Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 03:02 am GMT

PDB ID	:	2X4P
Title	:	Crystal structure of MHC CLass I HLA-A2.1 bound to a photocleavable peptide
Authors	:	Celie, P.H.N.; Toebes, M.; Rodenko, B.; Ovaa, H.; Perrakis, A.; Schumacher, T.N.M.
Deposited on	:	2010-02-02
Resolution	:	2.30 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:

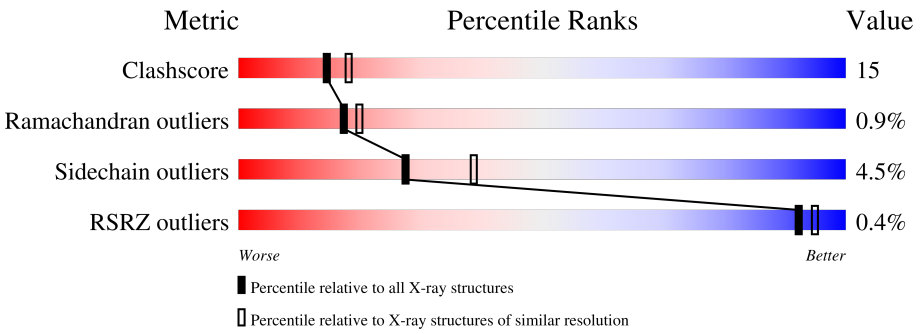
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	275	68% 31% .

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6920 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 HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	2292	1434	414	435	9	0	6	0
1	D	275	2262	1415	409	429	9	0	2	0

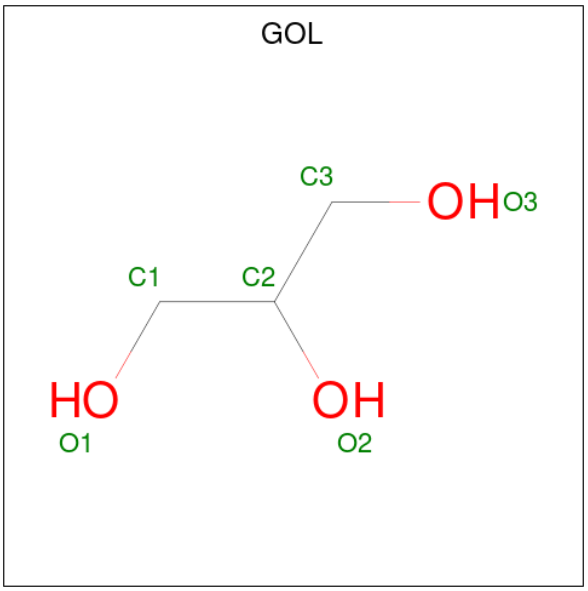
- Molecule 2 is a protein called BETA-2-MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	837	533	141	159	4	0	0	0
2	E	100	837	533	141	159	4	0	0	0

- Molecule 3 is a protein called HLA-A2.1-RESTRICTED INFLUENZA A MATRIX EPITOPE.

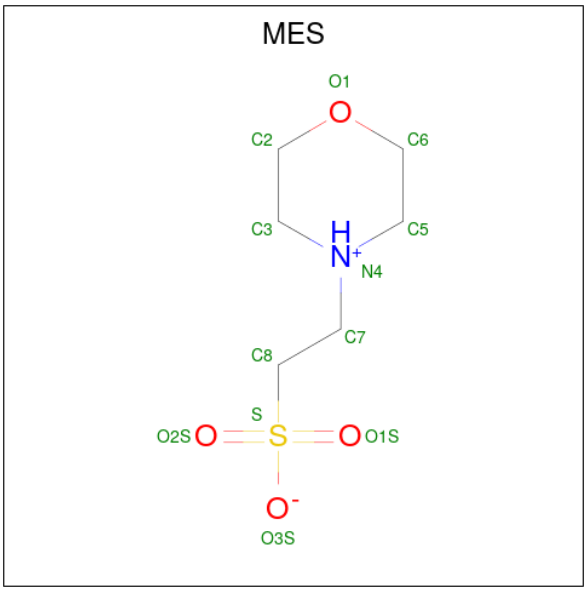
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
3	C	9	81	55	11	14	1	0	0	0
3	F	9	81	55	11	14	1	0	0	0

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



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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	B	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
5	B	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
5	D	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
5	D	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
5	E	1	12	6	1	4	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	143	143	143	0	0
			Total	O		
6	B	76	76	76	0	0
			Total	O		
6	C	5	5	5	0	0
			Total	O		
6	D	141	141	141	0	0
			Total	O		
6	E	64	64	64	0	0
			Total	O		
6	F	5	5	5	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.20Å 86.50Å 80.78Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	19.82 – 2.30 19.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.82-2.30) 99.4 (19.82-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.30Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.158 , 0.222 (Not available) , (Not available)	Depositor DCC
R_{free} test set	1921 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.360 for h,-k,-l	Xtriage
Reported twinning fraction	0.329 for -h,-k,l	Depositor
Outliers	0 of 37907 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6920	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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.

