Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 04:24 AM EDT

PDB ID	:	3CC5
Title	:	H-2Db complex with human gp100
Authors	:	Badia-Martinez, D.; Achour, A.
Deposited on	:	2008-02-24
Resolution	:	1.91 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 (1)) were used in the production of this report:

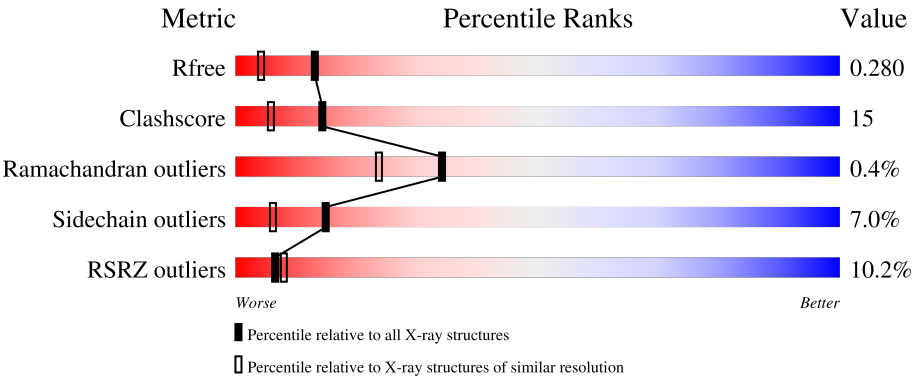
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	276	11% 78% 19%
1	D	276	11% 77% 20%
2	B	99	8% 80% 17%
2	E	99	6% 83% 14%
3	C	9	22% 44% 33% 22%

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Mol	Chain	Length	Quality of chain
3	F	9	22% 44% 33% 22%

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
5	GOL	A	279	-	-	X	-
5	GOL	B	100	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6994 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2265	1430	400	426	9			
1	D	276	Total	C	N	O	S	0	0	0
			2265	1430	400	426	9			

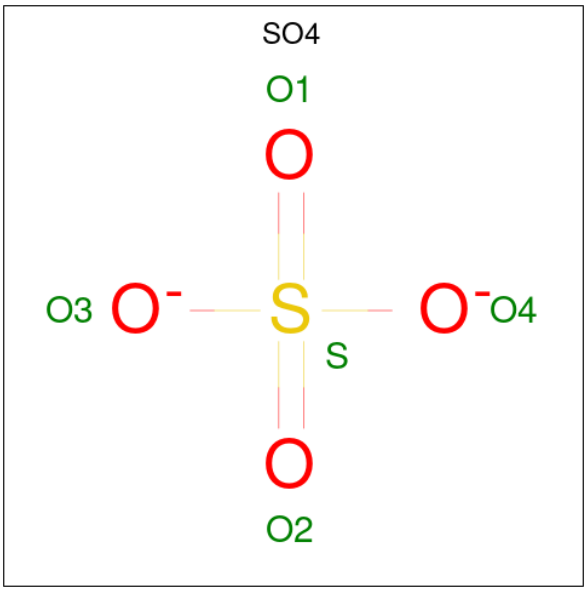
- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	E	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- Molecule 3 is a protein called nonameric peptide from Melanocyte protein Pmel 17.

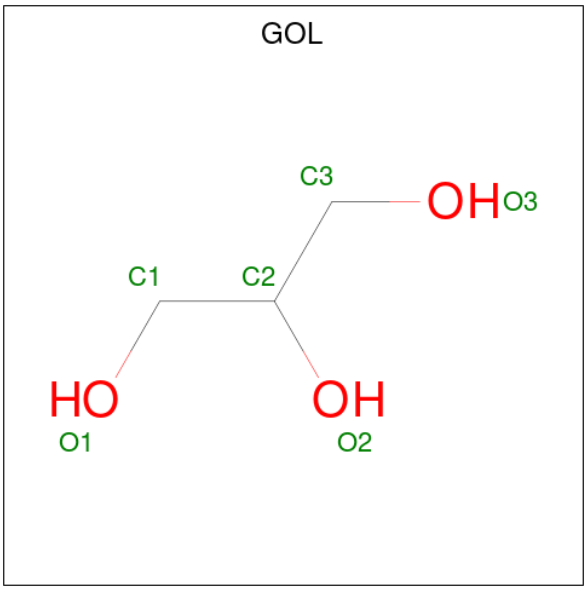
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			82	52	16	14			
3	F	9	Total	C	N	O	0	0	0
			82	52	16	14			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

