Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 07:44 am GMT

PDB ID	:	4AMW
Title	:	CRYSTAL STRUCTURE OF THE GRACILARIOPSIS LEMANEIFORMIS ALPHA-1,4- GLUCAN LYASE Covalent Intermediate Complex with 5-fluoro-idosyl- fluoride
Authors	:	Rozeboom, H.J.; Yu, S.; Madrid, S.; Kalk, K.H.; Dijkstra, B.W.
Deposited on	:	2012-03-14
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

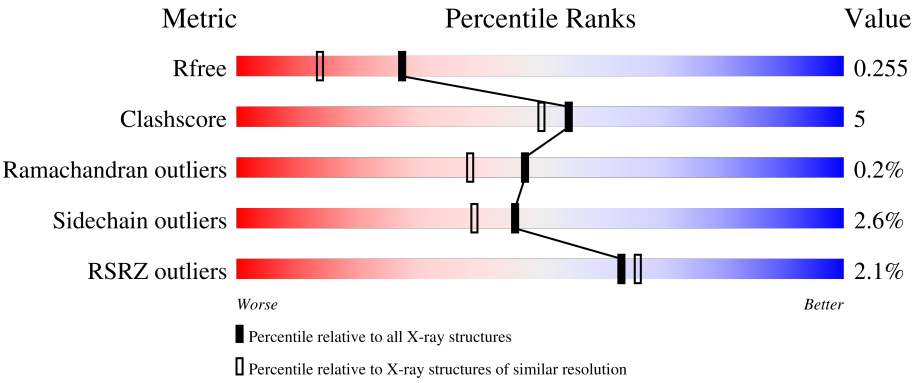
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1027	89% 11%
1	B	1027	3% 89% 10%
1	C	1027	4% 87% 12%
1	D	1027	86% 12%

2 Entry composition

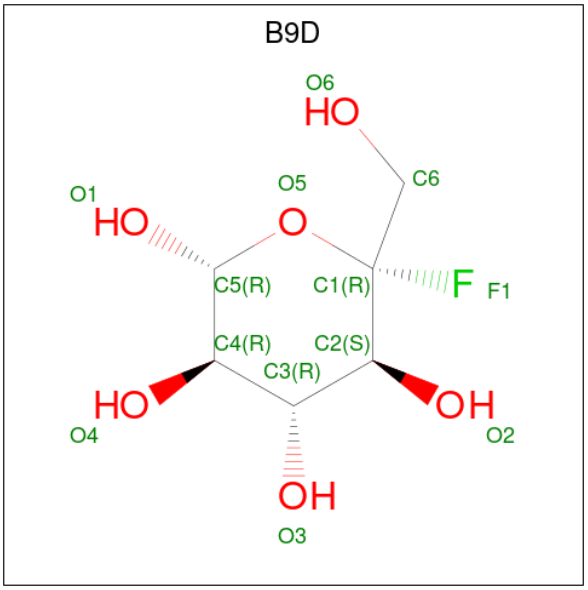
There are 5 unique types of molecules in this entry. The entry contains 35670 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALPHA-1,4-GLUCAN LYASE ISOZYME 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1025	Total	C	N	O	S	0	1	0
			8170	5140	1386	1596	48			
1	B	1025	Total	C	N	O	S	0	0	0
			8162	5135	1385	1595	47			
1	C	1025	Total	C	N	O	S	0	0	0
			8162	5135	1385	1595	47			
1	D	1025	Total	C	N	O	S	0	0	0
			8162	5135	1385	1595	47			

- Molecule 2 is 5-fluoro-alpha-L-idopyranose (three-letter code: B9D) (formula: $C_6H_{11}FO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	O	0	0
			12	6	1	5		
2	B	1	Total	C	F	O	0	0
			12	6	1	5		

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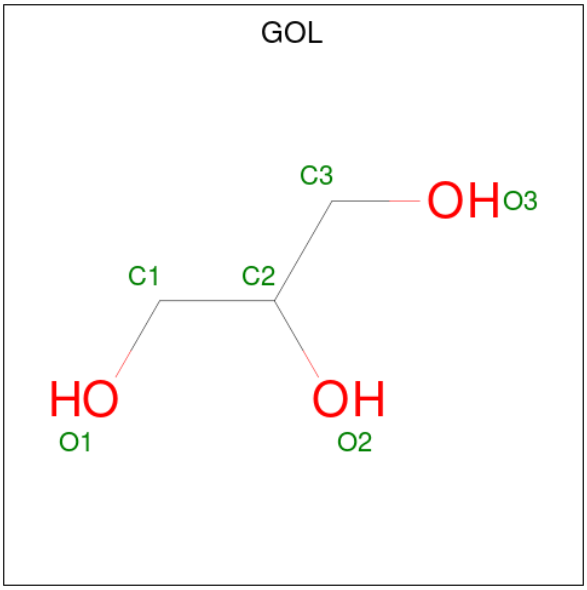
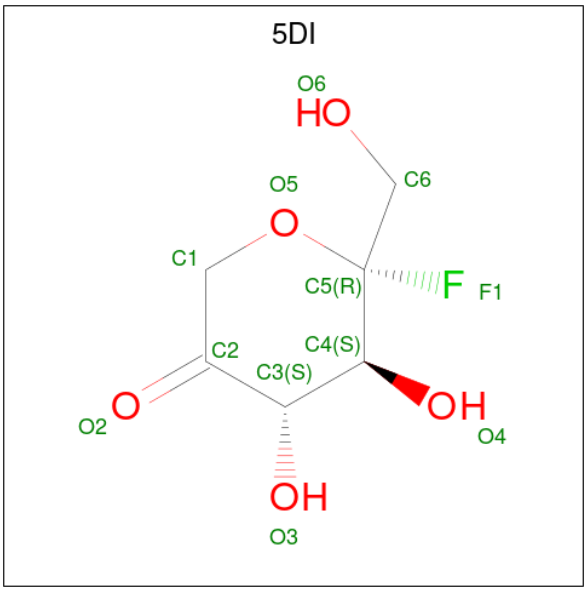
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C F O 12 6 1 5	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is alpha-D-threo-hexo-2,5-diulo-2,6-pyranosyl fluoride (three-letter code: 5DI) (formula: $C_6H_9FO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C F O 12 6 1 5	0	0

- Molecule 5 is water.

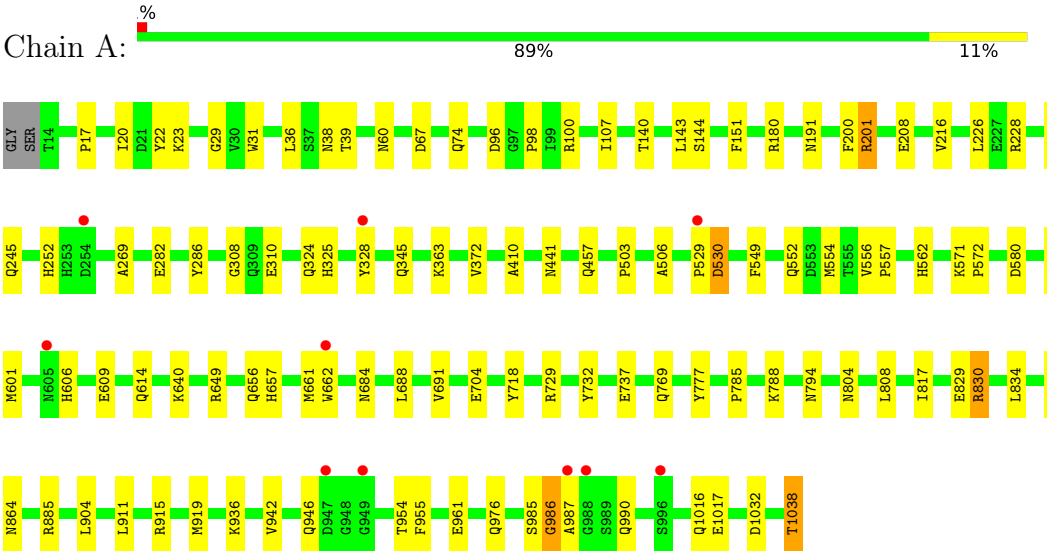
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	901	Total O 901 901	0	0
5	B	548	Total O 548 548	0	0
5	C	581	Total O 581 581	0	0
5	D	894	Total O 894 894	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

