



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:44 PM GMT

PDB ID : 1QFG
Title : E. COLI FERRIC HYDROXAMATE RECEPTOR (FHUA)
Authors : Ferguson, A.D.; Welte, W.; Hofmann, E.; Lindner, B.; Holst, O.; Coulton, J.W.; Diederichs, K.
Deposited on : 1999-04-10
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

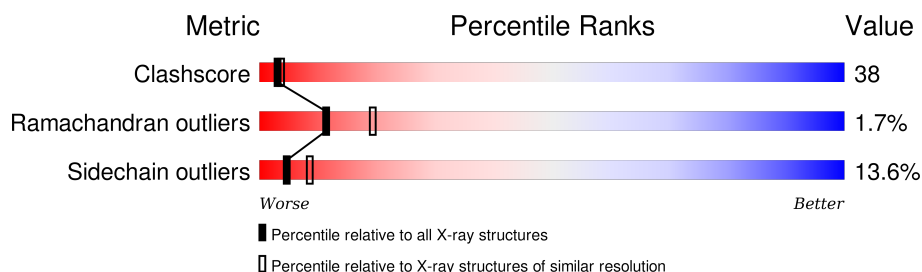
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	725	 46% 40% 9% ..

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
10	GOL	A	1105	-	-	X	-
10	GOL	A	1107	-	-	X	-
5	FTT	A	1013	-	-	X	-
7	MYR	A	1014	-	-	X	-
9	DPO	A	2000	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	DPO	A	2004	-	X	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 6077 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 PROTEIN (FERRIC HYDROXAMATE UPTAKE RECEPTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	707	Total	C	N	O	S	0	0	0
			5524	3475	944	1091	14			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	INTRACHAIN HIS TAG	UNP P06971
A	407	SER	-	INTRACHAIN HIS TAG	UNP P06971
A	408	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	409	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	410	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	411	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	412	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	413	HIS	-	INTRACHAIN HIS TAG	UNP P06971
A	414	GLY	-	INTRACHAIN HIS TAG	UNP P06971
A	415	SER	-	INTRACHAIN HIS TAG	UNP P06971
A	416	SER	-	INTRACHAIN HIS TAG	UNP P06971

- Molecule 2 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	9	Total	C	N	O	0	0
			110	60	2	48		

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

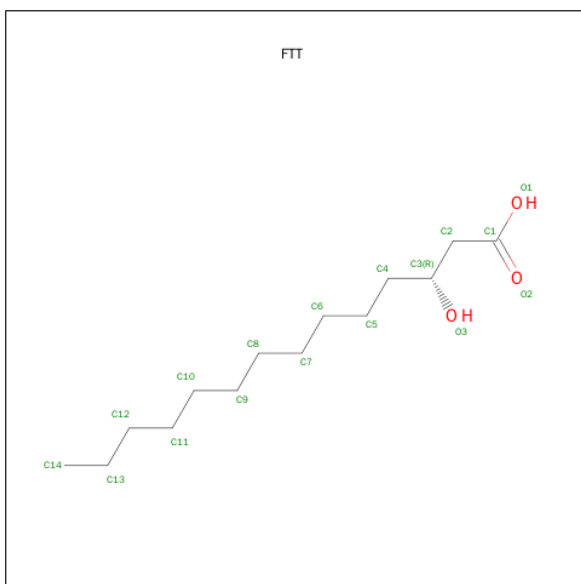
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			4	3	1		
4	A	1	Total	O	P	0	0
			4	3	1		

- Molecule 5 is 3-HYDROXY-TETRADECANOIC ACID (three-letter code: FTT) (formula: $C_{14}H_{28}O_3$).



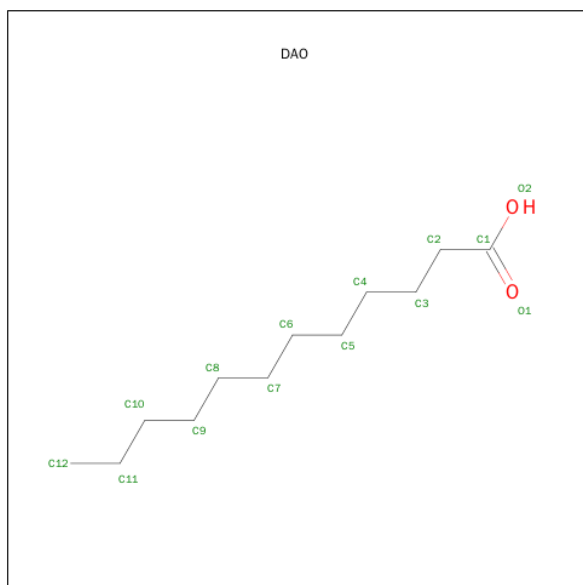
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	14	2		

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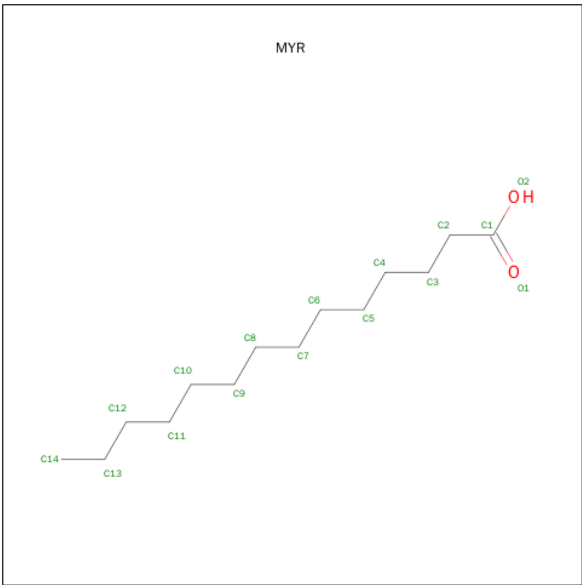
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			16	14	2		
5	A	1	Total	C	O	0	0
			17	14	3		

- Molecule 6 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).



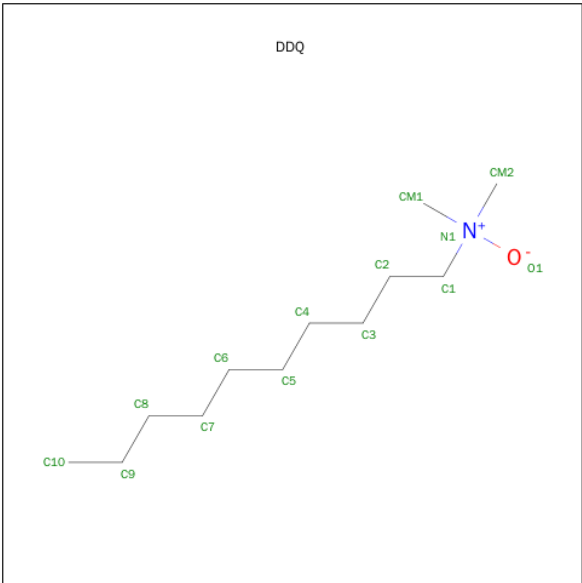
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	12	1		

- Molecule 7 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			15	14	1		

- Molecule 8 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula: C₁₂H₂₇NO).



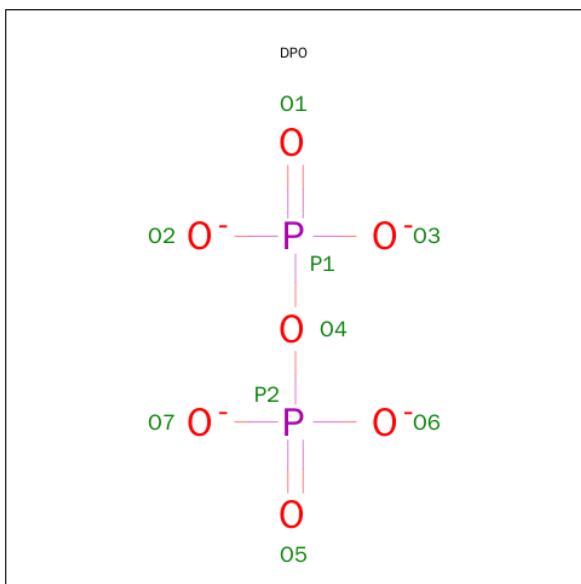
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	12	1	1		
8	A	1	Total	C	N	O	0	0
			14	12	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	12	1	1		

- Molecule 9 is DIPHOSPHATE (three-letter code: DPO) (formula: O_7P_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	P	0	0
			8	6	2		
9	A	1	Total	O	P	0	0
			8	6	2		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is water.

