



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:33 am BST

PDB ID : 3RIM
Title : Crystal structure of mycobacterium tuberculosis Transketolase (Rv1449c)
Authors : Pojer, F.; Fullam, E.; Jones, T.A.; Cole, S.T.
Deposited on : 2011-04-14
Resolution : 2.49 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 following versions of software and data (see [references](#) ⓘ) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

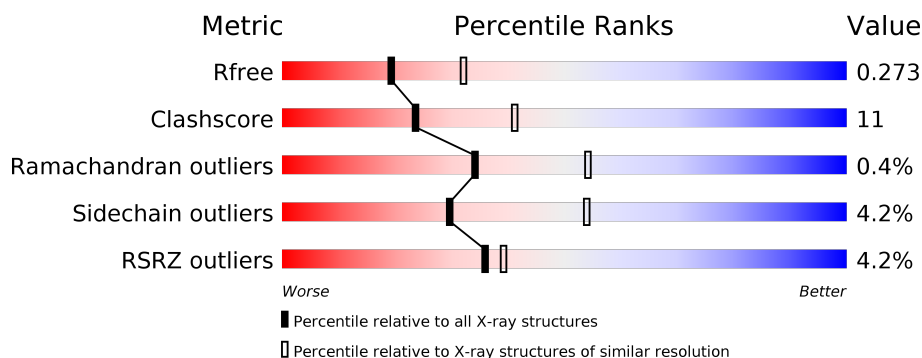
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	700	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>..</div> </div> </div>
1	B	700	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>..</div> </div> </div>
1	C	700	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>..</div> </div> </div>
1	D	700	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	D	701	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21767 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.

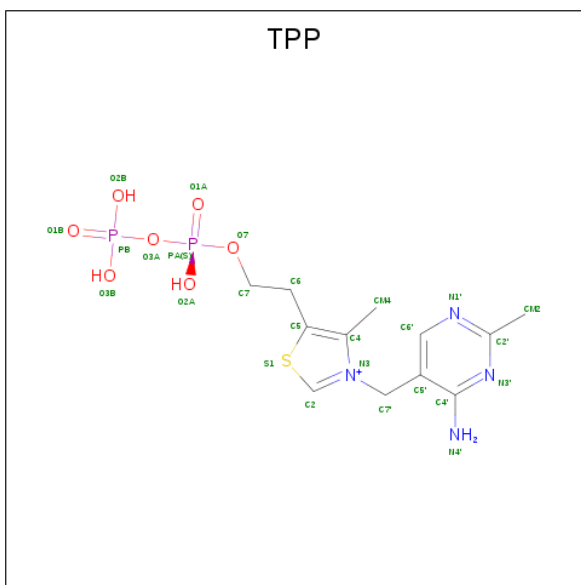
- Molecule 1 is a protein called Transketolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	694	Total	C	N	O	S	0	3	0
			5308	3343	935	1018	12			
1	B	694	Total	C	N	O	S	0	1	0
			5295	3334	935	1014	12			
1	C	694	Total	C	N	O	S	0	2	0
			5303	3339	938	1014	12			
1	D	694	Total	C	N	O	S	0	1	0
			5295	3334	935	1014	12			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

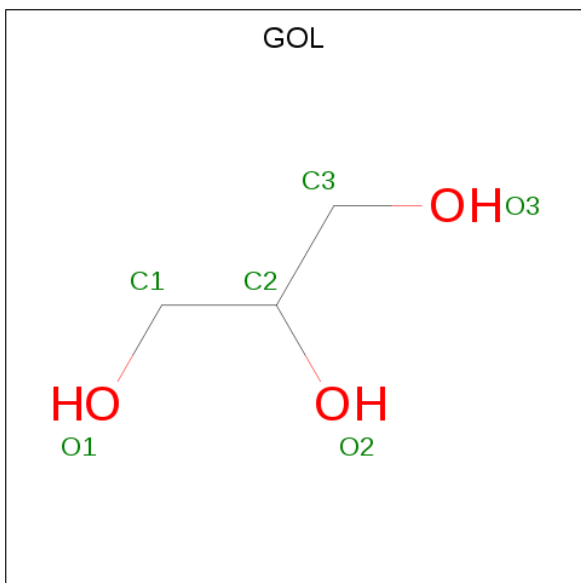
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

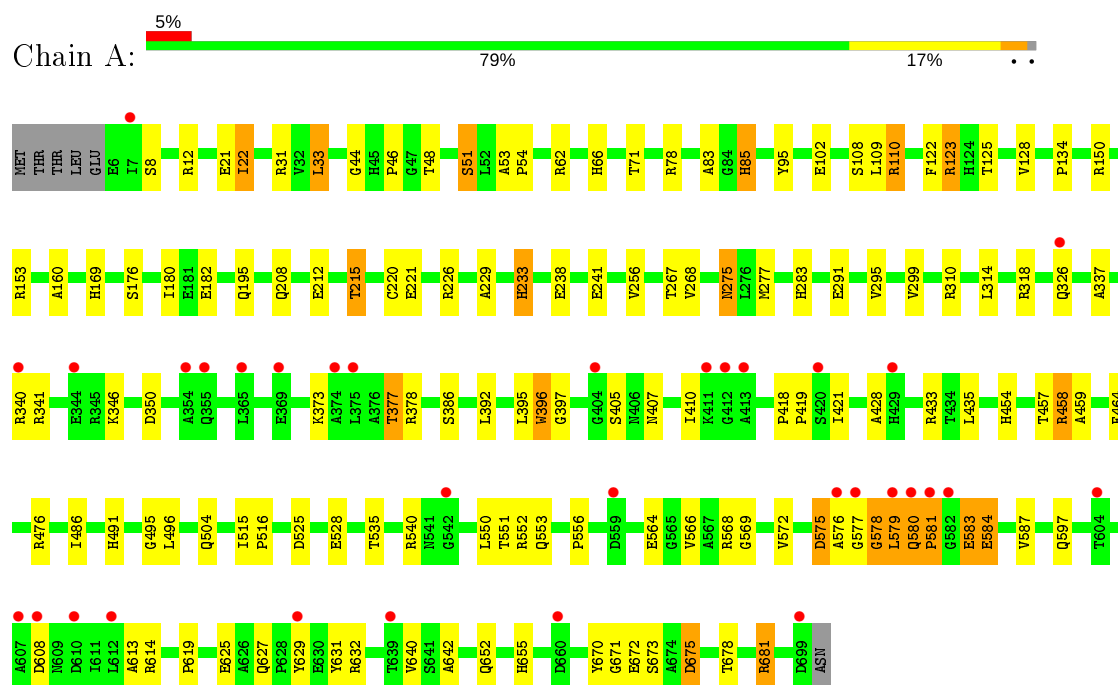
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	84	Total	O	0	0
			84	84		
5	B	128	Total	O	0	0
			128	128		
5	C	62	Total	O	0	0
			62	62		
5	D	136	Total	O	0	0
			136	136		

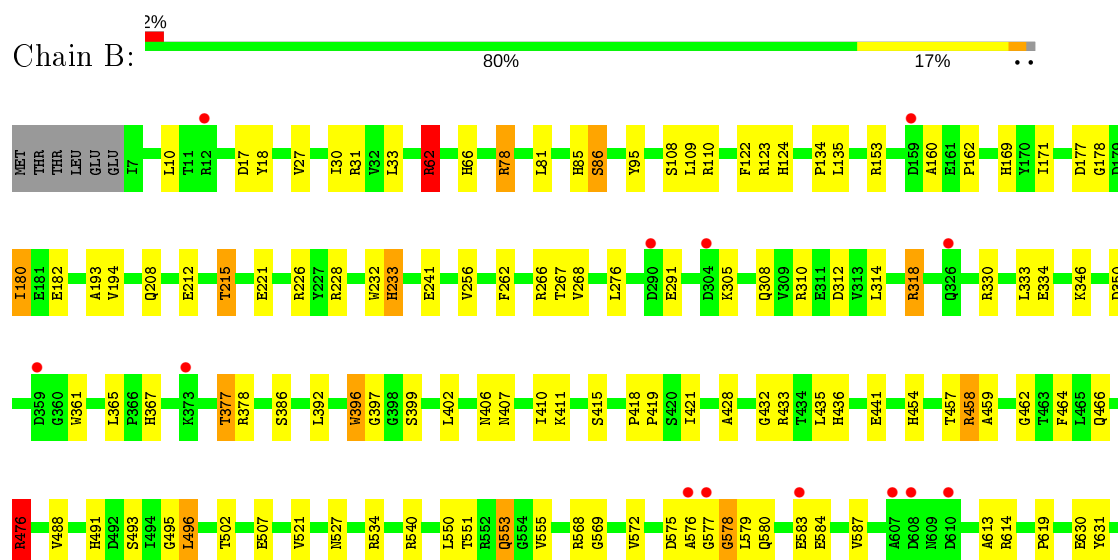
3 Residue-property plots [i](#)

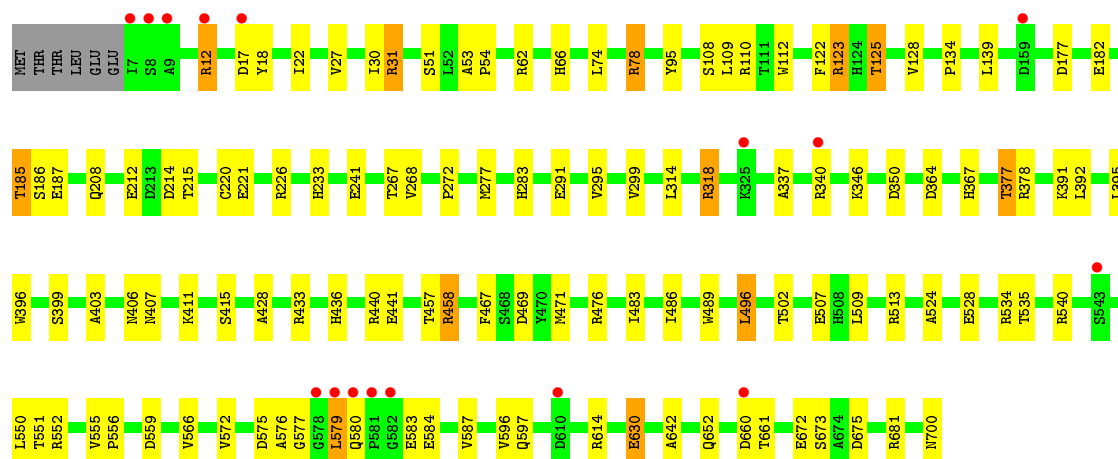
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Transketolase



• Molecule 1: Transketolase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.53Å 80.12Å 130.10Å 82.20° 81.16° 66.37°	Depositor
Resolution (Å)	19.81 – 2.49 19.81 – 2.49	Depositor EDS
% Data completeness (in resolution range)	96.7 (19.81-2.49) 96.9 (19.81-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.223 , 0.272 0.227 , 0.273	Depositor DCC
R_{free} test set	4579 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	21767	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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: GOL, MG, TPP

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	0.80	7/5445 (0.1%)	0.82	17/7425 (0.2%)
1	B	0.75	1/5426 (0.0%)	0.83	8/7401 (0.1%)
1	C	0.85	3/5437 (0.1%)	0.87	10/7415 (0.1%)
1	D	0.77	2/5426 (0.0%)	0.84	10/7401 (0.1%)
All	All	0.80	13/21734 (0.1%)	0.84	45/29642 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	577	GLY	C-N	6.21	1.44	1.33
1	C	78	ARG	CZ-NH1	-5.97	1.25	1.33
1	A	78	ARG	CZ-NH1	-5.91	1.25	1.33
1	A	340	ARG	CZ-NH1	-5.67	1.25	1.33
1	D	630	GLU	CD-OE2	-5.63	1.19	1.25
1	A	33	LEU	CG-CD1	-5.45	1.31	1.51
1	D	31	ARG	CZ-NH1	-5.42	1.25	1.33
1	A	238	GLU	CD-OE2	-5.40	1.19	1.25
1	A	326	GLN	CB-CG	-5.33	1.38	1.52
1	C	202	VAL	CB-CG1	5.32	1.64	1.52
1	B	476	ARG	CZ-NH2	-5.13	1.26	1.33
1	A	476	ARG	CG-CD	-5.09	1.39	1.51
1	A	632	ARG	CZ-NH1	-5.02	1.26	1.33