4 Model quality (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, GOL, PRV, PRQ

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	0.28	0/2370	0.46	0/3214
1	D	0.28	0/2334	0.46	0/3167
2	B	0.30	0/860	0.49	0/1162
2	E	0.30	0/860	0.47	0/1162
3	C	0.30	0/52	0.76	0/64
3	F	0.38	0/52	0.68	0/64
All	All	0.29	0/6528	0.47	0/8833

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
3	C	0	5
3	F	0	5
All	All	0	10

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	4	GLY	Peptide
3	C	5	PRV	Peptide,Mainchain
3	C	7	PHE	Mainchain
3	C	8	PRQ	Peptide
3	F	4	GLY	Peptide

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Mol	Chain	Res	Type	Group
3	F	5	PRV	Peptide,Mainchain
3	F	7	PHE	Mainchain
3	F	8	PRQ	Peptide

4.2 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	2292	0	2144	74	0
1	D	2262	0	2111	72	0
2	B	837	0	803	16	0
2	E	837	0	803	25	0
3	C	81	0	73	11	0
3	F	81	0	73	12	0
4	A	6	0	8	3	0
4	B	6	0	8	3	0
4	D	12	0	16	1	0
4	E	12	0	16	1	0
5	B	24	0	24	4	0
5	D	24	0	24	6	0
5	E	12	0	12	1	0
6	A	143	0	0	8	0
6	B	76	0	0	1	0
6	C	5	0	0	2	0
6	D	141	0	0	2	0
6	E	64	0	0	2	0
6	F	5	0	0	0	0
All	All	6920	0	6115	194	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 15.