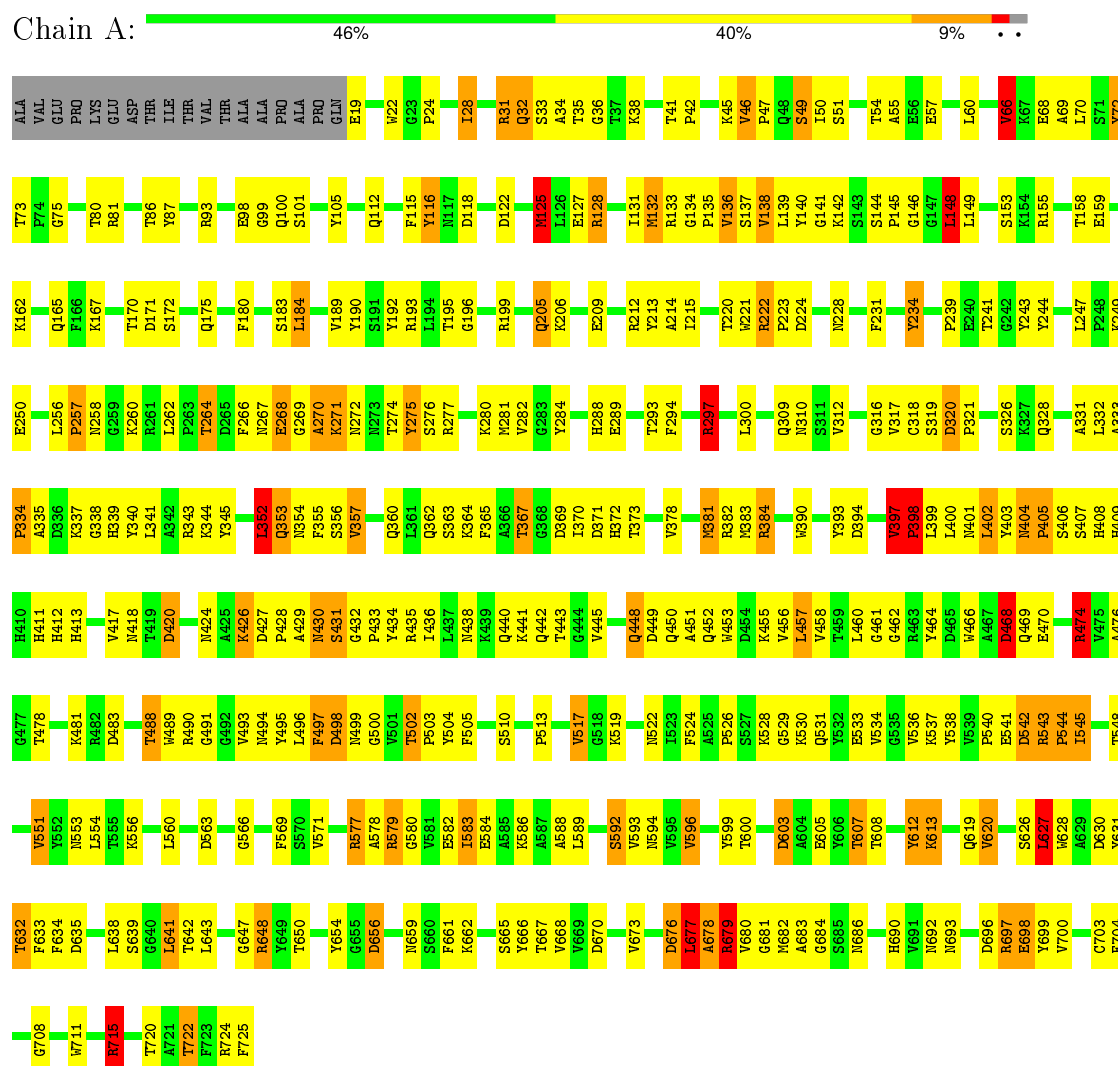
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	244	Total	O	0	0
			244	244		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: PROTEIN (FERRIC HYDROXAMATE UPTAKE RECEPTOR)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	171.55Å 171.55Å 87.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.30 – 2.50	Depositor
% Data completeness (in resolution range)	99.5 (42.30-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6077	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, DAO, FTT, NI, GLA, PO4, MYR, PA1, GCN, DPO, KDO, GLC, GMH, DDQ

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	1.21	9/5664 (0.2%)	1.28	31/7696 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	698	GLU	CG-CD	9.99	1.67	1.51
1	A	66	VAL	CB-CG2	-9.46	1.32	1.52
1	A	277	ARG	CZ-NH1	6.67	1.41	1.33
1	A	397	VAL	CA-CB	6.63	1.68	1.54
1	A	275	TYR	CE2-CZ	-6.09	1.30	1.38
1	A	698	GLU	CB-CG	6.08	1.63	1.52
1	A	698	GLU	CD-OE1	5.76	1.31	1.25
1	A	488	THR	CA-CB	5.69	1.68	1.53
1	A	697	ARG	CB-CG	-5.04	1.39	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	648	ARG	NE-CZ-NH1	-11.18	114.71	120.30
1	A	352	LEU	CA-CB-CG	9.23	136.52	115.30
1	A	125	MET	CG-SD-CE	-9.06	85.71	100.20
1	A	577	ARG	NE-CZ-NH1	-8.49	116.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	474	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	A	212	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	277	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	193	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	A	332	LEU	CA-CB-CG	6.96	131.32	115.30
1	A	297	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	656	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	145	PRO	C-N-CA	-6.31	109.06	122.30
1	A	199	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	A	400	LEU	CA-CB-CG	6.10	129.32	115.30
1	A	320	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	394	ASP	C-N-CA	-6.01	106.67	121.70
1	A	715	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	384	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	193	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	A	122	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	46	VAL	C-N-CD	-5.82	107.79	120.60
1	A	297	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	468	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	A	450	GLN	N-CA-C	-5.52	96.09	111.00
1	A	497	PHE	CB-CA-C	-5.52	99.36	110.40
1	A	566	GLY	N-CA-C	5.44	126.71	113.10
1	A	488	THR	N-CA-C	-5.40	96.43	111.00
1	A	627	LEU	CA-CB-CG	-5.40	102.89	115.30
1	A	715	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	563	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	148	LEU	CA-CB-CG	5.13	127.11	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	TYR	Sidechain
1	A	213	TYR	Sidechain
1	A	234	TYR	Sidechain
1	A	599	TYR	Sidechain
1	A	612	TYR	Sidechain
1	A	699	TYR	Sidechain
1	A	72	TYR	Sidechain

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	5524	0	5223	404	0
2	A	110	0	84	3	0
3	A	1	0	0	0	0
4	A	8	0	0	0	0
5	A	56	0	83	18	0
6	A	13	0	23	3	0
7	A	15	0	27	9	0
8	A	42	0	81	5	0
9	A	16	0	0	5	0
10	A	48	0	39	18	0
11	A	244	0	0	40	0
All	All	6077	0	5560	437	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 38.

