



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:27 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.; Toebe, 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

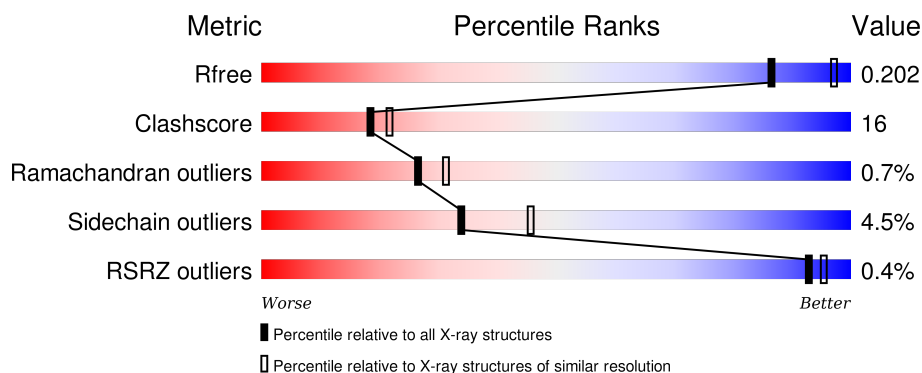
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*






The reported resolution of this entry is 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.



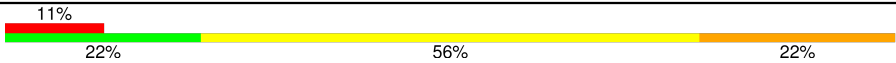
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	275	 68% 31% .
1	D	275	 66% 33% .
2	B	100	 77% 22% .
2	E	100	 72% 26% .
3	C	9	 11% 33% 22% 44%

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Mol	Chain	Length	Quality of chain
3	F	9	

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
4	GOL	D	1279	-	-	-	X
4	GOL	E	1102	-	-	-	X

## 2 Entry composition

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
1	A	275	Total	C	N	O	S	0	6	0
			2292	1434	414	435	9			
1	D	275	Total	C	N	O	S	0	2	0
			2262	1415	409	429	9			

- 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			
2	E	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

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

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

- 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	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
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		

- 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	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	B	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		
5	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

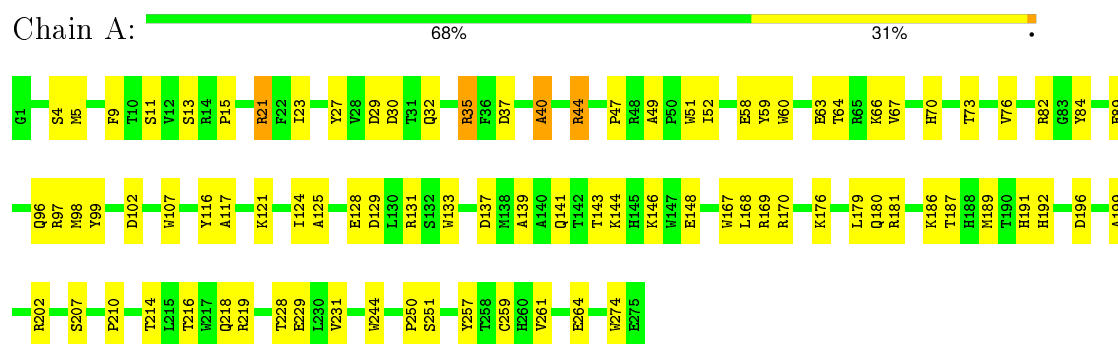
- Molecule 6 is water.

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

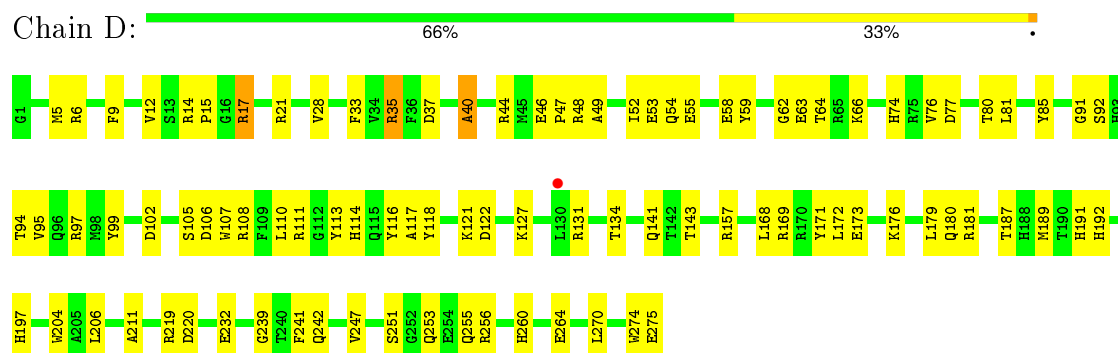
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

