



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:01 pm BST

PDB ID : 4JFQ  
Title : A2 HLA complex with L8A heteroclitic variant of Melanoma peptide  
Authors : Rizkallah, P.J.; Cole, D.K.; Madura, F.; Sewell, A.K.; Baker, B.M.  
Deposited on : 2013-02-28  
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](mailto: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.

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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 : 2.11  
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) : 2.11

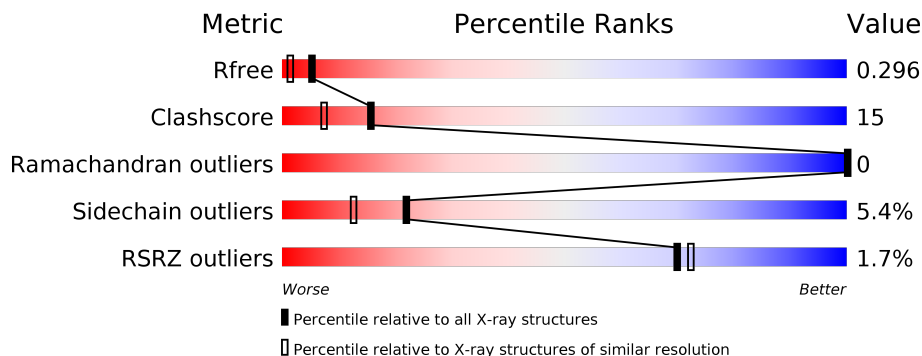
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	
1	D	276	
2	B	100	
2	E	100	
3	C	10	
3	F	10	

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	GOL	A	306	-	-	X	-
4	GOL	B	103	-	-	X	-
4	GOL	D	302	-	-	X	-
5	MES	A	308	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7301 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 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	Total	C	N	O	S	0	4	0
			2279	1422	417	431	9			
1	D	276	Total	C	N	O	S	0	2	0
			2269	1418	413	429	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	Total	C	N	O	S	0	1	0
			843	536	142	161	4			
2	E	100	Total	C	N	O	S	0	2	0
			855	545	145	161	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	INITIATING METHIONINE	UNP P61769
E	0	MET	-	INITIATING METHIONINE	UNP P61769

- Molecule 3 is a protein called L8A heteroclitic Melanoma peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	10	Total	C	N	O	0	0	0
			66	42	10	14			
3	F	10	Total	C	N	O	0	0	0
			66	42	10	14			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



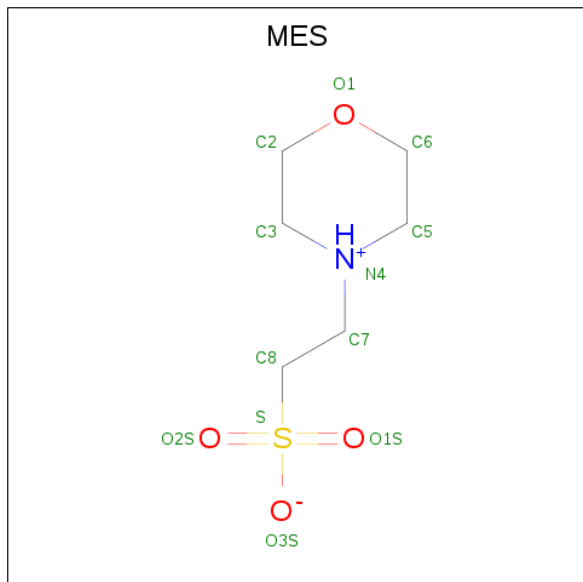
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0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

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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	265	Total	O	0	0
			265	265		
6	B	109	Total	O	0	0
			109	109		

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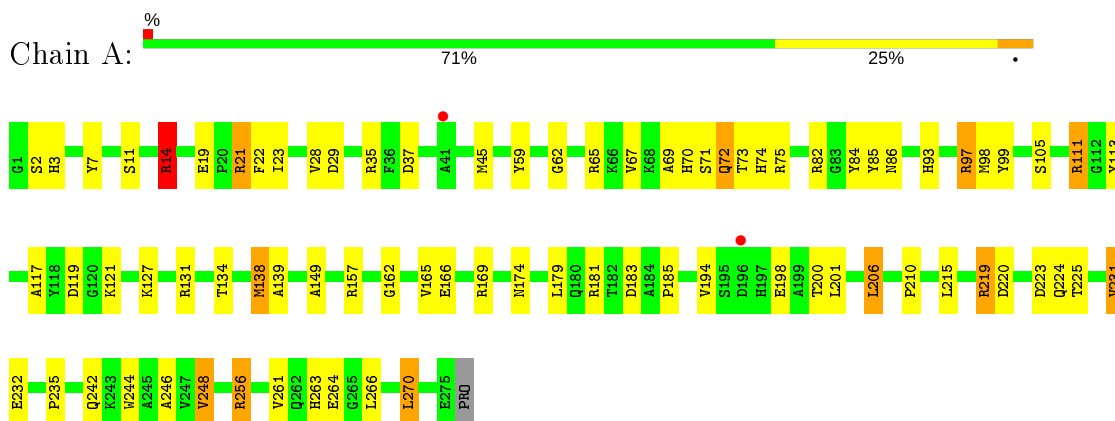
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
6	C	9	Total O 9 9	0	0
6	D	279	Total O 279 279	0	0
6	E	115	Total O 115 115	0	0
6	F	8	Total O 8 8	0	0

