



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2016 – 07:57 AM EDT

PDB ID : 5EJ7
Title : EcMenD-ThDP-Mn2+ complex soaked with 2-ketoglutarate for 21 s
Authors : Song, H.G.; Dong, C.; Chen, Y.Z.; Sun, Y.R.; Guo, Z.H.
Deposited on : 2015-11-01
Resolution : 1.56 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027790

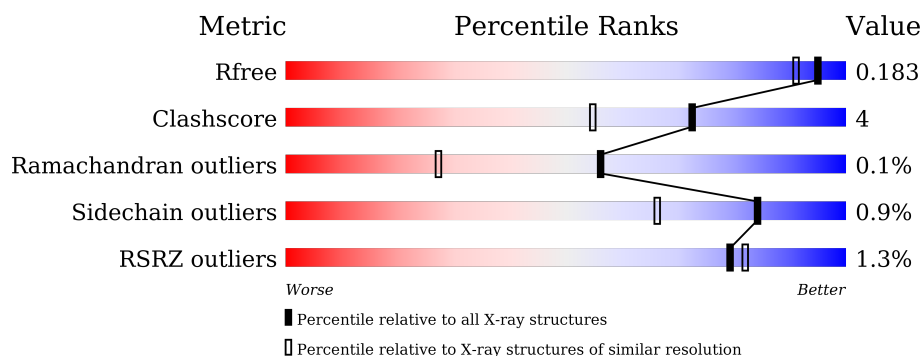
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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}	91344	1665 (1.58-1.54)
Clashscore	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

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.

Mol	Chain	Length	Quality of chain
1	A	556	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	B	556	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	C	556	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	D	556	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
1	E	556	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>7%</div> <div>.</div> </div> </div>
1	F	556	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	556	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	H	556	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>8%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	604	-	-	-	X
4	GOL	C	604	-	-	-	X
4	GOL	D	604	-	-	-	X
4	GOL	E	604	-	-	-	X
4	GOL	F	603	-	-	-	X
4	GOL	G	604	-	-	-	X
4	GOL	H	604	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 42054 atoms, of which 48 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 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	20	0
			4501	2847	820	820	14			
1	B	556	Total	C	N	O	S	0	11	0
			4424	2805	804	801	14			
1	C	556	Total	C	N	O	S	0	14	0
			4437	2810	804	809	14			
1	D	556	Total	C	N	O	S	0	11	0
			4433	2806	807	805	15			
1	E	556	Total	C	N	O	S	0	17	0
			4468	2828	815	811	14			
1	F	556	Total	C	N	O	S	0	8	0
			4387	2782	796	795	14			
1	G	556	Total	C	N	O	S	0	16	0
			4459	2827	811	807	14			
1	H	556	Total	C	N	O	S	0	12	0
			4429	2807	800	808	14			

- Molecule 2 is (4S)-4-{3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-5-(2-{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}ethyl)-4-methyl-1,3lambda 5 -thiazol-2-yl}-4-hydroxybutanoic acid (three-letter code: TD6) (formula: C₁₆H₂₅N₄O₁₀P₂S).



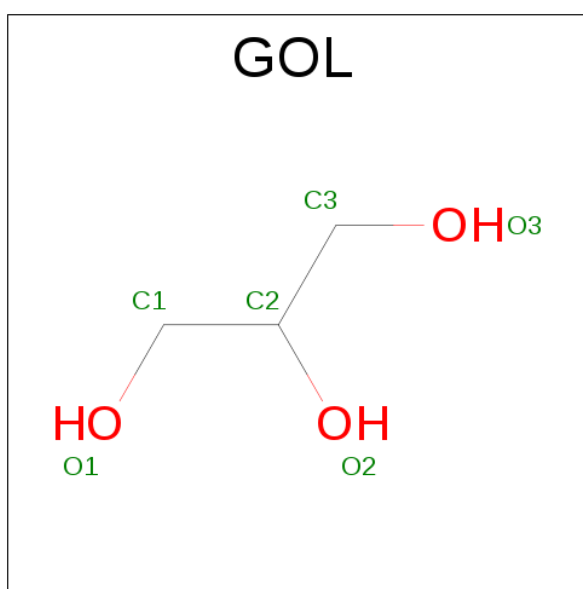
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	F	1	Total	Mn	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			6	3	3			
4	A	1	Total	C	H	O	0	0
			14	3	8	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	H	O	0	0
			14	3	8	3		
4	D	1	Total	C	O		0	0
			6	3	3			
4	D	1	Total	C	H	O	0	0
			14	3	8	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 6 3 3	0	0
4	E	1	Total C H O 14 3 8 3	0	0
4	F	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	G	1	Total C H O 14 3 8 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C H O 14 3 8 3	0	0

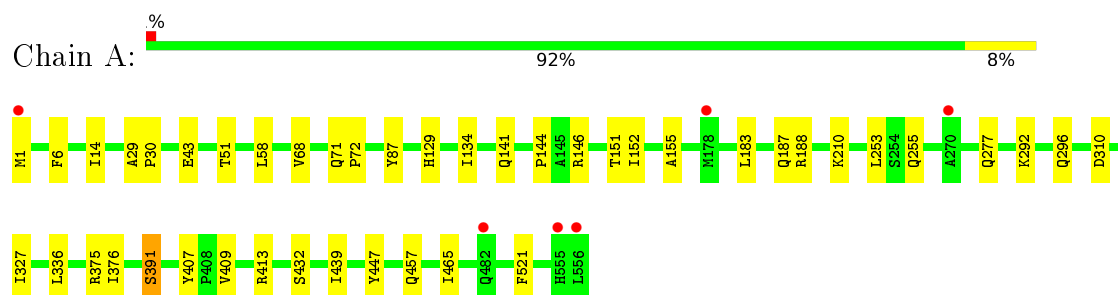
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	813	Total O 813 813	0	0
5	B	808	Total O 808 808	0	0
5	C	774	Total O 774 774	0	0
5	D	711	Total O 711 711	0	0
5	E	777	Total O 777 777	0	0
5	F	789	Total O 789 789	0	0
5	G	758	Total O 758 758	0	0
5	H	681	Total O 681 681	0	0

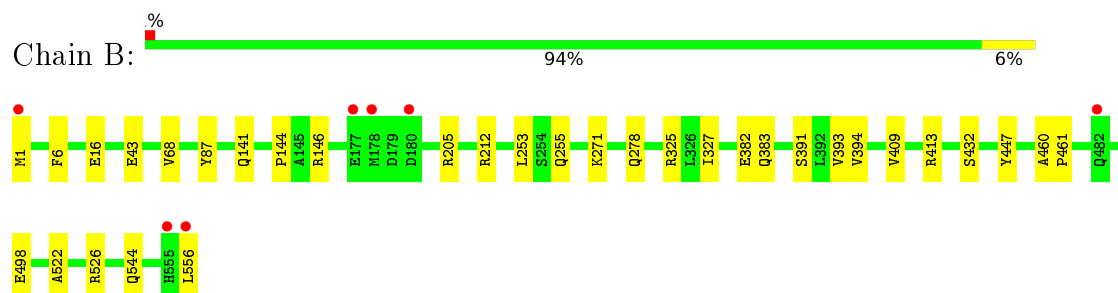
3 Residue-property plots

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.