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ARG	NE-CZ-NH2	10.31	125.46	120.30
1	C	78	ARG	NE-CZ-NH2	10.18	125.39	120.30
1	B	681	ARG	NE-CZ-NH2	10.17	125.39	120.30
1	C	310	ARG	NE-CZ-NH2	9.61	125.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	31	ARG	NE-CZ-NH2	8.75	124.67	120.30
1	A	123	ARG	NE-CZ-NH2	8.64	124.62	120.30
1	C	31	ARG	NE-CZ-NH2	8.51	124.56	120.30
1	B	476	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	C	340	ARG	NE-CZ-NH2	8.36	124.48	120.30
1	B	476	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	277	MET	CG-SD-CE	7.73	112.58	100.20
1	A	110	ARG	NE-CZ-NH2	7.70	124.15	120.30
1	A	373	LYS	CD-CE-NZ	7.64	129.26	111.70
1	A	123	ARG	NE-CZ-NH1	-7.61	116.49	120.30
1	A	632	ARG	NE-CZ-NH2	7.47	124.04	120.30
1	A	310	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	D	123	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	C	577	GLY	C-N-CA	-6.88	107.85	122.30
1	A	681	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	A	62	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	A	578	GLY	N-CA-C	-6.76	96.20	113.10
1	B	458	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	C	31	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	D	110	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	D	577	GLY	C-N-CA	-6.29	109.08	122.30
1	B	62	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	D	123	ARG	NE-CZ-NH1	-6.23	117.18	120.30
1	C	78	ARG	NE-CZ-NH1	-5.89	117.36	120.30
1	D	277	MET	CG-SD-CE	5.84	109.55	100.20
1	A	675	ASP	CB-CG-OD1	5.75	123.47	118.30
1	D	579	LEU	O-C-N	-5.74	113.52	122.70
1	A	564	GLU	OE1-CD-OE2	-5.72	116.44	123.30
1	B	228	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	C	277	MET	CG-SD-CE	5.69	109.30	100.20
1	A	12	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	B	110	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	C	123	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	D	675	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	78	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	D	78	ARG	CB-CG-CD	5.31	125.41	111.60
1	D	12	ARG	CG-CD-NE	5.29	122.91	111.80
1	A	340	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	B	78	ARG	CG-CD-NE	-5.16	100.96	111.80
1	A	632	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
1	C	110	ARG	NE-CZ-NH1	5.05	122.83	120.30

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	5308	0	5157	135	0
1	B	5295	0	5140	118	0
1	C	5303	0	5153	143	0
1	D	5295	0	5140	100	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
3	A	26	0	16	4	0
3	B	26	0	16	5	0
3	C	26	0	16	3	0
3	D	26	0	16	6	0
4	B	12	0	16	0	0
4	C	12	0	16	0	0
4	D	24	0	32	7	0
5	A	84	0	0	7	0
5	B	128	0	0	7	0
5	C	62	0	0	4	0
5	D	136	0	0	8	0
All	All	21767	0	20718	469	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 11.