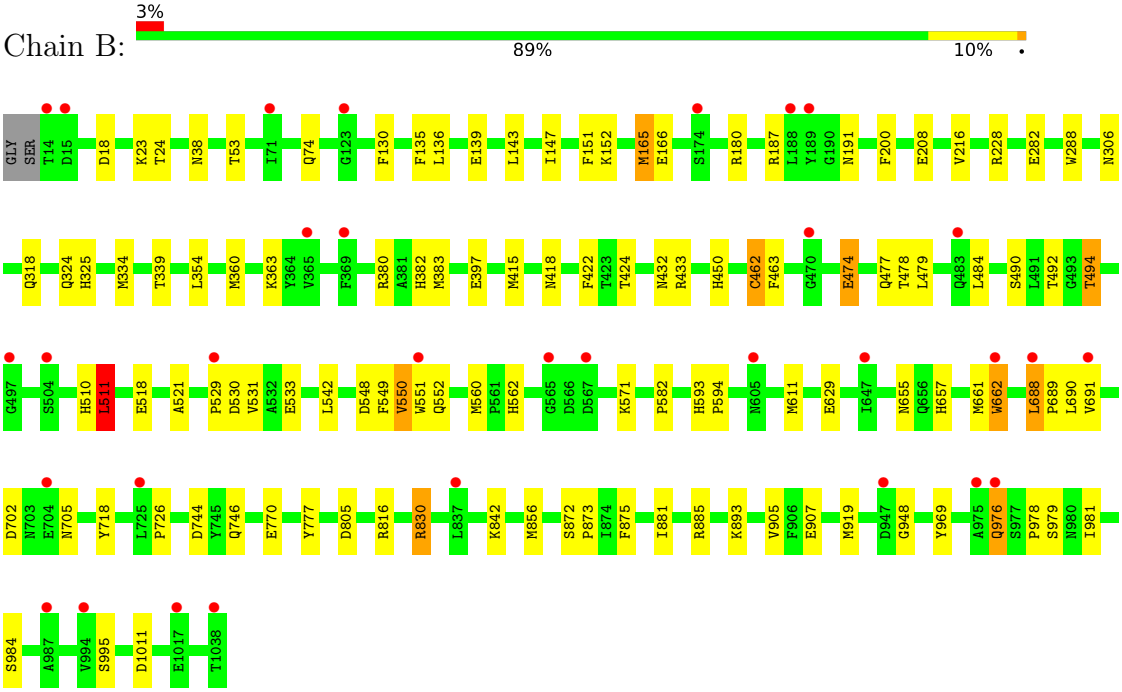
• Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1

Chain A:



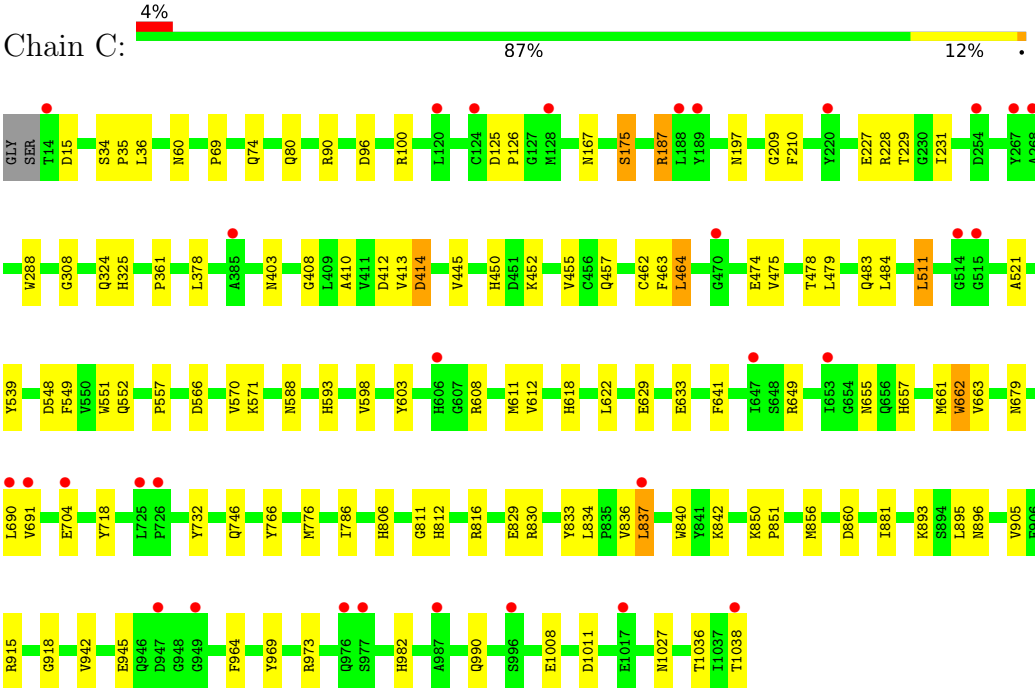
• Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1

Chain B:



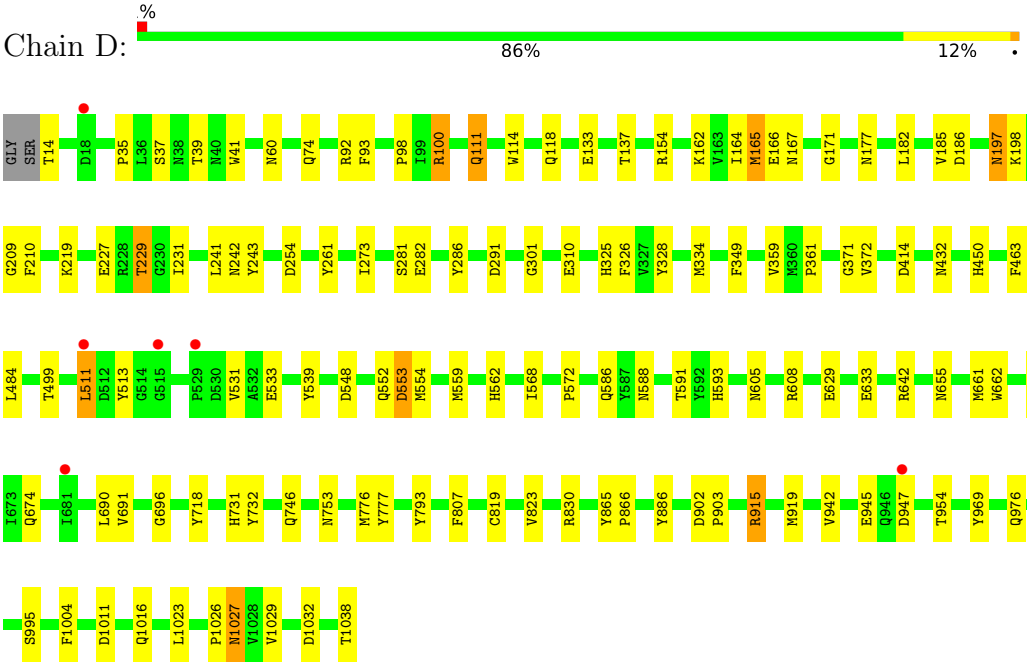
• Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1