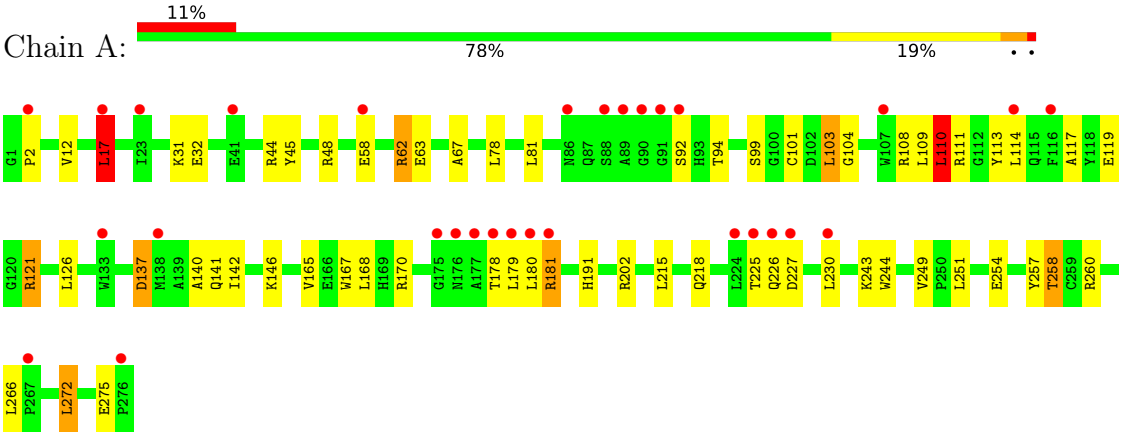
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	206	Total O 206 206	0	0
6	B	85	Total O 85 85	0	0
6	C	8	Total O 8 8	0	0
6	D	204	Total O 204 204	0	0
6	E	96	Total O 96 96	0	0
6	F	8	Total O 8 8	0	0

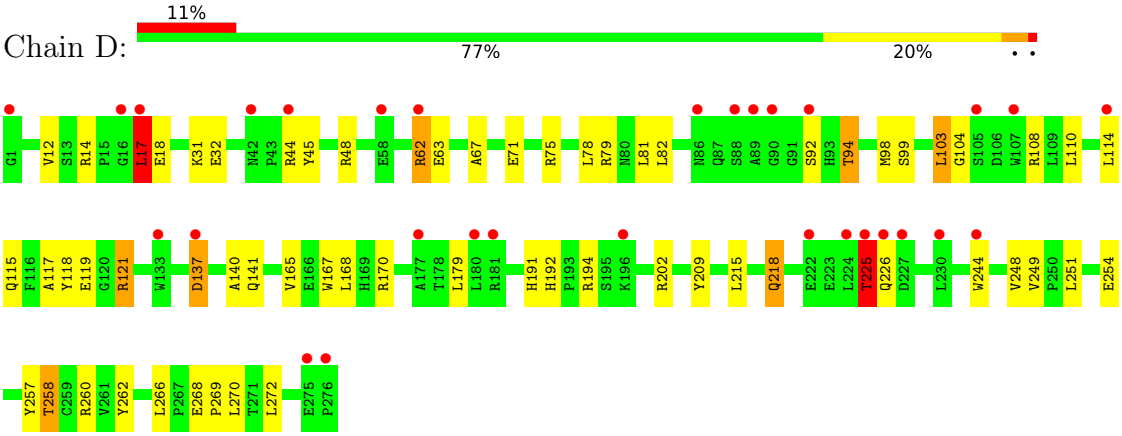
3 Residue-property plots (i)

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.

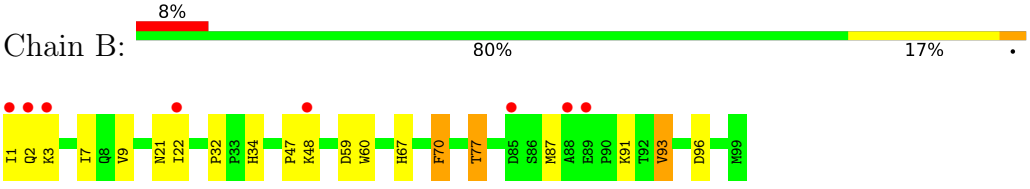
• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