All (469) 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)
3:A:1002:TPP:H2	5:C:748:HOH:O	1.39	1.23
1:A:44:GLY:HA2	1:A:110:ARG:HH21	1.06	1.14
1:C:491:HIS:CD2	1:C:552:ARG:HB2	1.86	1.10
1:A:583:GLU:HA	1:A:583:GLU:OE1	1.53	1.06
1:A:44:GLY:HA2	1:A:110:ARG:NH2	1.72	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:VAL:HA	5:C:733:HOH:O	1.56	1.03
1:A:580:GLN:O	1:A:583:GLU:HB2	1.58	1.03
1:A:580:GLN:H	1:A:583:GLU:CG	1.71	1.02
1:B:580:GLN:O	1:B:583:GLU:HB2	1.60	1.01
1:A:85:HIS:HD2	1:A:283:HIS:CE1	1.79	1.00
1:A:580:GLN:N	1:A:583:GLU:HG3	1.76	1.00
1:A:491:HIS:CD2	1:A:552:ARG:HB2	1.97	0.99
1:A:580:GLN:CB	1:A:583:GLU:HG2	1.93	0.98
1:D:552:ARG:HH21	4:D:701:GOL:H31	1.25	0.98
1:A:377:THR:HG22	1:A:551:THR:H	1.29	0.98
1:A:85:HIS:CD2	1:A:283:HIS:HE1	1.80	0.97
1:A:580:GLN:H	1:A:583:GLU:HG3	1.29	0.97
1:C:553:GLN:N	1:C:553:GLN:HE21	1.62	0.96
1:C:377:THR:HG22	1:C:551:THR:H	1.30	0.95
1:A:580:GLN:N	1:A:583:GLU:CG	2.30	0.94
1:B:377:THR:HG22	1:B:551:THR:H	1.33	0.94
3:B:1002:TPP:H2	5:D:811:HOH:O	1.65	0.93
1:C:580:GLN:HB2	1:C:583:GLU:CG	1.98	0.93
1:A:491:HIS:HD2	1:A:552:ARG:HB2	1.32	0.93
1:C:553:GLN:H	1:C:553:GLN:HE21	0.93	0.92
1:A:109:LEU:HG	1:A:110:ARG:HG3	1.50	0.91
1:B:62:ARG:HG2	1:B:62:ARG:HH11	1.31	0.91
1:C:553:GLN:NE2	1:C:553:GLN:H	1.69	0.91
1:B:652:GLN:HE21	1:D:652:GLN:HE21	1.12	0.91
1:A:580:GLN:HB3	1:A:583:GLU:HG2	1.51	0.90
1:C:464:PHE:CE1	1:C:491:HIS:CE1	2.59	0.89
1:D:377:THR:HG22	1:D:551:THR:H	1.36	0.89
1:A:580:GLN:CA	1:A:583:GLU:HG2	2.03	0.88
1:A:122:PHE:O	1:A:123:ARG:HB2	1.72	0.87
1:C:491:HIS:HD2	1:C:552:ARG:HB2	1.37	0.87
1:C:580:GLN:HB2	1:C:583:GLU:HG3	1.55	0.86
1:B:377:THR:HG21	5:B:814:HOH:O	1.76	0.85
1:A:377:THR:HG21	5:A:772:HOH:O	1.76	0.84
1:A:464:PHE:CE1	1:A:491:HIS:CE1	2.65	0.84
1:C:464:PHE:CE1	1:C:491:HIS:ND1	2.45	0.84
1:A:652:GLN:HE21	1:C:652:GLN:HE21	1.24	0.84
1:C:275:ASN:HD22	1:C:275:ASN:N	1.76	0.84
1:A:580:GLN:H	1:A:583:GLU:CB	1.90	0.84
1:C:314:LEU:HD11	1:C:318:ARG:NH1	1.93	0.82
1:A:580:GLN:CB	1:A:583:GLU:CG	2.57	0.81
1:A:580:GLN:O	1:A:583:GLU:CB	2.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:GLN:HE21	1:C:652:GLN:NE2	1.78	0.80
1:C:580:GLN:O	1:C:583:GLU:HB2	1.82	0.79
1:C:556:PRO:HD2	1:C:597:GLN:OE1	1.82	0.79
1:A:182:GLU:OE2	3:A:1002:TPP:HM23	1.81	0.79
1:D:471:MET:CE	1:D:489:TRP:HE1	1.95	0.79
1:B:652:GLN:HE21	1:D:652:GLN:NE2	1.80	0.79
1:B:551:THR:HB	1:B:553:GLN:NE2	1.98	0.79
1:A:580:GLN:CA	1:A:583:GLU:CG	2.60	0.79
1:B:576:ALA:HB2	1:B:613:ALA:O	1.82	0.78
1:C:291:GLU:O	1:C:295:VAL:HG23	1.85	0.77
1:C:377:THR:CG2	1:C:551:THR:H	1.97	0.77
1:A:652:GLN:NE2	1:C:652:GLN:HE21	1.84	0.76
1:C:378:ARG:HD2	1:C:407:ASN:ND2	2.00	0.76
1:D:580:GLN:O	1:D:583:GLU:HB2	1.85	0.76
1:D:122:PHE:O	1:D:123:ARG:HB2	1.85	0.76
1:C:295:VAL:O	1:C:299:VAL:HG22	1.84	0.76
1:C:580:GLN:HB2	1:C:583:GLU:HG2	1.67	0.76
1:D:139:LEU:HD23	1:D:185:THR:OG1	1.87	0.75
1:A:583:GLU:CA	1:A:583:GLU:OE1	2.30	0.75
1:D:471:MET:HE2	1:D:489:TRP:HE1	1.51	0.74
1:B:305:LYS:HD3	1:B:308:GLN:NE2	2.02	0.74
1:B:553:GLN:HE21	1:B:553:GLN:H	1.36	0.74
1:B:652:GLN:NE2	1:D:652:GLN:HE21	1.86	0.74
1:A:579:LEU:HD12	1:A:583:GLU:HB3	1.68	0.73
1:C:556:PRO:CD	1:C:597:GLN:OE1	2.36	0.73
1:B:580:GLN:O	1:B:583:GLU:CB	2.36	0.73
1:B:314:LEU:O	1:B:318:ARG:HB2	1.87	0.72
1:C:681[B]:ARG:HG3	1:C:681[B]:ARG:HH11	1.52	0.72
1:C:122:PHE:O	1:C:123:ARG:HB2	1.89	0.72
1:D:552:ARG:NH2	4:D:701:GOL:H31	2.02	0.72
1:D:208:GLN:HG3	5:D:808:HOH:O	1.90	0.72
1:A:579:LEU:CD1	1:A:583:GLU:HB3	2.21	0.71
1:B:233:HIS:CD2	1:B:256:VAL:HG21	2.25	0.71
1:B:464:PHE:CE1	1:B:491:HIS:CE1	2.78	0.71
1:A:580:GLN:C	1:A:583:GLU:HG2	2.11	0.71
3:D:1002:TPP:H2	5:D:738:HOH:O	1.90	0.71
1:D:346:LYS:HE3	1:D:350:ASP:OD2	1.91	0.71
1:A:575:ASP:OD1	1:A:614:ARG:HG3	1.90	0.71
1:C:681[B]:ARG:HG3	1:C:681[B]:ARG:NH1	2.06	0.71
1:A:576:ALA:O	1:A:578:GLY:HA3	1.90	0.71
1:B:553:GLN:HE21	1:B:553:GLN:N	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150[A]:ARG:NH1	1:C:430:TRP:O	2.24	0.71
1:A:83:ALA:HB1	1:A:85:HIS:HE1	1.56	0.70
1:D:283:HIS:HD2	3:D:1002:TPP:O1B	1.73	0.70
1:A:464:PHE:CE1	1:A:491:HIS:ND1	2.60	0.70
1:A:377:THR:CG2	1:A:551:THR:H	2.04	0.70
1:C:177:ASP:HB2	3:C:1002:TPP:O2A	1.91	0.70
1:D:552:ARG:HE	4:D:701:GOL:H12	1.56	0.70
1:D:580:GLN:O	1:D:583:GLU:CB	2.40	0.69
1:A:85:HIS:CD2	1:A:283:HIS:CE1	2.66	0.69
1:C:14:ARG:O	1:C:244:VAL:HG23	1.93	0.69
1:B:62:ARG:CG	1:B:62:ARG:HH11	2.05	0.69
1:B:433:ARG:NH1	5:B:719:HOH:O	2.26	0.68
1:C:377:THR:HG22	1:C:551:THR:N	2.05	0.68
1:A:569:GLY:O	1:A:619:PRO:HD2	1.94	0.68
1:C:96:LEU:HD22	1:C:317:THR:HG21	1.74	0.67
1:B:491:HIS:HB3	1:B:496:LEU:HD12	1.76	0.67
1:B:507:GLU:OE2	1:D:476:ARG:HD2	1.95	0.67
1:B:377:THR:HG23	1:B:550:LEU:CD2	2.25	0.67
1:D:267:THR:HG22	1:D:268:VAL:N	2.10	0.67
1:D:681[B]:ARG:HH11	1:D:681[B]:ARG:HG3	1.59	0.66
1:C:7:ILE:HG13	1:C:8:SER:OG	1.95	0.65
1:D:552:ARG:HH21	4:D:701:GOL:C3	2.06	0.65
1:A:464:PHE:CD1	1:A:491:HIS:ND1	2.64	0.65
1:C:411:LYS:O	1:C:411:LYS:HG3	1.95	0.65
1:A:208:GLN:HA	1:A:215:THR:OG1	1.97	0.65
1:B:377:THR:CG2	1:B:551:THR:H	2.08	0.64
1:D:509:LEU:O	1:D:513:ARG:HG3	1.98	0.63
1:A:102:GLU:HB3	5:A:736:HOH:O	1.96	0.63
1:A:95:TYR:O	1:A:318:ARG:NH1	2.31	0.63
1:C:314:LEU:HD11	1:C:318:ARG:HH12	1.63	0.63
1:B:551:THR:HB	1:B:553:GLN:HE22	1.64	0.63
1:C:551:THR:HB	1:C:553:GLN:NE2	2.13	0.63
1:D:559:ASP:HB2	5:D:760:HOH:O	1.99	0.62
1:A:464:PHE:HE1	1:A:491:HIS:CE1	2.17	0.62
1:B:476:ARG:HD3	1:D:507:GLU:OE2	1.99	0.62
1:C:397:GLY:HA2	1:C:435:LEU:HD12	1.81	0.62
1:B:579:LEU:HD22	1:B:583:GLU:HG3	1.81	0.62
1:A:495:GLY:HA3	1:A:553:GLN:OE1	2.00	0.62
1:B:122:PHE:O	1:B:123:ARG:HB2	1.99	0.62
1:B:386:SER:HA	1:B:410:ILE:HG23	1.81	0.62
1:C:697:ALA:HA	1:C:700:ASN:ND2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:THR:HG22	1:B:551:THR:N	2.09	0.61
1:D:314:LEU:O	1:D:318:ARG:HB2	1.99	0.61
1:D:314:LEU:HD11	1:D:318:ARG:NH1	2.15	0.61
1:B:212:GLU:OE1	1:D:436:HIS:HD2	1.84	0.61
1:B:276:LEU:HD12	1:B:291:GLU:HG2	1.82	0.61
1:C:156:PHE:O	1:C:345:ARG:HD3	2.00	0.61
1:D:95:TYR:O	1:D:318:ARG:NH1	2.33	0.61
1:D:283:HIS:CD2	3:D:1002:TPP:O1B	2.52	0.61
1:B:553:GLN:NE2	1:B:553:GLN:H	1.98	0.61
1:C:378:ARG:HD2	1:C:407:ASN:HD21	1.63	0.61
1:B:365:LEU:HD22	1:B:534[A]:ARG:HD2	1.82	0.61
1:B:476:ARG:CD	1:D:507:GLU:OE2	2.48	0.61
1:B:134:PRO:HD3	1:D:502:THR:HB	1.82	0.61
1:C:584:GLU:OE1	1:C:584:GLU:HA	2.01	0.61
1:D:337:ALA:HA	1:D:340:ARG:HH21	1.66	0.60
1:A:377:THR:HG22	1:A:551:THR:N	2.10	0.60
1:B:62:ARG:HG2	1:B:62:ARG:NH1	2.00	0.60
1:C:464:PHE:CD1	1:C:491:HIS:ND1	2.69	0.60
1:D:53:ALA:HB3	1:D:54:PRO:HD3	1.83	0.60
1:C:275:ASN:ND2	1:C:275:ASN:N	2.49	0.59
1:C:697:ALA:HA	1:C:700:ASN:HD22	1.67	0.59
1:A:83:ALA:HB1	1:A:85:HIS:CE1	2.36	0.59
1:B:177:ASP:HB2	3:B:1002:TPP:O2A	2.03	0.59
1:B:580:GLN:H	1:B:583:GLU:HG2	1.67	0.59
1:C:53:ALA:HB3	1:C:54:PRO:HD3	1.85	0.59
1:B:397:GLY:HA2	1:B:435:LEU:HD12	1.85	0.59
1:D:377:THR:HG22	1:D:551:THR:N	2.14	0.59
1:D:579:LEU:HD12	1:D:579:LEU:N	2.17	0.59
1:C:83:ALA:HB1	1:C:85:HIS:CE1	2.38	0.59
1:D:681[B]:ARG:HH11	1:D:681[B]:ARG:CG	2.15	0.59
1:D:221:GLU:OE2	1:D:226:ARG:NH1	2.36	0.59
1:C:169:HIS:HE1	1:C:454:HIS:NE2	2.00	0.58
1:A:226:ARG:HG3	1:C:226:ARG:HG3	1.85	0.58
1:B:18:TYR:CZ	1:B:62:ARG:NE	2.71	0.58
1:A:267:THR:HG22	1:A:268:VAL:N	2.18	0.58
1:B:124:HIS:CD2	5:B:755:HOH:O	2.56	0.58
1:B:346:LYS:HE3	1:B:350:ASP:OD2	2.02	0.58
1:D:458:ARG:NH1	1:D:486:ILE:HD11	2.19	0.58
1:C:208:GLN:HA	1:C:215:THR:OG1	2.04	0.58
1:C:85:HIS:HB3	5:C:747:HOH:O	2.04	0.58
1:D:377:THR:CG2	1:D:551:THR:H	2.14	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:681[B]:ARG:CG	1:C:681[B]:ARG:HH11	2.16	0.57
1:B:314:LEU:HD11	1:B:318:ARG:NH1	2.20	0.57
1:C:491:HIS:HD2	1:C:552:ARG:CB	2.15	0.57
1:B:367:HIS:ND1	1:B:527:ASN:ND2	2.52	0.57
1:B:221:GLU:OE2	1:B:226:ARG:NH1	2.36	0.57
1:B:568:ARG:HD2	1:B:631:TYR:CE1	2.40	0.57
1:B:436:HIS:HD2	1:D:212:GLU:OE1	1.88	0.56
1:A:122:PHE:O	1:A:123:ARG:CB	2.47	0.56
1:A:580:GLN:HB3	1:A:583:GLU:CG	2.30	0.56
1:D:268:VAL:HA	5:D:705:HOH:O	2.03	0.56
1:A:314:LEU:HD11	1:A:318:ARG:NH1	2.20	0.56
1:B:233:HIS:HD2	1:B:256:VAL:CB	2.17	0.56
1:C:491:HIS:CD2	1:C:552:ARG:CB	2.77	0.56
1:C:235:GLN:HE22	1:C:252:ASN:HB2	1.71	0.56
1:A:221:GLU:OE2	1:A:226:ARG:NH1	2.37	0.56
1:D:391:LYS:HD2	5:D:753:HOH:O	2.05	0.56
1:C:83:ALA:HB1	1:C:85:HIS:HE1	1.71	0.56
1:D:291:GLU:O	1:D:295:VAL:HG23	2.06	0.56
1:C:386:SER:HA	1:C:410:ILE:HG23	1.88	0.55
1:B:569:GLY:O	1:B:619:PRO:HD2	2.05	0.55
1:A:283:HIS:ND1	3:A:1002:TPP:O1B	2.39	0.55
1:A:212:GLU:OE1	1:C:436:HIS:HD2	1.90	0.55
1:A:169:HIS:HE1	1:A:454:HIS:NE2	2.04	0.55
1:C:346:LYS:HE3	1:C:350:ASP:OD2	2.07	0.55
1:C:377:THR:CG2	1:C:550:LEU:HA	2.36	0.55
1:D:31:ARG:NH2	1:D:241:GLU:OE2	2.40	0.55
1:A:577:GLY:HA2	1:A:578:GLY:C	2.25	0.55
1:B:169:HIS:HE1	1:B:454:HIS:NE2	2.04	0.55
1:A:110:ARG:HE	1:C:498:GLU:HB3	1.72	0.55
1:B:377:THR:HG23	1:B:550:LEU:HD22	1.89	0.54
1:A:378:ARG:HD2	1:A:407:ASN:ND2	2.22	0.54
1:A:652:GLN:NE2	1:C:652:GLN:NE2	2.46	0.54
1:A:169:HIS:HD2	5:A:767:HOH:O	1.89	0.54
1:A:31:ARG:HH22	1:A:241:GLU:CD	2.10	0.54
1:A:134:PRO:HD3	1:C:502:THR:HB	1.89	0.54
1:C:82:SER:OG	1:C:179:ASP:OD1	2.21	0.54
1:D:575:ASP:OD1	1:D:614:ARG:HG3	2.07	0.54
1:B:233:HIS:HD2	1:B:256:VAL:HB	1.72	0.54
1:C:233:HIS:HD2	1:C:256:VAL:HB	1.73	0.54
1:D:471:MET:HE3	1:D:489:TRP:HE1	1.73	0.54
1:A:458:ARG:NH1	1:A:486:ILE:HD11	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1002:TPP:H61	3:D:1002:TPP:O1A	2.08	0.53
1:B:267:THR:HG22	1:B:268:VAL:N	2.23	0.53
1:B:208:GLN:HA	1:B:215:THR:OG1	2.08	0.53
1:C:296:LYS:HD3	1:C:303:PRO:HA	1.91	0.53
1:C:524:ALA:HB2	1:C:596:VAL:HG21	1.91	0.53
1:D:177:ASP:HB2	3:D:1002:TPP:O2A	2.07	0.53
1:B:377:THR:HG23	1:B:550:LEU:HD23	1.91	0.53
1:B:333:LEU:HD23	5:B:806:HOH:O	2.08	0.53
1:C:31:ARG:HD3	1:C:272:PRO:HD3	1.90	0.53
1:C:523:PRO:O	1:C:593:GLY:HA2	2.09	0.53
1:C:590:ILE:O	1:C:645:ALA:HA	2.08	0.52
1:C:493:SER:HB2	5:C:721:HOH:O	2.09	0.52
1:D:377:THR:CG2	1:D:550:LEU:HA	2.39	0.52
1:A:53:ALA:HB3	1:A:54:PRO:HD3	1.89	0.52
1:B:169:HIS:HD2	5:B:821:HOH:O	1.92	0.52
1:D:125:THR:HB	1:D:128:VAL:HG23	1.92	0.52
1:D:528:GLU:HG2	1:D:566:VAL:CG2	2.40	0.52
1:B:579:LEU:CD2	1:B:583:GLU:HG3	2.38	0.51
1:D:18:TYR:OH	1:D:62:ARG:HD2	2.10	0.51
1:D:378:ARG:HH11	1:D:407:ASN:HD21	1.58	0.51
1:C:572:VAL:HG22	1:C:614:ARG:HD3	1.92	0.51
1:A:21:GLU:HA	1:A:21:GLU:OE1	2.11	0.51
1:A:397:GLY:HA2	1:A:435:LEU:HD12	1.93	0.51
1:C:73:TRP:O	1:C:76:ARG:HG2	2.10	0.51
1:A:346:LYS:HE3	1:A:350:ASP:OD2	2.11	0.51
1:C:135:LEU:HD11	3:C:1002:TPP:S1	2.51	0.51
1:D:483:ILE:HG22	4:D:704:GOL:H12	1.92	0.51