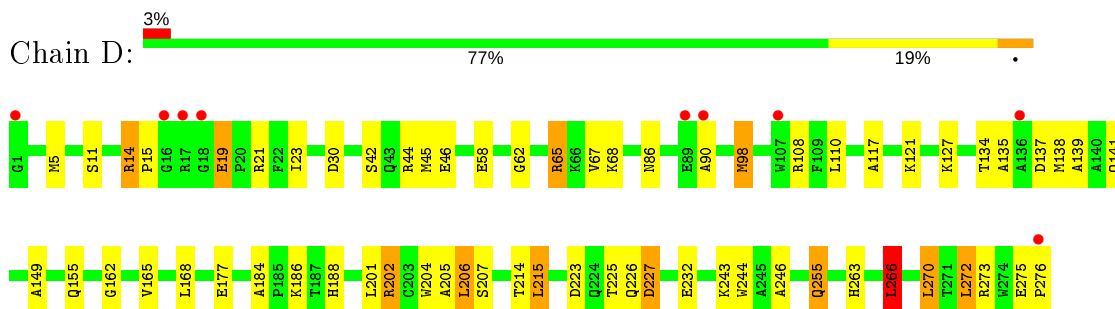
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

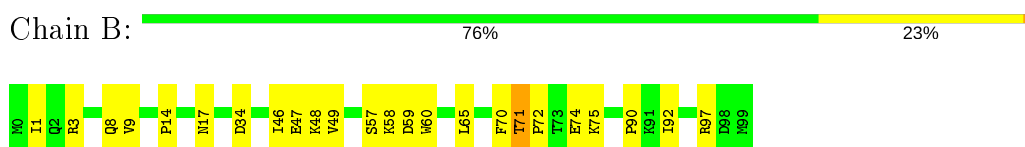
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



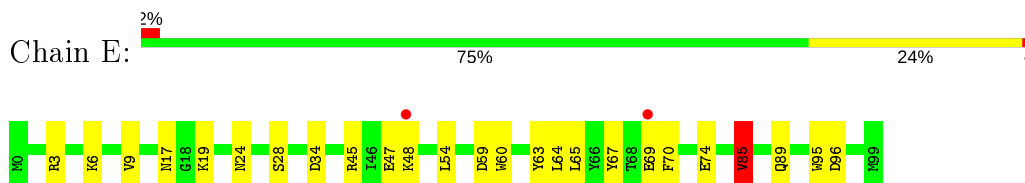
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin




- Molecule 2: Beta-2-microglobulin






- Molecule 3: L8A heteroclitic Melanoma peptide

Chain C:  90% 10%



- Molecule 3: L8A heteroclitic Melanoma peptide

Chain F:  90% 10%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.10Å 58.36Å 89.43Å 90.00° 109.82° 90.00°	Depositor
Resolution (Å)	84.22 – 1.90 19.91 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (84.22-1.90) 99.7 (19.91-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 1.90Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.216 , 0.297 0.218 , 0.296	Depositor DCC
$R_{free}$ test set	3275 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.9	Xtrriage
Anisotropy	0.779	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7301	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.96	2/2344 (0.1%)	1.05	11/3182 (0.3%)
1	D	0.92	0/2335	1.01	6/3171 (0.2%)
2	B	0.94	0/866	0.88	1/1170 (0.1%)
2	E	0.89	1/879 (0.1%)	0.84	1/1189 (0.1%)
3	C	1.06	0/65	0.89	0/86
3	F	0.80	0/65	0.75	0/86
All	All	0.93	3/6554 (0.0%)	0.98	19/8884 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	VAL	CB-CG1	-5.40	1.41	1.52
2	E	67	TYR	CD1-CE1	-5.16	1.31	1.39
1	A	59	TYR	CD1-CE1	5.04	1.47	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	202	ARG	NE-CZ-NH1	-16.79	111.91	120.30
1	D	202	ARG	NE-CZ-NH2	16.50	128.55	120.30
1	A	256	ARG	NE-CZ-NH1	-13.30	113.65	120.30
1	A	219	ARG	NE-CZ-NH1	-11.46	114.57	120.30
1	A	256	ARG	NE-CZ-NH2	11.18	125.89	120.30
1	A	219	ARG	NE-CZ-NH2	9.78	125.19	120.30
1	A	138	MET	CG-SD-CE	9.15	114.85	100.20
1	A	37	ASP	CB-CG-OD1	7.84	125.35	118.30
1	A	181	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	D	266	LEU	CB-CG-CD1	6.53	122.10	111.00
1	D	227	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	181	ARG	NE-CZ-NH2	-5.98	117.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	270	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	14	ARG	NE-CZ-NH2	5.49	123.04	120.30
2	B	34	ASP	CB-CG-OD1	5.38	123.14	118.30
1	D	202	ARG	CD-NE-CZ	5.17	130.84	123.60
2	E	85	VAL	CG1-CB-CG2	5.11	119.07	110.90
1	D	65	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	2279	0	2127	82	0
1	D	2269	0	2118	64	1
2	B	843	0	807	29	1
2	E	855	0	820	16	0
3	C	66	0	73	1	0
3	F	66	0	73	2	0
4	A	42	0	56	7	0
4	B	24	0	32	9	0
4	D	30	0	40	9	0
4	E	18	0	24	0	0
5	A	12	0	12	10	0
5	D	12	0	12	4	0
6	A	265	0	0	19	0
6	B	109	0	0	3	1
6	C	9	0	0	0	0
6	D	279	0	0	12	1
6	E	115	0	0	3	0
6	F	8	0	0	0	0
All	All	7301	0	6194	187	2