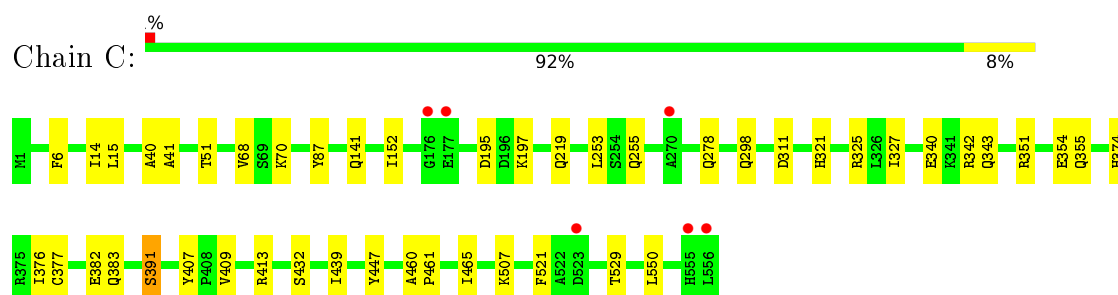
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



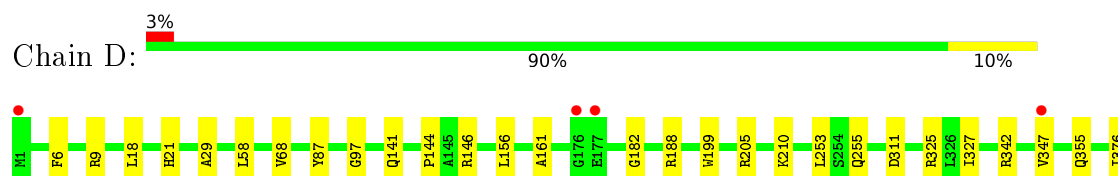
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

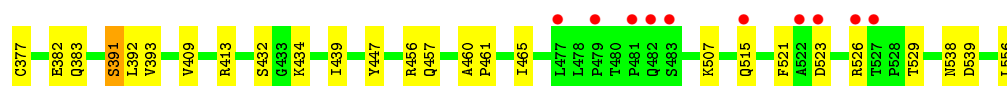


- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

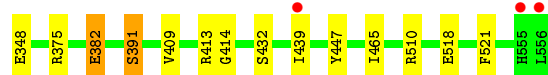


- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

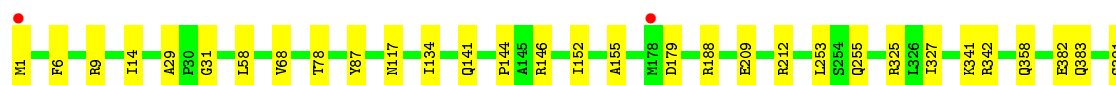




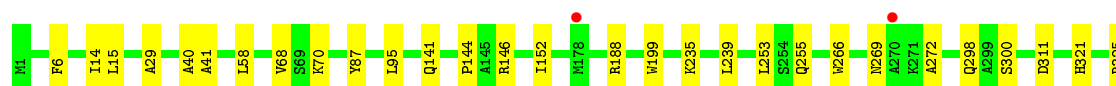
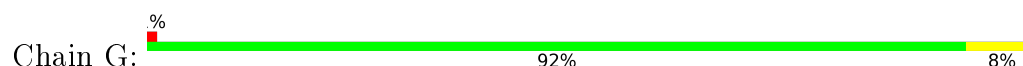
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



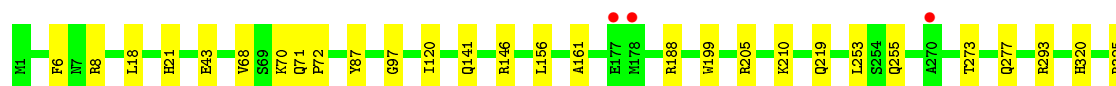
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.60Å 90.61Å 167.57Å 76.08° 83.45° 63.44°	Depositor
Resolution (Å)	32.45 – 1.56 32.45 – 1.56	Depositor EDS
% Data completeness (in resolution range)	96.0 (32.45-1.56) 88.3 (32.45-1.56)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 1.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.146 , 0.183 0.146 , 0.183	Depositor DCC
R_{free} test set	31886 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	10.5	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.030 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	42054	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MN, TD6

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	0.36	0/4610	0.54	2/6286 (0.0%)
1	B	0.33	0/4532	0.52	0/6179
1	C	0.33	0/4546	0.51	0/6201
1	D	0.31	0/4542	0.50	0/6191
1	E	0.34	0/4578	0.53	1/6243 (0.0%)
1	F	0.32	0/4495	0.51	0/6131
1	G	0.32	0/4568	0.50	0/6230
1	H	0.36	1/4539 (0.0%)	0.50	0/6192
All	All	0.33	1/36410 (0.0%)	0.51	3/49653 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	472	GLY	C-O	-5.50	1.14	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	375	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	E	375	ARG	NE-CZ-NH1	-5.19	117.70	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4501	0	4447	31	0
1	B	4424	0	4396	20	1
1	C	4437	0	4378	40	0
1	D	4433	0	4384	39	0
1	E	4468	0	4415	33	0
1	F	4387	0	4347	35	0
1	G	4459	0	4413	43	0
1	H	4429	0	4361	35	0
2	A	33	0	21	4	0
2	B	33	0	21	5	0
2	C	33	0	21	4	0
2	D	33	0	21	5	0
2	E	33	0	21	4	0
2	F	33	0	21	5	0
2	G	33	0	21	4	0
2	H	33	0	21	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
4	A	12	8	16	1	0
4	B	6	0	8	0	0
4	C	12	8	16	2	0
4	D	12	8	16	0	0
4	E	12	8	16	0	0
4	F	6	0	8	0	0
4	G	12	8	16	0	0
4	H	12	8	16	0	0
5	A	813	0	0	10	0
5	B	808	0	0	8	3
5	C	774	0	0	15	4
5	D	711	0	0	14	0
5	E	777	0	0	15	0
5	F	789	0	0	14	0
5	G	758	0	0	13	0
5	H	681	0	0	6	0
All	All	42006	48	35421	303	4

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 4.