1:B:464:PHE:CE1	1:B:491:HIS:ND1	2.79	0.51
1:C:170:TYR:HB2	1:C:172:TYR:CE2	2.46	0.51
1:B:418:PRO:O	1:B:421:ILE:HG12	2.11	0.51
1:C:125:THR:HB	1:C:128:VAL:HG23	1.93	0.51
1:A:491:HIS:HD2	1:A:552:ARG:CB	2.14	0.51
1:B:575:ASP:OD1	1:B:614:ARG:HG3	2.11	0.51
1:C:9:ALA:HA	1:C:12:ARG:HG3	1.92	0.51
1:C:53:ALA:HB3	1:C:54:PRO:CD	2.41	0.50
1:D:208:GLN:HA	1:D:215:THR:OG1	2.12	0.50
1:A:419:PRO:HA	1:A:428:ALA:O	2.12	0.50
1:B:579:LEU:HD22	1:B:583:GLU:CG	2.40	0.50
1:B:361:TRP:CH2	1:B:534[B]:ARG:HG2	2.47	0.50
1:D:378:ARG:HD2	1:D:407:ASN:ND2	2.26	0.50
1:A:275:ASN:N	1:A:275:ASN:HD22	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:TRP:CE3	1:C:262:PHE:HB2	2.46	0.50
3:A:1002:TPP:N1'	1:C:441:GLU:OE2	2.45	0.50
1:C:153:ARG:HH21	1:C:160:ALA:HB3	1.76	0.50
1:C:524:ALA:CB	1:C:596:VAL:HG21	2.42	0.49
1:A:153:ARG:HH21	1:A:160:ALA:HB3	1.77	0.49
1:A:396:TRP:O	1:A:459:ALA:HA	2.11	0.49
1:A:577:GLY:C	1:A:578:GLY:O	2.50	0.49
1:B:78:ARG:HB2	1:B:171:ILE:HD13	1.94	0.49
1:A:681:ARG:HH11	1:A:681:ARG:HG2	1.77	0.49
1:B:396:TRP:O	1:B:459:ALA:HA	2.11	0.49
1:C:528:GLU:HG2	1:C:566:VAL:CG2	2.43	0.49
1:C:578:GLY:H	1:C:612:LEU:HD22	1.77	0.49
1:A:670:TYR:HD2	1:C:517:ARG:HH21	1.61	0.49
1:B:365:LEU:HD22	1:B:534[A]:ARG:CD	2.43	0.49
1:B:672:GLU:HG2	1:D:112:TRP:CE3	2.48	0.49
1:D:535:THR:HG23	1:D:540:ARG:HB3	1.93	0.49
1:D:661:THR:HB	1:D:700:ASN:HB3	1.94	0.49
1:C:377:THR:HG21	1:C:550:LEU:HA	1.95	0.49
1:C:580:GLN:H	1:C:583:GLU:HG3	1.78	0.49
1:A:551:THR:HB	1:A:553:GLN:NE2	2.28	0.49
1:D:392:LEU:O	1:D:433:ARG:NH2	2.46	0.49
1:D:507:GLU:OE1	1:D:507:GLU:N	2.39	0.49
1:A:295:VAL:O	1:A:299:VAL:HG22	2.13	0.48
1:B:233:HIS:CD2	1:B:256:VAL:CG2	2.95	0.48
1:A:584:GLU:HG3	1:A:640:VAL:HG23	1.95	0.48
1:B:457:THR:HG23	5:B:825:HOH:O	2.13	0.48
1:B:462:GLY:HA2	1:B:488:VAL:O	2.13	0.48
1:B:568:ARG:HD2	1:B:631:TYR:CZ	2.48	0.48
1:C:672:GLU:HG3	1:C:673:SER:N	2.28	0.48
1:A:572:VAL:HG22	1:A:614:ARG:HD3	1.95	0.48
1:C:233:HIS:CE1	1:C:235:GLN:HE21	2.31	0.48
1:A:580:GLN:HB2	1:A:583:GLU:CG	2.42	0.48
1:C:31:ARG:NH2	1:C:241:GLU:OE2	2.46	0.48
1:A:675:ASP:OD1	1:A:678:THR:OG1	2.26	0.48
1:D:576:ALA:O	1:D:579:LEU:HD13	2.13	0.48
1:C:233:HIS:CD2	1:C:256:VAL:HG21	2.48	0.48
1:C:419:PRO:HA	1:C:428:ALA:O	2.12	0.48
1:A:535:THR:HG23	1:A:540:ARG:HB3	1.95	0.48
1:A:568:ARG:NH1	1:A:627:GLN:OE1	2.47	0.48
1:B:10:LEU:HD21	1:B:266:ARG:HG3	1.95	0.48
1:B:580:GLN:O	1:B:583:GLU:N	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:579:LEU:HD22	1:C:583:GLU:HB3	1.95	0.48
1:B:402:LEU:HD21	3:D:1002:TPP:H7'1	1.95	0.48
1:B:576:ALA:O	1:B:578:GLY:N	2.46	0.48
1:A:176:SER:HB2	5:A:779:HOH:O	2.14	0.47
1:A:580:GLN:O	1:A:583:GLU:CG	2.62	0.47
1:D:337:ALA:CA	1:D:340:ARG:HH21	2.26	0.47
1:D:403:ALA:HB1	4:D:702:GOL:H32	1.95	0.47
1:C:26:ALA:O	1:C:29:THR:HG22	2.14	0.47
1:C:644:VAL:HG22	1:C:663:GLU:HB2	1.95	0.47
1:B:660:ASP:OD2	1:D:660:ASP:HB2	2.14	0.47
1:A:569:GLY:O	1:A:619:PRO:CD	2.62	0.47
1:A:233:HIS:HD2	1:A:256:VAL:HB	1.79	0.47
1:D:31:ARG:HH22	1:D:241:GLU:CD	2.18	0.47
1:D:295:VAL:O	1:D:299:VAL:HG22	2.15	0.47
1:A:392:LEU:O	1:A:433:ARG:NH2	2.48	0.47
1:A:71:THR:HB	5:A:782:HOH:O	2.14	0.47
1:D:672:GLU:HG3	1:D:673:SER:N	2.30	0.47
1:B:476:ARG:HD2	1:D:507:GLU:OE2	2.14	0.47
1:B:675:ASP:OD1	1:B:678:THR:OG1	2.21	0.47
1:A:291:GLU:O	1:A:295:VAL:HG23	2.15	0.47
1:A:491:HIS:CD2	1:A:552:ARG:CB	2.85	0.47
1:D:267:THR:CG2	1:D:268:VAL:N	2.78	0.46
1:C:10:LEU:HD21	1:C:266:ARG:HG3	1.97	0.46
1:C:556:PRO:CG	1:C:597:GLN:OE1	2.63	0.46
1:A:51:SER:HB2	1:A:267:THR:HG21	1.98	0.46
5:B:737:HOH:O	1:D:186:SER:HB3	2.14	0.46
1:D:31:ARG:HD3	1:D:272:PRO:HD3	1.96	0.46
1:C:288:GLY:O	1:C:292:VAL:HG23	2.15	0.46
1:D:125:THR:HB	1:D:128:VAL:CG2	2.46	0.46
1:D:399:SER:OG	1:D:406:ASN:ND2	2.49	0.46
1:B:135:LEU:HD13	1:B:178:GLY:HA3	1.98	0.46
1:B:572:VAL:HG22	1:B:614:ARG:HD3	1.97	0.46
1:D:572:VAL:HG22	1:D:614:ARG:HD3	1.98	0.46
1:A:386:SER:HA	1:A:410:ILE:HG23	1.96	0.46
1:B:85:HIS:HD2	3:B:1002:TPP:S1	2.39	0.46
1:B:587:VAL:HG23	1:B:642:ALA:HB1	1.98	0.46
1:C:572:VAL:HG11	1:C:575:ASP:OD1	2.16	0.46
1:C:7:ILE:HA	1:C:8:SER:HA	1.68	0.45
1:B:466:GLN:HE22	1:D:476:ARG:NE	2.14	0.45
1:A:337:ALA:O	1:A:341[A]:ARG:HG3	2.16	0.45
1:C:209:ILE:HG21	1:C:269:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:GLU:HG3	1:A:673:SER:N	2.32	0.45
1:C:377:THR:HG23	1:C:550:LEU:CD2	2.47	0.45
1:A:233:HIS:CD2	1:A:256:VAL:HG21	2.52	0.45
1:A:377:THR:CG2	1:A:550:LEU:HA	2.47	0.45
1:A:48:THR:HB	5:A:781:HOH:O	2.16	0.45
1:B:31:ARG:HH22	1:B:241:GLU:CD	2.19	0.45
1:C:271:TYR:CE1	1:C:272:PRO:HB3	2.51	0.45
1:B:232:TRP:CE3	1:B:262:PHE:HB2	2.52	0.45
1:B:81:LEU:HD21	1:B:86:SER:O	2.17	0.45
1:A:580:GLN:O	1:A:583:GLU:N	2.49	0.45
1:B:521:VAL:HA	1:B:619:PRO:O	2.17	0.45
1:D:467:PHE:C	1:D:469:ASP:N	2.67	0.45
1:B:182:GLU:OE2	1:D:441:GLU:OE1	2.33	0.45
1:D:580:GLN:H	1:D:583:GLU:HG2	1.81	0.45
1:A:580:GLN:O	1:A:583:GLU:HG2	2.15	0.44
1:A:22:ILE:HA	1:A:22:ILE:HD13	1.82	0.44
1:B:95:TYR:O	1:B:318:ARG:NH1	2.50	0.44
1:C:568:ARG:HD2	1:C:631:TYR:CZ	2.53	0.44
1:A:580:GLN:HB2	1:A:583:GLU:HG3	1.99	0.44
1:B:378:ARG:HD2	1:B:407:ASN:ND2	2.31	0.44
1:C:271:TYR:CD1	1:C:272:PRO:HA	2.52	0.44
1:D:364:ASP:HB2	5:D:753:HOH:O	2.18	0.44
1:B:419:PRO:HA	1:B:428:ALA:O	2.17	0.44
1:C:246:ILE:O	1:C:250:ILE:HG13	2.18	0.44
1:C:337:ALA:HA	1:C:340:ARG:HH21	1.83	0.44
1:D:524:ALA:HB2	1:D:596:VAL:HG21	2.00	0.44
1:A:378:ARG:HH11	1:A:407:ASN:HD21	1.66	0.44
1:B:699:ASP:OD1	1:B:699:ASP:N	2.50	0.44
1:C:108:SER:O	1:C:109:LEU:C	2.57	0.44
1:C:504:GLN:OE1	1:C:671:GLY:HA3	2.17	0.44
1:A:226:ARG:O	1:A:229:ALA:HB3	2.17	0.44
1:A:580:GLN:CB	1:A:583:GLU:HG3	2.42	0.44
1:B:27:VAL:HA	1:B:30:ILE:HD12	1.99	0.44
1:B:180:ILE:HA	1:B:180:ILE:HD12	1.79	0.43
1:B:365:LEU:HD22	1:B:534[A]:ARG:HH11	1.83	0.43
1:C:657:LEU:C	1:C:657:LEU:HD23	2.39	0.43
1:A:267:THR:CG2	1:A:268:VAL:N	2.81	0.43
1:B:233:HIS:HD2	1:B:256:VAL:CG2	2.31	0.43
1:D:415:SER:O	1:D:428:ALA:HA	2.19	0.43
1:A:504:GLN:OE1	1:A:671:GLY:HA3	2.17	0.43
1:D:27:VAL:HA	1:D:30:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:THR:HG23	1:D:550:LEU:CD2	2.48	0.43
1:B:652:GLN:NE2	1:D:652:GLN:NE2	2.56	0.43
1:A:125:THR:HB	1:A:128:VAL:HG23	2.00	0.43
1:B:17:ASP:O	1:C:126:PRO:HD3	2.18	0.43
1:C:377:THR:HG23	1:C:550:LEU:HD22	2.00	0.43
1:C:271:TYR:HD1	1:C:277:MET:CE	2.31	0.43
1:C:308:GLN:HA	1:C:308:GLN:OE1	2.19	0.43
1:C:337:ALA:HA	1:C:340:ARG:NH2	2.33	0.43
1:C:406:ASN:HD21	1:C:463:THR:HA	1.83	0.43
1:B:153:ARG:HH21	1:B:160:ALA:HB3	1.83	0.43
1:B:502:THR:HB	1:D:134:PRO:HD3	2.01	0.43
1:A:123:ARG:HD3	1:A:123:ARG:HH11	1.63	0.43
1:C:150[B]:ARG:NH1	1:C:195:GLN:O	2.38	0.43
1:C:607:ALA:C	1:C:609:ASN:H	2.22	0.43
1:A:584:GLU:OE1	1:A:584:GLU:HA	2.18	0.43
1:D:108:SER:O	1:D:109:LEU:C	2.57	0.43
1:D:411:LYS:O	1:D:411:LYS:HG3	2.16	0.43
1:A:44:GLY:CA	1:A:110:ARG:NH2	2.62	0.42
1:A:21:GLU:CA	1:A:21:GLU:OE1	2.66	0.42
1:A:556:PRO:CD	1:A:597:GLN:OE1	2.67	0.42
1:B:579:LEU:HD22	1:B:583:GLU:HB3	2.01	0.42
1:B:584:GLU:HA	1:B:584:GLU:OE1	2.19	0.42
1:A:169:HIS:CE1	1:A:454:HIS:NE2	2.87	0.42
1:B:491:HIS:CD2	1:B:491:HIS:N	2.85	0.42
1:B:493:SER:O	1:B:496:LEU:HB3	2.19	0.42
1:C:235:GLN:OE1	1:C:249:ALA:HA	2.19	0.42
1:A:108:SER:O	1:A:109:LEU:C	2.58	0.42
1:B:193:ALA:O	1:B:194:VAL:C	2.54	0.42
1:C:173:VAL:HB	1:C:202:VAL:HG22	2.01	0.42
1:C:378:ARG:HB2	1:C:407:ASN:HD22	1.84	0.42
1:C:458:ARG:NH1	1:C:486:ILE:HD11	2.34	0.42
1:B:441:GLU:OE1	1:D:182:GLU:OE2	2.38	0.42
1:A:525:ASP:C	1:A:525:ASP:OD1	2.58	0.42
1:A:577:GLY:CA	1:A:578:GLY:O	2.67	0.42
1:C:92:ILE:HG22	1:C:96:LEU:HD12	2.00	0.42
1:D:208:GLN:O	1:D:214:ASP:HA	2.19	0.42
1:D:556:PRO:HD2	1:D:597:GLN:OE1	2.19	0.42
1:B:399:SER:OG	1:B:406:ASN:ND2	2.52	0.42
1:C:305:LYS:HD3	1:C:308:GLN:NE2	2.35	0.42
1:C:406:ASN:HA	1:C:490:THR:HG21	2.01	0.42
1:C:600:VAL:O	1:C:603:GLN:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ILE:O	1:A:516:PRO:C	2.57	0.42
1:B:169:HIS:CE1	1:B:454:HIS:NE2	2.85	0.42
1:C:145:MET:HG2	1:C:454:HIS:HB2	2.01	0.42
1:D:17:ASP:N	1:D:17:ASP:OD1	2.50	0.42
1:A:405:SER:HB3	1:A:491:HIS:HE1	1.84	0.41
1:A:584:GLU:HG3	1:A:640:VAL:CG2	2.50	0.41
1:A:568:ARG:HD2	1:A:631:TYR:CE1	2.55	0.41
1:B:226:ARG:HG3	1:D:226:ARG:HG3	2.01	0.41
1:C:596:VAL:O	1:C:599:ALA:HB3	2.20	0.41
1:A:655:HIS:CG	1:C:656:GLN:HB2	2.55	0.41
1:C:109:LEU:HG	1:C:110:ARG:HG3	2.02	0.41
1:C:142:ALA:CB	1:C:173:VAL:HG21	2.50	0.41
1:A:587:VAL:HG23	1:A:642:ALA:HB1	2.01	0.41
1:C:208:GLN:O	1:C:214:ASP:HA	2.19	0.41
1:A:528:GLU:HG2	1:A:566:VAL:CG2	2.50	0.41
1:B:334:GLU:HG2	1:B:334:GLU:H	1.68	0.41
1:D:580:GLN:C	1:D:583:GLU:HB2	2.39	0.41
1:A:44:GLY:CA	1:A:110:ARG:HH21	1.99	0.41
1:A:169:HIS:CD2	5:A:767:HOH:O	2.67	0.41
1:C:187:GLU:HB3	1:C:440:ARG:HD3	2.01	0.41
1:C:180:ILE:HG12	1:C:204:TYR:CD1	2.55	0.41
1:C:414:ASP:OD2	1:C:432:GLY:HA2	2.20	0.41
1:D:587:VAL:HG23	1:D:642:ALA:HB1	2.02	0.41
1:A:580:GLN:N	1:A:583:GLU:CB	2.70	0.41
1:B:108:SER:O	1:B:109:LEU:C	2.59	0.41
1:B:392:LEU:O	1:B:433:ARG:NH2	2.54	0.41
1:C:310:ARG:HH11	1:C:310:ARG:HD2	1.71	0.41
1:C:458:ARG:NH2	1:C:536:ILE:O	2.54	0.41
1:D:51:SER:HB2	1:D:267:THR:HG21	2.02	0.41
1:B:182:GLU:OE2	3:B:1002:TPP:HM23	2.20	0.41
1:D:187:GLU:HB3	1:D:440:ARG:HD3	2.02	0.41
1:A:577:GLY:CA	1:A:578:GLY:C	2.89	0.41
1:B:85:HIS:CD2	3:B:1002:TPP:S1	3.13	0.41
1:C:176:SER:OG	3:C:1002:TPP:O1A	2.34	0.41
1:C:384:VAL:HG21	1:C:530:ALA:HA	2.03	0.41
1:B:415:SER:O	1:B:432:GLY:HA3	2.20	0.41
1:B:466:GLN:HE22	1:D:476:ARG:CD	2.34	0.41
1:A:182:GLU:OE2	1:C:441:GLU:OE1	2.39	0.40
1:A:576:ALA:HB2	1:A:613:ALA:O	2.21	0.40
1:A:580:GLN:O	1:A:581:PRO:C	2.57	0.40
1:B:579:LEU:HD22	1:B:583:GLU:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:HIS:HD1	1:C:368:TRP:H	1.69	0.40
1:A:556:PRO:HD2	1:A:597:GLN:OE1	2.21	0.40
1:D:496:LEU:HD13	5:D:830:HOH:O	2.20	0.40
1:A:150:ARG:NH1	1:A:195:GLN:O	2.52	0.40
1:A:418:PRO:O	1:A:421:ILE:HG12	2.21	0.40
1:B:435:LEU:HA	1:B:435:LEU:HD23	1.86	0.40
1:D:403:ALA:O	4:D:702:GOL:H11	2.21	0.40
1:C:267:THR:CG2	1:C:268:VAL:N	2.85	0.40
1:D:681[B]:ARG:HB2	1:D:681[B]:ARG:NH1	2.37	0.40
1:B:310:ARG:HB3	1:B:312:ASP:OD1	2.21	0.40
1:C:250:ILE:HG22	1:C:254:GLN:NE2	2.36	0.40
1:C:419:PRO:O	1:C:422:SER:HB2	2.22	0.40
1:D:583:GLU:OE1	1:D:583:GLU:HA	2.22	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	695/700 (99%)	661 (95%)	32 (5%)	2 (0%)	41	61
1	B	693/700 (99%)	655 (94%)	34 (5%)	4 (1%)	25	43
1	C	694/700 (99%)	643 (93%)	47 (7%)	4 (1%)	25	43
1	D	693/700 (99%)	660 (95%)	33 (5%)	0	100	100
All	All	2775/2800 (99%)	2619 (94%)	146 (5%)	10 (0%)	34	54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	577	GLY
1	B	495	GLY