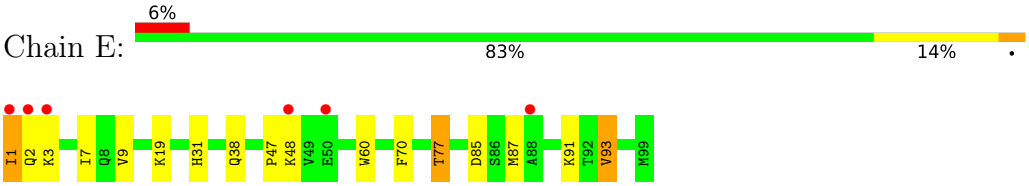


• Molecule 2: Beta-2-microglobulin



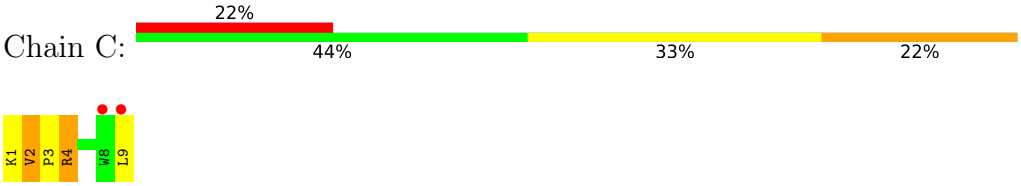
• Molecule 2: Beta-2-microglobulin

Chain E:



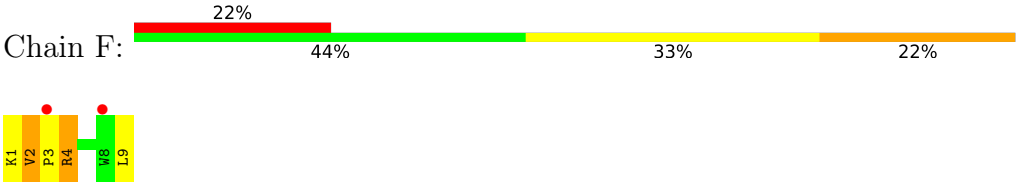
• Molecule 3: nonameric peptide from Melanocyte protein Pmel 17

Chain C:



• Molecule 3: nonameric peptide from Melanocyte protein Pmel 17

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	67.20Å 165.40Å 161.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.81 – 1.91 24.81 – 1.91	Depositor EDS
% Data completeness (in resolution range)	97.5 (24.81-1.91) 97.5 (24.81-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.228 , 0.268 0.243 , 0.280	Depositor DCC
R_{free} test set	3432 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 58.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6994	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1503e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: SO4, 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	0.56	0/2332	0.73	2/3166 (0.1%)
1	D	0.55	0/2332	0.68	1/3166 (0.0%)
2	B	0.56	0/847	0.68	0/1148
2	E	0.54	0/847	0.67	0/1148
3	C	0.61	0/84	0.64	0/112
3	F	0.60	0/84	0.68	0/112
All	All	0.56	0/6526	0.70	3/8852 (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	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	17	LEU	CA-CB-CG	5.65	128.28	115.30
1	A	110	LEU	CA-CB-CG	5.09	127.00	115.30
1	D	17	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	THR	Peptide
1	D	225	THR	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	2265	0	2136	70	0
1	D	2265	0	2136	67	0
2	B	821	0	796	27	0
2	E	821	0	796	18	0
3	C	82	0	83	10	0
3	F	82	0	83	11	0
4	A	10	0	0	1	0
4	D	5	0	0	1	0
5	A	12	0	16	6	0
5	B	6	0	8	6	0
5	D	18	0	24	2	0
6	A	206	0	0	14	0
6	B	85	0	0	3	0
6	C	8	0	0	1	0
6	D	204	0	0	10	0
6	E	96	0	0	7	0
6	F	8	0	0	3	0
All	All	6994	0	6078	193	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 (193) 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:A:121:ARG:HH11	1:A:121:ARG:CG	1.57	1.16
1:D:225:THR:H	1:D:226:GLN:HB3	1.06	1.11
1:D:121:ARG:HH11	1:D:121:ARG:CG	1.64	1.10
1:A:62:ARG:HH11	1:A:62:ARG:CG	1.65	1.09
1:D:121:ARG:HH11	1:D:121:ARG:HG2	0.92	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:ASP:H	5:B:100:GOL:H12	0.92	1.06
2:B:96:ASP:N	5:B:100:GOL:H12	1.71	1.05
1:D:62:ARG:HG2	1:D:62:ARG:HH11	0.89	1.05
1:D:62:ARG:HH11	1:D:62:ARG:CG	1.69	1.05
1:D:121:ARG:HG2	1:D:121:ARG:NH1	1.59	1.05
1:A:181:ARG:HG3	1:A:181:ARG:HH11	1.20	1.03
1:D:108:ARG:HG3	6:D:325:HOH:O	1.59	1.03
3:F:4:ARG:NH1	6:F:17:HOH:O	1.90	1.02
1:A:62:ARG:HG2	1:A:62:ARG:NH1	1.61	1.02
1:A:121:ARG:HG2	1:A:121:ARG:NH1	1.53	1.01
1:A:62:ARG:HH11	1:A:62:ARG:HG2	0.86	1.01
2:B:96:ASP:H	5:B:100:GOL:C1	1.76	0.98
1:D:62:ARG:HG2	1:D:62:ARG:NH1	1.64	0.98
1:A:121:ARG:HH11	1:A:121:ARG:HG2	0.83	0.97
1:D:225:THR:H	1:D:226:GLN:CB	1.78	0.96
1:D:225:THR:N	1:D:226:GLN:HB3	1.81	0.95
3:F:2:VAL:HG22	6:F:10:HOH:O	1.68	0.93
1:A:103:LEU:HG	1:A:168:LEU:HD23	1.50	0.92
6:A:485:HOH:O	3:C:2:VAL:HG22	1.71	0.91
1:D:103:LEU:HG	1:D:168:LEU:HD23	1.55	0.87
1:A:181:ARG:HH11	1:A:181:ARG:CG	1.87	0.87
3:C:4:ARG:NH1	6:C:10:HOH:O	1.99	0.86
2:B:1:ILE:H1	2:B:32:PRO:HD2	1.44	0.81
2:B:1:ILE:N	2:B:32:PRO:HD2	1.99	0.76
2:E:7:ILE:HD12	2:E:91:LYS:HD2	1.66	0.76
2:E:87:MET:HE3	2:E:91:LYS:HE3	1.66	0.76
3:C:4:ARG:HG2	3:C:4:ARG:HH11	1.50	0.76
2:E:87:MET:CE	2:E:91:LYS:HE3	2.15	0.76
1:D:191:HIS:HD2	6:D:445:HOH:O	1.69	0.75
2:B:87:MET:CE	2:B:91:LYS:HE3	2.17	0.75
1:A:126:LEU:O	5:A:279:GOL:H12	1.87	0.74
1:A:181:ARG:HG3	1:A:181:ARG:NH1	1.98	0.74
2:B:9:VAL:H	5:B:100:GOL:H32	1.51	0.74
3:C:4:ARG:HH11	3:C:4:ARG:CG	2.02	0.73
1:D:92:SER:HB2	6:D:319:HOH:O	1.89	0.72
3:F:4:ARG:HG2	3:F:4:ARG:HH11	1.55	0.71
1:A:226:GLN:HG2	1:A:226:GLN:O	1.89	0.71
2:B:7:ILE:HD12	2:B:91:LYS:HD2	1.72	0.70
2:E:19:LYS:HE3	6:E:139:HOH:O	1.90	0.70
2:B:1:ILE:N	2:B:32:PRO:CD	2.54	0.70