All (303) 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)
2:B:601:TD6:H11	2:B:601:TD6:HN4A	1.22	1.03
2:G:601:TD6:HN4A	2:G:601:TD6:H11	1.19	1.02
2:E:601:TD6:H11	2:E:601:TD6:HN4A	1.24	1.01
2:F:601:TD6:H11	2:F:601:TD6:HN4A	1.26	0.97
2:H:601:TD6:H11	2:H:601:TD6:HN4A	1.32	0.94
2:D:601:TD6:HN4A	2:D:601:TD6:H11	1.31	0.94
2:C:601:TD6:H11	2:C:601:TD6:HN4A	1.36	0.88
1:F:209:GLU:OE2	1:H:205:ARG:CZ	2.21	0.88
2:A:601:TD6:H11	2:A:601:TD6:HN4A	1.39	0.88
1:H:255:GLN:HE21	1:H:409:VAL:H	1.23	0.84
1:D:255:GLN:HE21	1:D:409:VAL:H	1.26	0.83
1:A:255:GLN:HE21	1:A:409:VAL:H	1.27	0.82
1:G:255:GLN:HE21	1:G:409:VAL:H	1.26	0.81
1:E:255:GLN:HE21	1:E:409:VAL:H	1.25	0.81
1:F:209:GLU:OE2	1:H:205:ARG:NH1	2.14	0.81
1:C:255:GLN:HE21	1:C:409:VAL:H	1.29	0.81
2:B:601:TD6:C11	2:B:601:TD6:HN4A	1.95	0.80
1:F:255:GLN:HE21	1:F:409:VAL:H	1.32	0.77
1:G:15[A]:LEU:HD12	1:G:40:ALA:HB3	1.66	0.77
2:G:601:TD6:HN4A	2:G:601:TD6:C11	1.96	0.77
2:F:601:TD6:C11	2:F:601:TD6:HN4A	1.98	0.75
2:H:601:TD6:C11	2:H:601:TD6:HN4A	1.99	0.75
1:G:15[B]:LEU:HD22	1:G:40:ALA:HB3	1.69	0.74
1:D:456:ARG:NH2	5:D:704:HOH:O	2.19	0.74
1:F:209:GLU:OE2	1:H:205:ARG:NE	2.20	0.74
2:G:601:TD6:N4'	2:G:601:TD6:H11	2.00	0.73
2:A:601:TD6:C11	2:A:601:TD6:HN4A	2.01	0.73
2:E:601:TD6:C11	2:E:601:TD6:HN4A	1.99	0.72
1:B:255:GLN:HE21	1:B:409:VAL:H	1.37	0.72
1:E:271:LYS:NZ	5:E:706:HOH:O	2.22	0.71
1:F:179:ASP:O	5:F:701:HOH:O	2.08	0.71
2:D:601:TD6:HN4A	2:D:601:TD6:C11	2.03	0.71
1:E:414:GLY:O	5:E:701:HOH:O	2.08	0.71
1:D:146[C]:ARG:HG2	1:D:199:TRP:CZ2	2.25	0.71
1:D:538:ASN:ND2	5:D:706:HOH:O	2.23	0.70
2:C:601:TD6:HN4A	2:C:601:TD6:C11	2.04	0.70
1:H:146[B]:ARG:HG2	1:H:199:TRP:CZ2	2.27	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:601:TD6:N4'	2:E:601:TD6:H11	2.05	0.69
1:F:146[B]:ARG:NH2	5:F:705:HOH:O	2.24	0.69
2:B:601:TD6:N4'	2:B:601:TD6:H11	2.02	0.69
1:F:212:ARG:NE	5:F:708:HOH:O	2.26	0.68
1:C:340:GLU:HG2	5:C:6308:HOH:O	1.93	0.68
1:E:134:ILE:HD11	1:E:155:ALA:HB2	1.74	0.68
1:E:518:GLU:HG3	5:E:717:HOH:O	1.92	0.68
1:G:6:PHE:CE1	1:G:141:GLN:HG2	2.28	0.68
1:G:15[B]:LEU:HD22	1:G:40:ALA:CB	2.24	0.68
1:G:146[C]:ARG:HH12	1:G:188:ARG:HB3	1.58	0.67
2:F:601:TD6:H11	2:F:601:TD6:N4'	2.06	0.67
1:C:354:GLU:OE1	5:C:6101:HOH:O	2.12	0.66
1:C:311:ASP:OD2	5:C:6102:HOH:O	2.13	0.65
1:E:43:GLU:HG3	5:E:1071:HOH:O	1.96	0.65
1:G:15[A]:LEU:HD12	1:G:40:ALA:CB	2.25	0.65
1:C:15[A]:LEU:HD12	1:C:40:ALA:HB3	1.78	0.65
1:A:1:MET:N	5:A:709:HOH:O	2.29	0.65
1:G:146[C]:ARG:HG2	1:G:199:TRP:CZ2	2.32	0.65
1:G:311:ASP:OD2	5:G:701:HOH:O	2.13	0.65
1:D:347:VAL:O	5:D:701:HOH:O	2.14	0.65
1:F:498:GLU:OE2	1:F:510[A]:ARG:NH2	2.30	0.64
1:H:6:PHE:CE1	1:H:141:GLN:HG2	2.32	0.64
1:C:382:GLU:HG2	1:C:383:GLN:HG2	1.79	0.63
1:G:269:ASN:HB3	1:G:352[B]:LEU:HD21	1.81	0.63
1:E:6:PHE:CE1	1:E:141:GLN:HG2	2.33	0.62
1:G:70:LYS:NZ	5:G:711:HOH:O	2.31	0.62
1:D:393:VAL:HG21	1:D:439[B]:ILE:HG12	1.82	0.62
1:H:18:LEU:HD22	1:H:156:LEU:HD21	1.82	0.62
1:D:507:LYS:NZ	1:D:529:THR:OG1	2.32	0.61
1:A:457:GLN:HG3	5:A:744:HOH:O	2.00	0.61
1:E:465:ILE:HD11	1:E:521:PHE:HZ	1.65	0.60
1:A:465:ILE:HD11	1:A:521:PHE:HZ	1.66	0.60
1:B:522:ALA:O	1:B:526[B]:ARG:NE	2.32	0.60
1:C:355:GLN:NE2	5:C:6119:HOH:O	2.34	0.60
1:D:18:LEU:HD22	1:D:156:LEU:HD21	1.84	0.60
1:H:18:LEU:CD2	1:H:156:LEU:HD21	2.32	0.60
2:D:601:TD6:H11	2:D:601:TD6:N4'	2.11	0.60
1:D:6:PHE:CE1	1:D:141:GLN:HG2	2.36	0.60
1:H:71[B]:GLN:HB3	1:H:72:PRO:HD2	1.84	0.60
1:F:188:ARG:NH2	5:F:715:HOH:O	2.33	0.59
1:F:358:GLN:OE1	5:F:702:HOH:O	2.16	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:VAL:HG11	1:C:432:SER:HB3	1.84	0.59
1:E:518:GLU:OE1	5:E:702:HOH:O	2.17	0.59
1:A:43:GLU:OE1	5:A:701:HOH:O	2.17	0.59
1:E:210:LYS:HG2	5:E:996:HOH:O	2.02	0.59
1:H:460:ALA:HB1	1:H:461:PRO:HD2	1.85	0.59
1:B:212:ARG:HD3	5:B:1250:HOH:O	2.02	0.58
1:C:351[A]:ARG:NH2	5:C:6122:HOH:O	2.36	0.58
1:B:6:PHE:CE1	1:B:141:GLN:HG2	2.38	0.58
1:C:354:GLU:OE2	5:C:6103:HOH:O	2.17	0.58
1:G:523:ASP:HB3	5:G:730:HOH:O	2.03	0.58
1:F:1:MET:N	5:F:716:HOH:O	2.35	0.58
1:B:544:GLN:NE2	5:B:709:HOH:O	2.36	0.58
1:H:210:LYS:HE2	1:H:336:LEU:CD1	2.34	0.58
2:H:601:TD6:N4'	2:H:601:TD6:H11	2.12	0.58
1:F:6:PHE:CE1	1:F:141:GLN:HG2	2.39	0.57
1:E:253:LEU:HD11	1:E:413:ARG:HG3	1.86	0.57
1:A:6:PHE:CE1	1:A:141:GLN:HG2	2.40	0.56
1:F:538:ASN:ND2	5:F:706:HOH:O	2.25	0.56
1:G:300:SER:OG	5:G:702:HOH:O	2.17	0.56
2:A:601:TD6:N4'	2:A:601:TD6:H11	2.17	0.56
1:D:376:ILE:HD11	1:D:439[A]:ILE:HD11	1.88	0.56
1:F:146[A]:ARG:NH2	5:F:715:HOH:O	2.37	0.56
1:G:14:ILE:HG12	1:G:152:ILE:HD11	1.88	0.56
1:E:510[A]:ARG:NH2	5:E:721:HOH:O	2.39	0.56
1:E:348:GLU:OE1	5:E:703:HOH:O	2.18	0.55
1:G:14:ILE:HA	1:G:152:ILE:CD1	2.36	0.55
1:B:43:GLU:HG3	5:B:1179:HOH:O	2.05	0.55
1:D:311[A]:ASP:OD2	5:D:702:HOH:O	2.18	0.55
1:H:343:GLN:NE2	1:H:344:PRO:HD2	2.22	0.55
1:A:71[B]:GLN:HB3	1:A:72:PRO:HD2	1.88	0.55
1:D:253:LEU:HD11	1:D:413:ARG:HG3	1.87	0.55
1:H:253:LEU:HD11	1:H:413:ARG:HG3	1.89	0.55
1:C:15[B]:LEU:HD23	1:C:41:ALA:HA	1.90	0.54
1:E:129:HIS:HD2	5:E:1159:HOH:O	1.90	0.54
1:G:235:LYS:NZ	5:G:707:HOH:O	2.26	0.54
1:G:377:CYS:HB2	5:G:1007:HOH:O	2.07	0.54
1:C:219:GLN:NE2	1:C:340:GLU:OE2	2.28	0.54
1:G:266:TRP:HB2	1:G:352[B]:LEU:HG	1.90	0.54
1:H:210:LYS:HE2	1:H:336:LEU:HD11	1.88	0.53
1:D:465:ILE:HD11	1:D:521:PHE:HZ	1.74	0.53
1:A:188:ARG:NH1	5:A:718:HOH:O	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:LYS:NZ	5:C:6118:HOH:O	2.33	0.53
1:H:97:GLY:HA2	1:H:161:ALA:HB1	1.90	0.53
1:E:177:GLU:O	5:E:705:HOH:O	2.19	0.53
1:D:29:ALA:HB2	1:D:58:LEU:HD22	1.90	0.53
1:A:129:HIS:HD2	5:A:1147:HOH:O	1.91	0.52
1:C:327:ILE:N	1:C:327:ILE:HD12	2.24	0.52
1:H:146[B]:ARG:HH22	1:H:188:ARG:HB3	1.73	0.52
1:B:253:LEU:HD11	1:B:413:ARG:HG3	1.90	0.52
1:C:15[A]:LEU:HD12	1:C:40:ALA:CB	2.40	0.52
1:D:68:VAL:HG11	1:D:432:SER:HB3	1.90	0.52
1:G:253:LEU:HD11	1:G:413:ARG:HG3	1.90	0.52
1:E:134:ILE:HD11	1:E:155:ALA:CB	2.40	0.52
1:G:188:ARG:NH2	5:G:726:HOH:O	2.42	0.52
1:G:298[B]:GLN:HG2	5:G:734:HOH:O	2.09	0.52
1:D:21:HIS:HB2	1:D:156:LEU:HD23	1.92	0.52
1:D:255:GLN:NE2	1:D:409:VAL:H	2.02	0.52
1:B:382:GLU:HG2	1:B:383:GLN:HG2	1.92	0.51
1:E:210:LYS:NZ	5:E:719:HOH:O	2.37	0.51
1:A:255:GLN:NE2	1:A:409:VAL:H	2.04	0.51
1:H:68:VAL:HG11	1:H:432:SER:HB3	1.91	0.51
1:D:523:ASP:OD1	1:D:526[B]:ARG:NE	2.43	0.51
1:B:68:VAL:HG11	1:B:432:SER:HB3	1.92	0.51
1:A:253:LEU:HD11	1:A:413:ARG:HG3	1.91	0.51
1:F:342:ARG:HD3	5:F:907:HOH:O	2.10	0.51
2:A:601:TD6:C2	2:A:601:TD6:HN4A	2.23	0.51
1:F:255:GLN:NE2	1:F:409:VAL:H	2.06	0.51
1:C:253:LEU:HD11	1:C:413:ARG:HG3	1.91	0.51
1:D:210:LYS:NZ	5:D:725:HOH:O	2.44	0.51
1:B:205:ARG:NE	5:B:713:HOH:O	2.44	0.50
1:C:197:LYS:NZ	5:C:6117:HOH:O	2.33	0.50
1:C:465:ILE:HD11	1:C:521:PHE:HZ	1.75	0.50
1:D:460:ALA:HB1	1:D:461:PRO:HD2	1.94	0.50
1:H:327:ILE:HD12	1:H:327:ILE:N	2.26	0.50
1:H:273:THR:O	1:H:277:GLN:HG3	2.12	0.50
1:A:465:ILE:HD11	1:A:521:PHE:CZ	2.47	0.50
1:F:68:VAL:HG11	1:F:432:SER:HB3	1.93	0.50
1:C:255:GLN:NE2	1:C:409:VAL:H	2.05	0.50
1:C:460:ALA:HB1	1:C:461:PRO:HD2	1.92	0.49
1:F:498:GLU:HG2	1:F:499:HIS:N	2.28	0.49
1:G:239[A]:LEU:HG	5:G:846:HOH:O	2.11	0.49
2:B:601:TD6:C2	2:B:601:TD6:HN4A	2.26	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:ASP:OD1	5:E:704:HOH:O	2.19	0.49