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Mol	Chain	Res	Type
1	B	578	GLY
1	C	162	PRO
1	A	608	ASP
1	C	46	PRO
1	C	608	ASP
1	B	162	PRO
1	C	218	ALA
1	A	46	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	542/545 (99%)	517 (95%)	25 (5%)	27	50
1	B	540/545 (99%)	521 (96%)	19 (4%)	36	62
1	C	541/545 (99%)	514 (95%)	27 (5%)	24	46
1	D	540/545 (99%)	519 (96%)	21 (4%)	32	57
All	All	2163/2180 (99%)	2071 (96%)	92 (4%)	30	53

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	22	ILE
1	A	33	LEU
1	A	51	SER
1	A	66	HIS
1	A	85	HIS
1	A	180	ILE
1	A	215	THR
1	A	220	CYS
1	A	233	HIS
1	A	275	ASN
1	A	377	THR
1	A	395	LEU

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Mol	Chain	Res	Type
1	A	396	TRP
1	A	457	THR
1	A	458	ARG
1	A	496	LEU
1	A	575	ASP
1	A	579	LEU
1	A	580	GLN
1	A	581	PRO
1	A	583	GLU
1	A	584	GLU
1	A	625	GLU
1	A	629	TYR
1	B	33	LEU
1	B	62	ARG
1	B	66	HIS
1	B	86	SER
1	B	180	ILE
1	B	215	THR
1	B	233	HIS
1	B	318	ARG
1	B	330	ARG
1	B	377	THR
1	B	396	TRP
1	B	411	LYS
1	B	458	ARG
1	B	476	ARG
1	B	496	LEU
1	B	540	ARG
1	B	553	GLN
1	B	555	VAL
1	B	630	GLU
1	C	22	ILE
1	C	51	SER
1	C	66	HIS
1	C	150[A]	ARG
1	C	150[B]	ARG
1	C	180	ILE
1	C	204	TYR
1	C	233	HIS
1	C	275	ASN
1	C	277	MET
1	C	299	VAL

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Mol	Chain	Res	Type
1	C	325	LYS
1	C	341	ARG
1	C	377	THR
1	C	396	TRP
1	C	414	ASP
1	C	422	SER
1	C	457	THR
1	C	458	ARG
1	C	496	LEU
1	C	510	SER
1	C	534	ARG
1	C	553	GLN
1	C	584	GLU
1	C	587	VAL
1	C	592	THR
1	C	625	GLU
1	D	12	ARG
1	D	22	ILE
1	D	66	HIS
1	D	74	LEU
1	D	78	ARG
1	D	125	THR
1	D	185	THR
1	D	220	CYS
1	D	233	HIS
1	D	318	ARG
1	D	367	HIS
1	D	377	THR
1	D	395	LEU
1	D	396	TRP
1	D	457	THR
1	D	458	ARG
1	D	496	LEU
1	D	534	ARG
1	D	555	VAL
1	D	584	GLU
1	D	630	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS

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Mol	Chain	Res	Type
1	A	169	HIS
1	A	233	HIS
1	A	275	ASN
1	A	283	HIS
1	A	308	GLN
1	A	326	GLN
1	A	355	GLN
1	A	406	ASN
1	A	407	ASN
1	A	436	HIS
1	A	669	HIS
1	B	85	HIS
1	B	119	HIS
1	B	169	HIS
1	B	196	GLN
1	B	233	HIS
1	B	275	ASN
1	B	308	GLN
1	B	355	GLN
1	B	406	ASN
1	B	407	ASN
1	B	436	HIS
1	B	466	GLN
1	B	491	HIS
1	B	527	ASN
1	B	553	GLN
1	C	169	HIS
1	C	233	HIS
1	C	254	GLN
1	C	275	ASN
1	C	316	HIS
1	C	355	GLN
1	C	406	ASN
1	C	407	ASN
1	C	436	HIS
1	C	553	GLN
1	C	603	GLN
1	C	652	GLN
1	C	669	HIS
1	C	700	ASN
1	D	45	HIS
1	D	208	GLN

