAS-CAV-CAT
4	D	601	6YT	OAB-CAS-CAV-CAT
5	B	702	EDO	O1-C1-C2-O2
4	F	601	6YT	C-CA-N-CAS
4	D	601	6YT	CAU-CAL-SAQ-CB
4	A	601	6YT	CA-CB-SAQ-CAL
4	B	601	6YT	CA-CB-SAQ-CAL
4	D	601	6YT	SAQ-CAL-CAU-CAK
4	A	601	6YT	C-CA-N-CAS
4	B	601	6YT	C-CA-N-CAS
4	D	601	6YT	C-CA-N-CAS
4	D	601	6YT	SAQ-CAL-CAU-NAN
5	A	703	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 18 short contacts:

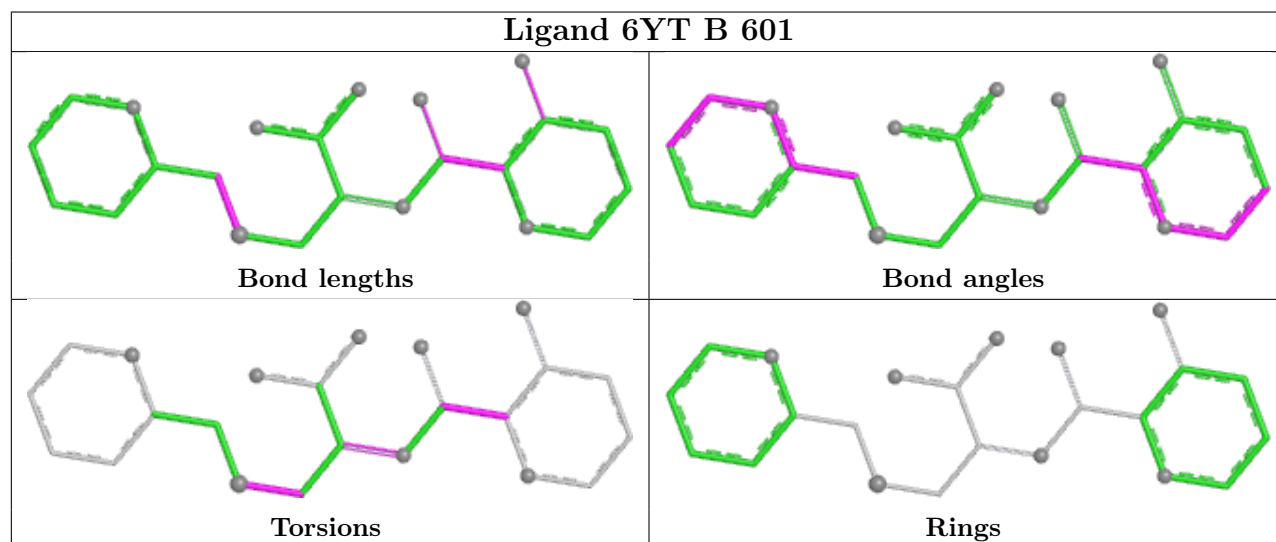
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	6YT	5	0

Continued on next page...