1:C:6:PHE:CE1	1:C:141:GLN:HG2	2.47	0.49
1:A:310:ASP:OD1	5:A:702:HOH:O	2.19	0.49
1:D:377:CYS:HB2	5:D:803:HOH:O	2.13	0.49
1:G:327:ILE:HD12	1:G:327:ILE:N	2.27	0.49
1:G:460:ALA:HB1	1:G:461:PRO:HD2	1.94	0.49
1:H:21:HIS:HB2	1:H:156:LEU:HD23	1.95	0.49
1:C:219:GLN:HB2	5:C:6483:HOH:O	2.12	0.48
1:C:507:LYS:NZ	1:C:529:THR:OG1	2.44	0.48
1:F:460:ALA:HB1	1:F:461:PRO:HD2	1.94	0.48
1:G:68:VAL:HG11	1:G:432:SER:HB3	1.94	0.48
1:D:342:ARG:HD3	5:D:904:HOH:O	2.12	0.48
1:A:210:LYS:HG2	1:A:336:LEU:HD13	1.95	0.48
2:F:601:TD6:C2	2:F:601:TD6:HN4A	2.27	0.48
1:G:272:ALA:HB2	1:G:352[B]:LEU:HD23	1.96	0.48
1:E:71[B]:GLN:HB3	1:E:72:PRO:HD2	1.95	0.48
2:C:601:TD6:N4'	2:C:601:TD6:H11	2.16	0.48
2:H:601:TD6:HN4A	2:H:601:TD6:C2	2.27	0.48
1:D:382:GLU:HG2	1:D:383:GLN:HG2	1.96	0.47
1:F:253:LEU:HD11	1:F:413:ARG:HG3	1.95	0.47
1:A:134:ILE:HD11	1:A:155:ALA:HB2	1.96	0.47
5:E:701:HOH:O	1:F:117:ASN:OD1	2.20	0.47
1:F:146[B]:ARG:NH1	5:F:723:HOH:O	2.47	0.47
1:H:210:LYS:CE	1:H:336:LEU:HD11	2.45	0.47
1:A:14:ILE:HG12	1:A:152[A]:ILE:HD11	1.96	0.47
1:F:327:ILE:N	1:F:327:ILE:HD12	2.30	0.47
1:G:342:ARG:HD3	5:G:803:HOH:O	2.14	0.47
1:H:70:LYS:NZ	5:H:729:HOH:O	2.48	0.47
1:D:9:ARG:HD2	1:D:182:GLY:C	2.35	0.46
1:D:18:LEU:CD2	1:D:156:LEU:HD21	2.45	0.46
1:D:434:LYS:NZ	5:D:732:HOH:O	2.48	0.46
1:D:97:GLY:HA2	1:D:161:ALA:HB1	1.97	0.46
1:G:95:LEU:HD11	1:H:120:ILE:HG22	1.96	0.46
1:F:134:ILE:HD11	1:F:155:ALA:HB2	1.98	0.46
1:A:51:THR:OG1	4:A:603:GOL:H12	2.15	0.46
1:B:1:MET:N	5:B:721:HOH:O	2.49	0.46
1:A:68:VAL:HG11	1:A:432:SER:HB3	1.97	0.46
1:H:343:GLN:CD	1:H:344:PRO:HD2	2.36	0.46
1:D:205:ARG:NH1	5:D:734:HOH:O	2.48	0.46
2:D:601:TD6:HN4A	2:D:601:TD6:C2	2.29	0.46
1:A:29:ALA:HB2	1:A:58:LEU:HD22	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:327:ILE:HD12	1:E:327:ILE:N	2.30	0.46
1:F:507:LYS:HD2	5:F:752:HOH:O	2.16	0.45
1:G:15[A]:LEU:CD1	1:G:40:ALA:HB3	2.41	0.45
1:G:68:VAL:HG21	1:G:428:VAL:HG13	1.98	0.45
1:B:460:ALA:HB1	1:B:461:PRO:HD2	1.98	0.45
1:H:255:GLN:NE2	1:H:409:VAL:H	2.02	0.45
1:B:327:ILE:N	1:B:327:ILE:HD12	2.31	0.45
1:G:15[B]:LEU:HD23	1:G:41:ALA:CA	2.46	0.45
1:C:376:ILE:HD11	1:C:439[A]:ILE:HD11	1.97	0.45
5:C:6751:HOH:O	1:E:382:GLU:HG3	2.15	0.45
1:C:342:ARG:HD3	5:C:6222:HOH:O	2.17	0.45
1:E:465:ILE:HD11	1:E:521:PHE:CZ	2.50	0.45
1:A:183:LEU:O	1:A:187:GLN:HG3	2.17	0.45
1:F:382:GLU:HG2	1:F:383:GLN:HG2	1.98	0.45
1:G:456[B]:ARG:NH1	1:G:505:GLU:OE1	2.50	0.45
1:A:376:ILE:HD11	1:A:439[A]:ILE:HD11	1.99	0.45
1:C:15[B]:LEU:HD23	1:C:41:ALA:CA	2.47	0.45
1:D:342:ARG:HD2	5:D:710:HOH:O	2.16	0.44
1:G:15[B]:LEU:HD23	1:G:41:ALA:HA	1.98	0.44
1:H:293:ARG:NH2	1:H:550[A]:LEU:HD11	2.33	0.44
1:H:71[B]:GLN:NE2	5:H:731:HOH:O	2.49	0.44
1:E:71[A]:GLN:NE2	5:E:710:HOH:O	2.30	0.44
1:F:341:LYS:NZ	5:F:727:HOH:O	2.49	0.44
1:B:43:GLU:OE1	5:B:701:HOH:O	2.20	0.43
1:C:507:LYS:HE3	5:C:6399:HOH:O	2.18	0.43
1:D:465:ILE:HD11	1:D:521:PHE:CZ	2.52	0.43
1:F:29:ALA:HB2	1:F:58:LEU:HD22	2.00	0.43
1:G:15[B]:LEU:CD2	1:G:41:ALA:N	2.81	0.43
1:G:15[B]:LEU:HD23	1:G:41:ALA:N	2.33	0.43
1:E:29:ALA:HB2	1:E:58:LEU:HD22	2.00	0.43
1:D:146[C]:ARG:HH22	1:D:188:ARG:HB3	1.83	0.43
1:H:8:ARG:NH2	1:H:43:GLU:OE2	2.51	0.43
1:D:327:ILE:N	1:D:327:ILE:HD12	2.33	0.43
1:A:292:LYS:HE2	1:A:296:GLN:NE2	2.33	0.43
1:C:550[B]:LEU:HD12	5:C:6195:HOH:O	2.18	0.43
1:A:255:GLN:HG2	1:A:407:TYR:O	2.19	0.43
2:C:601:TD6:C2	2:C:601:TD6:HN4A	2.31	0.43
1:G:298[A]:GLN:O	1:G:321:HIS:HE1	2.02	0.43
1:D:539:ASP:HB3	5:D:719:HOH:O	2.18	0.43
1:A:14:ILE:HA	1:A:152[A]:ILE:CD1	2.49	0.43
2:G:601:TD6:HN4A	2:G:601:TD6:C2	2.30	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:ILE:HG12	1:C:152:ILE:HD11	2.01	0.42
1:C:278[B]:GLN:OE1	5:C:6104:HOH:O	2.22	0.42
1:D:457:GLN:HG3	5:D:760:HOH:O	2.18	0.42
1:E:273:THR:O	1:E:277:GLN:HG3	2.18	0.42
1:E:9:ARG:HD2	1:E:182:GLY:C	2.40	0.42
1:F:9:ARG:NE	5:F:701:HOH:O	2.27	0.42
1:H:456:ARG:NH1	5:H:703:HOH:O	2.24	0.42
2:E:601:TD6:C2	2:E:601:TD6:HN4A	2.32	0.42
1:H:146[B]:ARG:HG3	5:H:951:HOH:O	2.19	0.42
1:A:210:LYS:HG3	5:A:1097:HOH:O	2.20	0.42
1:B:526[B]:ARG:HA	1:B:526[B]:ARG:HD3	1.87	0.42
1:G:29:ALA:HB2	1:G:58:LEU:HD22	2.02	0.42
1:C:374:HIS:NE2	4:C:604:GOL:H11	2.35	0.42
1:E:87:TYR:HB3	1:E:88:PRO:HD3	2.01	0.42
1:B:278:GLN:HG2	5:B:1344:HOH:O	2.20	0.42
1:F:14:ILE:HG12	1:F:152[A]:ILE:HD11	2.02	0.42
1:F:392:LEU:HB2	2:F:601:TD6:O2B	2.20	0.42
1:D:515:GLN:HG2	5:D:1131:HOH:O	2.20	0.42
1:F:146[B]:ARG:HD3	1:H:320:HIS:O	2.18	0.42
1:G:498:GLU:HB3	5:G:745:HOH:O	2.19	0.42
1:C:14:ILE:HA	1:C:152:ILE:CD1	2.50	0.41
1:C:15[B]:LEU:HD21	1:C:41:ALA:HB2	2.02	0.41
1:C:343[A]:GLN:CD	1:C:343[A]:GLN:H	2.23	0.41
1:A:144:PRO:HB2	1:A:146[A]:ARG:HG2	2.02	0.41
1:A:151:THR:HG21	5:A:1369:HOH:O	2.20	0.41
1:B:498[B]:GLU:HG2	5:B:1007:HOH:O	2.20	0.41
1:D:141:GLN:NE2	5:D:735:HOH:O	2.48	0.41
1:G:507:LYS:HD2	5:G:775:HOH:O	2.20	0.41
1:C:195:ASP:OD2	1:C:197:LYS:HE2	2.19	0.41
1:C:465:ILE:HD11	1:C:521:PHE:CZ	2.55	0.41
1:D:144:PRO:HB2	1:D:146[A]:ARG:HG2	2.01	0.41
1:E:255:GLN:NE2	1:E:409:VAL:H	2.04	0.41
1:D:355:GLN:HB3	1:D:556:LEU:HD13	2.03	0.41
1:F:144:PRO:HB2	1:F:146[A]:ARG:HG2	2.03	0.41
1:F:31:GLY:HA3	1:F:78:THR:HB	2.01	0.41
1:G:144:PRO:HB2	1:G:146[A]:ARG:HG2	2.01	0.41
1:A:146[A]:ARG:NH1	5:A:723:HOH:O	2.42	0.41
1:G:510:ARG:NH2	5:G:745:HOH:O	2.53	0.41
1:G:68:VAL:CG2	1:G:428:VAL:HG13	2.51	0.41
1:H:255:GLN:HG2	1:H:407:TYR:O	2.21	0.41
1:H:70:LYS:HE3	5:H:1149:HOH:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:VAL:HG13	1:B:394:VAL:N	2.36	0.41
1:C:377:CYS:HB2	5:C:6376:HOH:O	2.21	0.41
1:G:255:GLN:NE2	1:G:409:VAL:H	2.04	0.41
1:E:439[B]:ILE:O	1:E:439[B]:ILE:HG23	2.21	0.41
1:H:219:GLN:HG2	1:H:340[B]:GLU:OE2	2.21	0.41
1:A:277:GLN:HG2	5:A:1331:HOH:O	2.20	0.40
1:C:298:GLN:O	1:C:321:HIS:HE1	2.03	0.40
1:C:51:THR:OG1	4:C:603:GOL:H12	2.21	0.40
1:E:197:LYS:HE2	1:E:197:LYS:HB2	1.88	0.40
1:A:30:PRO:HG2	2:B:601:TD6:CM4	2.51	0.40
1:B:144:PRO:HB2	1:B:146[A]:ARG:HG2	2.04	0.40
1:D:392:LEU:HB2	2:D:601:TD6:O2B	2.22	0.40
1:E:298[B]:GLN:NE2	1:E:317:ASP:OD1	2.41	0.40
1:E:68:VAL:HG11	1:E:432:SER:HB3	2.03	0.40
1:B:271:LYS:NZ	1:B:556:LEU:OXT	2.54	0.40
1:C:255:GLN:HG2	1:C:407:TYR:O	2.21	0.40
1:A:327:ILE:HD12	1:A:327:ILE:N	2.36	0.40
1:E:312[A]:ILE:HG22	5:E:1172:HOH:O	2.21	0.40
1:F:341:LYS:NZ	5:F:720:HOH:O	2.41	0.40
1:H:377:CYS:HB2	5:H:776:HOH:O	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:GLU:OE2	5:C:6101:HOH:O[1_645]	2.14	0.06
5:B:1020:HOH:O	5:C:6101:HOH:O[1_645]	2.14	0.06
5:B:898:HOH:O	5:C:6101:HOH:O[1_645]	2.17	0.03
5:B:1380:HOH:O	5:C:6119:HOH:O[1_645]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	574/556 (103%)	561 (98%)	12 (2%)	1 (0%)	52	25
1	B	565/556 (102%)	551 (98%)	14 (2%)	0	100	100
1	C	568/556 (102%)	556 (98%)	11 (2%)	1 (0%)	52	25
1	D	566/556 (102%)	555 (98%)	10 (2%)	1 (0%)	52	25
1	E	571/556 (103%)	559 (98%)	11 (2%)	1 (0%)	52	25
1	F	562/556 (101%)	549 (98%)	13 (2%)	0	100	100
1	G	571/556 (103%)	557 (98%)	14 (2%)	0	100	100
1	H	567/556 (102%)	553 (98%)	13 (2%)	1 (0%)	52	25
All	All	4544/4448 (102%)	4441 (98%)	98 (2%)	5 (0%)	56	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	391	SER
1	A	391	SER
1	C	391	SER
1	D	391	SER
1	H	391	SER