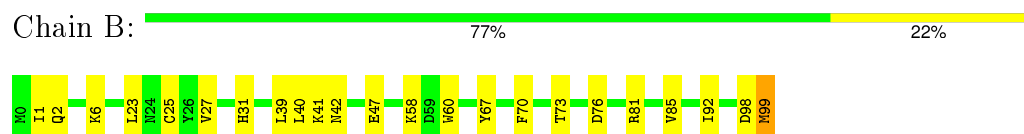
#### • Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2.1



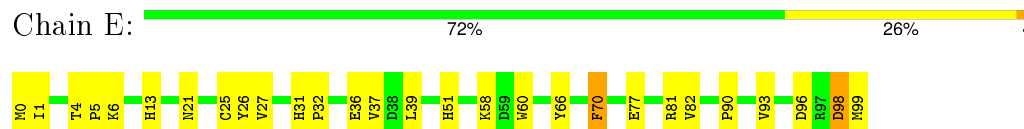
#### • Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2.1




#### • Molecule 2: BETA-2-MICROGLOBULIN

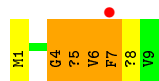


#### • Molecule 2: BETA-2-MICROGLOBULIN



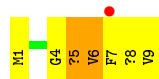
- Molecule 3: HLA-A2.1-RESTRICTED INFLUENZA A MATRIX EPITOPE

Chain C: 



- Molecule 3: HLA-A2.1-RESTRICTED INFLUENZA A MATRIX EPITOPE

Chain F: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 2.30Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.158 , 0.222 0.160 , 0.202	Depositor DCC
$R_{free}$ test set	1921 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.9	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.1	EDS
Estimated twinning fraction	0.329 for -H,-K,L 0.360 for h,-k,-l	Xtriage
Reported twinning fraction	0.329 for -H,-K,L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
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 <sup>2</sup> )	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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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, PRV, PRQ, 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	0.28	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	3
3	F	0	3
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	4	GLY	Peptide
3	C	5	PRV	Mainchain,Peptide
3	F	4	GLY	Peptide
3	F	5	PRV	Mainchain,Peptide

## 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	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	75	12	0
3	F	81	0	75	13	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	6119	196	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 16.