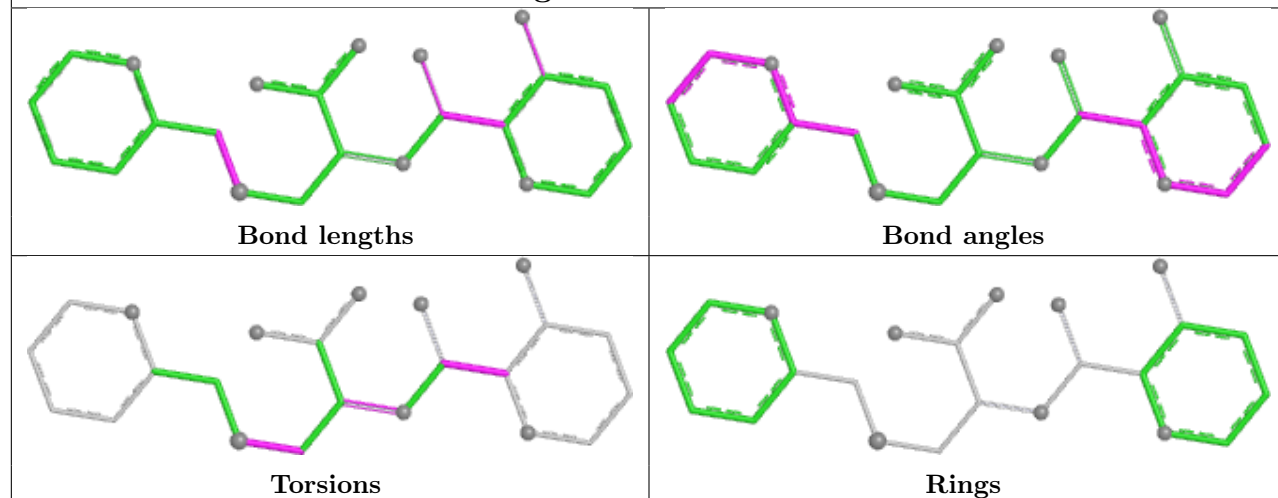
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	6YT	7	0
5	C	704	EDO	1	0
4	F	601	6YT	2	0
5	E	703	EDO	2	0
4	D	601	6YT	1	0

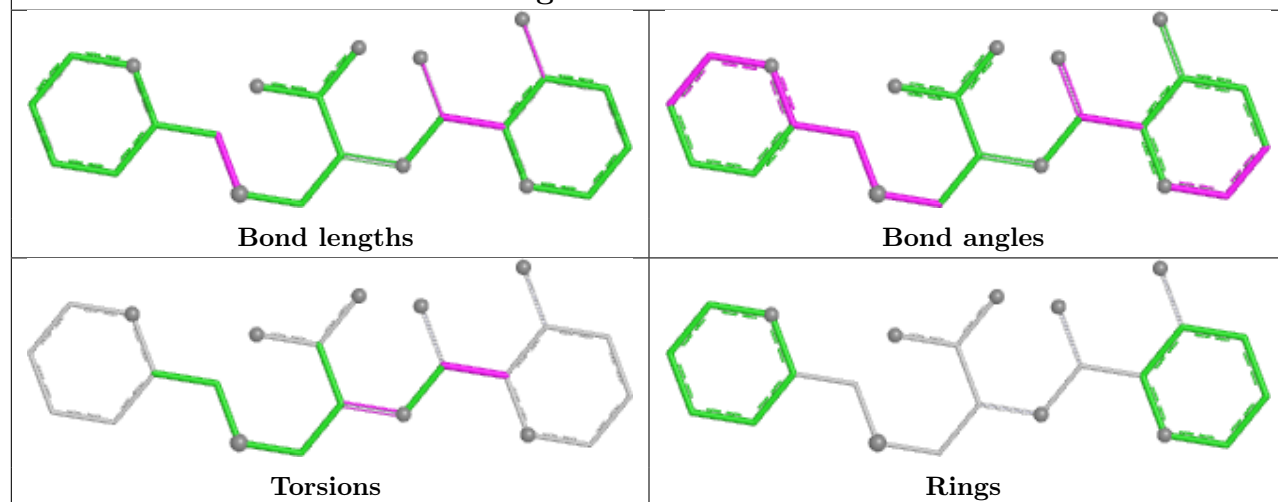
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