All (194) 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:E:58:LYS:HA	4:E:1102:GOL:H11	1.26	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:6:VAL:HG13	3:F:7:PHE:H	1.21	1.02
1:D:5:MET:HB2	1:D:168:LEU:HD13	1.45	0.96
1:A:44:ARG:HH11	1:A:44:ARG:HG3	1.33	0.94
3:F:6:VAL:O	3:F:7:PHE:HB2	1.72	0.89
5:D:1276:MES:H52	2:E:96:ASP:OD2	1.78	0.83
3:F:6:VAL:HG13	3:F:7:PHE:N	1.94	0.82
2:B:98:ASP:HA	2:B:99:MET:OXT	1.82	0.80
1:A:82:ARG:CZ	1:A:89:GLU:HG3	2.13	0.78
1:D:102:ASP:HB2	1:D:111:ARG:HG2	1.67	0.75
1:D:55:GLU:HG2	1:D:59:TYR:CG	2.21	0.74
1:A:30:ASP:HA	4:A:1276:GOL:H11	1.69	0.74
1:D:106:ASP:O	1:D:107:TRP:HB2	1.86	0.73
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.71	0.73
1:A:44:ARG:HH11	1:A:44:ARG:CG	2.03	0.72
2:E:96:ASP:O	2:E:99:MET:HG3	1.90	0.71
1:A:21:ARG:NH1	1:A:23:ILE:HD11	2.06	0.71
1:A:76:VAL:HB	3:C:8:PRQ:HAF	1.73	0.70
1:A:202:ARG:NH1	2:B:99:MET:HA	2.06	0.70
1:A:84:TYR:OH	1:A:146:LYS:HE3	1.93	0.69
1:D:28:VAL:HG11	1:D:179:LEU:HD13	1.74	0.69
1:A:144:LYS:O	1:A:148:GLU:HG3	1.91	0.69
3:C:6:VAL:HG22	3:C:7:PHE:H	1.58	0.69
1:D:189:MET:HE2	1:D:274:TRP:HE3	1.58	0.69
3:F:6:VAL:CG1	3:F:7:PHE:H	2.02	0.68
1:A:97:ARG:HH21	1:A:116[B]:TYR:HE2	1.41	0.68
1:D:74:HIS:HD1	1:D:95:VAL:HG11	1.58	0.68
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.76	0.67
1:D:169:ARG:O	1:D:173:GLU:HG3	1.95	0.65
1:A:49:ALA:O	1:A:52:ILE:HG22	1.96	0.65
1:A:58[B]:GLU:HB2	2:E:13:HIS:CD2	2.30	0.65
1:A:192:HIS:HD2	6:A:2105:HOH:O	1.80	0.65
1:D:15:PRO:O	1:D:17:ARG:HD3	1.96	0.64
1:D:191:HIS:HB2	1:D:274:TRP:CH2	2.32	0.64
1:A:189:MET:HE2	1:A:274:TRP:HE3	1.63	0.64
1:A:143:THR:HA	1:A:146:LYS:HD2	1.81	0.62
3:C:8:PRQ:HAI	1:D:54:GLN:HE22	1.64	0.62
1:A:167:TRP:CZ3	1:A:170:ARG:HD2	2.34	0.62
1:D:206:LEU:HD23	1:D:242:GLN:HB3	1.82	0.61
1:D:232[A]:GLU:HG3	5:D:1278:MES:O3S	2.00	0.61
1:D:12:VAL:HG22	1:D:94:THR:HG23	1.84	0.60
3:F:5:PRV:HA	3:F:5:PRV:O1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:ARG:HA	1:D:17:ARG:NH2	2.17	0.59
1:A:82:ARG:HD2	1:A:89:GLU:HA	1.84	0.59
1:D:99:TYR:HB3	1:D:114:HIS:HD2	1.68	0.59
2:E:25:CYS:HB2	2:E:39:LEU:HD21	1.85	0.59
3:C:5:PRV:O1	3:C:6:VAL:HB	2.02	0.58
1:A:66:LYS:NZ	3:C:1:MSE:HE3	2.19	0.58
1:D:28:VAL:HG23	1:D:33:PHE:CE1	2.39	0.57
1:D:99:TYR:HB3	1:D:114:HIS:CD2	2.38	0.57
1:A:73:THR:HG23	3:C:8:PRQ:CAH	2.35	0.57
1:A:121[A]:LYS:HG3	6:A:2064:HOH:O	2.06	0.56
1:A:202:ARG:HH12	5:B:1102:MES:H61	1.70	0.56
2:E:36:GLU:HB3	6:E:2022:HOH:O	2.05	0.56
1:A:70:HIS:CD2	6:C:2001:HOH:O	2.60	0.55
2:B:58:LYS:HA	4:B:1100:GOL:H2	1.89	0.55
1:D:176:LYS:HA	1:D:180:GLN:HG3	1.88	0.54
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.43	0.54
3:F:6:VAL:CG1	3:F:7:PHE:N	2.66	0.54
1:A:137:ASP:O	1:A:141:GLN:HG2	2.08	0.54
1:A:139:ALA:HB2	6:A:2076:HOH:O	2.07	0.54
2:E:98:ASP:HA	2:E:99:MET:OXT	2.07	0.54