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Mol	Chain	Res	Type
1	D	275	ASN
1	D	283	HIS
1	D	406	ASN
1	D	407	ASN
1	D	436	HIS
1	D	652	GLN
1	D	669	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 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	TPP	D	1002	2	22,27,27	2.55	3 (13%)	29,40,40	2.45	12 (41%)
3	TPP	C	1002	2	22,27,27	2.31	5 (22%)	29,40,40	2.06	9 (31%)
3	TPP	B	1002	2	22,27,27	1.85	5 (22%)	29,40,40	2.16	14 (48%)
3	TPP	A	1002	2	22,27,27	2.58	2 (9%)	29,40,40	1.87	10 (34%)
4	GOL	D	703	-	5,5,5	0.38	0	5,5,5	0.53	0
4	GOL	B	702	-	5,5,5	0.39	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	702	-	5,5,5	0.55	0	5,5,5	0.85	0
4	GOL	B	701	-	5,5,5	0.43	0	5,5,5	0.46	0
4	GOL	D	701	-	5,5,5	0.39	0	5,5,5	0.41	0
4	GOL	C	701	-	5,5,5	0.42	0	5,5,5	0.66	0
4	GOL	C	702	-	5,5,5	0.33	0	5,5,5	0.86	0
4	GOL	D	704	-	5,5,5	0.38	0	5,5,5	0.74	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
3	TPP	D	1002	2	-	1/16/17/17	0/2/2/2
3	TPP	C	1002	2	-	2/16/17/17	0/2/2/2
3	TPP	B	1002	2	-	1/16/17/17	0/2/2/2
3	TPP	A	1002	2	-	2/16/17/17	0/2/2/2
4	GOL	D	703	-	-	1/4/4/4	-
4	GOL	B	702	-	-	4/4/4/4	-
4	GOL	D	702	-	-	2/4/4/4	-
4	GOL	B	701	-	-	0/4/4/4	-
4	GOL	D	701	-	-	2/4/4/4	-
4	GOL	C	701	-	-	0/4/4/4	-
4	GOL	C	702	-	-	0/4/4/4	-
4	GOL	D	704	-	-	2/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	TPP	C6-C5	10.92	1.55	1.50
3	D	1002	TPP	C6-C5	10.25	1.55	1.50
3	C	1002	TPP	C6-C5	8.18	1.54	1.50
3	B	1002	TPP	C6-C5	5.04	1.53	1.50
3	B	1002	TPP	C4-N3	-4.05	1.36	1.39
3	C	1002	TPP	C4-N3	-3.84	1.36	1.39
3	D	1002	TPP	C4-N3	-3.38	1.36	1.39
3	A	1002	TPP	C4-N3	-2.52	1.37	1.39
3	C	1002	TPP	PB-O2B	2.51	1.64	1.54
3	B	1002	TPP	C5'-C4'	-2.39	1.38	1.42
3	C	1002	TPP	O7-C7	-2.38	1.35	1.44
3	D	1002	TPP	C5'-C4'	-2.24	1.39	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	TPP	C7'-N3	-2.05	1.44	1.48
3	B	1002	TPP	PA-O7	-2.05	1.51	1.59
3	C	1002	TPP	CM4-C4	2.01	1.54	1.49

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1002	TPP	CM2-C2'-N1'	5.30	122.97	117.14
3	B	1002	TPP	C6-C5-C4	5.27	131.66	127.43
3	C	1002	TPP	C5'-C7'-N3	-5.12	104.76	113.28
3	D	1002	TPP	CM4-C4-C5	-4.44	117.90	127.60
3	D	1002	TPP	C5-C4-N3	4.11	115.80	107.57
3	D	1002	TPP	PA-O3A-PB	-3.98	119.17	132.83
3	D	1002	TPP	C5'-C7'-N3	-3.94	106.72	113.28
3	C	1002	TPP	C5-C4-N3	3.80	115.18	107.57
3	D	1002	TPP	N1'-C2'-N3'	-3.77	119.05	125.54
3	A	1002	TPP	C5-C4-N3	3.71	114.99	107.57
3	A	1002	TPP	C5'-C7'-N3	-3.63	107.23	113.28
3	B	1002	TPP	N1'-C2'-N3'	-3.46	119.58	125.54
3	D	1002	TPP	C6'-N1'-C2'	3.36	121.67	115.96
3	C	1002	TPP	C6-C5-C4	3.33	130.10	127.43
3	B	1002	TPP	C5-C4-N3	3.22	114.02	107.57
3	D	1002	TPP	C7'-N3-C2	-3.22	119.54	125.35
3	B	1002	TPP	C6'-N1'-C2'	3.19	121.39	115.96
3	A	1002	TPP	C7'-N3-C2	-3.12	119.71	125.35
3	C	1002	TPP	CM2-C2'-N1'	3.11	120.56	117.14
3	C	1002	TPP	C5'-C6'-N1'	-3.07	118.71	123.82
3	C	1002	TPP	C6'-N1'-C2'	3.07	121.18	115.96
3	C	1002	TPP	CM4-C4-C5	-3.06	120.91	127.60
3	D	1002	TPP	CM4-C4-N3	2.95	126.29	122.53
3	A	1002	TPP	O3B-PB-O2B	-2.68	97.41	107.64
3	B	1002	TPP	C7'-N3-C2	-2.58	120.68	125.35
3	A	1002	TPP	CM4-C4-C5	-2.57	121.98	127.60
3	D	1002	TPP	O2B-PB-O3A	2.57	113.24	104.64
3	B	1002	TPP	O2B-PB-O3A	2.55	113.19	104.64
3	B	1002	TPP	C2'-N3'-C4'	2.52	122.01	118.08
3	C	1002	TPP	C7'-N3-C2	-2.50	120.83	125.35
3	A	1002	TPP	O2A-PA-O1A	2.45	124.34	112.24
3	B	1002	TPP	C5'-C7'-N3	-2.44	109.21	113.28
3	B	1002	TPP	CM2-C2'-N1'	2.40	119.78	117.14
3	A	1002	TPP	C6'-N1'-C2'	2.36	119.98	115.96
3	B	1002	TPP	O3B-PB-O1B	2.36	119.91	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1002	TPP	C6-C5-C4	2.34	129.31	127.43
3	D	1002	TPP	O3B-PB-O1B	2.33	119.79	110.68
3	A	1002	TPP	PA-O3A-PB	-2.32	124.86	132.83
3	A	1002	TPP	O2B-PB-O3A	2.29	112.33	104.64
3	A	1002	TPP	C7'-C5'-C6'	-2.26	116.37	120.69
3	B	1002	TPP	O2A-PA-O1A	2.25	123.35	112.24
3	B	1002	TPP	CM2-C2'-N3'	2.23	120.63	117.15
3	B	1002	TPP	PA-O3A-PB	-2.11	125.58	132.83
3	B	1002	TPP	CM4-C4-C5	-2.11	122.99	127.60
3	C	1002	TPP	C6'-C5'-C4'	2.03	118.49	115.72

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1002	TPP	C4-C5-C6-C7
3	C	1002	TPP	C4-C5-C6-C7
3	C	1002	TPP	C5-C6-C7-O7
4	B	702	GOL	O1-C1-C2-C3
4	B	702	GOL	C1-C2-C3-O3
4	D	701	GOL	O1-C1-C2-C3
4	D	704	GOL	C1-C2-C3-O3
4	B	702	GOL	O1-C1-C2-O2
4	B	702	GOL	O2-C2-C3-O3
4	D	701	GOL	O1-C1-C2-O2
4	D	704	GOL	O2-C2-C3-O3
3	A	1002	TPP	C5-C6-C7-O7
4	D	702	GOL	O1-C1-C2-O2
3	B	1002	TPP	C4-C5-C6-C7
3	A	1002	TPP	C4-C5-C6-C7
4	D	702	GOL	O1-C1-C2-C3
4	D	703	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 25 short contacts:

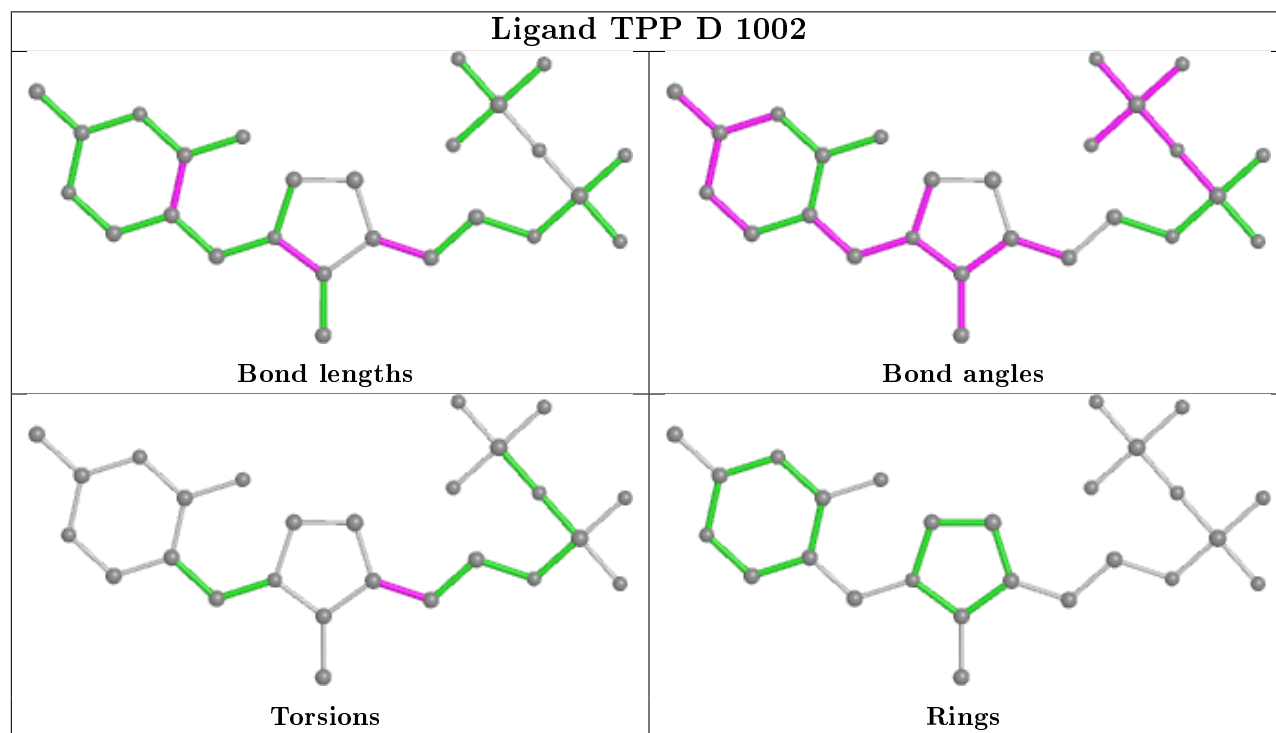
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1002	TPP	6	0
3	C	1002	TPP	3	0
3	B	1002	TPP	5	0
3	A	1002	TPP	4	0