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	469/452 (104%)	466 (99%)	3 (1%)	90	78
1	B	460/452 (102%)	456 (99%)	4 (1%)	84	66
1	C	461/452 (102%)	457 (99%)	4 (1%)	84	66
1	D	461/452 (102%)	457 (99%)	4 (1%)	84	66
1	E	465/452 (103%)	460 (99%)	5 (1%)	80	58
1	F	454/452 (100%)	450 (99%)	4 (1%)	84	66
1	G	463/452 (102%)	459 (99%)	4 (1%)	84	66
1	H	459/452 (102%)	455 (99%)	4 (1%)	84	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3692/3616 (102%)	3660 (99%)	32 (1%)	84	66

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	TYR
1	A	391	SER
1	A	447	TYR
1	B	87	TYR
1	B	325	ARG
1	B	391	SER
1	B	447	TYR
1	C	87	TYR
1	C	325	ARG
1	C	391	SER
1	C	447	TYR
1	D	87	TYR
1	D	325	ARG
1	D	391	SER
1	D	447	TYR
1	E	87	TYR
1	E	325	ARG
1	E	382	GLU
1	E	391	SER
1	E	447	TYR
1	F	87	TYR
1	F	325	ARG
1	F	391	SER
1	F	447	TYR
1	G	87	TYR
1	G	325	ARG
1	G	391	SER
1	G	447	TYR
1	H	87	TYR
1	H	325	ARG
1	H	391	SER
1	H	447	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	219	GLN
1	A	255	GLN
1	A	278	GLN
1	B	132	HIS
1	B	255	GLN
1	B	544	GLN
1	C	255	GLN
1	C	358	GLN
1	D	141	GLN
1	D	255	GLN
1	D	544	GLN
1	E	129	HIS
1	E	255	GLN
1	E	278	GLN
1	E	538	ASN
1	F	255	GLN
1	F	544	GLN
1	G	255	GLN
1	H	141	GLN
1	H	255	GLN
1	H	544	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 9 are monoatomic - leaving 22 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
2	TD6	A	601	3	24,34,34	1.39	6 (25%)	32,50,50	1.91	8 (25%)
4	GOL	A	603	-	5,5,5	0.35	0	5,5,5	0.51	0
4	GOL	A	604	-	5,5,5	0.37	0	5,5,5	0.28	0
2	TD6	B	601	3	24,34,34	1.36	4 (16%)	32,50,50	2.00	9 (28%)
4	GOL	B	603	-	5,5,5	0.43	0	5,5,5	0.43	0
2	TD6	C	601	3	24,34,34	1.35	5 (20%)	32,50,50	1.92	9 (28%)
4	GOL	C	603	-	5,5,5	0.28	0	5,5,5	0.36	0
4	GOL	C	604	-	5,5,5	0.42	0	5,5,5	0.53	0
2	TD6	D	601	3	24,34,34	1.32	4 (16%)	32,50,50	1.92	9 (28%)
4	GOL	D	603	-	5,5,5	0.35	0	5,5,5	0.40	0
4	GOL	D	604	-	5,5,5	0.31	0	5,5,5	0.19	0
2	TD6	E	601	3	24,34,34	1.31	3 (12%)	32,50,50	2.12	9 (28%)
4	GOL	E	603	-	5,5,5	0.33	0	5,5,5	0.49	0
4	GOL	E	604	-	5,5,5	0.36	0	5,5,5	0.33	0
2	TD6	F	601	3	24,34,34	1.30	3 (12%)	32,50,50	1.88	10 (31%)
4	GOL	F	603	-	5,5,5	0.29	0	5,5,5	0.40	0
2	TD6	G	601	3	24,34,34	1.32	4 (16%)	32,50,50	1.89	9 (28%)
4	GOL	G	603	-	5,5,5	0.32	0	5,5,5	0.26	0
4	GOL	G	604	-	5,5,5	0.31	0	5,5,5	0.30	0
2	TD6	H	601	3	24,34,34	1.87	9 (37%)	32,50,50	2.26	8 (25%)
4	GOL	H	603	-	5,5,5	0.38	0	5,5,5	0.27	0
4	GOL	H	604	-	5,5,5	0.33	0	5,5,5	0.23	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	TD6	A	601	3	-	0/19/26/26	0/2/2/2
4	GOL	A	603	-	-	0/4/4/4	0/0/0/0
4	GOL	A	604	-	-	0/4/4/4	0/0/0/0
2	TD6	B	601	3	-	0/19/26/26	0/2/2/2
4	GOL	B	603	-	-	0/4/4/4	0/0/0/0
2	TD6	C	601	3	-	0/19/26/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	603	-	-	0/4/4/4	0/0/0/0
4	GOL	C	604	-	-	0/4/4/4	0/0/0/0
2	TD6	D	601	3	-	0/19/26/26	0/2/2/2
4	GOL	D	603	-	-	0/4/4/4	0/0/0/0
4	GOL	D	604	-	-	0/4/4/4	0/0/0/0
2	TD6	E	601	3	-	0/19/26/26	0/2/2/2
4	GOL	E	603	-	-	0/4/4/4	0/0/0/0
4	GOL	E	604	-	-	0/4/4/4	0/0/0/0
2	TD6	F	601	3	-	0/19/26/26	0/2/2/2
4	GOL	F	603	-	-	0/4/4/4	0/0/0/0
2	TD6	G	601	3	-	0/19/26/26	0/2/2/2
4	GOL	G	603	-	-	0/4/4/4	0/0/0/0
4	GOL	G	604	-	-	0/4/4/4	0/0/0/0
2	TD6	H	601	3	-	0/19/26/26	0/2/2/2
4	GOL	H	603	-	-	0/4/4/4	0/0/0/0
4	GOL	H	604	-	-	0/4/4/4	0/0/0/0