1:D:110:LEU:HD23	1:D:111:ARG:NH2	2.23	0.53
1:A:186:LYS:HE2	1:A:207:SER:HB3	1.90	0.53
1:D:21:ARG:HG2	6:D:2012:HOH:O	2.08	0.53
2:B:98:ASP:HA	2:B:99:MET:C	2.26	0.53
1:A:98:MET:HE2	4:B:1100:GOL:H11	1.91	0.53
2:E:51:HIS:HB3	2:E:66:TYR:CD1	2.43	0.53
1:A:59:TYR:O	1:A:63:GLU:HG2	2.08	0.53
1:D:97:ARG:HD2	1:D:116[B]:TYR:CZ	2.44	0.53
1:D:106:ASP:CG	1:D:108:ARG:HD3	2.29	0.53
1:D:121:LYS:CG	2:E:1:ILE:HD11	2.39	0.53
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.44	0.52
2:B:85:VAL:HB	6:B:2013:HOH:O	2.08	0.52
1:A:121[B]:LYS:HB3	2:B:1:ILE:HD11	1.92	0.52
1:D:168:LEU:O	1:D:172:LEU:HG	2.08	0.52
1:A:47:PRO:HG3	1:A:60:TRP:CZ2	2.43	0.52
2:E:98:ASP:HA	2:E:99:MET:HB2	1.92	0.52
1:A:107:TRP:O	1:A:169:ARG:HD3	2.10	0.52
1:D:81:LEU:O	1:D:85:TYR:HD1	1.92	0.52
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.92	0.51
1:A:70:HIS:HD2	6:C:2001:HOH:O	1.91	0.51
1:A:35:ARG:O	1:A:35:ARG:HG3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:VAL:HB	3:F:8:PRQ:HAF	1.92	0.51
1:D:143:THR:HG23	3:F:9:VAL:HA	1.92	0.51
1:A:84:TYR:HB3	1:A:139:ALA:HB1	1.93	0.50
1:A:129:ASP:O	1:A:131:ARG:HG3	2.11	0.50
1:A:218:GLN:O	1:A:257:TYR:HA	2.11	0.50
1:D:62:GLY:O	1:D:66:LYS:HG3	2.11	0.50
1:D:114:HIS:HE1	1:D:116[B]:TYR:HE2	1.59	0.50
3:F:5:PRV:CD1	3:F:6:VAL:HB	2.42	0.50
1:D:37:ASP:HB3	1:D:40:ALA:HB2	1.94	0.50
1:A:44:ARG:HG3	1:A:44:ARG:NH1	2.14	0.50
2:E:37:VAL:HG11	2:E:66:TYR:CD2	2.46	0.49
1:D:6:ARG:NE	1:D:113:TYR:OH	2.46	0.49
2:E:31:HIS:ND1	2:E:32:PRO:HA	2.28	0.49
1:A:128:GLU:O	1:A:128:GLU:HG2	2.13	0.48
1:A:176:LYS:HA	1:A:180:GLN:HG3	1.95	0.48
1:D:17:ARG:HH22	1:D:92:SER:HB2	1.78	0.48
1:D:176:LYS:O	1:D:180:GLN:HB2	2.12	0.48
2:B:6:LYS:O	2:B:27:VAL:HA	2.13	0.48
1:A:44:ARG:CG	1:A:44:ARG:NH1	2.68	0.48
2:E:98:ASP:CG	2:E:98:ASP:O	2.51	0.48
1:D:52:ILE:O	1:D:55:GLU:HB2	2.14	0.48
1:D:121:LYS:HG2	2:E:1:ILE:HD11	1.94	0.48
1:A:63:GLU:OE2	3:C:1:MSE:HG2	2.14	0.48
1:A:98:MET:CE	4:B:1100:GOL:H11	2.43	0.48
1:D:260:HIS:HA	1:D:270:LEU:O	2.14	0.48
1:A:219:ARG:HD3	1:A:257:TYR:CZ	2.48	0.48
1:D:127:LYS:HE2	1:D:134:THR:OG1	2.13	0.48
2:E:21:ASN:HB3	2:E:70:PHE:CE2	2.49	0.48
1:A:9:PHE:HE2	1:A:99:TYR:CE2	2.32	0.47
1:A:13:SER:O	1:A:15:PRO:HD3	2.14	0.47
1:D:6:ARG:HD3	4:D:1277:GOL:H31	1.97	0.47
2:E:4:THR:HG22	2:E:5:PRO:HD2	1.95	0.47
1:D:114:HIS:CE1	1:D:116[B]:TYR:HE2	2.33	0.47
5:D:1276:MES:H51	5:D:1276:MES:H82	1.51	0.47
1:A:264:GLU:HB3	6:A:2135:HOH:O	2.15	0.47
3:F:5:PRV:CE1	3:F:6:VAL:HB	2.45	0.47
1:A:189:MET:SD	6:A:2133:HOH:O	2.61	0.47
1:D:106:ASP:HB2	1:D:108:ARG:HD3	1.96	0.47
3:C:6:VAL:O	3:C:7:PHE:HD2	1.98	0.47
1:D:110:LEU:HD23	1:D:111:ARG:HH21	1.79	0.47
2:E:0:MET:HB2	6:E:2001:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:PRO:HD2	1:D:17:ARG:NH1	2.29	0.46
1:D:192:HIS:CG	5:D:1276:MES:H72	2.49	0.46
1:A:96:GLN:NE2	2:B:31:HIS:NE2	2.63	0.46