All (437) 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)
10:A:1109:GOL:O1	10:A:1109:GOL:C1	1.64	1.44
10:A:1103:GOL:C1	10:A:1103:GOL:O1	1.65	1.44
10:A:1105:GOL:O1	10:A:1105:GOL:C1	1.66	1.43
10:A:1104:GOL:O1	10:A:1104:GOL:C1	1.65	1.42
10:A:1107:GOL:C1	10:A:1107:GOL:O1	1.65	1.41
10:A:1110:GOL:C1	10:A:1110:GOL:O1	1.68	1.40
1:A:648:ARG:HD2	11:A:2145:HOH:O	1.51	1.09
1:A:643:LEU:HD23	1:A:673:VAL:HG12	1.41	1.03
1:A:586:LYS:HG2	1:A:596:VAL:CG2	1.88	1.03
1:A:628:TRP:CH2	1:A:630:ASP:HB3	1.94	1.02
1:A:367:THR:HG22	1:A:370:ILE:HB	1.41	1.02
1:A:328:GLN:HB3	1:A:399:LEU:HD11	1.41	1.01
1:A:715:ARG:HH11	1:A:715:ARG:HG2	1.29	0.96
1:A:70:LEU:HD13	1:A:131:ILE:HD11	1.48	0.96
1:A:19:GLU:HG2	1:A:634:PHE:CZ	2.01	0.95
1:A:370:ILE:HG22	1:A:372:HIS:NE2	1.84	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:THR:OG1	1:A:57:GLU:HG3	1.68	0.92
1:A:722:THR:HG21	11:A:2114:HOH:O	1.68	0.92
1:A:274:THR:HG22	1:A:310:ASN:HB2	1.52	0.92
1:A:586:LYS:HG2	1:A:596:VAL:HG22	1.54	0.89
1:A:260:LYS:HB2	1:A:406:SER:OG	1.73	0.88
1:A:32:GLN:O	1:A:128:ARG:NH2	2.07	0.87
1:A:390:TRP:NE1	1:A:431:SER:OG	2.06	0.87
1:A:353:GLN:HG3	11:A:2030:HOH:O	1.75	0.87
1:A:93:ARG:HD2	1:A:582:GLU:OE2	1.75	0.86
1:A:430:ASN:HD22	1:A:430:ASN:C	1.78	0.85
1:A:300:LEU:HD12	1:A:357:VAL:HG13	1.56	0.85
1:A:42:PRO:HG3	10:A:1105:GOL:H12	1.58	0.84
1:A:241:THR:HG22	11:A:2016:HOH:O	1.78	0.84
1:A:500:GLY:O	1:A:538:TYR:HD1	1.59	0.83
1:A:589:LEU:HB2	1:A:593:VAL:HG12	1.62	0.81
1:A:538:TYR:CE2	1:A:545:ILE:HD11	2.16	0.80
1:A:381:MET:HG2	11:A:2097:HOH:O	1.79	0.80
1:A:162:LYS:HA	1:A:180:PHE:HD1	1.45	0.80
5:A:1013:FTT:H122	7:A:1014:MYR:H92	1.63	0.80
1:A:540:PRO:HG3	1:A:545:ILE:CD1	2.11	0.79
1:A:370:ILE:HG12	1:A:453:TRP:HB2	1.65	0.78
1:A:577:ARG:HD2	1:A:579:ARG:HG2	1.64	0.78
1:A:678:ALA:HA	1:A:683:ALA:HA	1.65	0.77
1:A:132:MET:HG2	1:A:136:VAL:HG11	1.66	0.77
1:A:494:ASN:ND2	1:A:504:TYR:HB3	1.99	0.77
1:A:99:GLY:O	1:A:100:GLN:HB2	1.84	0.77
1:A:381:MET:HE2	1:A:382:ARG:N	2.00	0.77
1:A:522:ASN:ND2	11:A:2085:HOH:O	2.18	0.76
1:A:540:PRO:HG3	1:A:545:ILE:HD11	1.68	0.76
1:A:86:THR:HG23	1:A:241:THR:HG21	1.68	0.76
1:A:365:PHE:HE1	1:A:372:HIS:HD1	1.34	0.75
1:A:390:TRP:CZ3	1:A:433:PRO:HG3	2.21	0.75
1:A:282:VAL:HG21	5:A:1013:FTT:H81	1.67	0.75
1:A:352:LEU:HB2	1:A:384:ARG:O	1.85	0.75
1:A:435:ARG:NH1	1:A:474:ARG:HD3	2.02	0.75
1:A:488:THR:HG23	11:A:2124:HOH:O	1.86	0.74
5:A:1013:FTT:H41	7:A:1014:MYR:H22	1.69	0.74
1:A:70:LEU:HD22	1:A:131:ILE:HG13	1.70	0.74
1:A:162:LYS:HA	1:A:180:PHE:CD1	2.22	0.73
1:A:390:TRP:CZ2	1:A:426:LYS:HB2	2.24	0.73
1:A:540:PRO:CG	1:A:545:ILE:HG12	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ASN:OD1	1:A:403:TYR:HB2	1.89	0.73
1:A:457:LEU:HD12	1:A:458:VAL:N	2.05	0.72
1:A:594:ASN:HB2	1:A:630:ASP:OD1	1.89	0.72
1:A:271:LYS:HG2	1:A:420:ASP:OD1	1.87	0.72
1:A:269:GLY:HA2	1:A:312:VAL:HG12	1.69	0.72
1:A:613:LYS:HD2	11:A:2066:HOH:O	1.89	0.72
1:A:51:SER:OG	1:A:133:ARG:NH2	2.23	0.72
1:A:451:ALA:HB3	1:A:458:VAL:HG12	1.71	0.72
1:A:497:PHE:HB3	1:A:499:ASN:OD1	1.90	0.72
5:A:1009:FTT:H101	6:A:1012:DAO:H62	1.72	0.72
1:A:586:LYS:HG2	1:A:596:VAL:HG23	1.72	0.71
1:A:676:ASP:O	1:A:678:ALA:N	2.25	0.70
1:A:367:THR:CG2	1:A:367:THR:O	2.40	0.70
1:A:474:ARG:HH11	1:A:474:ARG:HG2	1.55	0.70
5:A:1013:FTT:C4	7:A:1014:MYR:H22	2.22	0.69
1:A:650:THR:HB	1:A:666:TYR:CE1	2.27	0.69
1:A:159:GLU:N	1:A:159:GLU:OE1	2.18	0.69
1:A:633:PHE:HB3	1:A:638:LEU:O	1.92	0.69
1:A:28:ILE:HA	1:A:31:ARG:HG3	1.73	0.69
1:A:222:ARG:HH11	1:A:222:ARG:HG3	1.58	0.69
1:A:540:PRO:HG3	1:A:545:ILE:HG12	1.75	0.68
1:A:628:TRP:CZ2	11:A:2012:HOH:O	2.46	0.68
1:A:435:ARG:HH12	1:A:474:ARG:HD3	1.58	0.68
1:A:19:GLU:HG2	1:A:634:PHE:CE2	2.28	0.68
5:A:1013:FTT:H143	7:A:1014:MYR:H112	1.76	0.68
1:A:384:ARG:HG2	11:A:2234:HOH:O	1.93	0.68
1:A:343:ARG:O	1:A:397:VAL:HG13	1.93	0.68
1:A:316:GLY:O	1:A:341:LEU:HD12	1.94	0.68
1:A:370:ILE:CG2	1:A:372:HIS:NE2	2.58	0.67
1:A:189:VAL:HG23	1:A:223:PRO:HA	1.76	0.67
1:A:60:LEU:HD21	1:A:628:TRP:HH2	1.57	0.67
1:A:38:LYS:HG3	1:A:139:LEU:HD22	1.76	0.67
1:A:540:PRO:HG3	1:A:545:ILE:CG1	2.24	0.67
1:A:353:GLN:CG	11:A:2030:HOH:O	2.38	0.67
1:A:496:LEU:HD13	1:A:502:THR:HG23	1.76	0.67
1:A:367:THR:HG22	1:A:367:THR:O	1.94	0.66
1:A:633:PHE:HD2	1:A:641:LEU:HD23	1.59	0.66
1:A:496:LEU:HD13	1:A:502:THR:CG2	2.25	0.66
1:A:24:PRO:O	1:A:28:ILE:HG12	1.96	0.66
1:A:146:GLY:N	11:A:2164:HOH:O	2.04	0.66
9:A:2004:DPO:O3	11:A:2022:HOH:O	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLN:HG3	1:A:243:TYR:HB2	1.78	0.66
1:A:205:GLN:HG3	1:A:243:TYR:CB	2.26	0.66
1:A:50:ILE:HD12	1:A:132:MET:HE3	1.77	0.66
1:A:99:GLY:O	1:A:100:GLN:CB	2.43	0.65
1:A:222:ARG:HG3	1:A:222:ARG:NH1	2.09	0.65
1:A:686:ASN:ND2	11:A:2010:HOH:O	2.28	0.65
1:A:715:ARG:NH1	1:A:715:ARG:HG2	2.04	0.64
1:A:370:ILE:HG22	1:A:372:HIS:CD2	2.33	0.64
1:A:500:GLY:O	1:A:538:TYR:CD1	2.46	0.64