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	TD6	PB-O1B	-3.37	1.43	1.54
2	H	601	TD6	C4-N3	-3.01	1.32	1.39
2	H	601	TD6	PA-O2A	-2.99	1.42	1.55
2	H	601	TD6	PB-O2B	-2.69	1.42	1.50
2	B	601	TD6	C5'-C4'	-2.40	1.38	1.42
2	A	601	TD6	C5'-C4'	-2.35	1.38	1.42
2	H	601	TD6	C2-N3	-2.32	1.30	1.35
2	A	601	TD6	C4-N3	-2.28	1.34	1.39
2	C	601	TD6	C5'-C4'	-2.13	1.39	1.42
2	H	601	TD6	C5'-C4'	-2.05	1.39	1.42
2	D	601	TD6	C7'-C5'	2.01	1.55	1.51
2	C	601	TD6	C7'-C5'	2.02	1.55	1.51
2	A	601	TD6	C7'-C5'	2.05	1.55	1.51
2	H	601	TD6	C6-C7	2.09	1.57	1.50
2	G	601	TD6	C7'-C5'	2.13	1.55	1.51
2	A	601	TD6	C6-C7	2.15	1.57	1.50
2	F	601	TD6	C4'-N3'	2.18	1.38	1.35
2	B	601	TD6	C6-C7	2.27	1.57	1.50
2	C	601	TD6	C6-C7	2.29	1.57	1.50
2	E	601	TD6	C6-C7	2.31	1.57	1.50
2	F	601	TD6	CM2-C2'	2.37	1.57	1.49
2	G	601	TD6	C6-C7	2.38	1.58	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	TD6	C6-C7	2.40	1.58	1.50
2	H	601	TD6	CM2-C2'	2.42	1.57	1.49
2	C	601	TD6	CM2-C2'	2.56	1.57	1.49
2	A	601	TD6	CM4-C4	2.60	1.55	1.49
2	B	601	TD6	CM2-C2'	2.61	1.57	1.49
2	E	601	TD6	CM2-C2'	2.64	1.57	1.49
2	A	601	TD6	CM2-C2'	2.65	1.57	1.49
2	D	601	TD6	CM2-C2'	2.66	1.57	1.49
2	G	601	TD6	CM2-C2'	2.67	1.58	1.49
2	E	601	TD6	CM4-C4	2.92	1.56	1.49
2	D	601	TD6	CM4-C4	2.95	1.56	1.49
2	F	601	TD6	CM4-C4	3.00	1.56	1.49
2	H	601	TD6	C7'-C5'	3.00	1.57	1.51
2	G	601	TD6	CM4-C4	3.01	1.56	1.49
2	C	601	TD6	CM4-C4	3.17	1.56	1.49
2	B	601	TD6	CM4-C4	3.20	1.56	1.49