1:D:35:ARG:O	1:D:35:ARG:HG3	2.15	0.46
1:A:97:ARG:NH2	1:A:116[B]:TYR:HE2	2.11	0.46
1:D:74:HIS:HA	1:D:77:ASP:HB2	1.97	0.46
1:A:29:ASP:O	4:A:1276:GOL:H31	2.16	0.46
1:D:52:ILE:HD11	1:D:59:TYR:CZ	2.51	0.46
2:E:36:GLU:O	2:E:82:VAL:HA	2.16	0.46
1:A:58[A]:GLU:HB2	2:E:13:HIS:CD2	2.51	0.45
1:D:63:GLU:OE2	3:F:1:MSE:HG2	2.16	0.45
3:C:6:VAL:HG13	3:C:7:PHE:N	2.32	0.45
1:D:44:ARG:HA	1:D:64:THR:HG23	1.98	0.45
1:A:51:TRP:CZ2	1:A:179:LEU:HD11	2.52	0.45
1:A:192:HIS:HB2	5:B:1102:MES:H62	1.99	0.45
4:A:1276:GOL:O1	5:B:1101:MES:H22	2.17	0.44
1:A:231:VAL:HG11	1:A:244:TRP:CZ2	2.51	0.44
1:A:189:MET:HE2	1:A:274:TRP:CE3	2.48	0.44
3:C:7:PHE:C	3:C:8:PRQ:OAD	2.56	0.44
1:A:9:PHE:CE2	1:A:99:TYR:CE2	3.05	0.44
1:D:49:ALA:O	1:D:52:ILE:HG22	2.18	0.44
1:D:55:GLU:HG2	1:D:59:TYR:CD2	2.52	0.44
2:B:73:THR:OG1	2:B:76:ASP:HB2	2.18	0.43
3:C:1:MSE:HE2	3:C:1:MSE:HB3	1.89	0.43
1:D:35:ARG:HG2	1:D:48:ARG:HD3	1.99	0.43
1:D:46:GLU:HA	1:D:47:PRO:HD3	1.87	0.43
1:A:133:TRP:HB2	1:A:144:LYS:HG3	1.99	0.43
2:B:40:LEU:HD11	2:B:81:ARG:HB2	2.00	0.43
1:D:211:ALA:HB2	1:D:241:PHE:CD2	2.53	0.43
2:E:81:ARG:CG	2:E:90:PRO:HB2	2.48	0.43
1:A:37:ASP:HB3	1:A:40:ALA:HB2	1.99	0.43
2:B:41:LYS:O	2:B:42:ASN:HB2	2.18	0.43
2:B:99:MET:H	5:B:1102:MES:H51	1.84	0.43
1:D:253:GLN:NE2	1:D:256:ARG:HH11	2.17	0.43
1:A:176:LYS:HB2	1:A:180:GLN:NE2	2.33	0.43
2:B:2:GLN:HA	2:B:31:HIS:O	2.19	0.42
1:D:171:TYR:O	1:D:179:LEU:HD12	2.19	0.42
1:D:187:THR:HA	1:D:204:TRP:O	2.19	0.42
2:E:6:LYS:O	2:E:27:VAL:HA	2.19	0.42
1:A:27:TYR:CE1	1:A:32:GLN:HB2	2.55	0.42
1:A:44:ARG:HA	1:A:64:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:GLY:HA2	6:D:2128:HOH:O	2.19	0.42
1:A:176:LYS:HB2	1:A:180:GLN:HE21	1.85	0.42
1:D:55:GLU:HG2	1:D:59:TYR:CD1	2.54	0.42
1:D:106:ASP:CB	1:D:108:ARG:HD3	2.50	0.42
1:D:232[A]:GLU:HG3	5:D:1278:MES:H72	2.01	0.42
5:D:1278:MES:H52	5:D:1278:MES:H81	1.66	0.41
2:E:58:LYS:HG2	2:E:58:LYS:O	2.18	0.41
1:A:128:GLU:HG3	6:A:2061:HOH:O	2.20	0.41
2:B:23:LEU:O	2:B:67:TYR:HA	2.20	0.41
1:D:15:PRO:HD2	1:D:17:ARG:HH12	1.86	0.41
1:D:49:ALA:O	1:D:53:GLU:HG3	2.20	0.41
1:D:80:THR:HG21	3:F:9:VAL:HG23	2.01	0.41
1:D:121:LYS:HG3	2:E:1:ILE:HD11	2.01	0.41
1:D:255:GLN:HE21	1:D:275:GLU:HA	1.84	0.41
1:A:219:ARG:NH1	6:A:2112:HOH:O	2.52	0.41
1:A:259:CYS:N	6:A:2133:HOH:O	2.53	0.41
1:D:219:ARG:O	1:D:220:ASP:HB2	2.20	0.41
1:A:52:ILE:O	1:A:52:ILE:HG13	2.21	0.41
1:A:82:ARG:HH11	1:A:82:ARG:HG2	1.85	0.41
1:D:15:PRO:HG2	1:D:91:GLY:O	2.21	0.41
1:A:4:SER:HB3	1:A:102:ASP:OD1	2.21	0.41
2:E:26:TYR:OH	5:E:1100:MES:H61	2.22	0.40
1:A:124:ILE:HG12	1:A:125:ALA:N	2.36	0.40
1:A:191:HIS:CE1	1:A:199:ALA:HB1	2.56	0.40
1:A:228:THR:HG22	1:A:229:GLU:N	2.36	0.40
1:D:9:PHE:HE2	1:D:99:TYR:CE2	2.39	0.40
1:D:81:LEU:HD13	1:D:118:TYR:CD1	2.57	0.40
1:D:131:ARG:HD3	1:D:157:ARG:HH12	1.86	0.40
1:A:250:PRO:O	1:A:251:SER:C	2.60	0.40