Chain C:



• Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	92.10Å 97.30Å 136.28Å 80.31° 83.29° 85.21°	Depositor
Resolution (Å)	43.57 – 1.90 43.57 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.5 (43.57-1.90) 93.5 (43.57-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.207 , 0.254 0.208 , 0.255	Depositor DCC
R_{free} test set	17168 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	16.4	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	35670	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5DI, CSO, B9D, GOL

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	0.81	0/8382	0.79	4/11399 (0.0%)
1	B	0.61	1/8374 (0.0%)	0.66	1/11389 (0.0%)
1	C	0.61	0/8374	0.66	2/11389 (0.0%)
1	D	0.78	0/8374	0.78	5/11389 (0.0%)
All	All	0.71	1/33504 (0.0%)	0.73	12/45566 (0.0%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	976	GLN	CA-C	7.14	1.71	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	201	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	D	165	MET	CG-SD-CE	-6.47	89.85	100.20
1	C	464	LEU	CA-CB-CG	-5.95	101.62	115.30
1	D	464	LEU	CA-CB-CG	-5.85	101.85	115.30
1	A	830	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	C	511	LEU	CA-CB-CG	-5.71	102.16	115.30
1	D	291	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	830	ARG	NE-CZ-NH1	5.47	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	201	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	511	LEU	CA-CB-CG	-5.19	103.36	115.30
1	D	201	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	D	553	ASP	CB-CG-OD1	5.05	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	529	PRO	Peptide

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	8170	0	7614	79	0
1	B	8162	0	7606	71	0
1	C	8162	0	7606	81	0
1	D	8162	0	7606	98	0
2	A	12	0	9	0	0
2	B	12	0	9	1	0
2	C	12	0	8	0	0
3	A	24	0	32	1	0
3	B	6	0	8	1	0
3	D	12	0	16	1	0
4	D	12	0	9	4	0
5	A	901	0	0	17	0
5	B	548	0	0	14	0
5	C	581	0	0	7	0
5	D	894	0	0	27	0
All	All	35670	0	30523	328	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 5.