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:GLN:HA	4:B:103:GOL:H32	1.37	1.06
2:B:14:PRO:HD3	4:B:102:GOL:H12	1.39	1.03
2:B:8:GLN:HA	4:B:103:GOL:C3	1.90	1.01
1:D:149:ALA:HB2	4:D:302:GOL:H11	1.37	1.00
1:D:215[A]:LEU:HD12	1:D:215[A]:LEU:N	1.79	0.97
1:A:219:ARG:HD2	6:A:429:HOH:O	1.68	0.94
1:A:185:PRO:HD2	1:A:266:LEU:HD11	1.54	0.90
1:D:149:ALA:CB	4:D:302:GOL:H11	2.06	0.86
2:E:17:ASN:ND2	2:E:74:GLU:OE1	2.11	0.84
1:D:205:ALA:C	1:D:206:LEU:HD22	1.99	0.82
1:A:185:PRO:HD2	1:A:266:LEU:CD1	2.11	0.81
1:D:14:ARG:HD3	1:D:19:GLU:O	1.79	0.80
2:E:63:TYR:O	2:E:64[A]:LEU:HD12	1.81	0.80
4:B:103:GOL:H11	6:B:205:HOH:O	1.83	0.78
1:D:149:ALA:HA	4:D:302:GOL:H31	1.66	0.78
2:B:48:LYS:HG3	2:B:48:LYS:O	1.84	0.77
1:A:231[B]:VAL:HG11	2:B:8:GLN:OE1	1.86	0.75
1:A:165:VAL:HG12	1:A:169:ARG:NH1	2.02	0.75
1:D:149:ALA:CB	4:D:302:GOL:C1	2.65	0.74
1:D:215[A]:LEU:CD1	1:D:215[A]:LEU:N	2.49	0.74
1:A:21:ARG:NH2	1:A:23:ILE:HD11	2.03	0.72
2:E:3:ARG:NH1	2:E:59:ASP:O	2.23	0.71
2:E:54:LEU:HD12	2:E:64[A]:LEU:HD11	1.73	0.71
1:D:21:ARG:NH2	1:D:23:ILE:HD11	2.07	0.70
1:A:139:ALA:N	5:A:308:MES:O3S	2.25	0.69
4:B:103:GOL:C1	6:B:205:HOH:O	2.38	0.69
1:D:214:THR:C	1:D:215[A]:LEU:HD12	2.12	0.68
1:D:255:GLN:H	1:D:255:GLN:NE2	1.91	0.68
1:A:14:ARG:HD3	1:A:19:GLU:O	1.95	0.67
1:D:149:ALA:HB1	4:D:302:GOL:H12	1.76	0.67
1:A:206:LEU:HD12	1:A:242:GLN:HG2	1.78	0.66
1:A:232:GLU:HA	4:A:304:GOL:H12	1.75	0.66
1:A:210:PRO:HG3	4:A:306:GOL:H2	1.78	0.66
1:A:93:HIS:HE1	6:A:543:HOH:O	1.78	0.66
2:B:8:GLN:HA	4:B:103:GOL:H31	1.78	0.65
1:A:86[B]:ASN:HD22	5:A:308:MES:C6	2.09	0.65
2:B:75:LYS:HG2	6:B:250:HOH:O	1.97	0.65
2:B:92:ILE:H	4:B:104:GOL:H2	1.62	0.64
1:D:90:ALA:HB1	6:D:675:HOH:O	1.97	0.64
1:D:162:GLY:O	1:D:165:VAL:HG22	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLN:HB2	6:A:582:HOH:O	1.98	0.63
2:B:14:PRO:HD3	4:B:102:GOL:C1	2.24	0.63
1:A:65[B]:ARG:HB2	1:A:65[B]:ARG:CZ	2.28	0.62
1:A:121:LYS:HG3	2:B:1:ILE:CD1	2.30	0.62
1:A:194:VAL:CG1	1:A:200:THR:HG23	2.30	0.62
1:D:202:ARG:HD3	1:D:244:TRP:CE3	2.34	0.62
5:A:308:MES:H32	6:A:609:HOH:O	2.00	0.61
2:B:57[A]:SER:OG	2:B:59:ASP:OD1	2.18	0.61
1:A:84:TYR:O	5:A:308:MES:H51	2.01	0.60
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.37	0.60
1:D:215[A]:LEU:HD13	1:D:243:LYS:HD3	1.83	0.60
1:A:185:PRO:CD	1:A:266:LEU:HD11	2.29	0.59
5:D:306:MES:H62	6:D:443:HOH:O	2.00	0.59
1:A:86[B]:ASN:HD22	5:A:308:MES:H62	1.67	0.58
2:E:54:LEU:CD1	2:E:64[A]:LEU:HD11	2.33	0.58
1:D:149:ALA:HB1	4:D:302:GOL:C1	2.34	0.58
2:E:54:LEU:HD12	2:E:64[A]:LEU:CD1	2.34	0.58
1:A:231[B]:VAL:HG21	1:A:244:TRP:CZ2	2.40	0.57
1:D:110:LEU:HD23	1:D:110:LEU:O	2.04	0.57
1:D:110:LEU:C	1:D:110:LEU:HD23	2.25	0.57
1:A:263:HIS:HB3	1:A:266:LEU:HD13	1.87	0.56
1:D:90:ALA:C	6:D:675:HOH:O	2.43	0.56