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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	279/275 (102%)	261 (94%)	17 (6%)	1 (0%)	34	42
1	D	275/275 (100%)	256 (93%)	18 (6%)	1 (0%)	34	42
2	B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	E	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	C	5/9 (56%)	1 (20%)	1 (20%)	3 (60%)	0	0
3	F	5/9 (56%)	1 (20%)	2 (40%)	2 (40%)	0	0
All	All	760/768 (99%)	708 (93%)	45 (6%)	7 (1%)	17	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	6	VAL
3	F	7	PHE
3	C	7	PHE
1	D	40	ALA
1	A	40	ALA
3	C	4	GLY
3	F	6	VAL

4.3.2 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	237/231 (103%)	227 (96%)	10 (4%)	30	42
1	D	233/231 (101%)	222 (95%)	11 (5%)	26	37
2	B	95/95 (100%)	91 (96%)	4 (4%)	30	42
2	E	95/95 (100%)	91 (96%)	4 (4%)	30	42
3	C	6/5 (120%)	5 (83%)	1 (17%)	2	2
3	F	6/5 (120%)	6 (100%)	0	100	100
All	All	672/662 (102%)	642 (96%)	30 (4%)	27	39

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	21	ARG
1	A	35	ARG
1	A	44	ARG
1	A	67	VAL
1	A	181	ARG
1	A	196	ASP
1	A	210	PRO
1	A	214	THR
1	A	216	THR
2	B	47	GLU
2	B	70	PHE
2	B	92	ILE
2	B	99	MET
3	C	7	PHE
1	D	17	ARG
1	D	35	ARG
1	D	58	GLU
1	D	105	SER
1	D	122	ASP
1	D	141	GLN
1	D	181	ARG
1	D	197	HIS
1	D	247	VAL
1	D	251	SER
1	D	264	GLU
2	E	70	PHE
2	E	77	GLU
2	E	93	VAL
2	E	98	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	96	GLN
1	A	197	HIS
1	A	224	GLN
1	A	253	GLN
1	A	260	HIS
1	A	262	GLN
2	B	42	ASN
1	D	54	GLN

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Mol	Chain	Res	Type
1	D	96	GLN
1	D	114	HIS
1	D	141	GLN
1	D	197	HIS
1	D	226	GLN
1	D	253	GLN
1	D	260	HIS
2	E	42	ASN

4.3.3 RNA (i)

There are no RNA molecules in this entry.

4.4 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	$\#\|Z\| > 2$
3	PRQ	C	8	3	13,14,15	1.02	2 (15%)	12,18,20	1.32	3 (25%)
3	PRV	C	5	3	11,13,14	1.10	2 (18%)	9,17,19	1.43	2 (22%)
3	PRV	F	5	3	11,13,14	1.03	2 (18%)	9,17,19	1.56	3 (33%)
3	PRQ	F	8	3	13,14,15	0.94	1 (7%)	12,18,20	1.31	2 (16%)

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	PRQ	C	8	3	-	5/9/11/12	0/1/1/1
3	PRV	C	5	3	-	3/5/10/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PRV	F	5	3	-	3/5/10/12	0/1/1/1
3	PRQ	F	8	3	-	6/9/11/12	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	8	PRQ	CAL-NAN	-2.80	1.40	1.45
3	C	5	PRV	CD2-N1	-2.65	1.40	1.45
3	F	8	PRQ	CAL-NAN	-2.63	1.40	1.45
3	F	5	PRV	CD2-N1	-2.36	1.41	1.45
3	C	5	PRV	CG-CA	-2.25	1.49	1.52
3	F	5	PRV	CG-CA	-2.22	1.49	1.52
3	C	8	PRQ	CAK-CA	-2.04	1.48	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	5	PRV	CD1-CG-CD2	2.80	120.06	117.05
3	F	5	PRV	CE2-CD2-N1	2.77	119.44	116.47
3	C	5	PRV	CE2-CD2-N1	2.39	119.03	116.47
3	C	5	PRV	CD1-CG-CD2	2.36	119.58	117.05
3	C	8	PRQ	CAH-CAK-CAL	2.21	119.42	117.05
3	F	8	PRQ	CAH-CAK-CAL	2.18	119.39	117.05
3	F	8	PRQ	O-C-CAJ	-2.15	119.16	125.43
3	C	8	PRQ	O-C-CAJ	-2.06	119.44	125.43
3	C	8	PRQ	CAI-CAL-NAN	2.03	118.64	116.47
3	F	5	PRV	CE2-CD2-CG	-2.01	119.38	121.35

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	5	PRV	CG-CD2-N1-O2
3	C	5	PRV	CE2-CD2-N1-O2
3	C	5	PRV	N-CA-CG-CD2
3	F	5	PRV	N-CA-CG-CD2
3	C	8	PRQ	CAJ-CA-CAK-CAH
3	C	8	PRQ	N-CA-CAK-CAL
3	C	8	PRQ	CAK-CAL-NAN-OAC
3	C	8	PRQ	CAI-CAL-NAN-OAC
3	F	8	PRQ	N-CA-CAK-CAL

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Mol	Chain	Res	Type	Atoms
3	F	8	PRQ	CAK-CAL-NAN-OAC
3	F	8	PRQ	CAI-CAL-NAN-OAC
3	F	5	PRV	CE2-CD2-N1-O2
3	F	8	PRQ	CAJ-CA-CAK-CAH
3	C	8	PRQ	CAJ-CA-CAK-CAL
3	F	8	PRQ	CAJ-CA-CAK-CAL
3	F	5	PRV	CG-CD2-N1-O2
3	F	8	PRQ	N-CA-CAK-CAH

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	8	PRQ	4	0
3	C	5	PRV	1	0
3	F	5	PRV	3	0
3	F	8	PRQ	1	0