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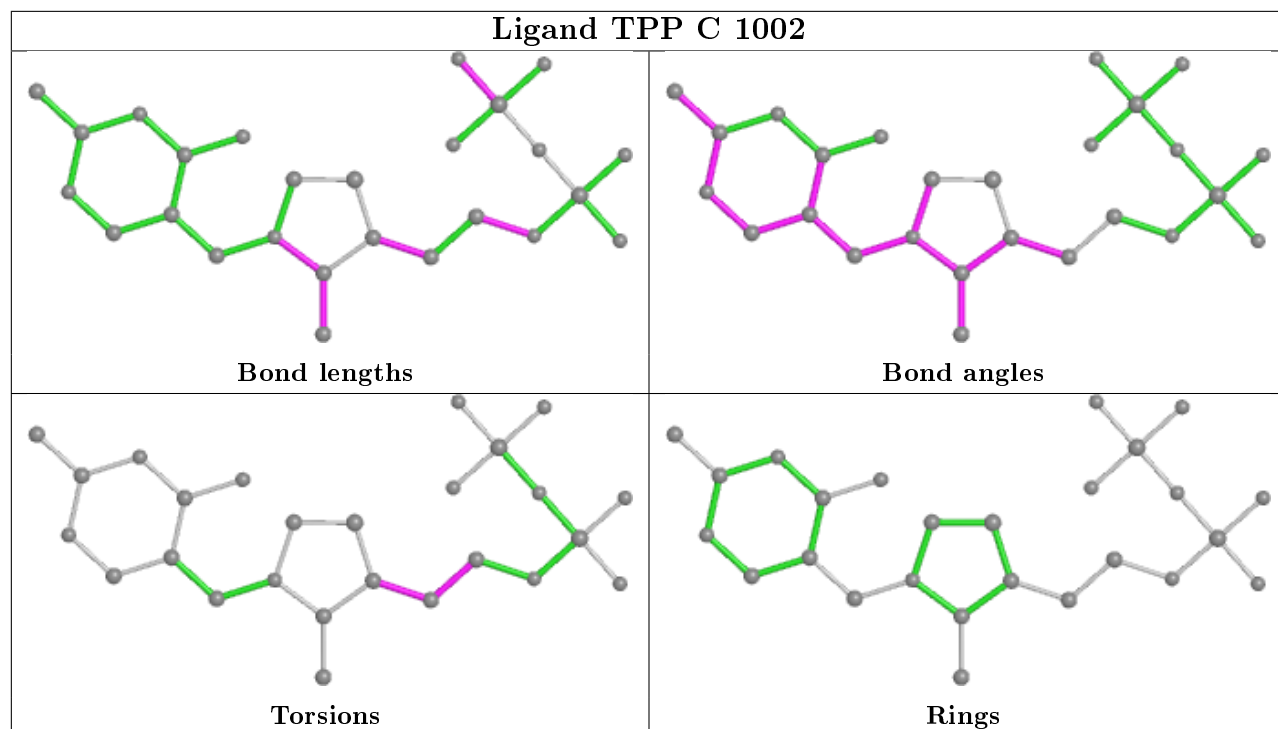
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	702	GOL	2	0
4	D	701	GOL	4	0
4	D	704	GOL	1	0

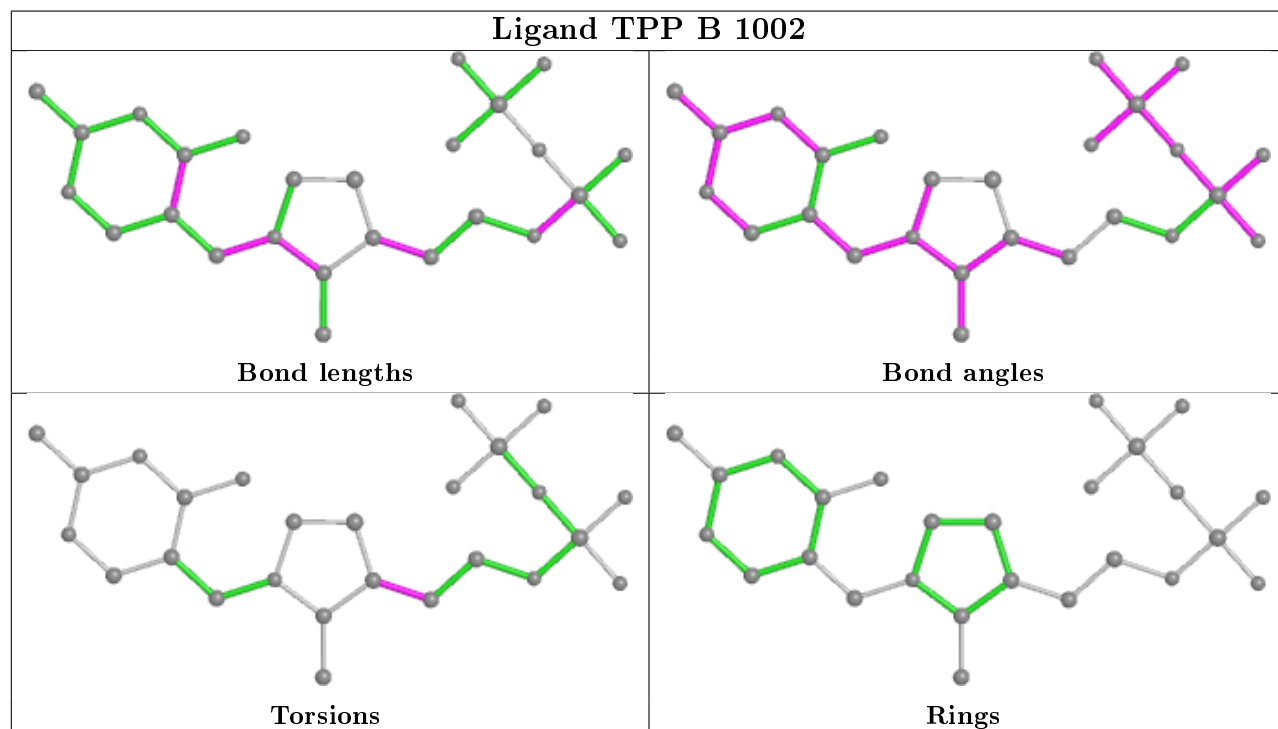
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

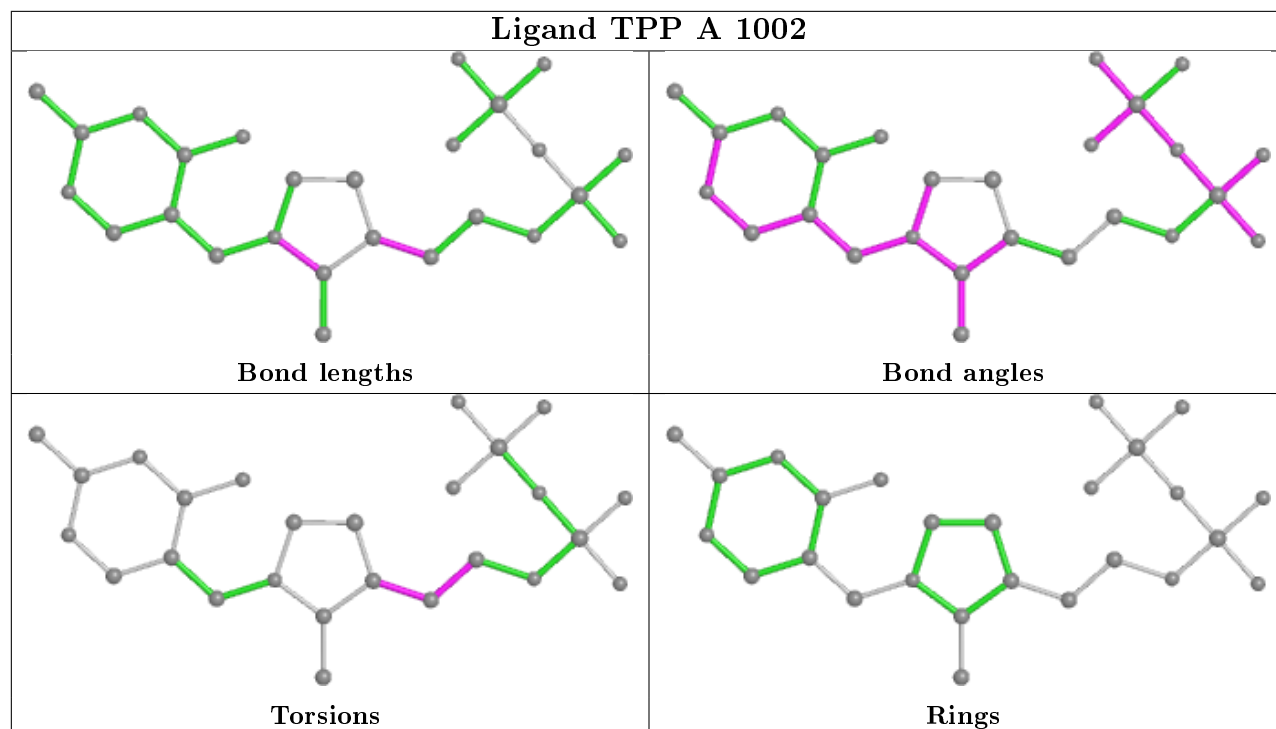


Ligand TPP C 1002



Ligand TPP B 1002





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	694/700 (99%)	0.24	33 (4%) 30 32	11, 26, 45, 61	0
1	B	694/700 (99%)	-0.04	17 (2%) 59 62	11, 26, 44, 60	0
1	C	694/700 (99%)	0.37	51 (7%) 15 15	11, 27, 46, 61	0
1	D	694/700 (99%)	-0.04	16 (2%) 60 63	11, 26, 43, 61	0
All	All	2776/2800 (99%)	0.13	117 (4%) 36 39	11, 26, 45, 61	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	579	LEU	6.0
1	A	629	TYR	5.8
1	A	582	GLY	5.5
1	C	582	GLY	5.3
1	B	699	ASP	5.2
1	C	17	ASP	5.0
1	C	164	ALA	4.5
1	C	300	GLY	4.2
1	C	7	ILE	4.1
1	A	412	GLY	4.1
1	A	581	PRO	4.0
1	C	608	ASP	4.0
1	B	700	ASN	4.0
1	A	610	ASP	3.9
1	D	582	GLY	3.9
1	C	581	PRO	3.9
1	D	579	LEU	3.9
1	A	580	GLN	3.9
1	C	299	VAL	3.9
1	C	329	GLU	3.8
1	C	575	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	18	TYR	3.6
1	A	607	ALA	3.6
1	C	305	LYS	3.6
1	A	579	LEU	3.6
1	A	411	LYS	3.5
1	B	577	GLY	3.4
1	C	12	ARG	3.4
1	A	577	GLY	3.4
1	A	576	ALA	3.4
1	D	581	PRO	3.4
1	A	699	ASP	3.3
1	C	610	ASP	3.3
1	C	248	GLU	3.3
1	C	14	ARG	3.2
1	C	330	ARG	3.2
1	C	364	ASP	3.2
1	C	20	THR	3.2
1	C	363	ALA	3.2
1	C	580	GLN	3.2
1	D	159	ASP	3.1
1	C	578	GLY	3.1
1	C	559	ASP	3.0
1	B	576	ALA	3.0
1	A	7	ILE	2.9
1	C	238	GLU	2.9
1	C	373	LYS	2.9
1	C	21	GLU	2.9
1	C	9	ALA	2.8
1	D	340	ARG	2.8
1	D	12	ARG	2.8
1	A	344	GLU	2.8
1	D	17	ASP	2.8
1	C	583	GLU	2.8
1	B	608	ASP	2.7
1	C	11	THR	2.7
1	C	255	ALA	2.7
1	C	285	ALA	2.7
1	C	316	HIS	2.7
1	C	22	ILE	2.6
1	C	660	ASP	2.6
1	A	542	GLY	2.6
1	B	159	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	365	LEU	2.5
1	A	420	SER	2.5
1	B	610	ASP	2.5
1	D	7	ILE	2.5
1	A	660	ASP	2.5
1	A	354	ALA	2.5
1	C	10	LEU	2.5
1	C	587	VAL	2.5
1	D	610	ASP	2.5
1	C	252	ASN	2.5
1	C	16	PRO	2.5
1	B	326	GLN	2.4
1	C	325	LYS	2.4
1	B	660	ASP	2.4
1	A	374	ALA	2.4
1	C	304	ASP	2.4
1	A	608	ASP	2.4
1	A	340	ARG	2.4
1	A	413	ALA	2.4
1	A	369	GLU	2.3
1	C	607	ALA	2.3
1	A	604	THR	2.3
1	D	578	GLY	2.3
1	A	429	HIS	2.3
1	B	583	GLU	2.3
1	C	612	LEU	2.3
1	D	8	SER	2.2
1	A	639	THR	2.2
1	C	19	TRP	2.2
1	C	609	ASN	2.2
1	D	580	GLN	2.2
1	B	659	GLY	2.2
1	A	612	LEU	2.2
1	C	336	ASP	2.1
1	C	163	GLY	2.1
1	C	13	PRO	2.1
1	B	359	ASP	2.1
1	C	344	GLU	2.1
1	B	304	ASP	2.1
1	C	15	HIS	2.1
1	D	9	ALA	2.1
1	A	375	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	325	LYS	2.1
1	D	660	ASP	2.1
1	B	290	ASP	2.1
1	A	355	GLN	2.1
1	B	12	ARG	2.1
1	A	559	ASP	2.0
1	A	404	GLY	2.0
1	B	607	ALA	2.0
1	C	334	GLU	2.0
1	B	373	LYS	2.0
1	A	326	GLN	2.0
1	D	543	SER	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 carbohydrates 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.

