Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 06:57 PM EDT

PDB ID	:	7RRG
Title	:	Crystal structure of human 0606T1-2 TCR bound to HLA-A*03:01 in complex with a mutant PIK3CA peptide
Authors	:	Ma, J.; Baker, B.M.
Deposited on	:	2021-08-09
Resolution	:	2.12 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 ⓘ 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 ⓘ) were used in the production of this report:

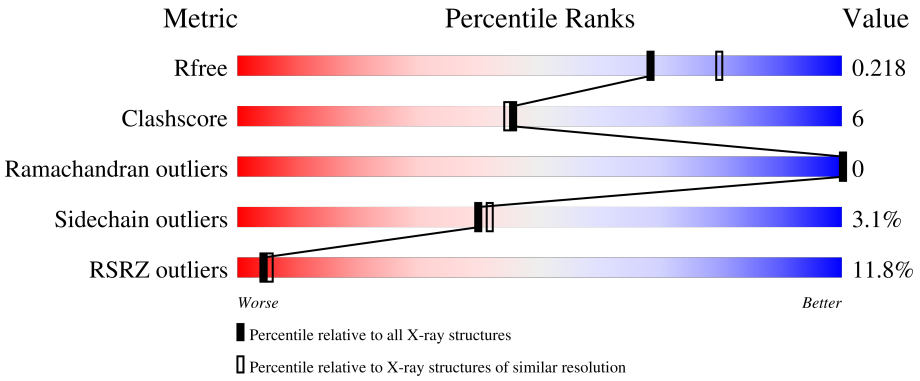
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	274	7% 89% 9%
2	B	100	94% 5%
3	D	207	9% 78% 11% 11%
4	E	245	23% 70% 26%
5	C	9	78% 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
6	GOL	A	303	-	-	X	-
6	GOL	B	103	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6912 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 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	1	0
			2208	1374	399	425	10			

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called T cell receptor, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	185	Total	C	N	O	S	0	1	0
			1416	893	234	281	8			

- Molecule 4 is a protein called T cell receptor, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	237	Total	C	N	O	S	0	0	0
			1890	1203	323	359	5			

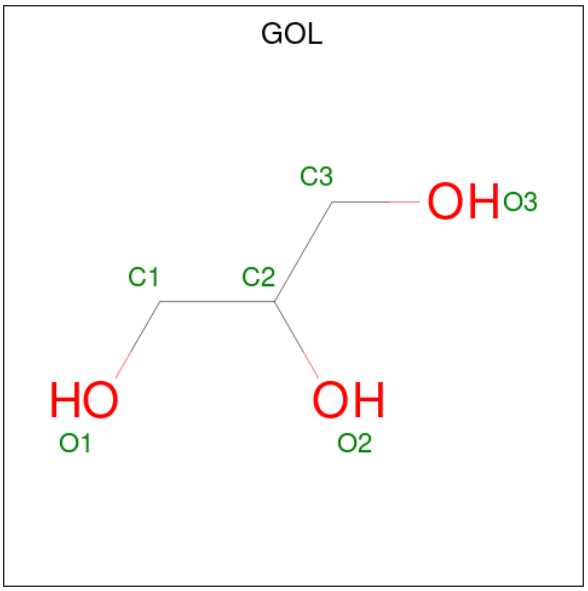
- Molecule 5 is a protein called Mutant PIK3CA peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	9	Total	C	N	O	0	0	0
			69	44	13	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	LEU	HIS	engineered mutation	UNP P42336

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 7 is water.

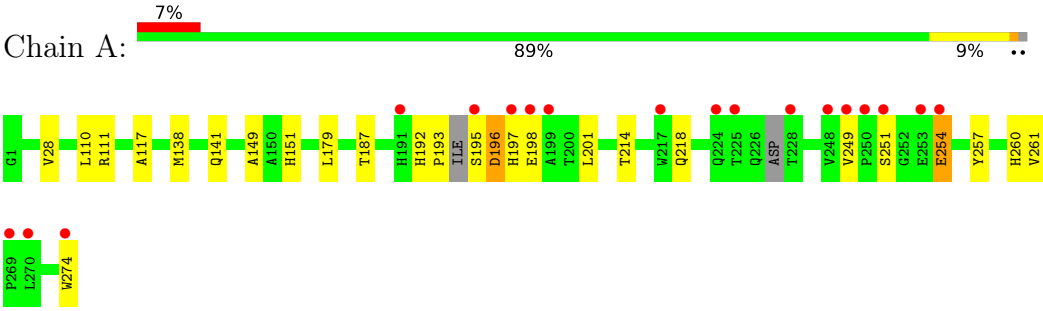
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	182	Total O 182 182	0	0
7	B	80	Total O 80 80	0	0
7	D	83	Total O 83 83	0	0
7	E	61	Total O 61 61	0	0
7	C	8	Total O 8 8	0	0

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.