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 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	$\#\|Z\| > 2$
5	MES	B	1102	-	12,12,12	2.14	1 (8%)	14,16,16	7.64	10 (71%)
4	GOL	E	1101	-	5,5,5	0.41	0	5,5,5	0.09	0
4	GOL	E	1102	-	5,5,5	0.43	0	5,5,5	0.11	0
5	MES	D	1278	-	12,12,12	2.20	1 (8%)	14,16,16	7.89	10 (71%)
5	MES	B	1101	-	12,12,12	2.09	1 (8%)	14,16,16	7.56	10 (71%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	A	1276	-	5,5,5	0.35	0	5,5,5	0.28	0
5	MES	E	1100	-	12,12,12	2.12	1 (8%)	14,16,16	7.60	10 (71%)
4	GOL	B	1100	-	5,5,5	0.41	0	5,5,5	0.17	0
4	GOL	D	1277	-	5,5,5	0.35	0	5,5,5	0.37	0
5	MES	D	1276	-	12,12,12	2.20	1 (8%)	14,16,16	7.74	10 (71%)
4	GOL	D	1279	-	5,5,5	0.39	0	5,5,5	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MES	B	1102	-	-	4/6/14/14	0/1/1/1
4	GOL	E	1101	-	-	2/4/4/4	-
4	GOL	E	1102	-	-	2/4/4/4	-
5	MES	D	1278	-	-	4/6/14/14	0/1/1/1
5	MES	B	1101	-	-	1/6/14/14	0/1/1/1
4	GOL	A	1276	-	-	0/4/4/4	-
5	MES	E	1100	-	-	1/6/14/14	0/1/1/1
4	GOL	B	1100	-	-	2/4/4/4	-
4	GOL	D	1277	-	-	2/4/4/4	-
5	MES	D	1276	-	-	1/6/14/14	0/1/1/1
4	GOL	D	1279	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1276	MES	C8-S	-7.21	1.67	1.77
5	D	1278	MES	C8-S	-7.19	1.67	1.77
5	B	1102	MES	C8-S	-7.06	1.67	1.77
5	E	1100	MES	C8-S	-6.99	1.67	1.77
5	B	1101	MES	C8-S	-6.87	1.67	1.77

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1278	MES	O1S-S-C8	-19.90	82.95	106.92
5	D	1276	MES	O1S-S-C8	-18.47	84.68	106.92
5	E	1100	MES	O1S-S-C8	-17.10	86.32	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1102	MES	O1S-S-C8	-17.05	86.39	106.92
5	D	1276	MES	O2S-S-C8	-17.02	86.42	106.92
5	B	1101	MES	O1S-S-C8	-17.00	86.44	106.92
5	D	1278	MES	O2S-S-C8	-16.99	86.46	106.92
5	B	1102	MES	O2S-S-C8	-16.96	86.49	106.92
5	B	1101	MES	O2S-S-C8	-16.43	87.13	106.92
5	E	1100	MES	O2S-S-C8	-16.03	87.62	106.92
5	E	1100	MES	O3S-S-C8	-12.37	85.76	105.77
5	B	1101	MES	O3S-S-C8	-12.17	86.09	105.77
5	B	1102	MES	O3S-S-C8	-11.59	87.03	105.77
5	D	1276	MES	O3S-S-C8	-10.40	88.94	105.77
5	D	1278	MES	O3S-S-C8	-9.92	89.72	105.77
5	D	1278	MES	C5-N4-C3	4.73	119.48	108.83
5	E	1100	MES	C5-N4-C3	4.63	119.25	108.83
5	D	1276	MES	C5-N4-C3	4.63	119.24	108.83
5	B	1101	MES	C5-N4-C3	4.34	118.60	108.83
5	B	1102	MES	C5-N4-C3	4.33	118.57	108.83
5	D	1276	MES	C2-C3-N4	-4.25	103.65	110.10
5	E	1100	MES	C7-N4-C5	4.02	121.52	111.23
5	B	1102	MES	C6-C5-N4	-4.00	104.03	110.10
5	B	1102	MES	C7-N4-C5	3.97	121.38	111.23
5	B	1101	MES	C7-N4-C5	3.95	121.34	111.23
5	D	1278	MES	O3S-S-O1S	3.89	120.78	111.27
5	E	1100	MES	C2-C3-N4	-3.88	104.22	110.10
5	E	1100	MES	O3S-S-O2S	3.71	120.34	111.27
5	E	1100	MES	O3S-S-O1S	3.66	120.21	111.27
5	D	1278	MES	C7-N4-C5	3.65	120.58	111.23
5	B	1102	MES	C2-C3-N4	-3.65	104.56	110.10
5	D	1276	MES	C7-N4-C3	3.64	120.54	111.23
5	B	1102	MES	O3S-S-O2S	3.64	120.16	111.27
5	E	1100	MES	C6-C5-N4	-3.61	104.62	110.10
5	D	1276	MES	C7-N4-C5	3.51	120.22	111.23
5	B	1101	MES	O3S-S-O2S	3.47	119.76	111.27
5	B	1101	MES	C7-N4-C3	3.45	120.06	111.23
5	B	1102	MES	C7-N4-C3	3.44	120.04	111.23
5	D	1276	MES	O3S-S-O1S	3.44	119.68	111.27
5	D	1278	MES	C7-N4-C3	3.40	119.93	111.23
5	B	1101	MES	O3S-S-O1S	3.38	119.53	111.27
5	B	1102	MES	O3S-S-O1S	3.37	119.52	111.27
5	D	1276	MES	O3S-S-O2S	3.27	119.26	111.27
5	B	1101	MES	C2-C3-N4	-3.23	105.21	110.10
5	E	1100	MES	C7-N4-C3	3.13	119.23	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1101	MES	C6-C5-N4	-2.88	105.73	110.10
5	D	1278	MES	C6-C5-N4	-2.83	105.82	110.10
5	D	1276	MES	C6-C5-N4	-2.60	106.16	110.10
5	D	1278	MES	O3S-S-O2S	2.60	117.63	111.27
5	D	1278	MES	C2-C3-N4	-2.30	106.62	110.10