1:A:46:VAL:O	1:A:537:LYS:NZ	2.29	0.64
1:A:264:THR:HA	1:A:711:TRP:CD1	2.32	0.64
1:A:378:VAL:HG12	1:A:445:VAL:HG12	1.79	0.63
1:A:643:LEU:CD2	1:A:673:VAL:HG12	2.21	0.63
1:A:28:ILE:O	1:A:31:ARG:HG3	1.98	0.63
1:A:189:VAL:HG23	1:A:222:ARG:O	1.98	0.63
1:A:148:LEU:HD23	1:A:148:LEU:C	2.20	0.63
1:A:205:GLN:HG3	1:A:243:TYR:CG	2.34	0.62
1:A:60:LEU:HD21	1:A:628:TRP:CH2	2.34	0.62
1:A:132:MET:CG	1:A:136:VAL:HG11	2.30	0.62
1:A:648:ARG:HG3	1:A:648:ARG:HH11	1.65	0.62
1:A:628:TRP:NE1	11:A:2012:HOH:O	2.32	0.61
1:A:328:GLN:CB	1:A:399:LEU:HD11	2.23	0.61
1:A:632:THR:HG23	1:A:642:THR:OG1	2.01	0.61
10:A:1103:GOL:C1	10:A:1103:GOL:HO1	2.08	0.61
1:A:241:THR:CG2	11:A:2016:HOH:O	2.44	0.61
1:A:142:LYS:HG2	1:A:442:GLN:OE1	2.00	0.61
1:A:679:ARG:NH1	1:A:679:ARG:HB3	2.16	0.60
1:A:155:ARG:HG3	1:A:155:ARG:HH11	1.65	0.60
10:A:1107:GOL:HO1	10:A:1107:GOL:C1	2.09	0.60
1:A:189:VAL:CG2	1:A:223:PRO:HA	2.32	0.60
1:A:171:ASP:O	1:A:172:SER:HB2	2.02	0.60
1:A:33:SER:OG	1:A:34:ALA:N	2.35	0.60
1:A:256:LEU:HD11	1:A:402:LEU:HB3	1.82	0.60
1:A:579:ARG:NH1	1:A:603:ASP:OD2	2.34	0.59
1:A:165:GLN:HG3	1:A:722:THR:HB	1.84	0.59
1:A:589:LEU:HB2	1:A:593:VAL:CG1	2.32	0.59
1:A:631:TYR:HE2	1:A:633:PHE:CE1	2.20	0.59
10:A:1109:GOL:HO1	10:A:1109:GOL:C1	2.08	0.59
1:A:293:THR:O	1:A:363:SER:HA	2.02	0.59
1:A:317:VAL:HA	1:A:340:TYR:O	2.03	0.59
1:A:22:TRP:HD1	11:A:2102:HOH:O	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:THR:HG22	1:A:608:THR:N	2.18	0.58
10:A:1105:GOL:C1	10:A:1105:GOL:HO1	2.10	0.58
1:A:538:TYR:CZ	1:A:545:ILE:HD11	2.39	0.58
1:A:579:ARG:HG3	1:A:603:ASP:OD2	2.04	0.58
1:A:260:LYS:NZ	11:A:2165:HOH:O	2.35	0.58
1:A:73:THR:HG22	11:A:2024:HOH:O	2.02	0.58
1:A:442:GLN:HA	1:A:466:TRP:O	2.04	0.58
1:A:192:TYR:CD1	1:A:192:TYR:C	2.77	0.58
1:A:722:THR:CG2	11:A:2010:HOH:O	2.51	0.57
1:A:294:PHE:HE1	1:A:363:SER:HG	1.52	0.57
1:A:54:THR:HG1	1:A:57:GLU:HG3	1.68	0.57
1:A:679:ARG:CB	1:A:679:ARG:HH11	2.17	0.57
1:A:593:VAL:HG23	1:A:631:TYR:CD1	2.40	0.57
1:A:448:GLN:HG2	1:A:449:ASP:N	2.18	0.57
1:A:167:LYS:HG3	1:A:720:THR:HG23	1.87	0.57
1:A:19:GLU:CG	1:A:634:PHE:CE2	2.88	0.57
1:A:650:THR:HB	1:A:666:TYR:CD1	2.38	0.57
1:A:458:VAL:O	1:A:458:VAL:CG1	2.52	0.56
1:A:260:LYS:CB	1:A:406:SER:OG	2.48	0.56
1:A:430:ASN:ND2	1:A:430:ASN:C	2.51	0.56
1:A:300:LEU:HB2	1:A:357:VAL:HG13	1.86	0.56
1:A:49:SER:HB2	11:A:2008:HOH:O	2.04	0.56
1:A:654:TYR:CE2	1:A:662:LYS:HD2	2.41	0.56
1:A:430:ASN:ND2	1:A:431:SER:HB3	2.20	0.56
1:A:593:VAL:HG12	1:A:593:VAL:O	2.05	0.56
1:A:628:TRP:HZ2	11:A:2012:HOH:O	1.87	0.56
1:A:541:GLU:CD	1:A:541:GLU:O	2.44	0.56
1:A:441:LYS:NZ	9:A:2000:DPO:O5	2.37	0.56
1:A:355:PHE:CZ	1:A:357:VAL:HG22	2.41	0.55
1:A:38:LYS:HD3	1:A:360:GLN:HE22	1.70	0.55
1:A:153:SER:O	1:A:155:ARG:HD3	2.05	0.55
1:A:670:ASP:OD1	1:A:692:ASN:HA	2.07	0.55
1:A:503:PRO:HA	1:A:536:VAL:HG12	1.88	0.55
10:A:1104:GOL:C1	10:A:1104:GOL:HO1	2.08	0.55
1:A:681:GLY:O	1:A:683:ALA:N	2.40	0.55
1:A:531:GLN:HB2	1:A:554:LEU:HD13	1.89	0.54
1:A:650:THR:CB	1:A:666:TYR:CE1	2.89	0.54
1:A:548:THR:HG22	1:A:584:GLU:HB3	1.89	0.54
1:A:693:ASN:O	1:A:715:ARG:HB2	2.08	0.54
1:A:612:TYR:O	1:A:613:LYS:C	2.45	0.54
1:A:441:LYS:HZ1	9:A:2000:DPO:P2	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:THR:CG2	1:A:46:VAL:HG23	2.38	0.53
1:A:93:ARG:HH11	1:A:582:GLU:CD	2.11	0.53
1:A:24:PRO:HG3	1:A:588:ALA:HB2	1.91	0.53
1:A:593:VAL:CG2	1:A:631:TYR:HD1	2.22	0.53
1:A:93:ARG:NH2	1:A:533:GLU:OE1	2.22	0.53
1:A:137:SER:OG	1:A:510:SER:HA	2.09	0.53
2:A:1002:KDO:H7	2:A:1004:GMH:C1	2.38	0.53
1:A:449:ASP:OD2	1:A:451:ALA:HB2	2.08	0.53
1:A:679:ARG:CB	1:A:679:ARG:NH1	2.72	0.53
1:A:495:TYR:O	1:A:503:PRO:HD2	2.07	0.53
1:A:247:LEU:HD21	1:A:268:GLU:HG3	1.91	0.53
1:A:458:VAL:O	1:A:458:VAL:HG13	2.08	0.53
1:A:402:LEU:O	1:A:406:SER:HB2	2.09	0.53
1:A:470:GLU:HG3	1:A:481:LYS:HG2	1.91	0.53
1:A:142:LYS:NZ	1:A:440:GLN:OE1	2.43	0.52
1:A:318:CYS:HB2	1:A:337:LYS:O	2.09	0.52
1:A:639:SER:HB3	1:A:679:ARG:HE	1.72	0.52
1:A:668:VAL:HG13	1:A:693:ASN:HA	1.90	0.52
1:A:404:ASN:HB3	1:A:405:PRO:HD3	1.90	0.52
1:A:648:ARG:CG	1:A:648:ARG:HH11	2.22	0.52
1:A:381:MET:HE1	1:A:383:MET:N	2.24	0.52
1:A:542:ASP:OD2	1:A:543:ARG:HG3	2.10	0.52
10:A:1110:GOL:HO1	10:A:1110:GOL:C1	2.11	0.51
1:A:390:TRP:CE3	1:A:426:LYS:NZ	2.79	0.51
1:A:50:ILE:HB	1:A:132:MET:CE	2.41	0.51
1:A:135:PRO:HA	11:A:2040:HOH:O	2.10	0.51
1:A:35:THR:O	1:A:140:TYR:OH	2.19	0.51
1:A:367:THR:HG22	1:A:370:ILE:CB	2.30	0.51
1:A:132:MET:SD	1:A:136:VAL:HG11	2.50	0.51
1:A:381:MET:HE2	1:A:381:MET:C	2.31	0.51
1:A:184:LEU:N	1:A:184:LEU:HD23	2.24	0.51
1:A:577:ARG:CG	1:A:578:ALA:N	2.72	0.51
1:A:620:VAL:HG22	1:A:620:VAL:O	2.09	0.51
1:A:586:LYS:HE3	11:A:2069:HOH:O	2.10	0.51
1:A:80:THR:CG2	1:A:619:GLN:NE2	2.74	0.51
1:A:284:TYR:CE2	1:A:300:LEU:HD22	2.45	0.51
1:A:538:TYR:CE2	1:A:545:ILE:CD1	2.89	0.51
1:A:148:LEU:HD23	1:A:149:LEU:N	2.26	0.51