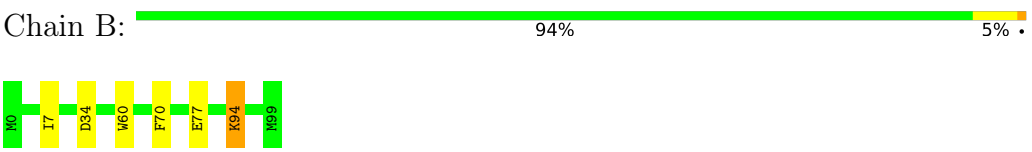
• Molecule 1: HLA class I histocompatibility antigen, A alpha chain

Chain A:



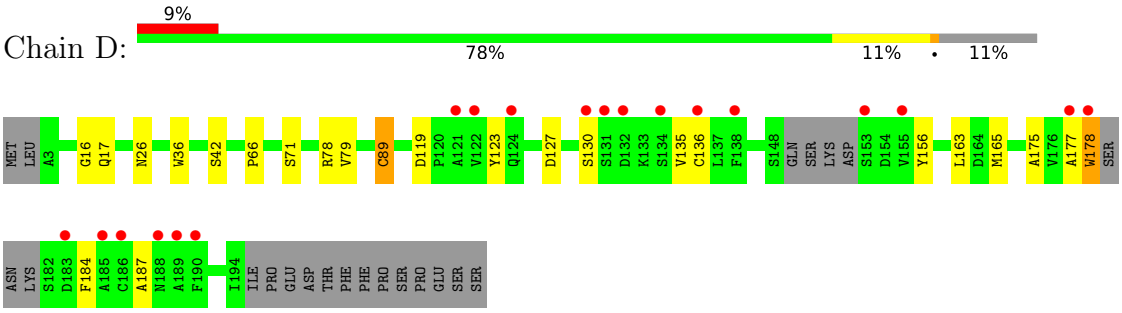
• Molecule 2: Beta-2-microglobulin

Chain B:



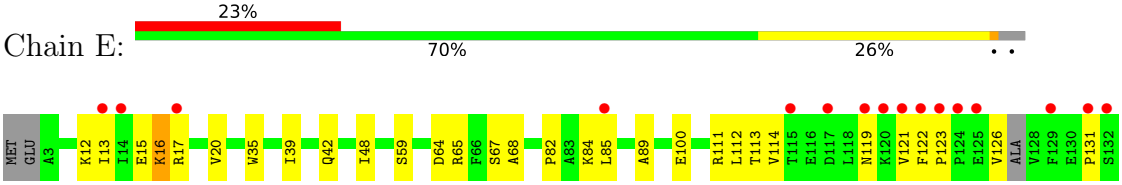
• Molecule 3: T cell receptor, alpha chain

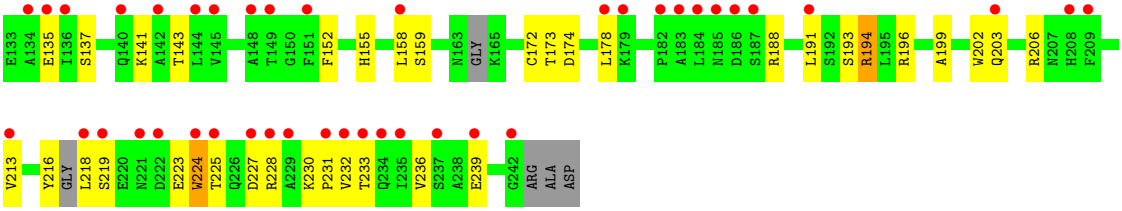
Chain D:



• Molecule 4: T cell receptor, beta chain

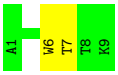
Chain E:





• Molecule 5: Mutant PIK3CA peptide

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	227.27Å 46.25Å 120.26Å 90.00° 118.67° 90.00°	Depositor
Resolution (Å)	49.85 – 2.12 49.85 – 2.12	Depositor EDS
% Data completeness (in resolution range)	95.0 (49.85-2.12) 94.5 (49.85-2.12)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.193 , 0.221 0.190 , 0.218	Depositor DCC
R_{free} test set	6144 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6912	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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: 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	0.27	0/2265	0.54	0/3070
2	B	0.25	0/860	0.48	0/1162
3	D	0.27	0/1445	0.52	0/1964
4	E	0.27	0/1939	0.51	0/2639
5	C	0.29	0/71	0.53	0/94
All	All	0.27	0/6580	0.52	0/8929

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2208	0	2056	17	0
2	B	837	0	803	8	0
3	D	1416	0	1326	14	0
4	E	1890	0	1811	45	0
5	C	69	0	68	1	0
6	A	24	0	32	4	0
6	B	36	0	48	7	0
6	C	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	12	0	16	0	0
7	A	182	0	0	0	0
7	B	80	0	0	0	0
7	C	8	0	0	0	0
7	D	83	0	0	0	0
7	E	61	0	0	0	0
All	All	6912	0	6168	81	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 6.