1:A:86[B]:ASN:ND2	5:A:308:MES:H62	2.20	0.56
1:A:183:ASP:OD1	6:A:661:HOH:O	2.18	0.56
1:D:68:LYS:NZ	6:D:504:HOH:O	2.38	0.56
1:D:255:GLN:H	1:D:255:GLN:HE21	1.53	0.56
2:E:85:VAL:HG22	6:E:254:HOH:O	2.05	0.56
1:D:204:TRP:HB3	1:D:206:LEU:HD21	1.88	0.56
2:B:17:ASN:ND2	2:B:74:GLU:CD	2.59	0.56
1:A:149:ALA:O	6:A:664:HOH:O	2.18	0.55
1:D:186:LYS:HE2	1:D:207:SER:HB2	1.87	0.55
1:D:19:GLU:HG3	6:D:486:HOH:O	2.05	0.55
1:A:105:SER:OG	4:A:305:GOL:O1	2.15	0.55
1:A:210:PRO:HG3	4:A:306:GOL:C2	2.37	0.54
1:D:206:LEU:N	1:D:206:LEU:HD22	2.21	0.54
4:D:302:GOL:C3	6:D:604:HOH:O	2.54	0.54
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.42	0.54
1:A:70:HIS:O	1:A:74:HIS:HD2	1.89	0.54
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.90	0.54
1:D:215[A]:LEU:CD1	1:D:243:LYS:HD3	2.37	0.54
1:A:174:ASN:ND2	6:A:657:HOH:O	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:THR:CG2	6:A:492:HOH:O	2.57	0.53
1:A:231[B]:VAL:CG1	2:B:8:GLN:CD	2.77	0.53
1:A:84:TYR:O	5:A:308:MES:C5	2.57	0.53
1:A:200:THR:HG21	6:A:492:HOH:O	2.09	0.52
2:B:17:ASN:HD21	2:B:74:GLU:CD	2.12	0.52
2:B:90:PRO:O	4:B:104:GOL:H31	2.09	0.52
1:D:42:SER:O	1:D:44:ARG:HG2	2.10	0.52
2:B:17:ASN:ND2	2:B:74:GLU:HG2	2.24	0.51
1:D:98:MET:O	1:D:98:MET:HE3	2.10	0.51
1:D:45:MET:CE	3:F:2:LEU:HD11	2.40	0.51
2:E:63:TYR:O	2:E:64[A]:LEU:CD1	2.55	0.51
1:D:138:MET:HB2	5:D:306:MES:H82	1.93	0.51
1:D:275:GLU:HB2	1:D:276:PRO:HD2	1.92	0.51
1:A:127:LYS:CG	1:A:134:THR:HG23	2.41	0.51
1:A:121:LYS:HG3	2:B:1:ILE:HD11	1.91	0.51
1:A:111:ARG:NH2	1:A:113:TYR:CE2	2.79	0.50
1:A:2:SER:O	4:A:306:GOL:H11	2.10	0.50
1:D:62:GLY:HA2	1:D:65:ARG:NH2	2.26	0.50
1:D:86[B]:ASN:OD1	1:D:86[B]:ASN:O	2.29	0.50
1:D:45:MET:HE2	1:D:67:VAL:HB	1.93	0.50
4:A:306:GOL:H32	6:A:510:HOH:O	2.11	0.50
1:A:127:LYS:HE3	1:A:134:THR:HG22	1.94	0.50
1:D:162:GLY:O	1:D:165:VAL:CG2	2.60	0.50
1:D:202:ARG:NH1	6:D:431:HOH:O	2.45	0.49
1:A:70:HIS:HE1	1:A:99:TYR:OH	1.96	0.49
1:A:121:LYS:HG3	2:B:1:ILE:HD12	1.93	0.49
1:D:155:GLN:HG3	6:D:645:HOH:O	2.12	0.49
1:A:223:ASP:HB3	1:A:225:THR:HG23	1.93	0.49
1:D:204:TRP:HB3	1:D:206:LEU:CD2	2.43	0.49
1:D:202:ARG:CD	1:D:244:TRP:CD2	2.96	0.49
4:D:302:GOL:H32	6:D:604:HOH:O	2.11	0.49
1:A:121:LYS:CG	2:B:1:ILE:HD11	2.42	0.48
1:A:45:MET:HE1	3:C:2:LEU:HD11	1.96	0.48
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.49	0.48
1:D:270:LEU:HD12	1:D:272:LEU:CD2	2.44	0.48
1:D:14:ARG:CD	1:D:19:GLU:O	2.58	0.47
1:A:266:LEU:O	6:A:658:HOH:O	2.20	0.47
1:A:69:ALA:O	1:A:73:THR:HG23	2.15	0.47
2:B:3:ARG:NH2	2:B:59:ASP:OD2	2.47	0.47
1:D:206:LEU:N	1:D:206:LEU:CD2	2.77	0.47
1:A:235:PRO:HG2	2:B:65:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:ALA:HB3	1:D:141:GLN:NE2	2.29	0.47
1:A:231[B]:VAL:HG11	2:B:8:GLN:CD	2.33	0.47
1:A:65[B]:ARG:CZ	1:A:65[B]:ARG:CB	2.92	0.46