1:D:71:GLU:OE2	6:D:482:HOH:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:LYS:NZ	6:D:331:HOH:O	2.19	0.69
3:F:4:ARG:HH11	3:F:4:ARG:CG	2.06	0.69
1:D:12:VAL:HG22	1:D:94:THR:HG22	1.74	0.68
1:A:167:TRP:CE3	1:A:170:ARG:HD3	2.29	0.68
1:D:167:TRP:CE3	1:D:170:ARG:HD3	2.29	0.68
1:D:104:GLY:N	1:D:110:LEU:CD1	2.57	0.67
1:A:113:TYR:HA	5:A:279:GOL:H11	1.76	0.67
1:A:111:ARG:HH21	5:A:279:GOL:H31	1.60	0.67
3:C:4:ARG:NH1	3:C:4:ARG:HG2	2.10	0.66
1:A:275:GLU:OE1	6:A:465:HOH:O	2.12	0.66
1:A:108:ARG:HG2	1:D:262:TYR:CD2	2.31	0.66
1:D:218:GLN:OE1	1:D:258:THR:HG22	1.97	0.65
1:A:218:GLN:OE1	1:A:258:THR:HG22	1.96	0.65
2:B:87:MET:HE3	2:B:91:LYS:HE3	1.77	0.65
1:D:75:ARG:HH12	1:D:79:ARG:NH1	1.94	0.65
1:A:167:TRP:CZ3	1:A:170:ARG:HD3	2.32	0.65
1:A:108:ARG:HD3	1:D:262:TYR:CE2	2.33	0.64
2:E:38:GLN:HG2	6:E:117:HOH:O	1.98	0.63
1:D:104:GLY:CA	1:D:110:LEU:CD1	2.77	0.63
3:F:4:ARG:NH1	3:F:4:ARG:HG2	2.13	0.63
2:E:2:GLN:NE2	2:E:3:LYS:HE3	2.12	0.63
1:A:103:LEU:HD21	1:A:165:VAL:HG22	1.80	0.62
1:A:108:ARG:HD3	1:D:262:TYR:CZ	2.34	0.62
1:D:167:TRP:CZ3	1:D:170:ARG:HD3	2.35	0.62
1:A:181:ARG:CG	1:A:181:ARG:NH1	2.58	0.61
1:A:104:GLY:N	1:A:110:LEU:HD23	2.16	0.61
2:B:1:ILE:H1	2:B:32:PRO:CD	2.13	0.60
1:D:103:LEU:HD21	1:D:165:VAL:HG22	1.83	0.60
1:D:104:GLY:N	1:D:110:LEU:HD13	2.16	0.60
6:A:485:HOH:O	3:C:2:VAL:CG2	2.40	0.60
1:D:75:ARG:HH12	1:D:79:ARG:HH12	1.49	0.59
1:D:104:GLY:HA3	1:D:110:LEU:HD11	1.85	0.59
3:F:2:VAL:CG2	6:F:10:HOH:O	2.39	0.59
1:A:17:LEU:HD12	6:A:325:HOH:O	2.03	0.58
1:D:31:LYS:HD2	1:D:209:TYR:OH	2.02	0.58
1:A:104:GLY:CA	1:A:110:LEU:HD21	2.33	0.58
1:A:179:LEU:CD2	6:A:304:HOH:O	2.52	0.58
1:A:12:VAL:HG22	1:A:94:THR:HG22	1.84	0.58
1:D:115:GLN:OE1	6:D:465:HOH:O	2.17	0.58
1:A:227:ASP:OD2	1:A:227:ASP:O	2.21	0.57
1:D:62:ARG:HD3	6:D:328:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:TYR:CE2	1:A:67:ALA:HB2	2.40	0.57
1:D:63:GLU:OE2	3:F:1:LYS:HG3	2.06	0.56
2:E:77:THR:CG2	6:E:104:HOH:O	2.52	0.56
1:D:104:GLY:CA	1:D:110:LEU:HD11	2.35	0.56
1:A:181:ARG:HG3	1:A:181:ARG:O	2.05	0.56
1:A:191:HIS:HE1	1:A:254:GLU:OE2	1.88	0.56
1:A:32:GLU:OE2	1:A:48:ARG:HD2	2.06	0.56
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.41	0.56
1:D:119:GLU:O	1:D:121:ARG:HD2	2.06	0.55
1:A:121:ARG:HH11	1:A:121:ARG:CB	2.19	0.55
1:A:104:GLY:HA3	1:A:110:LEU:HD21	1.87	0.55
2:B:87:MET:HE1	2:B:91:LYS:HE3	1.86	0.55
2:E:9:VAL:HG23	2:E:93:VAL:HG22	1.88	0.54
2:E:1:ILE:O	2:E:1:ILE:HD13	2.07	0.54
1:A:121:ARG:CG	1:A:121:ARG:NH1	2.30	0.54
2:E:1:ILE:HG12	2:E:85:ASP:O	2.08	0.53
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.43	0.53
1:A:119:GLU:O	1:A:121:ARG:HD2	2.08	0.53
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.43	0.53
1:A:178:THR:HG21	6:A:477:HOH:O	2.08	0.53
2:B:67:HIS:HE1	6:B:109:HOH:O	1.92	0.53
1:A:179:LEU:HD23	6:A:304:HOH:O	2.08	0.52
1:D:121:ARG:CG	1:D:121:ARG:NH1	2.36	0.52
1:D:192:HIS:HD2	6:E:128:HOH:O	1.91	0.52
1:A:58:GLU:HB2	6:A:340:HOH:O	2.09	0.52
1:A:126:LEU:O	5:A:279:GOL:C1	2.56	0.52
1:D:45:TYR:CE2	1:D:67:ALA:HB2	2.45	0.51
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.46	0.51
2:B:9:VAL:O	5:B:100:GOL:H11	2.10	0.51
1:A:62:ARG:HD3	6:A:484:HOH:O	2.10	0.51
2:E:19:LYS:CE	6:E:139:HOH:O	2.53	0.51
1:D:137:ASP:O	1:D:141:GLN:HG2	2.11	0.51
1:D:17:LEU:H	1:D:17:LEU:HD23	1.73	0.50
2:B:1:ILE:H3	2:B:32:PRO:HD3	1.76	0.50
1:D:62:ARG:CG	1:D:62:ARG:NH1	2.40	0.50
1:D:121:ARG:HH11	1:D:121:ARG:CB	2.22	0.50
3:C:2:VAL:HG22	3:C:3:PRO:HD2	1.92	0.49
1:A:137:ASP:O	1:A:141:GLN:HG2	2.12	0.49
2:B:21:ASN:C	2:B:22:ILE:HD12	2.33	0.49
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.48	0.49
1:A:101:CYS:HB2	1:A:109:LEU:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLY:N	1:A:110:LEU:CD2	2.75	0.49