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	TD6	C13-CLB-C11	-6.72	106.82	114.74
2	H	601	TD6	C13-CLB-C11	-6.63	106.93	114.74
2	E	601	TD6	C13-CLB-C11	-6.15	107.49	114.74
2	G	601	TD6	C13-CLB-C11	-5.25	108.55	114.74
2	C	601	TD6	C13-CLB-C11	-5.10	108.73	114.74
2	D	601	TD6	C13-CLB-C11	-4.82	109.06	114.74
2	F	601	TD6	C13-CLB-C11	-4.75	109.14	114.74
2	A	601	TD6	C13-CLB-C11	-4.48	109.46	114.74
2	H	601	TD6	OL1-C11-CLB	-4.10	99.73	109.73
2	H	601	TD6	CM4-C4-C5	-3.83	120.81	128.91
2	D	601	TD6	CM4-C4-C5	-3.50	121.51	128.91
2	H	601	TD6	C5'-C6'-N1'	-3.26	118.16	123.86
2	F	601	TD6	C5'-C6'-N1'	-3.13	118.39	123.86
2	A	601	TD6	CM4-C4-C5	-3.10	122.34	128.91
2	G	601	TD6	CM4-C4-C5	-3.10	122.36	128.91
2	C	601	TD6	CM4-C4-C5	-2.97	122.62	128.91
2	E	601	TD6	CM4-C4-C5	-2.96	122.65	128.91
2	E	601	TD6	C5'-C6'-N1'	-2.82	118.93	123.86
2	A	601	TD6	N1'-C2'-N3'	-2.80	120.25	125.50
2	D	601	TD6	C5'-C6'-N1'	-2.78	118.99	123.86
2	C	601	TD6	C5'-C6'-N1'	-2.77	119.01	123.86
2	G	601	TD6	N1'-C2'-N3'	-2.77	120.31	125.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	TD6	CM4-C4-C5	-2.71	123.17	128.91
2	F	601	TD6	C7'-N3-C2	-2.66	119.49	124.42
2	A	601	TD6	C5'-C6'-N1'	-2.65	119.24	123.86
2	E	601	TD6	N1'-C2'-N3'	-2.62	120.59	125.50
2	B	601	TD6	N1'-C2'-N3'	-2.55	120.71	125.50
2	F	601	TD6	CM4-C4-C5	-2.54	123.52	128.91
2	G	601	TD6	C5'-C6'-N1'	-2.52	119.45	123.86
2	C	601	TD6	C7'-N3-C2	-2.49	119.80	124.42
2	D	601	TD6	N1'-C2'-N3'	-2.48	120.85	125.50
2	A	601	TD6	OL1-C11-CLB	-2.45	103.75	109.73
2	C	601	TD6	N1'-C2'-N3'	-2.45	120.91	125.50
2	E	601	TD6	C7'-N3-C2	-2.39	119.97	124.42
2	B	601	TD6	C5'-C6'-N1'	-2.32	119.80	123.86
2	G	601	TD6	C7'-N3-C2	-2.19	120.36	124.42
2	F	601	TD6	N1'-C2'-N3'	-2.08	121.59	125.50
2	B	601	TD6	C7'-N3-C2	-2.05	120.62	124.42
2	H	601	TD6	CM2-C2'-N1'	2.12	119.67	117.05
2	F	601	TD6	CM2-C2'-N1'	2.13	119.68	117.05
2	D	601	TD6	C6'-C5'-C4'	2.16	118.70	115.65
2	D	601	TD6	CM2-C2'-N1'	2.39	120.00	117.05
2	E	601	TD6	CM2-C2'-N1'	2.42	120.04	117.05
2	B	601	TD6	C6'-N1'-C2'	2.45	120.58	115.92
2	C	601	TD6	CM2-C2'-N1'	2.46	120.08	117.05
2	F	601	TD6	C6'-C5'-C4'	2.50	119.18	115.65
2	D	601	TD6	C6'-N1'-C2'	2.76	121.17	115.92
2	G	601	TD6	C6'-N1'-C2'	2.80	121.24	115.92
2	A	601	TD6	C6'-N1'-C2'	2.84	121.31	115.92
2	C	601	TD6	C6'-N1'-C2'	2.87	121.37	115.92
2	F	601	TD6	C5-C4-N3	2.87	114.65	107.94
2	F	601	TD6	C6'-N1'-C2'	2.91	121.45	115.92
2	B	601	TD6	C5-C4-N3	2.95	114.82	107.94
2	G	601	TD6	CM2-C2'-N1'	2.97	120.71	117.05
2	B	601	TD6	CM2-C2'-N1'	2.98	120.73	117.05
2	C	601	TD6	C5-C4-N3	3.02	115.00	107.94
2	H	601	TD6	C6'-N1'-C2'	3.09	121.78	115.92
2	E	601	TD6	C5-C4-N3	3.12	115.23	107.94
2	E	601	TD6	C6'-N1'-C2'	3.13	121.87	115.92
2	G	601	TD6	C5-C4-N3	3.19	115.38	107.94
2	G	601	TD6	C6-C5-S1	3.24	124.77	120.24
2	A	601	TD6	C5-C4-N3	3.26	115.55	107.94
2	D	601	TD6	C5-C4-N3	3.28	115.61	107.94
2	B	601	TD6	C6-C5-S1	3.65	125.34	120.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	TD6	C6-C5-S1	3.67	125.38	120.24
2	A	601	TD6	C6-C5-S1	4.22	126.14	120.24
2	C	601	TD6	C6-C5-S1	4.29	126.24	120.24
2	H	601	TD6	C6-C5-S1	4.50	126.54	120.24
2	H	601	TD6	C5-C4-N3	4.56	118.61	107.94
2	D	601	TD6	C6-C5-S1	4.85	127.03	120.24
2	E	601	TD6	C6-C5-S1	5.38	127.77	120.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	TD6	4	0
4	A	603	GOL	1	0
2	B	601	TD6	5	0
2	C	601	TD6	4	0
4	C	603	GOL	1	0
4	C	604	GOL	1	0
2	D	601	TD6	5	0
2	E	601	TD6	4	0
2	F	601	TD6	5	0
2	G	601	TD6	4	0
2	H	601	TD6	4	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 ⓘ