5:A:1013:FTT:H91	7:A:1014:MYR:H81	1.93	0.50
1:A:722:THR:HG23	11:A:2010:HOH:O	2.12	0.50
1:A:115:PHE:H	10:A:1110:GOL:C3	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LEU:O	1:A:257:PRO:C	2.48	0.50
1:A:135:PRO:HB3	1:A:510:SER:HB3	1.94	0.50
1:A:628:TRP:CE2	11:A:2012:HOH:O	2.62	0.50
1:A:469:GLN:HG2	11:A:2051:HOH:O	2.12	0.50
1:A:367:THR:HB	1:A:372:HIS:CE1	2.47	0.50
1:A:684:GLY:O	1:A:724:ARG:HG3	2.11	0.50
2:A:1000:PA1:O1	9:A:2000:DPO:O6	2.29	0.50
1:A:320:ASP:OD1	1:A:321:PRO:HD2	2.11	0.50
1:A:73:THR:CG2	11:A:2024:HOH:O	2.60	0.50
1:A:133:ARG:NH1	11:A:2056:HOH:O	2.45	0.49
1:A:68:GLU:OE1	1:A:68:GLU:N	2.35	0.49
1:A:519:LYS:HG3	1:A:569:PHE:CD2	2.47	0.49
1:A:648:ARG:NH1	1:A:648:ARG:HG3	2.27	0.49
1:A:260:LYS:HB2	1:A:406:SER:HG	1.73	0.49
1:A:435:ARG:HH12	1:A:474:ARG:HB3	1.78	0.49
1:A:365:PHE:CE1	1:A:372:HIS:ND1	2.77	0.49
1:A:633:PHE:CB	1:A:638:LEU:O	2.58	0.49
1:A:577:ARG:HG2	1:A:578:ALA:N	2.21	0.49
5:A:1009:FTT:C10	6:A:1012:DAO:H62	2.41	0.49
1:A:93:ARG:NH1	1:A:582:GLU:OE1	2.46	0.49
1:A:50:ILE:HD12	1:A:132:MET:CE	2.43	0.49
1:A:45:LYS:HD3	1:A:457:LEU:CD2	2.43	0.49
1:A:86:THR:HG22	1:A:87:TYR:CE2	2.48	0.49
1:A:31:ARG:NH2	1:A:540:PRO:O	2.45	0.49
1:A:60:LEU:O	1:A:690:HIS:HE1	1.96	0.49
1:A:412:HIS:CD2	1:A:413:HIS:NE2	2.81	0.49
1:A:365:PHE:HE1	1:A:372:HIS:ND1	2.06	0.48
1:A:28:ILE:HG22	1:A:31:ARG:NH1	2.28	0.48
1:A:264:THR:CG2	1:A:698:GLU:HG2	2.43	0.48
1:A:138:VAL:HG23	1:A:489:TRP:HA	1.94	0.48
1:A:493:VAL:HG23	1:A:505:PHE:CZ	2.48	0.48
1:A:704:PHE:CE2	1:A:708:GLY:HA3	2.48	0.48
1:A:676:ASP:O	1:A:677:LEU:C	2.51	0.48
1:A:538:TYR:CD1	1:A:540:PRO:HD3	2.48	0.48
1:A:697:ARG:NH2	11:A:2070:HOH:O	2.46	0.48
1:A:344:LYS:O	1:A:345:TYR:HB3	2.13	0.48
1:A:70:LEU:HD22	1:A:131:ILE:CG1	2.43	0.48
1:A:650:THR:HG1	1:A:666:TYR:HE1	1.57	0.48
2:A:1000:PA1:N2	9:A:2000:DPO:O6	2.43	0.48
1:A:297:ARG:NH2	1:A:362:GLN:OE1	2.41	0.48
1:A:679:ARG:HH11	1:A:679:ARG:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLN:H	1:A:205:GLN:HG2	1.31	0.48
1:A:541:GLU:OE2	1:A:541:GLU:O	2.31	0.48
1:A:424:ASN:O	1:A:426:LYS:HG2	2.14	0.48
1:A:381:MET:CE	1:A:382:ARG:C	2.82	0.48
1:A:677:LEU:O	1:A:678:ALA:C	2.53	0.48
1:A:220:THR:HG22	1:A:221:TRP:N	2.26	0.48
1:A:409:HIS:O	1:A:413:HIS:N	2.36	0.48
1:A:412:HIS:CD2	1:A:413:HIS:CD2	3.02	0.48
1:A:457:LEU:C	1:A:457:LEU:HD12	2.34	0.47
1:A:159:GLU:H	1:A:159:GLU:CD	2.12	0.47
1:A:494:ASN:ND2	1:A:504:TYR:CB	2.73	0.47
1:A:72:TYR:CE2	1:A:628:TRP:HB2	2.50	0.47
1:A:596:VAL:HG12	1:A:628:TRP:HB3	1.96	0.47
1:A:627:LEU:HG	1:A:628:TRP:N	2.29	0.47
1:A:288:HIS:CD2	1:A:288:HIS:C	2.88	0.47
1:A:548:THR:HG23	11:A:2111:HOH:O	2.15	0.47
1:A:215:ILE:O	1:A:215:ILE:HG23	2.14	0.47
1:A:19:GLU:CG	1:A:634:PHE:CZ	2.86	0.47
1:A:271:LYS:HB2	1:A:417:VAL:CG2	2.45	0.47
1:A:220:THR:CG2	1:A:221:TRP:N	2.77	0.47
1:A:224:ASP:C	1:A:224:ASP:OD1	2.52	0.47
1:A:544:PRO:HG2	1:A:588:ALA:HB3	1.97	0.47
1:A:288:HIS:HD2	1:A:289:GLU:N	2.12	0.47
1:A:42:PRO:CG	10:A:1105:GOL:H12	2.38	0.47
1:A:300:LEU:HD12	1:A:357:VAL:CG1	2.37	0.47
1:A:397:VAL:O	1:A:398:PRO:O	2.33	0.47
1:A:435:ARG:NH1	1:A:474:ARG:CB	2.77	0.46
1:A:46:VAL:HA	1:A:47:PRO:HD2	1.27	0.46
1:A:267:ASN:O	1:A:418:ASN:ND2	2.49	0.46
1:A:631:TYR:HE2	1:A:633:PHE:CD1	2.33	0.46
1:A:427:ASP:HA	1:A:428:PRO:HD3	1.61	0.46
1:A:137:SER:O	1:A:138:VAL:C	2.51	0.46
1:A:36:GLY:HA2	1:A:132:MET:SD	2.56	0.46
1:A:538:TYR:CE1	1:A:540:PRO:HD3	2.51	0.45
1:A:650:THR:O	1:A:665:SER:HA	2.16	0.45
1:A:189:VAL:HG23	1:A:223:PRO:CA	2.46	0.45
1:A:528:LYS:O	1:A:556:LYS:HA	2.15	0.45
1:A:628:TRP:CZ3	1:A:630:ASP:HB3	2.48	0.45
1:A:328:GLN:HB2	1:A:328:GLN:HE21	1.59	0.45
1:A:677:LEU:HA	1:A:677:LEU:HD12	1.58	0.45
1:A:258:ASN:OD1	1:A:258:ASN:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:THR:HG21	1:A:46:VAL:HG23	1.98	0.45
1:A:125:MET:HE2	1:A:234:TYR:HE1	1.81	0.45
1:A:586:LYS:CG	1:A:596:VAL:HG23	2.42	0.45
1:A:633:PHE:O	1:A:639:SER:HA	2.16	0.45
1:A:294:PHE:HE1	1:A:363:SER:OG	1.98	0.45
1:A:390:TRP:CH2	1:A:433:PRO:HG3	2.52	0.45
1:A:648:ARG:NH1	1:A:648:ARG:CG	2.78	0.45
5:A:1013:FTT:C5	7:A:1014:MYR:H22	2.46	0.45
1:A:239:PRO:O	1:A:276:SER:HB3	2.17	0.45
1:A:228:ASN:OD1	1:A:228:ASN:C	2.55	0.45
1:A:656:ASP:OD1	1:A:659:ASN:N	2.49	0.45
1:A:155:ARG:NH1	1:A:155:ARG:HG3	2.32	0.45
1:A:28:ILE:HA	1:A:31:ARG:CG	2.44	0.45
1:A:404:ASN:HB2	11:A:2037:HOH:O	2.17	0.44
1:A:551:VAL:HA	1:A:580:GLY:O	2.17	0.44
1:A:430:ASN:HD22	1:A:431:SER:HB3	1.83	0.44
1:A:300:LEU:CD1	1:A:357:VAL:HG13	2.39	0.44
1:A:241:THR:O	1:A:241:THR:CG2	2.66	0.44
5:A:1009:FTT:H122	8:A:1100:DDQ:H92	1.99	0.44
1:A:495:TYR:O	1:A:503:PRO:CD	2.65	0.44
1:A:372:HIS:HB3	1:A:449:ASP:OD1	2.17	0.44
1:A:693:ASN:O	1:A:715:ARG:HD3	2.17	0.44
1:A:700:VAL:HG23	1:A:711:TRP:CZ3	2.53	0.44
1:A:528:LYS:NZ	11:A:2215:HOH:O	2.51	0.44
1:A:75:GLY:HA2	1:A:600:THR:HG21	1.98	0.44
1:A:137:SER:CB	1:A:510:SER:HA	2.48	0.44