All (328) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:SER:HB2	5:D:2028:HOH:O	1.27	1.34
1:B:462:CYS:HB2	5:B:2303:HOH:O	1.39	1.22
1:C:776:MET:HE2	1:C:786:ILE:HD11	1.25	1.16
1:D:586:GLN:HG2	5:D:2529:HOH:O	1.49	1.10
1:C:776:MET:CE	1:C:786:ILE:HD11	1.81	1.09
1:C:210:PHE:H	1:C:229:THR:HG22	1.19	1.07
1:D:219:LYS:HD2	5:D:2241:HOH:O	1.55	1.06
1:D:182:LEU:HB3	5:D:2208:HOH:O	1.55	1.05
1:A:562:HIS:HD2	1:A:593:HIS:HE1	1.08	1.01
1:D:41:TRP:CD1	5:D:2029:HOH:O	2.27	0.88
1:D:93:PHE:CE1	5:D:2208:HOH:O	2.28	0.85
1:B:38:ASN:HD21	1:B:180:ARG:HH11	1.24	0.84
1:A:562:HIS:HD2	1:A:593:HIS:CE1	1.95	0.82
1:D:210:PHE:H	1:D:229:THR:HG22	1.44	0.81
1:D:463:PHE:CE2	1:D:511:LEU:HD22	2.16	0.80
1:A:1038:THR:HG22	5:A:2863:HOH:O	1.82	0.79
1:C:325:HIS:HD2	5:C:2048:HOH:O	1.66	0.79
1:D:947:ASP:HB2	5:D:2774:HOH:O	1.83	0.79
1:A:38:ASN:HD21	1:A:180:ARG:HH11	1.34	0.76
1:A:601:MET:H	1:A:614:GLN:HE22	1.32	0.75
1:B:976:GLN:HB3	5:B:2527:HOH:O	1.85	0.75
1:C:210:PHE:H	1:C:229:THR:CG2	1.95	0.75
1:C:806:HIS:HE1	1:C:833:TYR:H	1.36	0.73
1:C:227:GLU:HG2	1:C:229:THR:HG23	1.71	0.72
1:B:24:THR:HG21	1:B:318:GLN:OE1	1.89	0.71
1:A:1017:GLU:OE2	5:A:2759:HOH:O	2.08	0.71
1:A:503:PRO:HG2	1:A:506:ALA:HB2	1.72	0.70
1:D:227:GLU:OE2	1:D:229:THR:CG2	2.41	0.69
1:D:513:TYR:HE1	1:D:554:MET:HE2	1.57	0.69
1:D:227:GLU:OE2	1:D:229:THR:HG21	1.92	0.69
1:B:995:SER:HB2	1:B:1011:ASP:HB3	1.75	0.67
1:D:450:HIS:HD2	5:D:2462:HOH:O	1.76	0.67
1:B:382:HIS:CD2	1:B:432:ASN:HB2	2.29	0.67
1:B:905:VAL:HG22	1:B:969:TYR:HB2	1.75	0.67
1:D:976:GLN:HE22	1:D:1016:GLN:HA	1.59	0.67
1:A:640:LYS:HE2	5:A:2599:HOH:O	1.94	0.67
1:D:753:ASN:ND2	5:D:2616:HOH:O	2.26	0.66
1:B:383:MET:HE1	5:B:2251:HOH:O	1.95	0.66
1:A:529:PRO:O	1:A:530:ASP:HB2	1.96	0.65
1:D:562:HIS:HD2	1:D:593:HIS:NE2	1.94	0.65
1:A:562:HIS:CD2	1:A:593:HIS:HE1	2.00	0.64
1:B:200:PHE:HB2	1:B:208:GLU:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:GLU:HB3	5:A:2322:HOH:O	1.97	0.63
1:B:288:TRP:NE1	1:B:324:GLN:OE1	2.30	0.63
1:C:776:MET:HE1	1:C:786:ILE:HD11	1.75	0.63
1:C:227:GLU:OE2	1:C:229:THR:HG21	1.98	0.63
1:D:629:GLU:HG3	1:D:633:GLU:OE2	1.98	0.63
1:C:209:GLY:HA2	1:C:229:THR:HG21	1.81	0.63
1:D:995:SER:HB2	1:D:1011:ASP:HB3	1.81	0.62
1:D:513:TYR:CE1	1:D:554:MET:HE2	2.35	0.62
1:D:513:TYR:CE1	1:D:554:MET:CE	2.83	0.62
1:A:23:LYS:H	1:A:191:ASN:HD21	1.47	0.61
1:A:457:GLN:NE2	1:A:729:ARG:HH11	1.97	0.61
1:B:38:ASN:HD21	1:B:180:ARG:NH1	1.96	0.61
1:A:704:GLU:HG3	5:A:2287:HOH:O	2.00	0.61
1:D:1016:GLN:OE1	5:D:2850:HOH:O	2.16	0.61
1:C:776:MET:CE	1:C:786:ILE:CD1	2.71	0.61
1:A:601:MET:H	1:A:614:GLN:NE2	1.97	0.61
1:A:961:GLU:HG2	5:A:2830:HOH:O	2.00	0.61
1:C:479:LEU:HD12	1:C:484:LEU:HB2	1.83	0.60
1:C:464:LEU:HD22	1:C:475:VAL:HG12	1.82	0.60
1:A:39:THR:HA	1:A:67:ASP:OD2	2.02	0.60
1:D:165:MET:HE1	1:D:326:PHE:CD1	2.36	0.60
1:A:410:ALA:HB2	1:A:457:GLN:HE21	1.67	0.60
1:C:210:PHE:N	1:C:229:THR:HG22	2.04	0.59
1:B:463:PHE:CD2	1:B:511:LEU:HD22	2.38	0.59
1:C:806:HIS:CE1	1:C:833:TYR:H	2.19	0.59
1:C:557:PRO:HD3	1:C:618:HIS:CE1	2.38	0.58
1:D:35:PRO:O	5:D:2029:HOH:O	2.17	0.58
1:D:197:ASN:ND2	5:D:2212:HOH:O	2.35	0.58
1:A:794:ASN:ND2	5:A:2325:HOH:O	2.35	0.58
1:B:657:HIS:HD2	5:B:2220:HOH:O	1.85	0.58
1:C:15:ASP:OD1	1:C:608:ARG:HD3	2.03	0.58
1:D:499:THR:HG23	1:D:568:ILE:HD12	1.86	0.58
1:C:457:GLN:HA	1:C:549:PHE:O	2.04	0.58
1:C:167:ASN:HA	1:C:197:ASN:HA	1.85	0.58
1:D:137:THR:HG21	5:D:2158:HOH:O	2.03	0.58
1:A:554[A]:MET:HE1	1:A:649:ARG:NH1	2.19	0.57
1:B:463:PHE:CE2	1:B:511:LEU:HD22	2.38	0.57
1:C:452:LYS:HE2	5:C:2302:HOH:O	2.04	0.57
1:C:80:GLN:HE22	1:C:90:ARG:HH11	1.51	0.57
1:D:137:THR:HG23	5:D:2154:HOH:O	2.03	0.57
1:D:209:GLY:HA2	1:D:229:THR:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:GLU:OE2	1:C:229:THR:CG2	2.53	0.56
1:C:566:ASP:HB3	1:C:570:VAL:CG2	2.35	0.56
1:C:464:LEU:HD22	1:C:475:VAL:CG1	2.35	0.56
1:D:539:TYR:OH	1:D:552:GLN:NE2	2.34	0.56
1:A:657:HIS:HE1	5:A:2370:HOH:O	1.88	0.56
1:D:165:MET:HG2	1:D:166:GLU:N	2.21	0.56
1:D:165:MET:CE	1:D:326:PHE:CD1	2.89	0.56
1:A:325:HIS:HE1	5:A:2112:HOH:O	1.89	0.56
1:A:554[A]:MET:HE1	1:A:649:ARG:HH12	1.71	0.56
1:B:339:THR:HG22	5:B:2042:HOH:O	2.06	0.55
1:B:560:MET:SD	1:B:571:LYS:HG3	2.46	0.55
1:D:93:PHE:CZ	5:D:2208:HOH:O	2.52	0.55
1:B:380:ARG:HD3	5:B:2237:HOH:O	2.07	0.55
1:D:642:ARG:HD3	5:D:2555:HOH:O	2.06	0.55
1:C:588:ASN:HB3	1:C:593:HIS:CE1	2.42	0.55
1:A:794:ASN:H	3:A:1043:GOL:H31	1.71	0.55
1:D:463:PHE:CD2	1:D:511:LEU:HD13	2.42	0.55
1:A:556:VAL:N	1:A:557:PRO:HA	2.21	0.55
1:D:777:TYR:HE2	1:D:919:MET:CE	2.20	0.55
1:B:463:PHE:CD1	1:B:511:LEU:HD13	2.42	0.54
1:B:842:LYS:HB2	1:B:856:MET:HE1	1.89	0.54
1:D:100:ARG:NH1	5:D:2115:HOH:O	2.40	0.54
1:C:96:ASP:OD1	1:C:187:ARG:HD2	2.08	0.54
1:A:785:PRO:O	1:A:788:LYS:HE3	2.07	0.54
1:B:594:PRO:HG3	5:B:2141:HOH:O	2.07	0.54
1:D:201:ARG:HD3	1:D:310:GLU:O	2.08	0.54
1:B:492:THR:HG23	1:B:494:THR:OG1	2.07	0.54
1:A:100:ARG:HD2	5:A:2054:HOH:O	2.07	0.54
1:C:60:ASN:HB3	1:C:74:GLN:OE1	2.09	0.53