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	556/556 (100%)	-0.29	6 (1%) 82 84	5, 11, 28, 48	0
1	B	556/556 (100%)	-0.35	7 (1%) 79 82	5, 11, 28, 46	0
1	C	556/556 (100%)	-0.30	6 (1%) 82 84	6, 12, 28, 54	0
1	D	556/556 (100%)	-0.12	14 (2%) 61 64	6, 15, 36, 56	0
1	E	556/556 (100%)	-0.29	7 (1%) 79 82	6, 11, 30, 48	0
1	F	556/556 (100%)	-0.32	5 (0%) 85 87	6, 12, 27, 50	0
1	G	556/556 (100%)	-0.31	5 (0%) 85 87	6, 12, 29, 45	0
1	H	556/556 (100%)	-0.16	10 (1%) 71 75	7, 14, 34, 62	0
All	All	4448/4448 (100%)	-0.27	60 (1%) 79 82	5, 12, 31, 62	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	347	VAL	4.3
1	E	178	MET	3.8
1	B	1	MET	3.6
1	H	555	HIS	3.6
1	A	556	LEU	3.5
1	D	482	GLN	3.3
1	E	556	LEU	3.3
1	A	178	MET	3.3
1	G	555	HIS	3.2
1	D	1	MET	3.1
1	A	1	MET	3.1
1	D	523	ASP	3.0
1	F	1	MET	3.0
1	H	523[A]	ASP	3.0
1	D	522	ALA	3.0
1	H	522	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	555	HIS	2.9
1	H	178	MET	2.9
1	C	176	GLY	2.9
1	D	479	PRO	2.8
1	B	556	LEU	2.8
1	C	177	GLU	2.8
1	H	270	ALA	2.7
1	G	178	MET	2.7
1	D	526[A]	ARG	2.6
1	E	270	ALA	2.6
1	G	556	LEU	2.6
1	H	556	LEU	2.6
1	B	177	GLU	2.5
1	H	343	GLN	2.5
1	G	526	ARG	2.5
1	D	481	PRO	2.4
1	E	1	MET	2.4
1	H	526	ARG	2.4
1	B	482	GLN	2.4
1	C	555	HIS	2.4
1	B	555	HIS	2.4
1	D	515	GLN	2.4
1	F	526	ARG	2.3
1	E	555	HIS	2.3
1	D	177	GLU	2.3
1	B	178	MET	2.2
1	E	439[A]	ILE	2.2
1	C	523	ASP	2.2
1	C	556	LEU	2.2
1	A	482	GLN	2.2
1	G	270	ALA	2.2
1	C	270	ALA	2.2
1	D	176	GLY	2.2
1	H	351	ARG	2.2
1	D	483	SER	2.1
1	F	556	LEU	2.1
1	F	178	MET	2.1
1	A	270	ALA	2.1
1	H	177	GLU	2.1
1	D	527	THR	2.1
1	D	477	LEU	2.1
1	F	482	GLN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	177	GLU	2.0
1	B	180	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	G	604	6/6	0.90	0.17	10.62	24,29,33,35	0
4	GOL	C	604	6/6	0.89	0.17	5.93	23,30,34,36	0
4	GOL	D	604	6/6	0.80	0.16	5.00	31,37,40,42	0
4	GOL	E	604	6/6	0.83	0.16	4.17	33,40,41,43	0
4	GOL	A	604	6/6	0.88	0.15	3.61	28,33,37,38	0
4	GOL	H	604	6/6	0.72	0.17	3.21	33,39,43,44	0
4	GOL	F	603	6/6	0.96	0.09	2.26	15,18,19,19	0
4	GOL	G	603	6/6	0.92	0.13	1.69	18,21,22,24	0
4	GOL	B	603	6/6	0.95	0.08	1.46	15,19,20,20	0
4	GOL	H	603	6/6	0.94	0.09	1.16	17,19,20,22	0
4	GOL	D	603	6/6	0.94	0.10	1.11	19,21,23,24	0
4	GOL	C	603	6/6	0.93	0.10	1.06	15,20,22,22	0
3	MN	G	605	1/1	1.00	0.08	1.00	36,36,36,36	0
2	TD6	H	601	33/33	0.97	0.08	0.62	8,12,21,26	0
4	GOL	A	603	6/6	0.96	0.08	0.57	12,15,16,16	0
3	MN	H	602	1/1	1.00	0.08	0.56	16,16,16,16	0
2	TD6	G	601	33/33	0.98	0.07	0.43	8,10,21,27	0
2	TD6	C	601	33/33	0.98	0.07	0.20	7,10,16,21	0
2	TD6	D	601	33/33	0.97	0.07	0.03	9,11,21,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	TD6	B	601	33/33	0.98	0.07	-0.15	7,10,17,22	0
3	MN	D	602	1/1	1.00	0.07	-0.20	18,18,18,18	0
2	TD6	A	601	33/33	0.98	0.07	-0.22	5,8,17,22	0
2	TD6	E	601	33/33	0.98	0.07	-0.24	6,9,20,26	0
3	MN	C	602	1/1	1.00	0.06	-0.39	15,15,15,15	0
3	MN	G	602	1/1	1.00	0.06	-0.46	15,15,15,15	0
3	MN	B	602	1/1	1.00	0.06	-0.60	13,13,13,13	0
4	GOL	E	603	6/6	0.97	0.06	-0.62	12,15,15,16	0
2	TD6	F	601	33/33	0.98	0.07	-0.75	7,10,20,24	0
3	MN	A	602	1/1	1.00	0.06	-0.86	12,12,12,12	0
3	MN	E	602	1/1	1.00	0.05	-1.27	13,13,13,13	0
3	MN	F	602	1/1	1.00	0.04	-1.49	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.