2:E:24:ASN:HB3	2:E:65:LEU:HD11	1.97	0.46
1:A:215:LEU:HD23	1:A:261:VAL:HG13	1.98	0.46
1:D:11:SER:HA	1:D:21:ARG:O	2.16	0.46
1:D:5:MET:HB2	1:D:168:LEU:HD13	1.98	0.46
1:A:224:GLN:NE2	6:A:488:HOH:O	2.49	0.46
1:A:127:LYS:HG2	1:A:134:THR:HG23	1.97	0.46
1:A:21:ARG:HH22	1:A:23:ILE:HD11	1.80	0.46
1:A:105:SER:HG	4:A:305:GOL:HO1	1.54	0.45
1:A:75:ARG:NH2	6:A:632:HOH:O	2.50	0.45
1:A:194:VAL:HG11	1:A:200:THR:HG23	1.99	0.45
1:D:137:ASP:CG	5:D:306:MES:O2S	2.55	0.44
1:D:270:LEU:CD1	1:D:272:LEU:HD22	2.47	0.44
1:D:202:ARG:CD	1:D:244:TRP:CE3	3.00	0.44
1:A:86[B]:ASN:ND2	5:A:308:MES:O1	2.51	0.44
2:B:17:ASN:ND2	2:B:74:GLU:CG	2.81	0.43
2:E:96:ASP:C	2:E:96:ASP:OD1	2.55	0.43
1:A:131:ARG:NH1	6:A:633:HOH:O	2.51	0.43
1:A:111:ARG:HD3	1:A:113:TYR:CZ	2.53	0.43
2:E:45:ARG:NH1	2:E:47:GLU:OE1	2.52	0.43
2:E:17:ASN:ND2	2:E:74:GLU:CD	2.71	0.43
1:A:62:GLY:HA2	1:A:65[B]:ARG:HE	1.82	0.43
1:A:198:GLU:OE2	6:A:660:HOH:O	2.21	0.43
1:D:184:ALA:HB1	1:D:266:LEU:HD13	2.00	0.43
1:A:215:LEU:CD2	1:A:261:VAL:HG22	2.49	0.43
1:A:201:LEU:O	1:A:246:ALA:HA	2.19	0.43
1:A:266:LEU:N	1:A:266:LEU:CD1	2.81	0.43
1:A:74:HIS:CE1	1:A:97:ARG:HE	2.37	0.43
1:D:139:ALA:H	5:D:306:MES:H82	1.84	0.43
1:A:169:ARG:NH1	6:A:525:HOH:O	2.50	0.43
1:A:266:LEU:HD12	1:A:266:LEU:N	2.34	0.42
1:D:45:MET:HE1	3:F:2:LEU:HD11	2.01	0.42
2:B:46:ILE:O	2:B:49:VAL:HG23	2.20	0.42
2:E:19:LYS:HE3	6:E:309:HOH:O	2.18	0.42
1:D:263:HIS:HB3	1:D:266:LEU:HD22	2.00	0.42
2:E:9:VAL:HG13	2:E:95:TRP:HA	2.02	0.42
1:A:127:LYS:CE	1:A:134:THR:HG22	2.50	0.42
1:A:231[B]:VAL:CG1	2:B:8:GLN:OE1	2.62	0.42
1:A:264:GLU:HG3	6:A:594:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:TYR:O	1:A:98:MET:HA	2.20	0.42
2:B:9:VAL:HG13	2:B:9:VAL:O	2.19	0.42
1:D:227:ASP:HB2	6:D:414:HOH:O	2.20	0.42
1:A:220:ASP:OD1	1:A:256:ARG:HD2	2.21	0.41
1:D:273:ARG:NH1	6:D:663:HOH:O	2.53	0.41
1:D:201:LEU:O	1:D:246:ALA:HA	2.20	0.41
1:A:82:ARG:HD3	6:A:491:HOH:O	2.19	0.41
1:D:108:ARG:NH1	6:D:495:HOH:O	2.53	0.41
1:D:42:SER:OG	1:D:46:GLU:OE2	2.23	0.41
2:B:17:ASN:OD1	2:B:97:ARG:NH2	2.49	0.41
1:D:30:ASP:HA	4:D:301:GOL:H32	2.03	0.41
1:D:188:HIS:HE1	6:E:205:HOH:O	2.04	0.41
1:A:157:ARG:NH1	6:A:557:HOH:O	2.54	0.41
1:A:11:SER:HA	1:A:21:ARG:O	2.21	0.41
1:A:28:VAL:HG11	1:A:179:LEU:HD13	2.03	0.41
1:A:22:PHE:CD2	1:A:71:SER:HB2	2.56	0.41
1:A:162:GLY:O	1:A:166:GLU:HG3	2.22	0.40
2:B:71:THR:HA	2:B:72:PRO:HD2	1.87	0.40
1:D:127:LYS:NZ	1:D:134:THR:OG1	2.51	0.40
2:E:6:LYS:NZ	2:E:28:SER:OG	2.53	0.40
1:A:3:HIS:HA	1:A:29:ASP:OD1	2.21	0.40
1:A:85:TYR:HA	5:A:308:MES:H52	2.03	0.40
1:A:86[B]:ASN:ND2	5:A:308:MES:C6	2.77	0.40
1:D:177:GLU:H	1:D:177:GLU:CD	2.25	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:LYS:NZ	1:D:15:PRO:O[1_554]	1.72	0.48
6:B:256:HOH:O	6:D:421:HOH:O[1_554]	2.19	0.01