1:D:325:HIS:HE1	5:D:2101:HOH:O	1.90	0.53
1:B:479:LEU:HD12	1:B:484:LEU:HB2	1.90	0.53
1:D:154:ARG:HG2	1:D:166:GLU:HG2	1.90	0.53
1:A:737:GLU:HG3	5:A:2415:HOH:O	2.08	0.53
1:A:20:ILE:HD11	1:A:96:ASP:HB3	1.90	0.53
1:A:226:LEU:H	1:A:804:ASN:ND2	2.06	0.53
1:B:136:LEU:HD23	1:B:147:ILE:HD12	1.89	0.53
1:B:490:SER:HB2	1:B:492:THR:HG22	1.91	0.53
1:C:905:VAL:HG22	1:C:969:TYR:HB2	1.90	0.53
1:A:345:GLN:NE2	1:A:656:GLN:HE22	2.07	0.53
1:A:834:LEU:O	1:A:859:GLY:N	2.30	0.53
1:C:69:PRO:HB2	1:C:175:SER:OG	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:669:THR:HG1	1:D:672:TYR:HD2	1.57	0.53
1:A:22:TYR:OH	1:A:609:GLU:OE1	2.25	0.52
1:B:463:PHE:HB2	1:B:521:ALA:HB1	1.92	0.52
1:B:744:ASP:OD2	3:B:1040:GOL:H31	2.09	0.52
1:A:74:GLN:NE2	5:A:2086:HOH:O	2.42	0.52
1:D:696:GLY:HA3	5:D:2579:HOH:O	2.10	0.52
1:B:510:HIS:C	1:B:511:LEU:HG	2.29	0.52
1:C:464:LEU:HD13	1:C:479:LEU:HD22	1.90	0.52
1:D:450:HIS:HE1	1:D:548:ASP:OD1	1.92	0.52
1:B:978:PRO:HG3	1:B:981:ILE:HD11	1.92	0.52
1:B:562:HIS:ND1	1:B:593:HIS:HE1	2.08	0.51
1:D:286:TYR:HB3	1:D:328:TYR:CD2	2.46	0.51
1:C:641:PHE:CZ	1:C:896:ASN:HB2	2.44	0.51
1:D:165:MET:HE2	1:D:326:PHE:CE1	2.45	0.51
1:D:1026:PRO:O	1:D:1029:VAL:HG22	2.10	0.51
1:C:484:LEU:HB3	1:C:531:VAL:HG22	1.92	0.51
1:B:165:MET:HG2	1:B:166:GLU:N	2.26	0.51
1:B:325:HIS:HD2	5:B:2041:HOH:O	1.93	0.51
1:D:661:MET:O	1:D:691:VAL:HA	2.11	0.51
1:A:441:ASN:ND2	1:C:403:ASN:HD22	2.08	0.51
1:C:378:LEU:HD13	1:C:445:VAL:HG23	1.93	0.51
1:C:452:LYS:CE	5:C:2302:HOH:O	2.59	0.50
1:B:770:GLU:HG2	1:B:885:ARG:HG2	1.93	0.50
1:C:100:ARG:HG3	1:C:603:TYR:CE1	2.46	0.50
1:C:850:LYS:HB2	1:C:851:PRO:HD2	1.92	0.50
1:D:533:GLU:HA	1:D:629:GLU:HG2	1.93	0.50
1:D:986:GLY:O	1:D:987:ALA:HB3	2.12	0.50
1:D:371:GLY:C	1:D:731:HIS:HD2	2.15	0.50
1:D:111:GLN:HE21	1:D:111:GLN:HA	1.78	0.49
1:A:252:HIS:HE1	1:A:580:ASP:OD1	1.95	0.49
1:A:657:HIS:HD2	5:A:2388:HOH:O	1.96	0.49
1:C:982:HIS:HB3	1:C:1036:THR:CG2	2.42	0.49
1:D:111:GLN:HE22	1:D:349:PHE:H	1.60	0.49
1:A:363:LYS:NZ	1:A:769:GLN:HE21	2.10	0.49
1:A:961:GLU:CG	5:A:2830:HOH:O	2.59	0.49
1:C:915:ARG:NH1	1:C:945:GLU:OE2	2.45	0.49
1:D:114:TRP:O	1:D:118:GLN:HG2	2.12	0.49
1:C:412:ASP:HB3	1:C:414:ASP:OD1	2.12	0.49
1:D:746:GLN:CD	5:D:2579:HOH:O	2.51	0.49
1:B:511:LEU:O	1:B:518:GLU:HB2	2.13	0.48
1:C:881:ILE:HB	1:C:918:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:SER:O	1:A:986:GLY:C	2.51	0.48
1:A:777:TYR:HE2	1:A:919:MET:CE	2.26	0.48
1:A:885:ARG:HD2	1:A:904:LEU:HA	1.96	0.48
1:B:777:TYR:HE2	1:B:919:MET:HE3	1.77	0.48
1:C:361:PRO:CD	1:C:776:MET:HG2	2.42	0.48
1:C:661:MET:HB2	1:C:691:VAL:HG23	1.95	0.48
1:C:1008:GLU:O	1:C:1011:ASP:HB2	2.12	0.48
1:A:829:GLU:OE1	1:A:864:ASN:HA	2.14	0.48
1:B:777:TYR:CE2	1:B:919:MET:CE	2.97	0.48
1:C:598:VAL:HG11	1:C:611:MET:CE	2.44	0.48
1:A:457:GLN:HE22	1:A:729:ARG:HH11	1.60	0.48
1:A:529:PRO:O	1:A:530:ASP:CB	2.61	0.48
1:B:593:HIS:HD2	5:B:2348:HOH:O	1.95	0.48
1:A:216:VAL:O	1:A:228:ARG:NH2	2.40	0.48
1:A:556:VAL:N	1:A:557:PRO:CA	2.77	0.48
1:C:325:HIS:HE1	5:C:2053:HOH:O	1.96	0.48
1:B:474:GLU:HA	1:B:477:GLN:HB2	1.95	0.48
1:D:553:ASP:OD2	4:D:1041:5DI:H12C	2.12	0.48
1:A:976:GLN:HE22	1:A:1016:GLN:HG2	1.77	0.47
1:C:539:TYR:OH	1:C:552:GLN:NE2	2.46	0.47
1:C:812:HIS:CE1	5:C:2470:HOH:O	2.67	0.47
1:D:200:PHE:HB2	1:D:208:GLU:HG3	1.96	0.47
1:C:526:TRP:CZ2	1:C:622:LEU:HD13	2.48	0.47
1:C:842:LYS:HB2	1:C:856:MET:HE1	1.96	0.47
1:B:463:PHE:HB2	1:B:521:ALA:CB	2.43	0.47
1:C:410:ALA:HB2	1:C:457:GLN:HE21	1.78	0.47
1:A:325:HIS:HD2	5:A:2099:HOH:O	1.98	0.47
1:A:976:GLN:HE22	1:A:1016:GLN:HA	1.78	0.47
1:B:422:PHE:HA	1:B:542:LEU:HD11	1.95	0.47
1:B:380:ARG:NH2	1:B:397:GLU:OE1	2.32	0.47
1:D:915:ARG:NH1	1:D:945:GLU:OE2	2.47	0.47
1:A:661:MET:HG2	1:A:688:LEU:HD11	1.96	0.47
1:C:612:VAL:O	5:C:2195:HOH:O	2.21	0.47
1:C:463:PHE:CD1	1:C:511:LEU:HD13	2.50	0.47
1:D:185:VAL:HG12	1:D:186:ASP:O	2.14	0.47
1:D:553:ASP:OD1	4:D:1041:5DI:H12C	2.15	0.47
1:A:976:GLN:NE2	1:A:1016:GLN:HG2	2.30	0.46
1:B:139:GLU:HB2	1:B:143:LEU:O	2.15	0.46
1:A:661:MET:HG3	1:A:688:LEU:HG	1.97	0.46
1:A:245:GLN:HE21	1:A:590:LYS:NZ	2.12	0.46
1:A:661:MET:O	1:A:691:VAL:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:942:VAL:HA	1:D:954:THR:O	2.15	0.46
1:B:450:HIS:HE1	1:B:548:ASP:OD1	1.98	0.46
1:B:484:LEU:HB3	1:B:531:VAL:HG22	1.97	0.46
1:B:661:MET:O	1:B:691:VAL:HA	2.15	0.46
1:A:226:LEU:H	1:A:804:ASN:HD22	1.62	0.46
1:D:281:SER:HA	5:D:2647:HOH:O	2.16	0.46
1:B:474:GLU:O	1:B:474:GLU:HG2	2.16	0.46
1:B:805:ASP:CG	1:B:830:ARG:HH22	2.19	0.46
1:D:60:ASN:HB3	1:D:74:GLN:HE21	1.80	0.46
1:D:696:GLY:CA	5:D:2579:HOH:O	2.63	0.46
1:A:201:ARG:HD3	1:A:310:GLU:O	2.16	0.46
1:B:23:LYS:H	1:B:191:ASN:HD21	1.64	0.46
1:C:80:GLN:NE2	1:C:90:ARG:HH11	2.14	0.46
1:D:865:TYR:HA	1:D:866:PRO:HD3	1.85	0.46
1:A:777:TYR:CE2	1:A:919:MET:CE	2.99	0.46
1:B:661:MET:HG3	1:B:688:LEU:HG	1.96	0.46
1:D:201:ARG:NH1	1:D:301:GLY:O	2.49	0.45
1:D:227:GLU:OE2	1:D:229:THR:HG23	2.14	0.45
1:D:793:TYR:HA	3:D:1040:GOL:H31	1.98	0.45