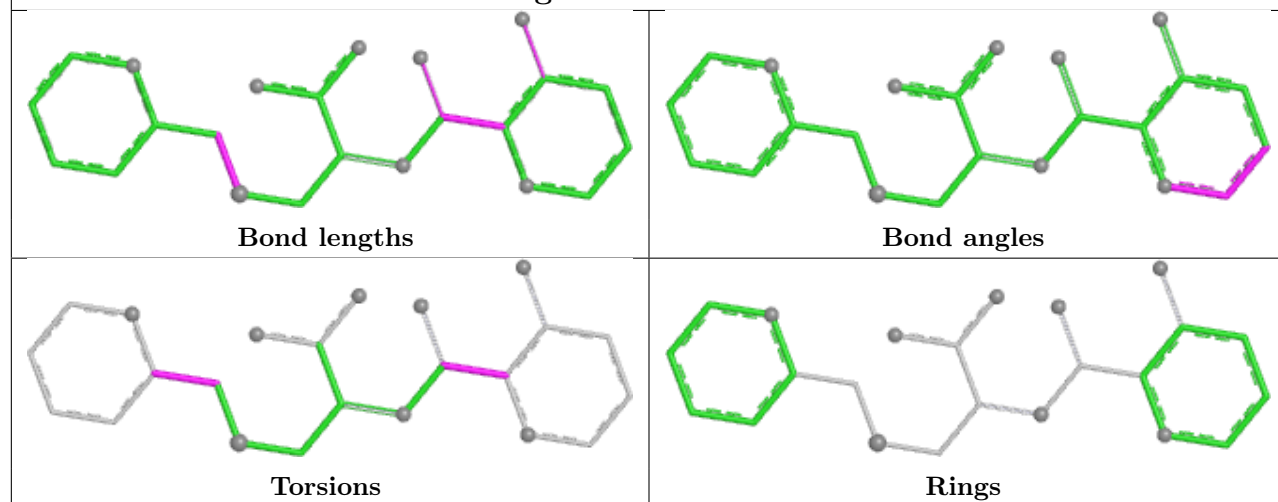
Ligand 6YT A 601

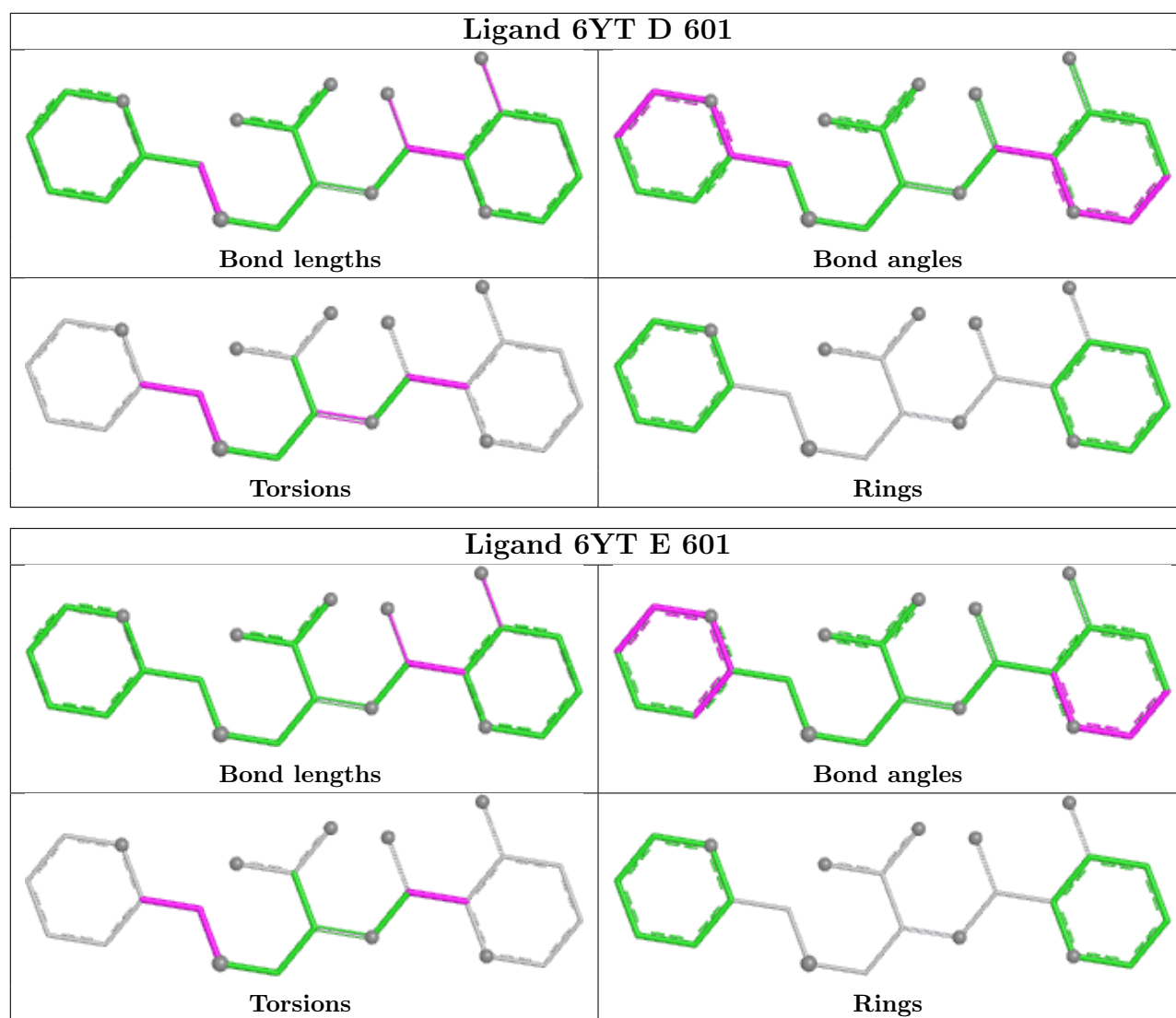


Ligand 6YT F 601



Ligand 6YT C 601





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	384/388 (98%)	-0.10	3 (0%)	82 75	36, 55, 80, 95	0
1	B	384/388 (98%)	-0.13	1 (0%)	90 86	34, 53, 76, 91	0
1	C	384/388 (98%)	0.07	4 (1%)	79 72	27, 61, 82, 109	0
1	D	384/388 (98%)	0.16	7 (1%)	67 58	33, 65, 98, 113	1 (0%)
1	E	384/388 (98%)	0.18	3 (0%)	82 75	43, 72, 103, 113	0
1	F	384/388 (98%)	0.12	1 (0%)	90 86	40, 64, 85, 98	1 (0%)
All	All	2304/2328 (98%)	0.05	19 (0%)	82 75	27, 61, 90, 113	2 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	209	HIS	5.0
1	F	209	HIS	4.7
1	C	194	TYR	2.7
1	C	12	ASP	2.7
1	B	354	ALA	2.5
1	D	24	GLU	2.4
1	D	4	THR	2.4
1	C	262	ILE	2.4
1	D	130	VAL	2.3
1	C	264	VAL	2.2
1	D	1	MET	2.2
1	A	189	ALA	2.2
1	A	12	ASP	2.2
1	A	184	GLN	2.1
1	D	28	LEU	2.1
1	D	291	PHE	2.1
1	E	2	ALA	2.1
1	E	13	GLY	2.1
1	E	78	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
5	EDO	E	702	4/4	0.73	0.15	72,76,77,79	0
5	EDO	C	704	4/4	0.79	0.12	62,63,64,65	0