## 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	277/276 (100%)	271 (98%)	6 (2%)	0	100	100
1	D	276/276 (100%)	269 (98%)	7 (2%)	0	100	100
2	B	99/100 (99%)	98 (99%)	1 (1%)	0	100	100
2	E	100/100 (100%)	99 (99%)	1 (1%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
3	F	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
All	All	768/772 (100%)	752 (98%)	16 (2%)	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	235/232 (101%)	223 (95%)	12 (5%)	24	14
1	D	234/232 (101%)	218 (93%)	16 (7%)	16	7
2	B	96/95 (101%)	92 (96%)	4 (4%)	30	20
2	E	97/95 (102%)	91 (94%)	6 (6%)	18	9
3	C	6/6 (100%)	6 (100%)	0	100	100
3	F	6/6 (100%)	6 (100%)	0	100	100
All	All	674/666 (101%)	636 (94%)	38 (6%)	22	11

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	21	ARG
1	A	35	ARG
1	A	67	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	72	GLN
1	A	111	ARG
1	A	138	MET
1	A	206	LEU
1	A	231[A]	VAL
1	A	231[B]	VAL
1	A	248	VAL
1	A	270	LEU
2	B	47	GLU
2	B	58	LYS
2	B	70	PHE
2	B	71	THR
1	D	14	ARG
1	D	19	GLU
1	D	58	GLU
1	D	98	MET
1	D	121	LYS
1	D	206	LEU
1	D	215[A]	LEU
1	D	215[B]	LEU
1	D	223	ASP
1	D	225	THR
1	D	226	GLN
1	D	232	GLU
1	D	255	GLN
1	D	266	LEU
1	D	270	LEU
1	D	272	LEU
2	E	34	ASP
2	E	48	LYS
2	E	69	GLU
2	E	70	PHE
2	E	85	VAL
2	E	89	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	32	GLN
1	A	70	HIS
1	A	74	HIS
1	A	93	HIS