All (81) 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)
3:D:165:MET:HE1	4:E:196:ARG:HG2	1.51	0.92
3:D:135:VAL:HG12	3:D:178:TRP:HB3	1.56	0.86
2:B:94:LYS:HB3	6:B:103:GOL:H11	1.68	0.74
4:E:16:LYS:HE3	4:E:85:LEU:HD23	1.74	0.70
3:D:136:CYS:HB3	3:D:177:ALA:HB3	1.73	0.69
4:E:17:ARG:HA	4:E:82:PRO:HB2	1.73	0.69
4:E:119:ASN:HA	4:E:224:TRP:HZ3	1.57	0.68
4:E:158:LEU:HD13	4:E:213:VAL:HG22	1.79	0.65
1:A:201:LEU:HD12	1:A:249:VAL:HG11	1.80	0.63
2:B:77:GLU:HA	6:B:102:GOL:H32	1.80	0.63
2:B:94:LYS:HE3	6:B:103:GOL:H32	1.79	0.63
3:D:163:LEU:HB3	4:E:172:CYS:HB2	1.80	0.61
4:E:158:LEU:HD12	4:E:159:SER:H	1.66	0.61
4:E:121:VAL:HG23	4:E:231:PRO:HG2	1.81	0.60
3:D:184:PHE:CZ	3:D:187:ALA:HA	2.35	0.60
2:B:77:GLU:HG2	6:B:102:GOL:H12	1.84	0.59
3:D:16:GLY:HA2	3:D:78:ARG:HG3	1.86	0.58
4:E:39:ILE:HG22	4:E:89:ALA:HB2	1.85	0.57
4:E:113:THR:HG1	4:E:155:HIS:HE2	1.49	0.57
4:E:199:ALA:O	4:E:203:GLN:HG2	2.06	0.55
1:A:151:HIS:H	6:A:303:GOL:H12	1.72	0.54
4:E:227:ASP:OD1	4:E:228:ARG:N	2.37	0.53
4:E:39:ILE:HD11	4:E:42:GLN:HE21	1.74	0.53
1:A:214:THR:HB	1:A:262:GLN:HB2	1.90	0.52
4:E:173:THR:HG23	4:E:193:SER:HB2	1.90	0.52
6:A:303:GOL:O1	6:A:303:GOL:O3	2.22	0.51
3:D:156:TYR:O	3:D:177:ALA:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:12:LYS:HB3	4:E:112:LEU:HD12	1.93	0.51
4:E:111:ARG:HH11	4:E:111:ARG:HG2	1.76	0.51
4:E:131:PRO:HD2	4:E:202:TRP:CZ2	2.46	0.51
4:E:224:TRP:O	4:E:225:THR:OG1	2.25	0.50
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.94	0.50
1:A:138:MET:HA	1:A:141:GLN:HG2	1.94	0.49
1:A:151:HIS:ND1	6:A:303:GOL:H12	2.27	0.49
4:E:48:ILE:HD13	4:E:68:ALA:HB3	1.93	0.49
4:E:158:LEU:HD12	4:E:159:SER:N	2.28	0.48
4:E:84:LYS:HE2	4:E:84:LYS:HB3	1.76	0.48
2:B:7:ILE:H	6:B:106:GOL:H2	1.79	0.48
3:D:36:TRP:CZ2	3:D:89:CYS:HB2	2.49	0.48
1:A:149:ALA:O	6:A:303:GOL:H11	2.15	0.47
1:A:28:VAL:HG11	1:A:179:LEU:HD13	1.97	0.47
4:E:174:ASP:HB2	4:E:191:LEU:HD12	1.98	0.46
3:D:175:ALA:HA	4:E:194:ARG:HH21	1.81	0.46
1:A:197:HIS:HA	1:A:251:SER:HB3	1.98	0.45
1:A:218:GLN:HG3	1:A:260:HIS:ND1	2.32	0.45
4:E:84:LYS:O	4:E:114:VAL:HG11	2.15	0.45
4:E:216:TYR:HA	4:E:233:THR:HB	1.98	0.45
4:E:39:ILE:HG13	4:E:42:GLN:HG3	1.98	0.45
4:E:121:VAL:HG12	4:E:152:PHE:CD2	2.52	0.45
4:E:121:VAL:O	4:E:231:PRO:HG3	2.16	0.45
3:D:127:ASP:HB3	3:D:130:SER:O	2.18	0.44
4:E:12:LYS:HG2	4:E:20:VAL:HG21	2.00	0.44
4:E:141:LYS:CB	4:E:196:ARG:HD2	2.48	0.44
4:E:224:TRP:HD1	4:E:225:THR:N	2.16	0.44
4:E:100:GLU:H	4:E:100:GLU:CD	2.21	0.44
2:B:77:GLU:HG2	6:B:103:GOL:H31	1.99	0.44
3:D:66:PRO:HD2	3:D:71:SER:O	2.17	0.43
4:E:121:VAL:HA	4:E:152:PHE:HD2	1.82	0.43
3:D:184:PHE:H	3:D:184:PHE:HD1	1.65	0.43
4:E:143:THR:HA	4:E:196:ARG:HA	1.99	0.43
4:E:126:VAL:HG22	4:E:236:VAL:HG12	2.00	0.43
4:E:230:LYS:O	4:E:232:VAL:N	2.51	0.43
1:A:249:VAL:HG12	1:A:257:TYR:CE2	2.54	0.42
1:A:195:SER:OG	1:A:196:ASP:N	2.50	0.42
4:E:111:ARG:HG2	4:E:111:ARG:NH1	2.35	0.42
4:E:223:GLU:HA	4:E:230:LYS:NZ	2.35	0.42
3:D:17:GLN:O	3:D:79:VAL:HG22	2.20	0.41
4:E:122:PHE:HB3	4:E:188:ARG:HH21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:6:TRP:CG	5:C:7:THR:N	2.88	0.41
1:A:254:GLU:HB3	1:A:274:TRP:HD1	1.84	0.41
2:B:94:LYS:HG2	6:B:103:GOL:H32	2.02	0.41
4:E:121:VAL:HG23	4:E:231:PRO:CG	2.49	0.41
4:E:123:PRO:HD3	4:E:231:PRO:HB3	2.03	0.41
1:A:110:LEU:HB3	1:A:111:ARG:HH11	1.85	0.41
4:E:13:ILE:HG23	4:E:218:LEU:HD23	2.02	0.41
1:A:198:GLU:HA	1:A:249:VAL:O	2.21	0.41
3:D:123:TYR:CE2	4:E:135:GLU:HA	2.57	0.40
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.56	0.40
4:E:35:TRP:HB2	4:E:48:ILE:HG22	2.03	0.40
4:E:64:ASP:OD1	4:E:65:ARG:N	2.55	0.40
1:A:192:HIS:HA	1:A:193:PRO:HD2	1.87	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	267/274 (97%)	265 (99%)	2 (1%)	0	100	100
2	B	98/100 (98%)	98 (100%)	0	0	100	100
3	D	180/207 (87%)	170 (94%)	10 (6%)	0	100	100
4	E	229/245 (94%)	215 (94%)	14 (6%)	0	100	100
5	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	781/835 (94%)	754 (96%)	27 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	227/231 (98%)	225 (99%)	2 (1%)	78 83
2	B	95/95 (100%)	92 (97%)	3 (3%)	39 40
3	D	154/184 (84%)	149 (97%)	5 (3%)	39 40
4	E	207/213 (97%)	196 (95%)	11 (5%)	22 20
5	C	6/6 (100%)	6 (100%)	0	100 100
All	All	689/729 (94%)	668 (97%)	21 (3%)	40 43