All (196) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	1:A:44:ARG:HH11	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
3:C:8:PRQ:HAI	1:D:54:GLN:HE22	1.64	0.62
1:A:143:THR:HA	1:A:146:LYS:HD2	1.81	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:O1	3:F:5:PRV:HA	2.01	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:21:ARG:HG2	6:D:2012:HOH:O	2.08	0.53
1:A:186:LYS:HE2	1:A:207:SER:HB3	1.90	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:106:ASP:CG	1:D:108:ARG:HD3	2.29	0.53
1:D:97:ARG:HD2	1:D:116[B]:TYR:CZ	2.44	0.53
1:D:121:LYS:CG	2:E:1:ILE:HD11	2.39	0.53
2:B:85:VAL:HB	6:B:2013:HOH:O	2.08	0.52
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.44	0.52
1:D:168:LEU:O	1:D:172:LEU:HG	2.08	0.52
1:A:121[B]:LYS:HB3	2:B:1:ILE:HD11	1.92	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:D:81:LEU:O	1:D:85:TYR:HD1	1.92	0.52
1:A:107:TRP:O	1:A:169:ARG:HD3	2.10	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:D:76:VAL:HB	3:F:8:PRQ:HAF	1.92	0.51
1:A:35:ARG:HG3	1:A:35:ARG:O	2.09	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:D:62:GLY:O	1:D:66:LYS:HG3	2.11	0.50
1:A:218:GLN:O	1:A:257:TYR:HA	2.11	0.50
1:D:114:HIS:HE1	1:D:116[B]:TYR:HE2	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
3:F:8:PRQ:HAH	3:F:8:PRQ:HAJ1	1.52	0.48
2:E:21:ASN:HB3	2:E:70:PHE:CE2	2.49	0.48
1:D:127:LYS:HE2	1:D:134:THR:OG1	2.13	0.48
1:A:9:PHE:HE2	1:A:99:TYR:CE2	2.32	0.47
1:D:6:ARG:HD3	4:D:1277:GOL:H31	1.97	0.47
1:A:13:SER:O	1:A:15:PRO:HD3	2.14	0.47
2:E:4:THR:HG22	2:E:5:PRO:HD2	1.95	0.47
5:D:1276:MES:H51	5:D:1276:MES:H82	1.51	0.47
1:D:114:HIS:CE1	1:D:116[B]:TYR:HE2	2.33	0.47
3:F:5:PRV:CE1	3:F:6:VAL:HB	2.45	0.47
1:A:264:GLU:HB3	6:A:2135:HOH:O	2.15	0.47
1:D:106:ASP:HB2	1:D:108:ARG:HD3	1.96	0.47
3:C:8:PRQ:HAH	3:C:8:PRQ:HAJ1	1.62	0.47
1:A:189:MET:SD	6:A:2133:HOH:O	2.61	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
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:D:35:ARG:O	1:D:35:ARG:HG3	2.15	0.46
1:A:96:GLN:NE2	2:B:31:HIS:NE2	2.63	0.46
1:A:97:ARG:NH2	1:A:116[B]:TYR:HE2	2.11	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:HIS:HA	1:D:77:ASP:HB2	1.97	0.46
1:D:52:ILE:HD11	1:D:59:TYR:CZ	2.51	0.46
1:A:29:ASP:O	4:A:1276:GOL:H31	2.16	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:D:49:ALA:O	1:D:52:ILE:HG22	2.18	0.44
1:A:9:PHE:CE2	1:A:99:TYR:CE2	3.05	0.44
1:D:55:GLU:HG2	1:D:59:TYR:CD2	2.52	0.44
3:C:1:MSE:HB3	3:C:1:MSE:HE2	1.89	0.43
1:D:35:ARG:HG2	1:D:48:ARG:HD3	1.99	0.43
2:B:73:THR:OG1	2:B:76:ASP:HB2	2.18	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
2:B:99:MET:H	5:B:1102:MES:H51	1.84	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
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
1:D:171:TYR:O	1:D:179:LEU:HD12	2.19	0.42
2:B:2:GLN:HA	2:B:31:HIS:O	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:44:ARG:HA	1:A:64:THR:HG23	2.01	0.42
1:A:27:TYR:CE1	1:A:32:GLN:HB2	2.55	0.42
1:D:239:GLY:HA2	6:D:2128:HOH:O	2.19	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:A:176:LYS:HB2	1:A:180:GLN:HE21	1.85	0.42
1:D:232[A]:GLU:HG3	5:D:1278:MES:H72	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1278:MES:H52	5:D:1278:MES:H81	1.66	0.41
2:E:58:LYS:O	2:E:58:LYS:HG2	2.18	0.41
1:D:49:ALA:O	1:D:53:GLU:HG3	2.20	0.41
1:D:15:PRO:HD2	1:D:17:ARG:HH12	1.86	0.41
1:D:121:LYS:HG3	2:E:1:ILE:HD11	2.01	0.41
1:D:80:THR:HG21	3:F:9:VAL:HG23	2.01	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:255:GLN:HE21	1:D:275:GLU:HA	1.84	0.41
1:A:259:CYS:N	6:A:2133:HOH:O	2.53	0.41
1:A:219:ARG:NH1	6:A:2112:HOH:O	2.52	0.41
1:D:219:ARG:O	1:D:220:ASP:HB2	2.20	0.41
1:A:82:ARG:HH11	1:A:82:ARG:HG2	1.85	0.41
1:A:52:ILE:O	1:A:52:ILE:HG13	2.21	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:D:9:PHE:HE2	1:D:99:TYR:CE2	2.39	0.40
1:A:228:THR:HG22	1:A:229:GLU:N	2.36	0.40
1:A:191:HIS:CE1	1:A:199:ALA:HB1	2.56	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.

## 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	279/275 (102%)	261 (94%)	17 (6%)	1 (0%)	39 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	275/275 (100%)	256 (93%)	18 (6%)	1 (0%)	39	48
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	4/9 (44%)	1 (25%)	1 (25%)	2 (50%)	0	0
3	F	4/9 (44%)	1 (25%)	2 (50%)	1 (25%)	0	0
All	All	758/768 (99%)	708 (93%)	45 (6%)	5 (1%)	26	31

All (5) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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%)	36	49
1	D	233/231 (101%)	222 (95%)	11 (5%)	32	43
2	B	95/95 (100%)	91 (96%)	4 (4%)	36	49
2	E	95/95 (100%)	91 (96%)	4 (4%)	36	49
3	C	6/5 (120%)	5 (83%)	1 (17%)	3	2
3	F	6/5 (120%)	6 (100%)	0	100	100
All	All	672/662 (102%)	642 (96%)	30 (4%)	34	46

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

Mol	Chain	Res	Type
1	A	11	SER

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Mol	Chain	Res	Type
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