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Mol	Chain	Res	Type
1	A	115	GLN
2	B	13	HIS
2	B	83	ASN
1	D	32	GLN
1	D	70	HIS
1	D	141	GLN
1	D	174	ASN
1	D	188	HIS
1	D	192	HIS
1	D	255	GLN
2	E	83	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](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

21 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	$\# Z  > 2$
4	GOL	A	306	-	5,5,5	0.61	0	5,5,5	0.66	0
4	GOL	B	104	-	5,5,5	0.41	0	5,5,5	0.30	0
4	GOL	A	302	-	5,5,5	0.37	0	5,5,5	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	D	304	-	5,5,5	0.45	0	5,5,5	0.42	0
5	MES	A	308	-	12,12,12	1.86	1 (8%)	14,16,16	2.76	8 (57%)
4	GOL	D	303	-	5,5,5	0.42	0	5,5,5	0.25	0
4	GOL	E	103	-	5,5,5	0.44	0	5,5,5	0.50	0
4	GOL	A	307	-	5,5,5	0.44	0	5,5,5	0.25	0
4	GOL	B	103	-	5,5,5	0.88	0	5,5,5	1.32	0
4	GOL	A	301	-	5,5,5	0.33	0	5,5,5	0.26	0
4	GOL	A	304	-	5,5,5	0.68	0	5,5,5	1.23	0
4	GOL	A	303	-	5,5,5	0.47	0	5,5,5	0.96	0
4	GOL	D	302	-	5,5,5	0.61	0	5,5,5	0.69	0
5	MES	D	306	-	12,12,12	2.36	1 (8%)	14,16,16	4.14	8 (57%)
4	GOL	D	301	-	5,5,5	0.38	0	5,5,5	0.85	0
4	GOL	B	102	-	5,5,5	0.51	0	5,5,5	0.89	0
4	GOL	A	305	-	5,5,5	0.21	0	5,5,5	0.52	0
4	GOL	D	305	-	5,5,5	0.32	0	5,5,5	0.40	0
4	GOL	E	101	-	5,5,5	0.47	0	5,5,5	0.48	0
4	GOL	B	101	-	5,5,5	0.45	0	5,5,5	0.42	0
4	GOL	E	102	-	5,5,5	0.64	0	5,5,5	0.53	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
4	GOL	A	306	-	-	4/4/4/4	-
4	GOL	B	104	-	-	2/4/4/4	-
4	GOL	A	302	-	-	2/4/4/4	-
4	GOL	D	304	-	-	4/4/4/4	-
5	MES	A	308	-	-	4/6/14/14	0/1/1/1
4	GOL	D	303	-	-	2/4/4/4	-
4	GOL	E	103	-	-	2/4/4/4	-
4	GOL	A	307	-	-	0/4/4/4	-
4	GOL	B	103	-	-	4/4/4/4	-
4	GOL	A	301	-	-	0/4/4/4	-
4	GOL	A	304	-	-	4/4/4/4	-
4	GOL	A	303	-	-	2/4/4/4	-
4	GOL	D	302	-	-	2/4/4/4	-
5	MES	D	306	-	-	2/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	301	-	-	4/4/4/4	-
4	GOL	B	102	-	-	4/4/4/4	-
4	GOL	A	305	-	-	3/4/4/4	-
4	GOL	D	305	-	-	2/4/4/4	-
4	GOL	E	101	-	-	2/4/4/4	-
4	GOL	B	101	-	-	0/4/4/4	-
4	GOL	E	102	-	-	1/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	306	MES	C8-S	-7.54	1.66	1.77
5	A	308	MES	C8-S	-5.95	1.69	1.77

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	306	MES	O1S-S-C8	9.10	117.87	106.92
5	D	306	MES	C6-C5-N4	-6.23	100.66	110.10
5	D	306	MES	O2S-S-C8	-6.11	99.55	106.92
5	D	306	MES	C7-N4-C3	5.14	124.39	111.23
5	A	308	MES	C5-N4-C3	4.59	119.17	108.83
5	A	308	MES	C7-N4-C3	4.21	122.01	111.23
5	D	306	MES	C5-N4-C3	4.08	118.01	108.83
5	A	308	MES	O1S-S-C8	3.75	111.43	106.92
5	A	308	MES	C2-C3-N4	-3.66	104.55	110.10
5	D	306	MES	O3S-S-C8	3.65	111.68	105.77
5	D	306	MES	O1-C6-C5	-3.35	104.42	111.80
5	A	308	MES	O2S-S-C8	3.29	110.88	106.92
5	A	308	MES	C6-C5-N4	2.96	114.59	110.10
5	A	308	MES	C7-N4-C5	2.89	118.62	111.23
5	A	308	MES	C6-O1-C2	-2.48	101.62	109.89
5	D	306	MES	C7-N4-C5	2.44	117.47	111.23