1:A:200:PHE:HB2	1:A:208:GLU:HG3	1.97	0.45
1:A:942:VAL:HA	1:A:954:THR:O	2.16	0.45
1:B:550:VAL:HG21	1:B:552:GLN:HE21	1.82	0.45
1:B:533:GLU:HA	1:B:629:GLU:HG2	1.99	0.45
1:B:689:PRO:O	1:B:726:PRO:HG2	2.17	0.45
1:C:657:HIS:HD2	5:C:2237:HOH:O	1.99	0.45
1:C:732:TYR:CD1	1:C:746:GLN:HB3	2.52	0.44
1:C:811:GLY:HA3	1:C:816:ARG:HG3	2.00	0.44
1:C:1038:THR:HG22	1:C:1038:THR:OXT	2.18	0.44
1:D:243:TYR:OH	1:D:666:ASN:HB3	2.17	0.44
1:A:286:TYR:HB3	1:A:328:TYR:CD2	2.52	0.44
1:B:383:MET:CE	5:B:2251:HOH:O	2.61	0.44
1:C:964:PHE:O	1:C:1027:ASN:HB2	2.17	0.44
1:A:20:ILE:CD1	1:A:96:ASP:HB3	2.48	0.44
1:C:408:GLY:HA3	1:C:455:VAL:O	2.17	0.44
1:C:34:SER:HA	1:C:35:PRO:HD2	1.92	0.44
1:A:29:GLY:HA3	1:A:31:TRP:CE2	2.53	0.44
1:D:182:LEU:CB	5:D:2208:HOH:O	2.35	0.44
1:D:886:TYR:O	1:D:902:ASP:HB3	2.17	0.44
1:D:1032:ASP:CG	1:D:1032:ASP:O	2.55	0.44
1:D:98:PRO:HD2	5:D:2115:HOH:O	2.17	0.44
1:D:969:TYR:HA	1:D:1023:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:702:ASP:HB3	1:B:705:ASN:O	2.18	0.44
1:D:133:GLU:CD	1:D:133:GLU:H	2.21	0.44
1:B:152:LYS:HZ2	1:B:166:GLU:HB2	1.83	0.43
1:C:811:GLY:HA3	1:C:816:ARG:CG	2.48	0.43
1:A:98:PRO:HG2	1:A:100:ARG:NH1	2.34	0.43
1:C:766:TYR:CE2	1:C:895:LEU:HG	2.54	0.43
1:D:93:PHE:HE1	5:D:2208:HOH:O	1.86	0.43
1:D:162:LYS:HE2	1:D:282:GLU:OE1	2.19	0.43
1:C:450:HIS:HE1	1:C:548:ASP:OD1	2.01	0.43
1:C:36:LEU:HD12	1:C:308:GLY:HA2	2.01	0.43
1:D:903:PRO:HG2	1:D:1004:PHE:CD2	2.54	0.43
1:A:808:LEU:HA	1:A:817:ILE:O	2.18	0.43
1:C:836:VAL:HG22	1:C:837:LEU:N	2.34	0.43
1:B:662:TRP:HZ2	2:B:1039:B9D:H4	1.84	0.43
1:D:241:LEU:O	1:D:242:ASN:HB2	2.19	0.43
1:B:433:ARG:HD3	5:B:2278:HOH:O	2.19	0.42
1:D:559:MET:HG3	1:D:591:THR:HA	2.01	0.42
1:B:130:PHE:HA	1:B:135:PHE:O	2.19	0.42
1:C:776:MET:HE1	1:C:786:ILE:CD1	2.46	0.42
1:D:553:ASP:CG	4:D:1041:5DI:H12C	2.39	0.42
1:A:554[A]:MET:CE	1:A:649:ARG:NH1	2.81	0.42
1:C:463:PHE:HB2	1:C:521:ALA:HB1	2.02	0.42
1:D:1027:ASN:N	1:D:1027:ASN:HD22	2.17	0.42
1:B:777:TYR:CE2	1:B:919:MET:HE3	2.53	0.42
1:D:210:PHE:H	1:D:229:THR:CG2	2.23	0.42
1:D:231:ILE:HB	1:D:261:TYR:CD1	2.54	0.42
1:D:361:PRO:CD	1:D:776:MET:HG2	2.50	0.42
1:A:17:PRO:HG3	1:A:606:HIS:O	2.20	0.42
1:C:474:GLU:OE2	1:C:478:THR:HG21	2.19	0.42
1:C:649:ARG:HB2	1:C:662:TRP:CH2	2.55	0.42
1:C:463:PHE:CG	1:C:511:LEU:HD13	2.54	0.42
1:D:273:ILE:HG21	1:D:334:MET:HG2	2.01	0.42
1:A:785:PRO:O	1:A:788:LYS:CE	2.67	0.42
1:B:380:ARG:NH1	5:B:2237:HOH:O	2.08	0.42
1:D:39:THR:HG21	5:D:2018:HOH:O	2.18	0.42
1:B:582:PRO:HG3	5:B:2345:HOH:O	2.20	0.42
1:D:483:GLN:HE21	1:D:483:GLN:HB2	1.52	0.42
1:A:372:VAL:HG22	1:A:732:TYR:CE1	2.55	0.41
1:B:415:MET:SD	1:B:424:THR:HG22	2.60	0.41
1:C:288:TRP:HE1	1:C:324:GLN:CD	2.24	0.41
1:C:361:PRO:HD3	1:C:776:MET:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:ASN:HA	1:D:197:ASN:HA	2.01	0.41
1:D:484:LEU:HB3	1:D:531:VAL:HG22	2.02	0.41
1:B:593:HIS:CD2	5:B:2348:HOH:O	2.72	0.41
1:D:372:VAL:HG22	1:D:732:TYR:CE1	2.55	0.41
1:A:60:ASN:HB3	1:A:74:GLN:HE21	1.85	0.41
1:A:955:PHE:O	1:A:1032:ASP:HA	2.20	0.41
1:A:990:GLN:HB3	5:A:2870:HOH:O	2.20	0.41
1:B:363:LYS:NZ	1:B:770:GLU:OE2	2.44	0.41
1:A:688:LEU:HD12	1:A:691:VAL:HB	2.02	0.41
1:C:834:LEU:HB3	1:C:840:TRP:CD1	2.55	0.41
1:A:140:THR:OG1	1:A:143:LEU:HB2	2.21	0.41
1:C:629:GLU:HG3	1:C:633:GLU:OE2	2.20	0.41
1:D:171:GLY:HA2	1:D:177:ASN:HD22	1.86	0.41
1:D:807:PHE:CE1	1:D:819:CYS:HB2	2.56	0.41
1:B:777:TYR:HE2	1:B:919:MET:CE	2.33	0.41
1:C:228:ARG:HB3	1:C:231:ILE:HD11	2.02	0.41
1:D:165:MET:HG2	1:D:166:GLU:H	1.85	0.41
1:D:674:GLN:HG3	1:D:823:VAL:HB	2.01	0.41
1:A:684:ASN:C	5:A:2620:HOH:O	2.58	0.41
1:A:911:LEU:HD12	1:A:946:GLN:HB2	2.02	0.41
1:B:881:ILE:HA	1:B:907:GLU:O	2.21	0.41
1:D:513:TYR:CE1	1:D:554:MET:HE3	2.55	0.41
1:A:36:LEU:HD12	1:A:308:GLY:HA2	2.03	0.41
1:A:235:ASN:ND2	1:A:269:ALA:H	2.19	0.41
1:B:872:SER:HA	1:B:873:PRO:HD3	1.96	0.40
1:D:777:TYR:CE2	1:D:919:MET:CE	3.01	0.40
1:C:907:GLU:OE2	1:C:973:ARG:NE	2.45	0.40
1:A:562:HIS:CD2	1:A:593:HIS:CE1	2.88	0.40
1:B:474:GLU:O	1:B:478:THR:HG23	2.21	0.40
1:D:553:ASP:OD2	4:D:1041:5DI:C1	2.69	0.40
1:D:588:ASN:HB3	1:D:593:HIS:CE1	2.56	0.40
1:B:216:VAL:O	1:B:228:ARG:NH2	2.53	0.40
1:B:354:LEU:HD21	1:B:360:MET:HG3	2.03	0.40
1:C:125:ASP:HA	1:C:126:PRO:HD2	1.98	0.40
1:C:663:VAL:HG11	1:C:679:ASN:ND2	2.36	0.40
1:D:182:LEU:CA	5:D:2208:HOH:O	2.67	0.40
1:B:334:MET:HB3	1:B:334:MET:HE2	1.95	0.40
1:B:856:MET:HE1	1:B:875:PHE:HE1	1.86	0.40
1:C:598:VAL:HG11	1:C:611:MET:HE1	2.03	0.40
1:C:776:MET:HE2	1:C:786:ILE:CD1	2.19	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	1023/1027 (100%)	981 (96%)	38 (4%)	4 (0%)	34	24
1	B	1022/1027 (100%)	980 (96%)	39 (4%)	3 (0%)	41	31
1	C	1022/1027 (100%)	988 (97%)	34 (3%)	0	100	100
1	D	1022/1027 (100%)	977 (96%)	44 (4%)	1 (0%)	51	42
All	All	4089/4108 (100%)	3926 (96%)	155 (4%)	8 (0%)	47	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	530	ASP
1	B	948	GLY
1	D	986	GLY
1	A	530	ASP
1	A	986	GLY
1	B	746	GLN
1	A	239	ASP
1	A	987	ALA