1:A:583:ILE:HD11	11:A:2174:HOH:O	2.17	0.44
1:A:524:PHE:CD2	1:A:560:LEU:HD11	2.53	0.44
1:A:55:ALA:HB2	1:A:127:GLU:O	2.18	0.44
1:A:249:LYS:HD2	1:A:661:PHE:CE2	2.52	0.44
1:A:462:GLY:HA2	1:A:489:TRP:HA	1.99	0.44
1:A:80:THR:HG23	1:A:619:GLN:NE2	2.32	0.44
1:A:626:SER:HA	1:A:647:GLY:O	2.17	0.44
1:A:639:SER:O	1:A:679:ARG:CD	2.66	0.44
1:A:264:THR:HG21	1:A:698:GLU:HG2	2.00	0.44
1:A:424:ASN:O	1:A:426:LYS:N	2.51	0.44
1:A:352:LEU:HD13	1:A:383:MET:HG2	2.00	0.44
1:A:505:PHE:CD1	1:A:505:PHE:C	2.90	0.44
1:A:427:ASP:CG	1:A:429:ALA:HB3	2.38	0.44
1:A:468:ASP:HB3	1:A:483:ASP:OD1	2.18	0.43
5:A:1009:FTT:H72	8:A:1100:DDQ:H51	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:TYR:CD1	1:A:148:LEU:HG	2.54	0.43
1:A:258:ASN:HB3	1:A:403:TYR:CE1	2.54	0.43
1:A:703:CYS:HA	1:A:708:GLY:O	2.17	0.43
1:A:319:SER:HB3	1:A:338:GLY:N	2.33	0.43
1:A:452:GLN:HA	1:A:456:VAL:O	2.18	0.43
1:A:430:ASN:HD22	1:A:431:SER:N	2.15	0.43
1:A:162:LYS:HB3	1:A:725:PHE:HB2	2.00	0.43
1:A:264:THR:HA	1:A:711:TRP:CG	2.54	0.43
1:A:494:ASN:HD22	1:A:504:TYR:HB3	1.78	0.43
1:A:517:VAL:HA	1:A:522:ASN:O	2.18	0.43
1:A:141:GLY:O	1:A:142:LYS:C	2.57	0.43
1:A:75:GLY:N	11:A:2068:HOH:O	2.51	0.43
10:A:1107:GOL:C2	10:A:1107:GOL:O1	2.52	0.43
1:A:434:TYR:CZ	1:A:436:ILE:HG13	2.53	0.43
1:A:41:THR:HG22	1:A:46:VAL:HG23	2.01	0.43
1:A:407:SER:O	1:A:411:HIS:HD2	2.01	0.43
5:A:1013:FTT:C9	7:A:1014:MYR:H81	2.48	0.43
8:A:1100:DDQ:H21	8:A:1100:DDQ:HM13	1.59	0.43
1:A:148:LEU:CD2	1:A:148:LEU:C	2.86	0.43
1:A:196:GLY:HA2	1:A:214:ALA:O	2.19	0.43
1:A:293:THR:OG1	1:A:364:LYS:O	2.28	0.42
1:A:577:ARG:O	1:A:605:GLU:N	2.36	0.42
1:A:382:ARG:NH1	5:A:1011:FTT:H21	2.34	0.42
1:A:438:ASN:HB3	11:A:2088:HOH:O	2.19	0.42
1:A:586:LYS:HE2	11:A:2122:HOH:O	2.18	0.42
1:A:339:HIS:O	1:A:339:HIS:CD2	2.72	0.42
1:A:24:PRO:HD2	11:A:2154:HOH:O	2.18	0.42
1:A:381:MET:HE2	1:A:382:ARG:CA	2.48	0.42
1:A:343:ARG:C	1:A:397:VAL:HG13	2.40	0.42
1:A:589:LEU:HD23	1:A:589:LEU:HA	1.69	0.42
1:A:345:TYR:CD1	1:A:345:TYR:C	2.92	0.42
1:A:270:ALA:HB1	1:A:272:ASN:OD1	2.19	0.42
1:A:476:ALA:O	1:A:478:THR:HG23	2.19	0.42
1:A:22:TRP:CD1	1:A:60:LEU:HD22	2.55	0.42
5:A:1009:FTT:H51	8:A:1100:DDQ:H31	2.02	0.42
1:A:66:VAL:O	1:A:69:ALA:HB3	2.20	0.42
1:A:81:ARG:HG3	1:A:81:ARG:O	2.20	0.42
1:A:42:PRO:HG2	1:A:45:LYS:HG3	2.01	0.42
1:A:231:PHE:CE1	5:A:1013:FTT:H131	2.55	0.42
1:A:680:VAL:HG12	1:A:680:VAL:O	2.19	0.42
1:A:317:VAL:HG12	1:A:340:TYR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:SER:C	1:A:184:LEU:HD23	2.40	0.42
1:A:262:LEU:HD22	1:A:266:PHE:CD2	2.55	0.42
1:A:274:THR:O	1:A:309:GLN:HA	2.20	0.42
1:A:529:GLY:O	1:A:530:LYS:HD3	2.20	0.42
1:A:244:TYR:OH	10:A:1107:GOL:H31	2.20	0.41
5:A:1013:FTT:H52	7:A:1014:MYR:H22	2.02	0.41
1:A:461:GLY:O	1:A:489:TRP:HB2	2.20	0.41
1:A:28:ILE:CA	1:A:31:ARG:HG3	2.46	0.41
1:A:577:ARG:HH11	1:A:577:ARG:HD3	1.51	0.41
1:A:496:LEU:HD13	1:A:502:THR:HG21	2.02	0.41
1:A:134:GLY:C	11:A:2164:HOH:O	2.58	0.41
1:A:247:LEU:CD2	1:A:268:GLU:HG3	2.49	0.41
1:A:257:PRO:HD2	1:A:339:HIS:HB3	2.02	0.41
1:A:435:ARG:NH1	1:A:474:ARG:HB3	2.35	0.41
1:A:51:SER:OG	1:A:73:THR:HG23	2.21	0.41
1:A:397:VAL:HG23	1:A:398:PRO:HD2	2.03	0.41
1:A:86:THR:CG2	1:A:241:THR:HG21	2.45	0.41
1:A:167:LYS:HB2	1:A:175:GLN:HB3	2.03	0.41
1:A:249:LYS:HG2	1:A:250:GLU:OE1	2.21	0.41
1:A:673:VAL:O	1:A:673:VAL:HG23	2.20	0.41
1:A:195:THR:O	1:A:215:ILE:HD12	2.21	0.41
1:A:373:THR:O	1:A:449:ASP:HA	2.21	0.41
1:A:586:LYS:CG	1:A:596:VAL:CG2	2.78	0.41
1:A:381:MET:HE1	1:A:382:ARG:C	2.40	0.41
5:A:1009:FTT:H82	6:A:1012:DAO:H42	2.03	0.41
1:A:531:GLN:HA	1:A:553:ASN:O	2.21	0.41
1:A:371:ASP:O	1:A:451:ALA:HA	2.20	0.41
1:A:22:TRP:NE1	1:A:630:ASP:OD2	2.38	0.41
1:A:678:ALA:O	1:A:680:VAL:N	2.52	0.41
1:A:648:ARG:O	1:A:667:THR:HA	2.21	0.41
1:A:628:TRP:HH2	1:A:630:ASP:HB3	1.70	0.41
5:A:1013:FTT:H91	7:A:1014:MYR:C8	2.51	0.41
1:A:189:VAL:HG13	1:A:190:TYR:CD2	2.56	0.41
1:A:137:SER:HB2	1:A:510:SER:HA	2.03	0.41
1:A:356:SER:HB3	11:A:2074:HOH:O	2.20	0.41
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.54	0.40
1:A:390:TRP:NE1	1:A:426:LYS:HB3	2.36	0.40
1:A:435:ARG:C	1:A:436:ILE:HG12	2.40	0.40
1:A:333:ALA:O	1:A:335:ALA:N	2.54	0.40
1:A:639:SER:HB3	1:A:679:ARG:NE	2.34	0.40
1:A:592:SER:O	1:A:632:THR:N	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:TYR:CE2	1:A:466:TRP:CZ2	3.09	0.40
1:A:490:ARG:HG2	1:A:491:GLY:N	2.35	0.40
1:A:393:TYR:OH	1:A:432:GLY:HA3	2.21	0.40
1:A:364:LYS:HA	1:A:372:HIS:O	2.22	0.40
1:A:407:SER:OG	1:A:409:HIS:HB3	2.21	0.40
1:A:98:GLU:HG3	1:A:513:PRO:O	2.21	0.40
1:A:116:TYR:OH	10:A:1108:GOL:H12	2.21	0.40
1:A:435:ARG:HH12	1:A:474:ARG:CB	2.34	0.40
1:A:443:THR:OG1	8:A:1100:DDQ:HM11	2.21	0.40
1:A:493:VAL:HG23	1:A:505:PHE:CE2	2.56	0.40
1:A:498:ASP:OD1	1:A:498:ASP:N	2.53	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	705/725 (97%)	639 (91%)	54 (8%)	12 (2%)	11 19