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	306	GOL	C1-C2-C3-O3
4	A	302	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	D	304	GOL	O1-C1-C2-O2
4	D	304	GOL	O1-C1-C2-C3
5	A	308	MES	C7-C8-S-O1S
4	E	103	GOL	O1-C1-C2-C3
4	B	103	GOL	O1-C1-C2-O2
4	B	103	GOL	O1-C1-C2-C3
4	A	304	GOL	O1-C1-C2-C3
4	A	303	GOL	C1-C2-C3-O3
4	D	302	GOL	O1-C1-C2-C3
5	D	306	MES	N4-C7-C8-S
4	D	301	GOL	O1-C1-C2-O2
4	D	301	GOL	O1-C1-C2-C3
4	B	102	GOL	C1-C2-C3-O3
4	E	101	GOL	O1-C1-C2-C3
5	A	308	MES	C7-C8-S-O3S
4	A	306	GOL	O1-C1-C2-C3
4	B	104	GOL	C1-C2-C3-O3
4	D	305	GOL	C1-C2-C3-O3
4	D	304	GOL	C1-C2-C3-O3
4	D	303	GOL	O1-C1-C2-C3
4	B	103	GOL	C1-C2-C3-O3
4	A	304	GOL	C1-C2-C3-O3
4	D	301	GOL	C1-C2-C3-O3
4	B	102	GOL	O1-C1-C2-C3
4	A	305	GOL	C1-C2-C3-O3
4	A	306	GOL	O2-C2-C3-O3
4	D	305	GOL	O2-C2-C3-O3
4	A	302	GOL	O2-C2-C3-O3
4	E	103	GOL	O1-C1-C2-O2
4	B	103	GOL	O2-C2-C3-O3
4	A	304	GOL	O1-C1-C2-O2
4	A	303	GOL	O2-C2-C3-O3
4	D	302	GOL	O1-C1-C2-O2
4	B	102	GOL	O1-C1-C2-O2
4	B	102	GOL	O2-C2-C3-O3
4	A	305	GOL	O2-C2-C3-O3
4	A	306	GOL	O1-C1-C2-O2
4	B	104	GOL	O2-C2-C3-O3
4	D	303	GOL	O1-C1-C2-O2
4	A	304	GOL	O2-C2-C3-O3
4	E	101	GOL	O1-C1-C2-O2
4	A	305	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	308	MES	C8-C7-N4-C3
5	D	306	MES	C8-C7-N4-C5
4	D	304	GOL	O2-C2-C3-O3
4	D	301	GOL	O2-C2-C3-O3
5	A	308	MES	C7-C8-S-O2S
4	E	102	GOL	O1-C1-C2-C3

There are no ring outliers.

10 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	306	GOL	4	0
4	B	104	GOL	2	0
5	A	308	MES	10	0
4	B	103	GOL	5	0
4	A	304	GOL	1	0
4	D	302	GOL	8	0
5	D	306	MES	4	0
4	D	301	GOL	1	0
4	B	102	GOL	2	0
4	A	305	GOL	2	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 [i](#)

### 6.1 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	275/276 (99%)	0.18	2 (0%) 87 88	5, 16, 31, 41	0
1	D	276/276 (100%)	0.25	9 (3%) 46 49	6, 17, 32, 45	0
2	B	100/100 (100%)	0.09	0 100 100	7, 16, 30, 36	0
2	E	100/100 (100%)	0.18	2 (2%) 65 68	7, 17, 33, 39	0
3	C	10/10 (100%)	-0.01	0 100 100	12, 14, 19, 25	0
3	F	10/10 (100%)	0.28	0 100 100	12, 23, 28, 30	0
All	All	771/772 (99%)	0.19	13 (1%) 70 72	5, 17, 32, 45	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	GLY	5.3
1	D	276	PRO	4.8
1	D	16	GLY	3.3
1	A	196	ASP	3.0
1	D	90	ALA	2.8
1	D	107	TRP	2.6
1	D	89	GLU	2.4
1	D	17	ARG	2.3
1	D	136	ALA	2.3
1	A	41	ALA	2.2
2	E	69	GLU	2.2
1	D	18	GLY	2.1
2	E	48	LYS	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	GOL	D	303	6/6	0.62	0.31	39,39,40,40	0
4	GOL	D	305	6/6	0.63	0.34	32,35,36,38	0
4	GOL	B	101	6/6	0.64	0.22	36,42,42,45	0
4	GOL	D	301	6/6	0.66	0.18	28,30,32,36	0
4	GOL	E	102	6/6	0.72	0.23	26,30,31,31	0
4	GOL	A	307	6/6	0.74	0.27	40,42,44,45	0
5	MES	D	306	12/12	0.75	0.28	36,39,41,42	0
4	GOL	A	302	6/6	0.75	0.21	33,39,39,41	0
4	GOL	A	301	6/6	0.76	0.21	44,46,46,46	0
4	GOL	A	305	6/6	0.77	0.17	39,41,42,43	0
4	GOL	B	104	6/6	0.77	0.20	34,38,39,41	0
4	GOL	A	304	6/6	0.78	0.26	23,30,31,31	0
4	GOL	D	304	6/6	0.79	0.26	28,29,30,31	0
4	GOL	E	103	6/6	0.79	0.18	36,40,41,41	0
4	GOL	A	303	6/6	0.80	0.23	30,32,32,33	0
5	MES	A	308	12/12	0.81	0.28	31,34,42,43	0
4	GOL	B	102	6/6	0.82	0.25	25,28,30,31	0
4	GOL	A	306	6/6	0.88	0.28	27,31,32,34	0
4	GOL	E	101	6/6	0.89	0.12	28,35,35,36	0
4	GOL	D	302	6/6	0.90	0.17	10,24,25,26	0
4	GOL	B	103	6/6	0.93	0.15	13,20,21,22	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.