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	ASP
1	A	254	GLU
2	B	34	ASP
2	B	70	PHE
2	B	94	LYS
3	D	26	ASN
3	D	42	SER
3	D	89	CYS
3	D	119	ASP
3	D	178	TRP
4	E	15	GLU
4	E	16	LYS
4	E	59	SER
4	E	67	SER
4	E	137	SER
4	E	178	LEU
4	E	194	ARG
4	E	206	ARG
4	E	219	SER
4	E	224	TRP
4	E	239	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
4	E	42	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

13 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	$\#\|Z\| > 2$
6	GOL	A	302	-	5,5,5	0.99	0	5,5,5	0.84	0
6	GOL	B	102	-	5,5,5	0.94	0	5,5,5	0.93	0
6	GOL	D	302	-	5,5,5	0.89	0	5,5,5	0.96	0
6	GOL	B	104	-	5,5,5	0.90	0	5,5,5	1.02	0
6	GOL	C	101	-	5,5,5	0.95	0	5,5,5	0.95	0
6	GOL	A	301	-	5,5,5	0.84	0	5,5,5	1.02	0
6	GOL	B	103	-	5,5,5	0.91	0	5,5,5	0.90	0
6	GOL	B	106	-	5,5,5	0.91	0	5,5,5	0.95	0
6	GOL	D	301	-	5,5,5	0.89	0	5,5,5	0.88	0
6	GOL	B	101	-	5,5,5	0.91	0	5,5,5	1.00	0
6	GOL	A	303	-	5,5,5	0.84	0	5,5,5	0.98	0
6	GOL	A	304	-	5,5,5	0.88	0	5,5,5	1.00	0
6	GOL	B	105	-	5,5,5	0.90	0	5,5,5	0.98	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
6	GOL	A	302	-	-	4/4/4/4	-
6	GOL	B	102	-	-	3/4/4/4	-
6	GOL	D	302	-	-	1/4/4/4	-
6	GOL	B	104	-	-	0/4/4/4	-
6	GOL	C	101	-	-	2/4/4/4	-
6	GOL	A	301	-	-	0/4/4/4	-
6	GOL	B	103	-	-	2/4/4/4	-
6	GOL	B	106	-	-	2/4/4/4	-
6	GOL	D	301	-	-	0/4/4/4	-
6	GOL	B	101	-	-	4/4/4/4	-
6	GOL	A	303	-	-	0/4/4/4	-
6	GOL	A	304	-	-	2/4/4/4	-
6	GOL	B	105	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	302	GOL	C1-C2-C3-O3
6	A	304	GOL	C1-C2-C3-O3
6	A	304	GOL	O2-C2-C3-O3
6	B	102	GOL	O2-C2-C3-O3
6	A	302	GOL	O1-C1-C2-O2
6	C	101	GOL	O1-C1-C2-O2
6	A	302	GOL	O1-C1-C2-C3
6	B	101	GOL	O1-C1-C2-C3
6	B	101	GOL	C1-C2-C3-O3
6	B	102	GOL	C1-C2-C3-O3
6	B	103	GOL	C1-C2-C3-O3
6	B	106	GOL	O1-C1-C2-C3
6	C	101	GOL	O1-C1-C2-C3
6	A	302	GOL	O2-C2-C3-O3
6	B	106	GOL	O1-C1-C2-O2
6	B	101	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	B	101	GOL	O1-C1-C2-O2
6	B	103	GOL	O2-C2-C3-O3
6	D	302	GOL	O1-C1-C2-C3
6	B	102	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	102	GOL	2	0
6	B	103	GOL	4	0
6	B	106	GOL	1	0
6	A	303	GOL	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	272/274 (99%)	0.40	19 (6%) 16 20	15, 35, 102, 118	0
2	B	100/100 (100%)	-0.16	0 100 100	18, 33, 59, 65	0
3	D	185/207 (89%)	0.70	19 (10%) 6 8	20, 46, 131, 145	0
4	E	237/245 (96%)	1.02	57 (24%) 0 0	20, 81, 121, 152	0
5	C	9/9 (100%)	0.20	0 100 100	19, 20, 22, 25	0
All	All	803/835 (96%)	0.58	95 (11%) 4 5	15, 46, 117, 152	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	136	CYS	16.0
3	D	185	ALA	13.8
3	D	177	ALA	8.5
3	D	186	CYS	8.5
4	E	122	PHE	7.2
4	E	183	ALA	5.9
4	E	225	THR	5.8
1	A	199	ALA	5.4
4	E	191	LEU	5.4
3	D	190	PHE	5.2
3	D	130	SER	5.0
3	D	134	SER	4.6
3	D	132	ASP	4.5
3	D	131	SER	4.3
1	A	249	VAL	4.2
4	E	218	LEU	4.2
1	A	197	HIS	4.2
4	E	233	THR	4.0
4	E	129	PHE	4.0
4	E	184	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
4	E	187	SER	3.8
1	A	248	VAL	3.8
4	E	151	PHE	3.8
4	E	234	GLN	3.8
4	E	13	ILE	3.7
3	D	178	TRP	3.7
3	D	189	ALA	3.6
4	E	186	ASP	3.4
4	E	237	SER	3.4
4	E	179	LYS	3.4
3	D	155	VAL	3.4
4	E	235	ILE	3.3
3	D	122	VAL	3.3
4	E	134	ALA	3.2
4	E	178	LEU	3.2
4	E	227	ASP	3.2
4	E	132	SER	3.1
3	D	124	GLN	3.1
4	E	124	PRO	3.1
1	A	224	GLN	3.1
1	A	198	GLU	3.0
4	E	17	ARG	3.0
4	E	120	LYS	3.0
4	E	185	ASN	3.0
4	E	142	ALA	3.0
1	A	269	PRO	3.0
3	D	153	SER	3.0
4	E	14	ILE	2.9
1	A	250	PRO	2.9
3	D	121	ALA	2.9
4	E	136	ILE	2.9
4	E	148	ALA	2.8
1	A	225	THR	2.8
4	E	224	TRP	2.8
4	E	115	THR	2.8
4	E	221	ASN	2.8
4	E	219	SER	2.8
3	D	183	ASP	2.7
1	A	254	GLU	2.7
4	E	209	PHE	2.7
1	A	274	TRP	2.6
1	A	195	SER	2.6