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	ALA
1	A	420	ASP
1	A	677	LEU
1	A	679	ARG
1	A	682	MET
1	A	264	THR
1	A	331	ALA
1	A	398	PRO
1	A	676	ASP
1	A	696	ASP

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Mol	Chain	Res	Type
1	A	678	ALA
1	A	334	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	587/601 (98%)	507 (86%)	80 (14%)	5 8

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	31	ARG
1	A	32	GLN
1	A	49	SER
1	A	66	VAL
1	A	101	SER
1	A	112	GLN
1	A	118	ASP
1	A	125	MET
1	A	128	ARG
1	A	132	MET
1	A	136	VAL
1	A	138	VAL
1	A	144	SER
1	A	148	LEU
1	A	158	THR
1	A	170	THR
1	A	184	LEU
1	A	205	GLN
1	A	206	LYS
1	A	209	GLU
1	A	222	ARG
1	A	257	PRO
1	A	268	GLU

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Mol	Chain	Res	Type
1	A	271	LYS
1	A	275	TYR
1	A	280	LYS
1	A	281	MET
1	A	297	ARG
1	A	326	SER
1	A	334	PRO
1	A	352	LEU
1	A	353	GLN
1	A	354	ASN
1	A	357	VAL
1	A	367	THR
1	A	369	ASP
1	A	381	MET
1	A	397	VAL
1	A	398	PRO
1	A	402	LEU
1	A	404	ASN
1	A	405	PRO
1	A	408	HIS
1	A	426	LYS
1	A	430	ASN
1	A	431	SER
1	A	448	GLN
1	A	455	LYS
1	A	457	LEU
1	A	460	LEU
1	A	468	ASP
1	A	474	ARG
1	A	498	ASP
1	A	502	THR
1	A	517	VAL
1	A	526	PRO
1	A	534	VAL
1	A	542	ASP
1	A	543	ARG
1	A	544	PRO
1	A	545	ILE
1	A	551	VAL
1	A	571	VAL
1	A	579	ARG
1	A	583	ILE

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Mol	Chain	Res	Type
1	A	592	SER
1	A	596	VAL
1	A	603	ASP
1	A	607	THR
1	A	613	LYS
1	A	620	VAL
1	A	627	LEU
1	A	632	THR
1	A	635	ASP
1	A	641	LEU
1	A	677	LEU
1	A	679	ARG
1	A	715	ARG
1	A	722	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	44	GLN
1	A	112	GLN
1	A	165	GLN
1	A	205	GLN
1	A	288	HIS
1	A	310	ASN
1	A	328	GLN
1	A	339	HIS
1	A	388	ASN
1	A	404	ASN
1	A	410	HIS
1	A	412	HIS
1	A	418	ASN
1	A	430	ASN
1	A	448	GLN
1	A	494	ASN
1	A	522	ASN
1	A	619	GLN
1	A	690	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 ⓘ

9 carbohydrates are modelled in this entry.

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$
2	PA1	A	1000	9,2,5	11,11,12	0.85	0	11,15,17	1.37	2 (18%)
2	GCN	A	1001	2,5	10,10,11	1.42	3 (30%)	10,13,15	3.68	4 (40%)
2	KDO	A	1002	2	12,15,16	1.15	0	12,21,24	1.39	1 (8%)
2	KDO	A	1003	2	12,15,16	1.12	1 (8%)	12,21,24	1.51	2 (16%)
2	GMH	A	1004	2	13,13,14	1.50	1 (7%)	17,18,20	1.46	2 (11%)
2	GMH	A	1005	2	13,13,14	2.67	7 (53%)	17,18,20	1.61	4 (23%)
2	GLC	A	1006	2	11,11,12	0.66	0	14,15,17	1.49	3 (21%)
2	GLC	A	1007	2	11,11,12	1.38	2 (18%)	14,15,17	1.10	1 (7%)
2	GLA	A	1008	2	11,11,12	0.83	0	14,15,17	0.70	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
2	PA1	A	1000	9,2,5	-	0/2/18/22	0/1/1/1
2	GCN	A	1001	2,5	-	0/2/15/18	0/1/1/1
2	KDO	A	1002	2	-	0/6/26/30	0/1/1/1
2	KDO	A	1003	2	-	0/6/26/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GMH	A	1004	2	-	0/6/23/26	0/1/1/1
2	GMH	A	1005	2	-	0/6/23/26	1/1/1/1
2	GLC	A	1006	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1007	2	-	0/2/19/22	0/1/1/1
2	GLA	A	1008	2	-	0/2/19/22	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	GCN	C4-C5	-2.79	1.46	1.52
2	A	1003	KDO	C4-C5	-2.51	1.49	1.52
2	A	1001	GCN	O5-C1	-2.37	1.39	1.43
2	A	1005	GMH	C1-C2	-2.11	1.47	1.52
2	A	1001	GCN	C3-C2	2.14	1.58	1.53
2	A	1007	GLC	C1-C2	2.52	1.58	1.52
2	A	1005	GMH	C4-C3	2.58	1.59	1.52
2	A	1007	GLC	C4-C5	2.73	1.58	1.53
2	A	1005	GMH	C7-C6	2.85	1.60	1.52
2	A	1005	GMH	C4-C5	3.05	1.61	1.52
2	A	1005	GMH	O5-C5	3.71	1.48	1.43
2	A	1005	GMH	O4-C4	3.88	1.52	1.43
2	A	1004	GMH	C2-C3	4.34	1.58	1.52
2	A	1005	GMH	C2-C3	5.41	1.59	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1002	KDO	C3-C4-C5	-4.14	104.92	110.56
2	A	1003	KDO	O5-C5-C4	-3.00	104.57	110.00
2	A	1003	KDO	C3-C4-C5	-2.78	106.78	110.56
2	A	1006	GLC	C6-C5-C4	-2.26	107.44	113.02
2	A	1005	GMH	C3-C4-C5	-2.20	104.77	109.60
2	A	1005	GMH	C1-C2-C3	2.01	111.91	109.54
2	A	1005	GMH	O7-C7-C6	2.15	115.76	111.10
2	A	1000	PA1	O1-C1-C2	2.47	114.65	109.02
2	A	1007	GLC	O2-C2-C1	2.49	114.20	109.21
2	A	1000	PA1	C1-O5-C5	2.72	118.51	113.47
2	A	1006	GLC	C1-C2-C3	2.74	112.78	109.54
2	A	1001	GCN	C3-C2-N2	2.95	116.32	110.64
2	A	1001	GCN	O5-C5-C4	3.02	114.82	109.63
2	A	1004	GMH	O5-C5-C6	3.03	110.09	106.04
2	A	1004	GMH	C1-C2-C3	3.20	113.32	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1006	GLC	C1-O5-C5	3.29	116.42	112.25
2	A	1005	GMH	C1-O5-C5	3.96	117.96	111.52
2	A	1001	GCN	C3-C2-C1	6.11	115.42	109.60
2	A	1001	GCN	C1-O5-C5	8.64	123.21	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1005	GMH	C1-C2-C3-C4-C5-O5

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	PA1	2	0
2	A	1002	KDO	1	0
2	A	1004	GMH	1	0