1:A:137:ASP:HB3	1:A:140:ALA:H	1.76	0.49
2:B:1:ILE:N	2:B:32:PRO:HD3	2.28	0.49
1:A:62:ARG:HD3	4:A:278:SO4:O3	2.14	0.48
3:F:2:VAL:HG22	3:F:3:PRO:HD2	1.94	0.48
1:D:191:HIS:HE1	1:D:254:GLU:OE2	1.96	0.48
2:E:87:MET:HE1	2:E:91:LYS:HE3	1.94	0.48
1:A:113:TYR:CD2	5:A:279:GOL:H32	2.49	0.48
2:B:9:VAL:HG23	2:B:93:VAL:HG22	1.96	0.47
1:A:167:TRP:CZ3	1:A:170:ARG:CD	2.97	0.47
1:A:44:ARG:HH11	1:A:44:ARG:HG3	1.79	0.47
1:A:63:GLU:OE2	3:C:1:LYS:HG3	2.14	0.47
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.50	0.47
2:B:77:THR:CG2	6:B:127:HOH:O	2.62	0.47
1:D:62:ARG:CD	6:D:328:HOH:O	2.62	0.47
2:E:9:VAL:CG2	2:E:93:VAL:HG22	2.45	0.47
1:D:103:LEU:C	1:D:110:LEU:HD13	2.35	0.46
1:D:44:ARG:HG3	1:D:44:ARG:HH11	1.80	0.46
1:D:119:GLU:HG3	5:D:280:GOL:H32	1.96	0.46
2:E:7:ILE:CD1	2:E:91:LYS:HD2	2.41	0.46
1:A:260:ARG:NH1	6:A:409:HOH:O	2.40	0.46
2:B:1:ILE:H3	2:B:32:PRO:CD	2.29	0.45
1:A:17:LEU:HD12	1:A:17:LEU:H	1.80	0.45
2:E:77:THR:HG22	6:E:104:HOH:O	2.12	0.45
2:B:34:HIS:O	6:B:121:HOH:O	2.21	0.45
1:D:167:TRP:CZ3	1:D:170:ARG:CD	2.99	0.45
1:A:191:HIS:HD2	6:A:327:HOH:O	1.99	0.45
1:A:226:GLN:O	1:A:227:ASP:HB3	2.16	0.44
1:A:103:LEU:CD2	1:A:165:VAL:HG22	2.46	0.44
1:A:17:LEU:CD1	6:A:325:HOH:O	2.62	0.44
1:A:81:LEU:HD11	3:C:9:LEU:CD1	2.48	0.44
1:D:137:ASP:HB3	1:D:140:ALA:H	1.82	0.44
2:E:31:HIS:ND1	6:E:113:HOH:O	2.36	0.44
2:B:9:VAL:CG2	2:B:93:VAL:HG22	2.47	0.44
1:D:62:ARG:NE	6:D:328:HOH:O	2.51	0.44
1:D:249:VAL:HG22	1:D:257:TYR:CZ	2.52	0.44
1:D:225:THR:N	1:D:226:GLN:CB	2.57	0.43
1:D:98:MET:HG3	2:E:60:TRP:CZ3	2.53	0.43
1:D:32:GLU:OE2	1:D:48:ARG:HD2	2.19	0.43
1:D:75:ARG:NH1	1:D:79:ARG:NH1	2.65	0.43
1:D:31:LYS:HB3	6:D:339:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:LEU:HD11	3:F:9:LEU:CD1	2.49	0.43
2:B:59:ASP:O	2:B:60:TRP:HB2	2.18	0.43
1:D:118:TYR:HD2	5:D:280:GOL:H12	1.84	0.43
1:A:142:ILE:O	1:A:146:LYS:HG3	2.19	0.43
2:B:9:VAL:O	5:B:100:GOL:C1	2.66	0.43
1:A:45:TYR:HE2	1:A:67:ALA:HB2	1.84	0.42
1:D:260:ARG:HA	1:D:270:LEU:O	2.20	0.42
1:A:178:THR:CG2	6:A:477:HOH:O	2.65	0.42
1:D:170:ARG:HD2	4:D:277:SO4:O3	2.20	0.42
1:A:230:LEU:HD13	1:A:243:LYS:HE3	2.01	0.42
3:F:4:ARG:HH11	3:F:4:ARG:CB	2.33	0.42
1:A:272:LEU:HD23	1:A:272:LEU:N	2.35	0.42
2:B:2:GLN:HG3	2:B:3:LYS:HG3	2.01	0.41
3:C:4:ARG:HH11	3:C:4:ARG:CB	2.33	0.41
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.72	0.41
1:A:119:GLU:O	1:A:121:ARG:CD	2.68	0.41
1:D:14:ARG:HB2	1:D:18:GLU:HB2	2.03	0.41
3:F:4:ARG:HH11	3:F:4:ARG:HB3	1.86	0.41
1:A:227:ASP:HB2	6:A:454:HOH:O	2.20	0.41
1:D:82:LEU:HD12	1:D:82:LEU:HA	1.88	0.41
1:D:194:ARG:HD2	1:D:248:VAL:HG22	2.03	0.41
1:D:268:GLU:HB2	1:D:269:PRO:HD2	2.03	0.41
1:A:111:ARG:NH2	5:A:279:GOL:H31	2.33	0.40
1:D:119:GLU:O	1:D:121:ARG:CD	2.70	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	274/276 (99%)	261 (95%)	12 (4%)	1 (0%)	34 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	274/276 (99%)	266 (97%)	8 (3%)	0	100 100
2	B	97/99 (98%)	95 (98%)	1 (1%)	1 (1%)	15 6
2	E	97/99 (98%)	95 (98%)	1 (1%)	1 (1%)	15 6
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100 100
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100 100
All	All	756/768 (98%)	729 (96%)	24 (3%)	3 (0%)	34 24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	47	PRO
1	A	2	PRO
2	B	47	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	234/234 (100%)	217 (93%)	17 (7%)	14 5
1	D	234/234 (100%)	217 (93%)	17 (7%)	14 5
2	B	94/94 (100%)	90 (96%)	4 (4%)	29 18
2	E	94/94 (100%)	89 (95%)	5 (5%)	22 12
3	C	9/9 (100%)	7 (78%)	2 (22%)	1 0
3	F	9/9 (100%)	7 (78%)	2 (22%)	1 0
All	All	674/674 (100%)	627 (93%)	47 (7%)	15 6