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Mol	Chain	Res	Type	RSRZ
4	E	121	VAL	2.6
4	E	229	ALA	2.6
4	E	149	THR	2.6
1	A	191	HIS	2.5
1	A	270	LEU	2.5
4	E	239	GLU	2.5
1	A	228	THR	2.4
4	E	182	PRO	2.4
4	E	228	ARG	2.4
4	E	123	PRO	2.4
4	E	222	ASP	2.3
4	E	232	VAL	2.3
4	E	242	GLY	2.3
1	A	267	PRO	2.2
3	D	138	PHE	2.2
1	A	251	SER	2.2
4	E	131	PRO	2.2
4	E	231	PRO	2.2
1	A	217	TRP	2.2
4	E	85	LEU	2.2
4	E	125	GLU	2.1
4	E	213	VAL	2.1
1	A	253	GLU	2.1
4	E	119	ASN	2.1
4	E	140	GLN	2.1
4	E	203	GLN	2.1
4	E	144	LEU	2.1
3	D	188	ASN	2.0
4	E	117	ASP	2.0
4	E	158	LEU	2.0
4	E	208	HIS	2.0
4	E	145	VAL	2.0
4	E	135	GLU	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
6	GOL	B	103	6/6	0.56	0.35	60,69,73,74	0
6	GOL	B	105	6/6	0.68	0.21	56,61,66,69	0
6	GOL	B	102	6/6	0.71	0.32	39,60,63,74	0
6	GOL	A	304	6/6	0.73	0.38	53,66,69,69	0
6	GOL	A	303	6/6	0.77	0.23	36,48,52,57	0
6	GOL	B	101	6/6	0.78	0.27	44,50,66,68	0
6	GOL	B	106	6/6	0.81	0.24	43,50,61,65	0
6	GOL	D	302	6/6	0.82	0.24	42,49,59,61	0
6	GOL	A	302	6/6	0.85	0.24	53,57,61,63	0
6	GOL	D	301	6/6	0.88	0.12	26,34,38,39	0
6	GOL	A	301	6/6	0.91	0.16	34,40,48,49	0
6	GOL	B	104	6/6	0.91	0.11	34,38,42,44	0
6	GOL	C	101	6/6	0.93	0.19	37,44,46,50	0

6.5 Other polymers (i)

There are no such residues in this entry.