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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	FTT	A	1009	2	14,15,16	0.45	0	15,15,17	1.04	1 (6%)
5	FTT	A	1010	2	3,6,16	0.63	0	3,7,17	1.13	0
5	FTT	A	1011	2,6	14,15,16	0.62	0	15,15,17	1.18	2 (13%)
6	DAO	A	1012	5	12,12,13	1.18	1 (8%)	11,11,13	0.79	0
5	FTT	A	1013	2,7	13,16,16	1.96	1 (7%)	13,17,17	1.96	4 (30%)
7	MYR	A	1014	5	14,14,15	0.97	1 (7%)	13,13,15	0.78	0
8	DDQ	A	1100	-	13,13,13	0.98	1 (7%)	14,15,15	0.78	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	DDQ	A	1101	-	13,13,13	0.78	0	14,15,15	1.13	1 (7%)
8	DDQ	A	1102	-	13,13,13	1.33	1 (7%)	14,15,15	1.25	2 (14%)
10	GOL	A	1103	-	5,5,5	4.65	5 (100%)	5,5,5	0.27	0
10	GOL	A	1104	-	5,5,5	4.62	5 (100%)	5,5,5	0.22	0
10	GOL	A	1105	-	5,5,5	4.43	3 (60%)	5,5,5	0.53	0
10	GOL	A	1106	-	5,5,5	4.76	5 (100%)	5,5,5	0.29	0
10	GOL	A	1107	-	5,5,5	4.35	4 (80%)	5,5,5	0.74	0
10	GOL	A	1108	-	5,5,5	4.47	5 (100%)	5,5,5	0.47	0
10	GOL	A	1109	-	5,5,5	4.90	5 (100%)	5,5,5	0.24	0
10	GOL	A	1110	-	5,5,5	4.46	3 (60%)	5,5,5	0.77	0
9	DPO	A	2000	2	4,7,8	2.72	3 (75%)	6,10,13	1.46	0
4	PO4	A	2001	-	0,3,4	0.00	-	0,3,6	0.00	-
9	DPO	A	2004	-	5,7,8	4.97	5 (100%)	6,10,13	3.27	4 (66%)
4	PO4	A	2005	3	0,3,4	0.00	-	0,3,6	0.00	-

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	FTT	A	1009	2	-	0/14/14/15	0/0/0/0
5	FTT	A	1010	2	-	0/2/4/15	0/0/0/0
5	FTT	A	1011	2,6	-	0/14/14/15	0/0/0/0
6	DAO	A	1012	5	-	0/10/10/11	0/0/0/0
5	FTT	A	1013	2,7	-	0/13/15/15	0/0/0/0
7	MYR	A	1014	5	-	0/12/12/13	0/0/0/0
8	DDQ	A	1100	-	-	0/11/11/11	0/0/0/0
8	DDQ	A	1101	-	-	0/11/11/11	0/0/0/0
8	DDQ	A	1102	-	-	0/11/11/11	0/0/0/0
10	GOL	A	1103	-	-	0/4/4/4	0/0/0/0
10	GOL	A	1104	-	-	0/4/4/4	0/0/0/0
10	GOL	A	1105	-	-	0/4/4/4	0/0/0/0
10	GOL	A	1106	-	-	0/4/4/4	0/0/0/0
10	GOL	A	1107	-	-	0/4/4/4	0/0/0/0
10	GOL	A	1108	-	-	0/4/4/4	0/0/0/0
10	GOL	A	1109	-	-	0/4/4/4	0/0/0/0
10	GOL	A	1110	-	-	0/4/4/4	0/0/0/0
9	DPO	A	2000	2	-	0/3/5/6	0/0/0/0
4	PO4	A	2001	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	DPO	A	2004	-	-	0/3/5/6	0/0/0/0
4	PO4	A	2005	3	-	0/0/0/0	0/0/0/0

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1106	GOL	C3-C2	-8.00	1.21	1.52
10	A	1109	GOL	C3-C2	-7.70	1.22	1.52
10	A	1104	GOL	C3-C2	-7.47	1.23	1.52
10	A	1103	GOL	C3-C2	-7.39	1.24	1.52
10	A	1105	GOL	C3-C2	-7.08	1.25	1.52
10	A	1108	GOL	C3-C2	-6.93	1.25	1.52
10	A	1110	GOL	C3-C2	-6.61	1.27	1.52
10	A	1107	GOL	C3-C2	-6.36	1.28	1.52
5	A	1013	FTT	C2-C3	-6.17	1.46	1.53
9	A	2004	DPO	P1-O4	-5.68	1.45	1.63
8	A	1102	DDQ	CM1-N1	-4.17	1.43	1.49
6	A	1012	DAO	O2-C1	-3.75	1.21	1.42
9	A	2000	DPO	P2-O4	-3.63	1.51	1.62
10	A	1109	GOL	O2-C2	-3.46	1.33	1.43
9	A	2000	DPO	P2-O6	-3.15	1.46	1.51
10	A	1106	GOL	C1-C2	-3.06	1.40	1.52
10	A	1109	GOL	C1-C2	-2.99	1.40	1.52
7	A	1014	MYR	O2-C1	-2.85	1.26	1.42
10	A	1103	GOL	C1-C2	-2.76	1.41	1.52
10	A	1104	GOL	C1-C2	-2.59	1.42	1.52
10	A	1107	GOL	C1-C2	-2.58	1.42	1.52
10	A	1108	GOL	C1-C2	-2.53	1.42	1.52
10	A	1104	GOL	O2-C2	-2.38	1.36	1.43
10	A	1106	GOL	O2-C2	-2.29	1.36	1.43
9	A	2000	DPO	P2-O7	-2.23	1.48	1.51
10	A	1108	GOL	O2-C2	-2.21	1.36	1.43
10	A	1103	GOL	O2-C2	-2.21	1.36	1.43
8	A	1100	DDQ	CM1-N1	-2.20	1.46	1.49
9	A	2004	DPO	P2-O4	-2.03	1.56	1.62
10	A	1104	GOL	O3-C3	3.27	1.56	1.42
10	A	1106	GOL	O3-C3	3.47	1.57	1.42
10	A	1105	GOL	O3-C3	3.48	1.57	1.42
10	A	1103	GOL	O3-C3	3.68	1.58	1.42
10	A	1109	GOL	O3-C3	3.73	1.58	1.42
9	A	2004	DPO	P2-O5	3.80	1.59	1.51
10	A	1110	GOL	O3-C3	4.05	1.59	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1107	GOL	O3-C3	4.12	1.60	1.42
9	A	2004	DPO	P2-O6	4.31	1.59	1.51
10	A	1108	GOL	O3-C3	4.48	1.61	1.42
10	A	1108	GOL	O1-C1	4.52	1.61	1.42
10	A	1106	GOL	O1-C1	4.74	1.62	1.42
10	A	1109	GOL	O1-C1	5.09	1.64	1.42
10	A	1103	GOL	O1-C1	5.25	1.65	1.42
10	A	1104	GOL	O1-C1	5.28	1.65	1.42
10	A	1107	GOL	O1-C1	5.43	1.65	1.42
10	A	1105	GOL	O1-C1	5.56	1.66	1.42
10	A	1110	GOL	O1-C1	6.01	1.68	1.42
9	A	2004	DPO	P2-O7	7.35	1.64	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2004	DPO	O6-P2-O5	-5.53	99.91	112.76
8	A	1102	DDQ	O1-N1-C1	-3.14	106.73	110.27
9	A	2004	DPO	O7-P2-O6	-3.04	106.11	112.85
8	A	1101	DDQ	O1-N1-C1	-2.99	106.91	110.27
5	A	1013	FTT	C4-C3-C2	-2.78	103.33	112.25
5	A	1013	FTT	O3-C3-C2	-2.78	103.34	109.21
5	A	1011	FTT	O2-C1-C2	-2.43	116.37	125.24
5	A	1009	FTT	C4-C3-C2	-2.14	105.14	112.23
8	A	1100	DDQ	O1-N1-C1	-2.09	107.92	110.27
8	A	1102	DDQ	CM2-N1-C1	2.23	116.97	109.77
5	A	1011	FTT	O3-C3-C2	2.56	115.92	109.32
9	A	2004	DPO	O7-P2-O5	2.81	119.30	112.76
5	A	1013	FTT	C5-C4-C3	3.02	125.36	115.07
9	A	2004	DPO	O6-P2-O4	3.98	117.40	105.18
5	A	1013	FTT	O3-C3-C4	4.79	122.95	109.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1009	FTT	6	0
5	A	1011	FTT	1	0
6	A	1012	DAO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1013	FTT	11	0
7	A	1014	MYR	9	0
8	A	1100	DDQ	5	0
10	A	1103	GOL	2	0
10	A	1104	GOL	2	0
10	A	1105	GOL	4	0
10	A	1107	GOL	4	0
10	A	1108	GOL	1	0
10	A	1109	GOL	2	0
10	A	1110	GOL	3	0
9	A	2000	DPO	4	0
9	A	2004	DPO	1	0

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.