5	EDO	E	701	4/4	0.79	0.19	72,72,73,73	0
5	EDO	C	701	4/4	0.79	0.25	73,73,73,74	0
4	6YT	B	601	23/23	0.80	0.20	98,100,100,101	0
4	6YT	E	601	23/23	0.81	0.15	94,97,101,101	0
5	EDO	B	702	4/4	0.81	0.13	62,64,64,65	0
4	6YT	F	601	23/23	0.83	0.20	94,97,100,101	0
4	6YT	C	601	23/23	0.84	0.17	98,100,100,101	0
5	EDO	A	701	4/4	0.85	0.13	61,63,64,65	0
5	EDO	C	702	4/4	0.85	0.18	82,83,84,84	0
5	EDO	C	703	4/4	0.85	0.13	71,72,72,73	0
5	EDO	E	703	4/4	0.86	0.12	54,58,59,60	0
5	EDO	F	701	4/4	0.87	0.15	78,79,79,80	0
5	EDO	B	701	4/4	0.88	0.15	62,63,63,63	0
5	EDO	A	703	4/4	0.88	0.12	60,62,62,63	0
5	EDO	A	702	4/4	0.90	0.13	68,68,69,70	0
4	6YT	D	601	23/23	0.90	0.14	80,84,91,91	0
4	6YT	A	601	23/23	0.90	0.14	98,100,100,101	0
5	EDO	F	702	4/4	0.92	0.18	63,65,65,65	0
2	NI	A	501	1/1	0.99	0.03	76,76,76,76	0
2	NI	B	501	1/1	0.99	0.03	70,70,70,70	0
2	NI	D	501	1/1	0.99	0.03	54,54,54,54	0
2	NI	E	501	1/1	0.99	0.03	81,81,81,81	0
2	NI	F	501	1/1	0.99	0.03	49,49,49,49	0
3	ZN	A	502	1/1	0.99	0.02	52,52,52,52	0
3	ZN	B	502	1/1	0.99	0.05	55,55,55,55	0

Continued on next page...