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	31	LYS
1	A	62	ARG

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Mol	Chain	Res	Type
1	A	78	LEU
1	A	92	SER
1	A	99	SER
1	A	103	LEU
1	A	110	LEU
1	A	114	LEU
1	A	121	ARG
1	A	137	ASP
1	A	181	ARG
1	A	215	LEU
1	A	251	LEU
1	A	258	THR
1	A	266	LEU
1	A	272	LEU
2	B	48	LYS
2	B	70	PHE
2	B	77	THR
2	B	93	VAL
3	C	2	VAL
3	C	4	ARG
1	D	17	LEU
1	D	62	ARG
1	D	78	LEU
1	D	94	THR
1	D	99	SER
1	D	103	LEU
1	D	114	LEU
1	D	121	ARG
1	D	137	ASP
1	D	179	LEU
1	D	215	LEU
1	D	218	GLN
1	D	225	THR
1	D	251	LEU
1	D	258	THR
1	D	266	LEU
1	D	272	LEU
2	E	1	ILE
2	E	48	LYS
2	E	70	PHE
2	E	77	THR
2	E	93	VAL

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Mol	Chain	Res	Type
3	F	2	VAL
3	F	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	54	GLN
1	A	86	ASN
1	A	149	GLN
1	A	191	HIS
1	A	192	HIS
1	A	256	ASN
2	B	2	GLN
2	B	38	GLN
2	B	67	HIS
1	D	54	GLN
1	D	115	GLN
1	D	149	GLN
1	D	191	HIS
1	D	192	HIS
2	E	38	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