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	878/878 (100%)	863 (98%)	15 (2%)	60	57
1	B	877/878 (100%)	850 (97%)	27 (3%)	40	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	877/878 (100%)	855 (98%)	22 (2%)	47 41
1	D	877/878 (100%)	850 (97%)	27 (3%)	40 32
All	All	3509/3512 (100%)	3418 (97%)	91 (3%)	46 39

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ILE
1	A	144	SER
1	A	151	PHE
1	A	324	GLN
1	A	549	PHE
1	A	552	GLN
1	A	571	LYS
1	A	572	PRO
1	A	662	TRP
1	A	718	TYR
1	A	830	ARG
1	A	838	THR
1	A	915	ARG
1	A	936	LYS
1	A	1038	THR
1	B	18	ASP
1	B	53	THR
1	B	74	GLN
1	B	151	PHE
1	B	165	MET
1	B	187	ARG
1	B	282	GLU
1	B	306	ASN
1	B	418	ASN
1	B	462	CYS
1	B	474	GLU
1	B	494	THR
1	B	511	LEU
1	B	549	PHE
1	B	550	VAL
1	B	551	TRP
1	B	611	MET
1	B	655	ASN
1	B	662	TRP

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Mol	Chain	Res	Type
1	B	688	LEU
1	B	690	LEU
1	B	718	TYR
1	B	816	ARG
1	B	830	ARG
1	B	893	LYS
1	B	979	SER
1	B	984	SER
1	C	175	SER
1	C	187	ARG
1	C	282	GLU
1	C	413	VAL
1	C	414	ASP
1	C	462	CYS
1	C	483	GLN
1	C	551	TRP
1	C	571	LYS
1	C	655	ASN
1	C	662	TRP
1	C	688	LEU
1	C	690	LEU
1	C	704	GLU
1	C	718	TYR
1	C	829	GLU
1	C	830	ARG
1	C	837	LEU
1	C	860	ASP
1	C	893	LYS
1	C	942	VAL
1	C	990	GLN
1	D	14	THR
1	D	92	ARG
1	D	100	ARG
1	D	111	GLN
1	D	164	ILE
1	D	197	ASN
1	D	198	LYS
1	D	229	THR
1	D	254	ASP
1	D	359	VAL
1	D	414	ASP
1	D	432	ASN

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Mol	Chain	Res	Type
1	D	474	GLU
1	D	483	GLN
1	D	511	LEU
1	D	572	PRO
1	D	605	ASN
1	D	608	ARG
1	D	655	ASN
1	D	662	TRP
1	D	690	LEU
1	D	718	TYR
1	D	830	ARG
1	D	915	ARG
1	D	990	GLN
1	D	1027	ASN
1	D	1038	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	74	GLN
1	A	191	ASN
1	A	202	ASN
1	A	235	ASN
1	A	245	GLN
1	A	252	HIS
1	A	325	HIS
1	A	345	GLN
1	A	441	ASN
1	A	457	GLN
1	A	483	GLN
1	A	510	HIS
1	A	552	GLN
1	A	562	HIS
1	A	586	GLN
1	A	593	HIS
1	A	614	GLN
1	A	657	HIS
1	A	769	GLN
1	A	804	ASN
1	A	930	ASN
1	A	934	ASN

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Mol	Chain	Res	Type
1	A	957	ASN
1	A	976	GLN
1	B	38	ASN
1	B	191	ASN
1	B	217	ASN
1	B	221	GLN
1	B	242	ASN
1	B	325	HIS
1	B	418	ASN
1	B	450	HIS
1	B	552	GLN
1	B	593	HIS
1	B	657	HIS
1	B	671	ASN
1	B	839	GLN
1	B	930	ASN
1	B	934	ASN
1	B	946	GLN
1	C	80	GLN
1	C	207	GLN
1	C	242	ASN
1	C	325	HIS
1	C	382	HIS
1	C	450	HIS
1	C	457	GLN
1	C	483	GLN
1	C	552	GLN
1	C	605	ASN
1	C	655	ASN
1	C	657	HIS
1	C	671	ASN
1	C	806	HIS
1	C	812	HIS
1	C	930	ASN
1	C	934	ASN
1	D	74	GLN
1	D	75	HIS
1	D	111	GLN
1	D	177	ASN
1	D	217	ASN
1	D	242	ASN
1	D	325	HIS

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Mol	Chain	Res	Type
1	D	432	ASN
1	D	450	HIS
1	D	483	GLN
1	D	552	GLN
1	D	562	HIS
1	D	655	ASN
1	D	679	ASN
1	D	731	HIS
1	D	864	ASN
1	D	896	ASN
1	D	930	ASN
1	D	934	ASN
1	D	946	GLN
1	D	957	ASN
1	D	976	GLN
1	D	990	GLN
1	D	1027	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSO	D	336	1	3,6,7	0.67	0	0,6,8	-	-
1	CSO	A	336	1	3,6,7	0.49	0	0,6,8	-	-
1	CSO	C	336	1	3,6,7	0.64	0	0,6,8	-	-
1	CSO	B	336	1	3,6,7	0.64	0	0,6,8	-	-

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
1	CSO	D	336	1	-	0/1/5/7	-
1	CSO	A	336	1	-	0/1/5/7	-
1	CSO	C	336	1	-	0/1/5/7	-
1	CSO	B	336	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