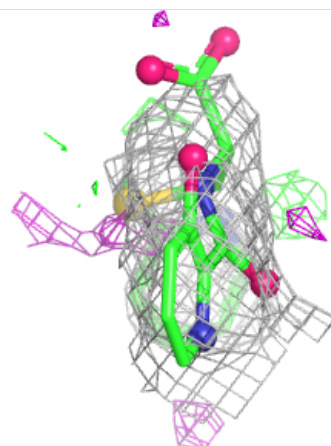
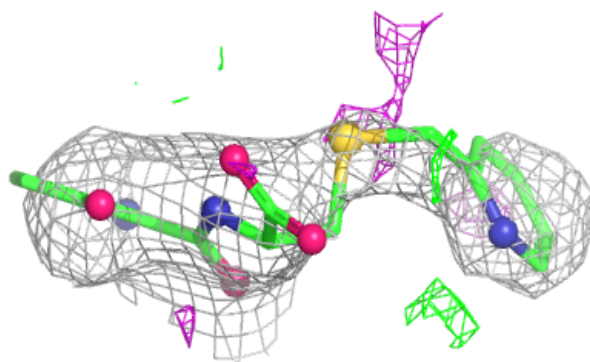
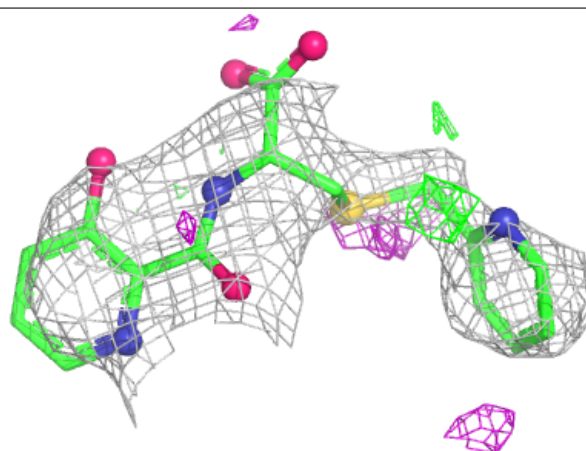
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	C	502	1/1	0.99	0.04	63,63,63,63	0
3	ZN	D	502	1/1	0.99	0.03	67,67,67,67	0
3	ZN	E	502	1/1	0.99	0.07	95,95,95,95	0
2	NI	C	501	1/1	1.00	0.02	67,67,67,67	0
3	ZN	F	502	1/1	1.00	0.03	63,63,63,63	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.

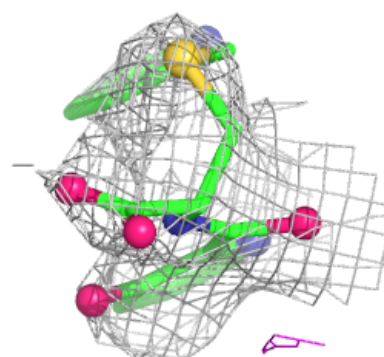
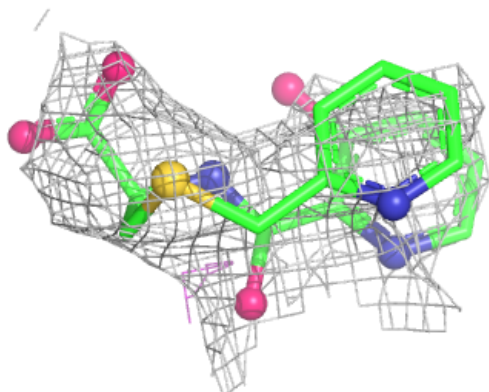
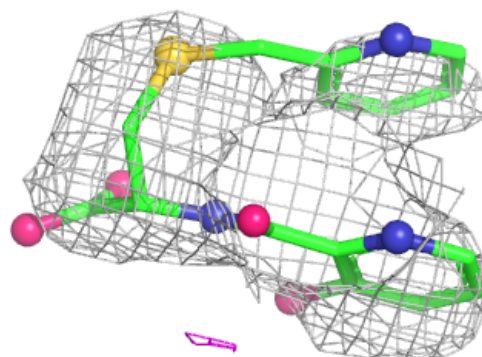
Electron density around 6YT B 601:

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

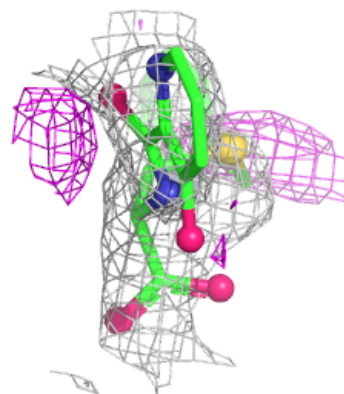
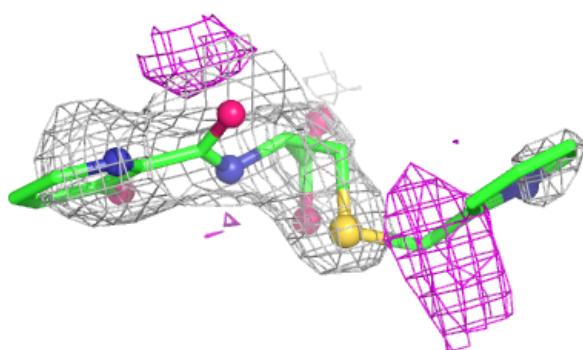
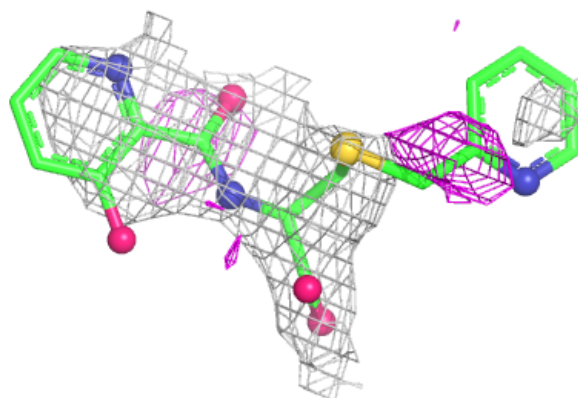


Electron density around 6YT E 601:

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

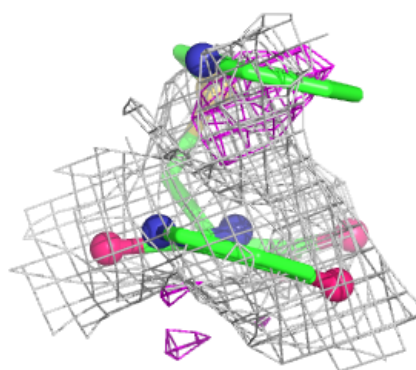
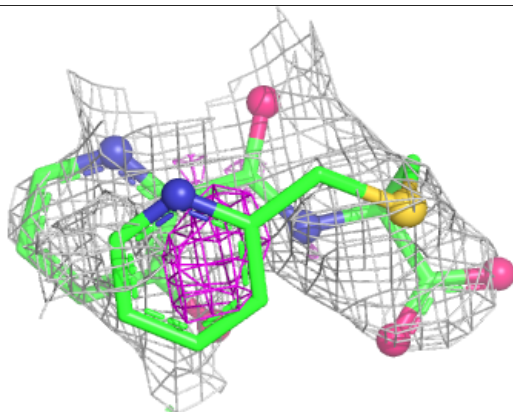
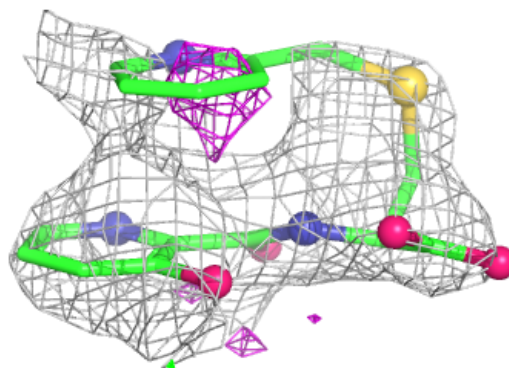
**Electron density around 6YT F 601:**