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1277	GOL	C1-C2-C3-O3
4	D	1279	GOL	C1-C2-C3-O3
4	E	1102	GOL	C1-C2-C3-O3
5	B	1101	MES	C8-C7-N4-C5
5	B	1102	MES	C7-C8-S-O1S
5	D	1276	MES	C8-C7-N4-C5
5	D	1278	MES	C8-C7-N4-C5
5	D	1278	MES	C7-C8-S-O1S
5	D	1278	MES	C7-C8-S-O3S
5	E	1100	MES	C8-C7-N4-C5
4	B	1100	GOL	O2-C2-C3-O3
5	B	1102	MES	C7-C8-S-O3S
4	B	1100	GOL	C1-C2-C3-O3
4	D	1277	GOL	O2-C2-C3-O3
4	D	1279	GOL	O2-C2-C3-O3
4	E	1102	GOL	O2-C2-C3-O3
5	B	1102	MES	C8-C7-N4-C3
5	B	1102	MES	C7-C8-S-O2S
5	D	1278	MES	C7-C8-S-O2S
4	E	1101	GOL	C1-C2-C3-O3
4	E	1101	GOL	O2-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1102	MES	3	0
4	E	1102	GOL	1	0
5	D	1278	MES	3	0
5	B	1101	MES	1	0
4	A	1276	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1100	MES	1	0
4	B	1100	GOL	3	0
4	D	1277	GOL	1	0
5	D	1276	MES	3	0

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

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	275/275 (100%)	-0.14	0 100 100	21, 42, 73, 112	0
1	D	275/275 (100%)	-0.04	1 (0%) 92 95	15, 46, 73, 89	0
2	B	100/100 (100%)	-0.29	0 100 100	21, 35, 61, 86	0
2	E	100/100 (100%)	-0.34	0 100 100	21, 37, 63, 74	0
3	C	6/9 (66%)	1.42	1 (16%) 1 2	37, 70, 91, 119	0
3	F	6/9 (66%)	0.77	1 (16%) 1 2	40, 58, 77, 103	0
All	All	762/768 (99%)	-0.13	3 (0%) 92 95	15, 42, 73, 119	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	7	PHE	5.0
3	F	7	PHE	4.1
1	D	130	LEU	2.1

5.2 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PRQ	C	8	14/15	0.72	0.37	93,128,142,146	0
3	PRV	C	5	13/14	0.81	0.29	85,101,111,111	0
3	PRV	F	5	13/14	0.87	0.16	65,70,75,76	0
3	PRQ	F	8	14/15	0.90	0.20	46,94,106,106	0

5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

5.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	B	1100	6/6	0.88	0.17	56,63,65,65	0
5	MES	B	1102	12/12	0.88	0.18	48,64,150,151	0
4	GOL	D	1279	6/6	0.90	0.16	48,52,56,59	0
4	GOL	A	1276	6/6	0.90	0.14	44,49,50,55	0
4	GOL	E	1102	6/6	0.91	0.24	35,48,56,59	0
4	GOL	D	1277	6/6	0.92	0.17	46,47,50,51	0
5	MES	E	1100	12/12	0.92	0.15	61,65,68,68	0
5	MES	B	1101	12/12	0.93	0.13	62,71,91,95	0
4	GOL	E	1101	6/6	0.94	0.12	27,32,39,50	0
5	MES	D	1278	12/12	0.96	0.15	25,30,38,40	0
5	MES	D	1276	12/12	0.97	0.14	27,44,47,48	0

5.5 Other polymers (i)

There are no such residues in this entry.