11 ligands 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	$\#\|Z\| > 2$
3	GOL	A	1042	-	5,5,5	0.37	0	5,5,5	0.30	0
3	GOL	D	1039	-	5,5,5	0.51	0	5,5,5	0.49	0
2	B9D	B	1039	1	9,12,13	1.25	1 (11%)	14,18,20	0.87	0
3	GOL	A	1041	-	5,5,5	0.24	0	5,5,5	0.69	0
4	5DI	D	1041	-	9,12,12	6.01	4 (44%)	10,18,18	1.01	0
3	GOL	B	1040	-	5,5,5	0.48	0	5,5,5	0.43	0
3	GOL	A	1040	-	5,5,5	0.43	0	5,5,5	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	B9D	A	1039	1	9,12,13	1.20	1 (11%)	14,18,20	1.20	2 (14%)
2	B9D	C	1039	1	9,12,13	1.33	1 (11%)	14,18,20	0.95	0
3	GOL	A	1043	-	5,5,5	0.29	0	5,5,5	0.53	0
3	GOL	D	1040	-	5,5,5	0.32	0	5,5,5	0.30	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	GOL	A	1042	-	-	2/4/4/4	-
3	GOL	D	1039	-	-	2/4/4/4	-
2	B9D	B	1039	1	-	0/2/23/26	0/1/1/1
3	GOL	A	1041	-	-	3/4/4/4	-
4	5DI	D	1041	-	-	0/2/23/23	0/1/1/1
3	GOL	B	1040	-	-	4/4/4/4	-
3	GOL	A	1040	-	-	0/4/4/4	-
2	B9D	A	1039	1	-	0/2/23/26	0/1/1/1
2	B9D	C	1039	1	-	0/2/23/26	0/1/1/1
3	GOL	A	1043	-	-	0/4/4/4	-
3	GOL	D	1040	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1041	5DI	C1-C2	-16.07	1.34	1.51
4	D	1041	5DI	O2-C2	7.10	1.33	1.21
2	C	1039	B9D	O5-C1	3.73	1.45	1.37
2	A	1039	B9D	O5-C1	3.19	1.44	1.37
2	B	1039	B9D	O5-C1	3.04	1.43	1.37
4	D	1041	5DI	O5-C1	2.72	1.46	1.43
4	D	1041	5DI	O5-C5	2.53	1.42	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1039	B9D	O2-C2-C1	3.00	116.12	110.14
2	A	1039	B9D	O4-C4-C5	2.18	113.62	109.15

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1041	GOL	C1-C2-C3-O3
3	A	1042	GOL	C1-C2-C3-O3
3	B	1040	GOL	C1-C2-C3-O3
3	B	1040	GOL	O2-C2-C3-O3
3	D	1039	GOL	C1-C2-C3-O3
3	D	1039	GOL	O2-C2-C3-O3
3	B	1040	GOL	O1-C1-C2-C3
3	A	1042	GOL	O2-C2-C3-O3
3	B	1040	GOL	O1-C1-C2-O2
3	A	1041	GOL	O2-C2-C3-O3
3	A	1041	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1039	B9D	1	0
4	D	1041	5DI	4	0
3	B	1040	GOL	1	0
3	A	1043	GOL	1	0
3	D	1040	GOL	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

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, 95^{th} 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	1024/1027 (99%)	-0.17	10 (0%)	82	84	9, 16, 31, 46	0
1	B	1024/1027 (99%)	0.18	32 (3%)	49	51	13, 29, 49, 69	0
1	C	1024/1027 (99%)	0.20	36 (3%)	44	47	13, 29, 45, 72	0
1	D	1024/1027 (99%)	-0.17	6 (0%)	89	90	8, 17, 36, 59	0
All	All	4096/4108 (99%)	0.01	84 (2%)	63	66	8, 22, 44, 72	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	14	THR	5.7
1	A	987	ALA	5.3
1	C	14	THR	4.4
1	B	529	PRO	4.4
1	D	529	PRO	4.3
1	B	188	LEU	4.2
1	B	189	TYR	3.8
1	B	976	GLN	3.6
1	C	120	LEU	3.6
1	C	837	LEU	3.4
1	B	365	VAL	3.3
1	C	977	SER	3.3
1	B	691	VAL	3.2
1	B	647	ILE	3.1
1	C	514	GLY	3.0
1	C	947	ASP	2.9
1	B	123	GLY	2.9
1	B	704	GLU	2.9
1	A	605	ASN	2.7
1	B	174	SER	2.7
1	C	515	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	18	ASP	2.6
1	B	565	GLY	2.6
1	A	949	GLY	2.6
1	C	691	VAL	2.6
1	C	470	GLY	2.6
1	C	949	GLY	2.6
1	B	975	ALA	2.5
1	A	254	ASP	2.5
1	B	470	GLY	2.5
1	C	647	ILE	2.5
1	A	529	PRO	2.5
1	C	1017	GLU	2.5
1	B	551	TRP	2.5
1	C	653	ILE	2.5
1	B	837	LEU	2.5
1	C	726	PRO	2.4
1	C	268	ALA	2.4
1	C	220	TYR	2.4
1	A	947	ASP	2.4
1	B	15	ASP	2.4
1	B	947	ASP	2.4
1	C	690	LEU	2.4
1	B	369	PHE	2.3
1	A	662	TRP	2.3
1	B	662	TRP	2.3
1	B	1038	THR	2.3
1	C	913	ASN	2.3
1	B	987	ALA	2.3
1	B	504	SER	2.3
1	C	987	ALA	2.2
1	C	124	CYS	2.2
1	C	1038	THR	2.2
1	D	511	LEU	2.2
1	C	267	TYR	2.2
1	C	188	LEU	2.2
1	C	725	LEU	2.2
1	B	994	VAL	2.2
1	D	681	ILE	2.2
1	A	996	SER	2.2
1	C	269	ALA	2.2
1	C	688	LEU	2.1
1	B	567	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	483	GLN	2.1
1	C	976	GLN	2.1
1	C	270	PRO	2.1
1	C	606	HIS	2.1
1	D	947	ASP	2.1
1	A	988	GLY	2.1
1	C	996	SER	2.1
1	C	254	ASP	2.1
1	C	385	ALA	2.1
1	C	189	TYR	2.1
1	C	128	MET	2.1
1	C	686	SER	2.1
1	B	605	ASN	2.1
1	B	71	ILE	2.1
1	B	688	LEU	2.1
1	B	497	GLY	2.1
1	C	704	GLU	2.0
1	D	515	GLY	2.0
1	B	725	LEU	2.0
1	A	328	TYR	2.0
1	B	1017	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
1	CSO	A	336	7/8	0.91	0.16	18,20,28,32	0
1	CSO	C	336	7/8	0.92	0.10	25,26,33,34	0
1	CSO	B	336	7/8	0.93	0.09	23,24,31,32	0
1	CSO	D	336	7/8	0.94	0.12	13,15,25,28	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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
3	GOL	B	1040	6/6	0.81	0.25	56,57,57,57	0
3	GOL	D	1039	6/6	0.81	0.18	37,37,38,41	0
2	B9D	C	1039	12/13	0.83	0.13	36,38,40,40	0
3	GOL	D	1040	6/6	0.84	0.18	37,41,44,44	0
4	5DI	D	1041	12/12	0.88	0.18	38,41,43,43	0
3	GOL	A	1043	6/6	0.89	0.13	35,38,38,40	0
2	B9D	B	1039	12/13	0.90	0.16	40,42,42,45	0
3	GOL	A	1042	6/6	0.92	0.12	28,34,35,37	0
3	GOL	A	1040	6/6	0.92	0.14	35,36,37,39	0
3	GOL	A	1041	6/6	0.93	0.14	31,36,37,37	0
2	B9D	A	1039	12/13	0.94	0.12	25,28,29,30	0

6.5 Other polymers (i)

There are no such residues in this entry.