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

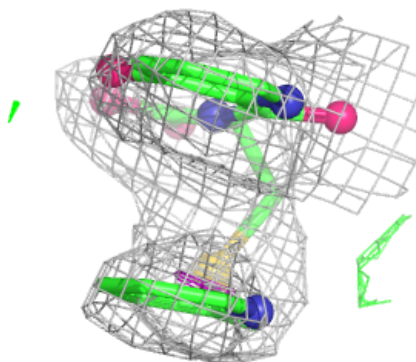
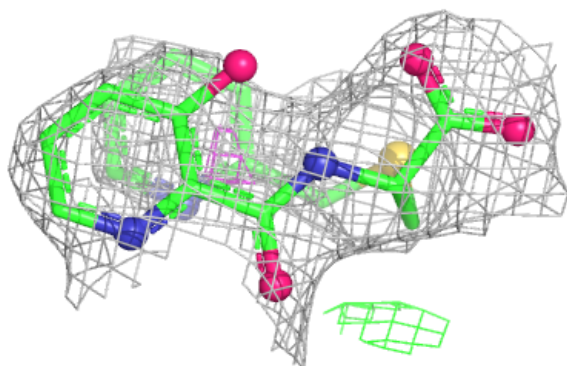
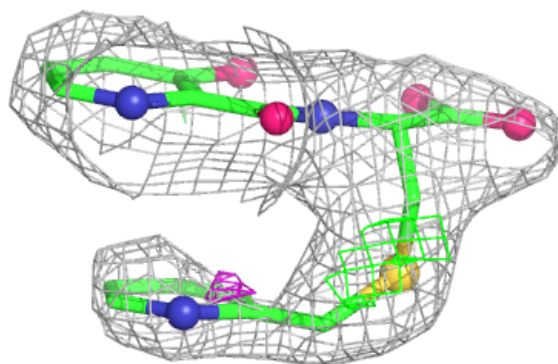


Electron density around 6YT C 601:

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

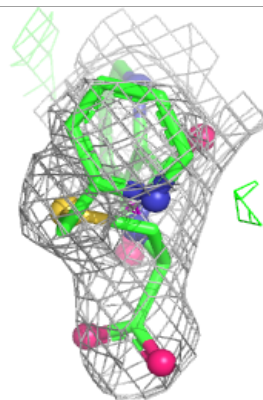
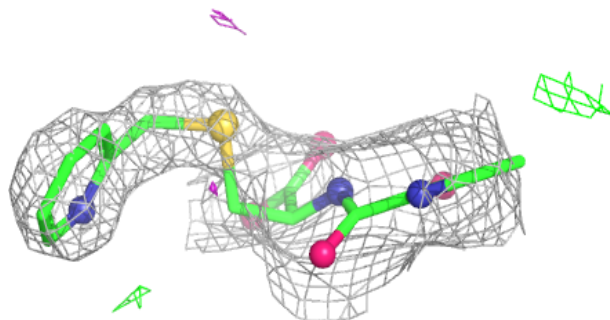
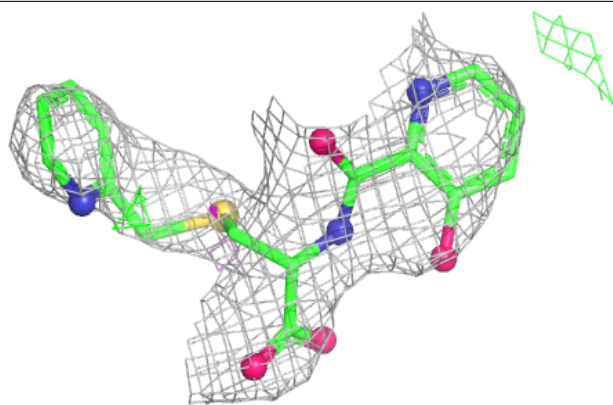
**Electron density around 6YT D 601:**

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



Electron density around 6YT A 601:

$2mF_o-DF_c$ (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.