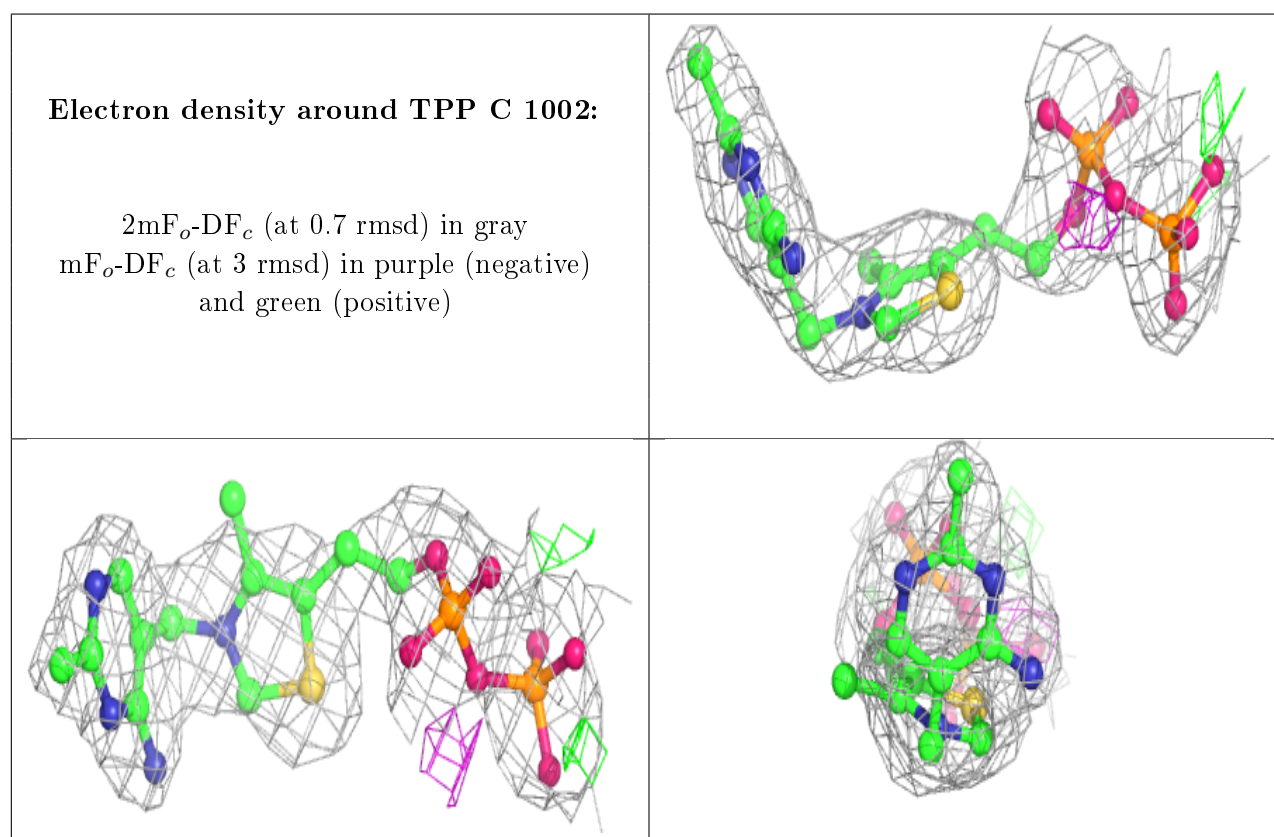
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	701	6/6	0.78	0.16	56,57,58,58	0
4	GOL	D	703	6/6	0.79	0.30	39,45,45,46	0
4	GOL	C	702	6/6	0.82	0.21	36,39,40,40	0
4	GOL	B	702	6/6	0.83	0.22	39,42,44,44	0
4	GOL	D	701	6/6	0.84	0.17	30,33,36,36	0
4	GOL	D	702	6/6	0.84	0.31	34,37,38,39	0
4	GOL	C	701	6/6	0.87	0.18	43,44,45,45	0
2	MG	C	1001	1/1	0.90	0.06	22,22,22,22	0
4	GOL	D	704	6/6	0.91	0.21	36,39,40,42	0
2	MG	D	1001	1/1	0.94	0.10	7,7,7,7	0
3	TPP	C	1002	26/26	0.95	0.13	23,31,34,36	0

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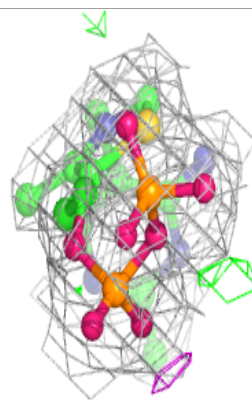
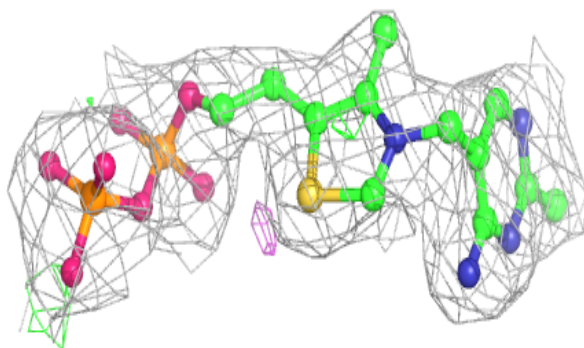
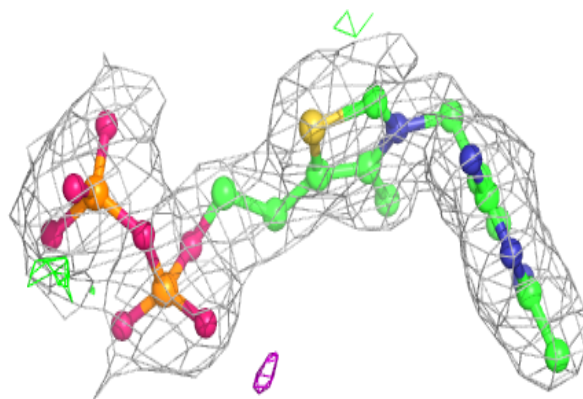
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	TPP	A	1002	26/26	0.96	0.12	13,18,25,26	0
3	TPP	B	1002	26/26	0.97	0.10	11,19,26,29	0
2	MG	A	1001	1/1	0.97	0.09	9,9,9,9	0
2	MG	B	1001	1/1	0.98	0.10	2,2,2,2	0
3	TPP	D	1002	26/26	0.98	0.10	5,21,25,27	0

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.

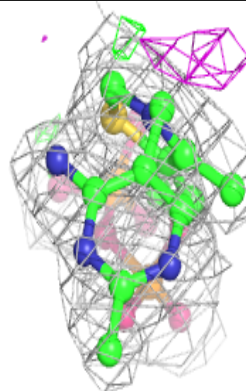
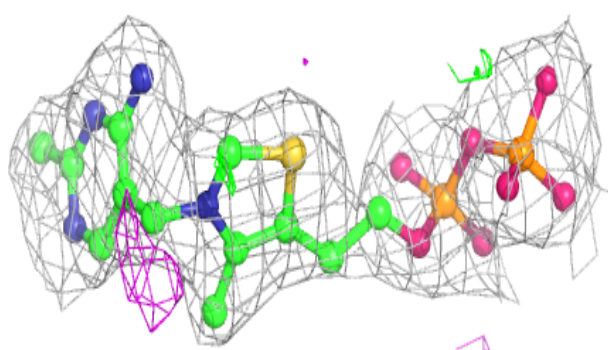
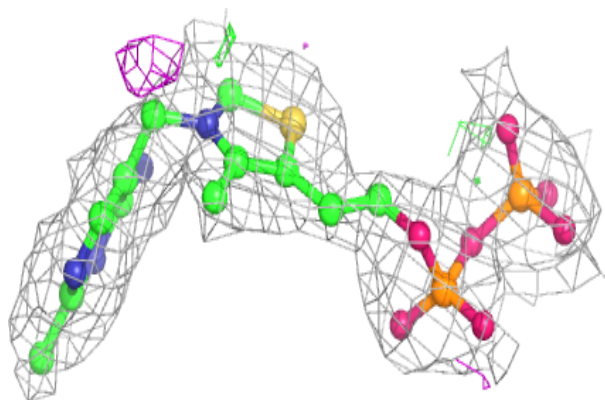


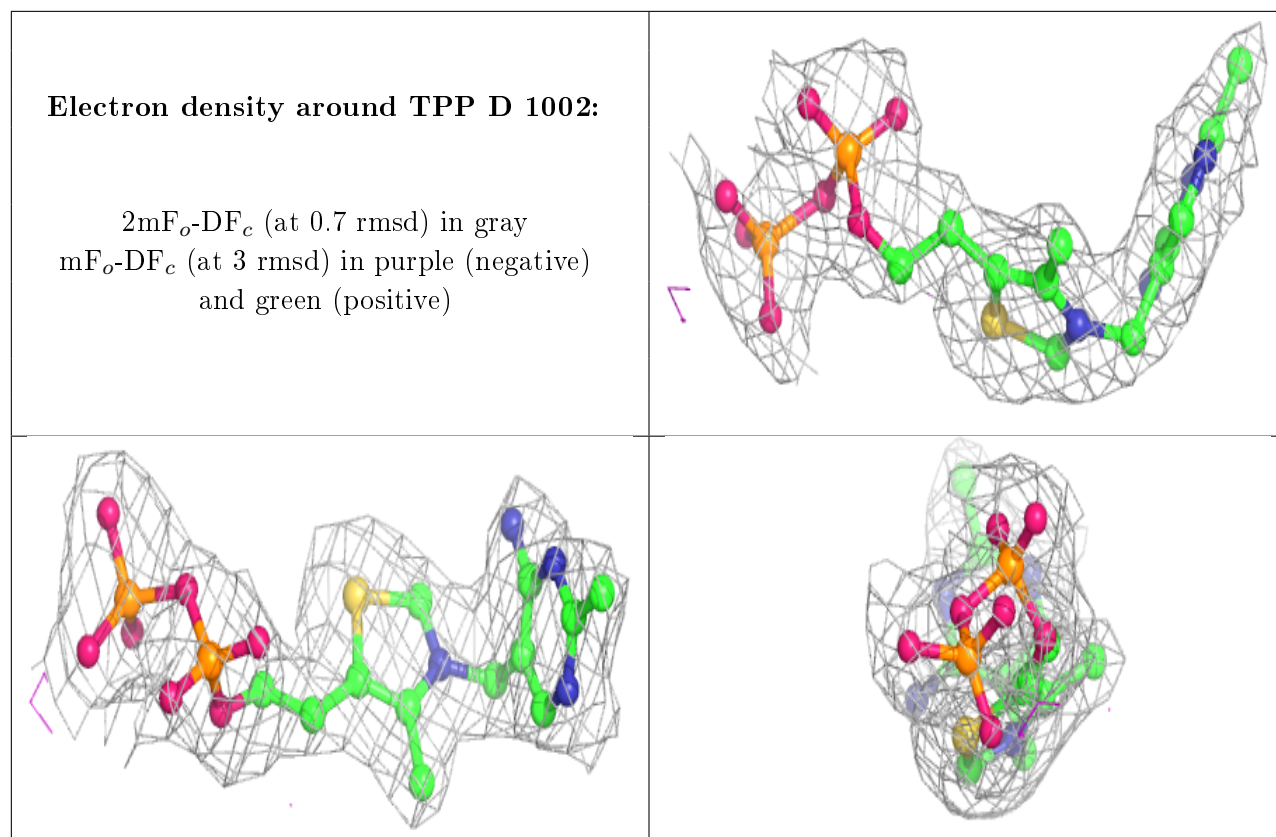
Electron density around TPP A 1002:

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

**Electron density around TPP B 1002:**

$2mF_o-DF_c$ (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.