9 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	GOL	D	280	-	5,5,5	0.37	0	5,5,5	0.20	0
5	GOL	D	279	-	5,5,5	0.21	0	5,5,5	0.26	0
5	GOL	A	279	-	5,5,5	0.35	0	5,5,5	0.57	0
5	GOL	A	280	-	5,5,5	0.37	0	5,5,5	0.39	0
4	SO4	D	277	-	4,4,4	0.13	0	6,6,6	0.09	0
5	GOL	D	278	-	5,5,5	0.41	0	5,5,5	0.53	0
4	SO4	A	277	-	4,4,4	0.34	0	6,6,6	0.15	0
4	SO4	A	278	-	4,4,4	0.14	0	6,6,6	0.04	0
5	GOL	B	100	-	5,5,5	0.78	0	5,5,5	0.72	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	GOL	D	280	-	-	4/4/4/4	-
5	GOL	D	279	-	-	1/4/4/4	-
5	GOL	A	279	-	-	2/4/4/4	-
5	GOL	A	280	-	-	0/4/4/4	-
5	GOL	D	278	-	-	0/4/4/4	-
5	GOL	B	100	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	279	GOL	O1-C1-C2-C3
5	D	280	GOL	O1-C1-C2-O2
5	D	280	GOL	O1-C1-C2-C3
5	B	100	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	279	GOL	O1-C1-C2-O2
5	D	280	GOL	O2-C2-C3-O3
5	D	280	GOL	C1-C2-C3-O3
5	D	279	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	280	GOL	2	0
5	A	279	GOL	6	0
4	D	277	SO4	1	0
4	A	278	SO4	1	0
5	B	100	GOL	6	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	276/276 (100%)	0.84	30 (10%) 5 6	6, 13, 30, 38	0
1	D	276/276 (100%)	0.75	30 (10%) 5 6	6, 13, 27, 38	0
2	B	99/99 (100%)	0.73	8 (8%) 12 14	8, 14, 26, 35	0
2	E	99/99 (100%)	0.74	6 (6%) 21 24	8, 14, 26, 37	0
3	C	9/9 (100%)	1.41	2 (22%) 0 0	15, 19, 24, 25	0
3	F	9/9 (100%)	1.39	2 (22%) 0 0	15, 19, 24, 26	0
All	All	768/768 (100%)	0.79	78 (10%) 6 8	6, 14, 28, 38	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	ILE	11.6
2	E	1	ILE	10.3
1	D	17	LEU	10.0
1	A	17	LEU	6.7
1	A	89	ALA	6.2
1	A	225	THR	5.7
1	D	225	THR	5.5
1	D	227	ASP	5.4
1	A	90	GLY	4.8
2	E	48	LYS	4.5
1	D	230	LEU	4.3
2	B	2	GLN	4.3
2	E	2	GLN	4.2
1	A	227	ASP	4.2
1	A	92	SER	4.2
1	A	226	GLN	4.2
1	D	89	ALA	4.2
1	D	90	GLY	3.8
1	D	226	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	88	ALA	3.5
1	A	86	ASN	3.4
1	D	105	SER	3.2
1	D	177	ALA	3.1
1	A	276	PRO	3.1
1	A	267	PRO	3.0
2	E	88	ALA	3.0
1	D	107	TRP	3.0
1	D	58	GLU	2.9
1	A	177	ALA	2.9
1	D	1	GLY	2.9
1	D	16	GLY	2.8
1	A	178	THR	2.8
2	B	3	LYS	2.8
1	D	224	LEU	2.8
1	A	91	GLY	2.8
1	D	114	LEU	2.7
1	A	181	ARG	2.6
1	D	276	PRO	2.6
2	B	85	ASP	2.6
1	D	196	LYS	2.6
2	B	48	LYS	2.6
2	B	89	GLU	2.6
1	D	42	ASN	2.6
1	A	116	PHE	2.6
1	D	44	ARG	2.5
1	D	222	GLU	2.5
1	A	41	GLU	2.5
1	D	92	SER	2.5
1	A	88	SER	2.4
1	D	244	TRP	2.4
1	D	275	GLU	2.4
1	D	86	ASN	2.4
1	A	58	GLU	2.4
1	A	224	LEU	2.3
1	A	114	LEU	2.3
1	A	138	MET	2.3
1	D	181	ARG	2.3
2	B	22	ILE	2.3
1	A	2	PRO	2.3
3	F	8	TRP	2.3
2	E	3	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	107	TRP	2.3
3	F	3	PRO	2.3
1	D	88	SER	2.3
1	D	180	LEU	2.3
1	A	176	ASN	2.2
1	A	23	ILE	2.2
1	A	179	LEU	2.2
1	D	133	TRP	2.2
3	C	8	TRP	2.2
3	C	9	LEU	2.2
1	A	133	TRP	2.1
2	E	50	GLU	2.1
1	D	62	ARG	2.1
1	A	230	LEU	2.1
1	A	175	GLY	2.0
1	D	137	ASP	2.0
1	A	180	LEU	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 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
5	GOL	D	280	6/6	0.61	0.23	50,52,52,52	0
4	SO4	D	277	5/5	0.83	0.32	83,83,83,83	0
5	GOL	B	100	6/6	0.85	0.24	30,30,31,32	0
4	SO4	A	277	5/5	0.85	0.36	89,89,89,89	0
5	GOL	A	279	6/6	0.89	0.20	27,32,33,34	0
5	GOL	D	278	6/6	0.90	0.20	23,28,29,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	278	5/5	0.90	0.23	73,73,74,74	0
5	GOL	D	279	6/6	0.91	0.21	29,30,30,30	0
5	GOL	A	280	6/6	0.95	0.17	32,33,33,34	0

6.5 Other polymers (i)

There are no such residues in this entry.