Some 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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	PRV	C	5	3	10,13,14	0.92	1 (10%)	10,17,19	1.25	1 (10%)
3	PRQ	C	8	3	12,14,15	0.70	0	10,18,20	1.48	2 (20%)
3	PRV	F	5	3	10,13,14	0.90	1 (10%)	10,17,19	1.42	2 (20%)
3	PRQ	F	8	3	12,14,15	0.61	0	10,18,20	1.47	2 (20%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5	PRV	CG-CA	-2.63	1.49	1.52
3	F	5	PRV	CG-CA	-2.60	1.49	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	8	PRQ	CAJ-CAM-CAK	-2.63	104.68	111.65
3	F	8	PRQ	CAJ-CAM-CAK	-2.24	105.70	111.65
3	F	8	PRQ	CAH-CAK-CAL	2.16	119.39	117.00
3	C	8	PRQ	CAH-CAK-CAL	2.20	119.42	117.00
3	F	5	PRV	CE2-CD2-N1	2.20	119.44	116.59
3	C	5	PRV	CD1-CG-CD2	2.34	119.58	117.00
3	F	5	PRV	CD1-CG-CD2	2.77	120.06	117.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	5	PRV	1	0
3	C	8	PRQ	5	0
3	F	5	PRV	3	0
3	F	8	PRQ	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	A	1276	-	5,5,5	0.33	0	5,5,5	0.22	0
4	GOL	B	1100	-	5,5,5	0.38	0	5,5,5	0.16	0
5	MES	B	1101	-	11,12,12	0.70	0	14,16,16	9.28	9 (64%)
5	MES	B	1102	-	11,12,12	0.70	0	14,16,16	9.48	9 (64%)
5	MES	D	1276	-	11,12,12	0.74	0	14,16,16	9.84	9 (64%)
4	GOL	D	1277	-	5,5,5	0.32	0	5,5,5	0.36	0
5	MES	D	1278	-	11,12,12	0.75	0	14,16,16	10.18	9 (64%)
4	GOL	D	1279	-	5,5,5	0.37	0	5,5,5	0.31	0
5	MES	E	1100	-	11,12,12	0.71	0	14,16,16	9.27	9 (64%)
4	GOL	E	1101	-	5,5,5	0.39	0	5,5,5	0.09	0
4	GOL	E	1102	-	5,5,5	0.40	0	5,5,5	0.15	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	1276	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1100	-	-	0/4/4/4	0/0/0/0
5	MES	B	1101	-	-	0/6/14/14	0/1/1/1
5	MES	B	1102	-	-	0/6/14/14	0/1/1/1
5	MES	D	1276	-	-	0/6/14/14	0/1/1/1
4	GOL	D	1277	-	-	0/4/4/4	0/0/0/0
5	MES	D	1278	-	-	0/6/14/14	0/1/1/1
4	GOL	D	1279	-	-	0/4/4/4	0/0/0/0
5	MES	E	1100	-	-	0/6/14/14	0/1/1/1
4	GOL	E	1101	-	-	0/4/4/4	0/0/0/0
4	GOL	E	1102	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1278	MES	O1S-S-C8	-28.07	82.95	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1276	MES	O1S-S-C8	-26.05	84.68	106.91
5	E	1100	MES	O1S-S-C8	-24.12	86.32	106.91
5	B	1102	MES	O1S-S-C8	-24.04	86.39	106.91
5	D	1276	MES	O2S-S-C8	-24.01	86.42	106.91
5	B	1101	MES	O1S-S-C8	-23.98	86.44	106.91
5	D	1278	MES	O2S-S-C8	-23.96	86.46	106.91
5	B	1102	MES	O2S-S-C8	-23.93	86.49	106.91
5	B	1101	MES	O2S-S-C8	-23.17	87.13	106.91
5	E	1100	MES	O2S-S-C8	-22.60	87.62	106.91
5	D	1276	MES	C2-C3-N4	-4.27	103.65	110.12
5	B	1102	MES	C6-C5-N4	-4.02	104.03	110.12
5	E	1100	MES	C2-C3-N4	-3.90	104.22	110.12
5	B	1102	MES	C2-C3-N4	-3.67	104.56	110.12
5	E	1100	MES	C6-C5-N4	-3.63	104.62	110.12
5	B	1101	MES	C2-C3-N4	-3.24	105.21	110.12
5	B	1101	MES	C6-C5-N4	-2.90	105.73	110.12
5	D	1278	MES	C6-C5-N4	-2.84	105.82	110.12
5	D	1276	MES	C6-C5-N4	-2.62	106.16	110.12
5	D	1278	MES	C2-C3-N4	-2.31	106.62	110.12
5	D	1278	MES	O3S-S-O2S	2.59	117.63	111.61
5	E	1100	MES	C7-N4-C3	3.11	119.23	111.27
5	D	1276	MES	O3S-S-O2S	3.29	119.26	111.61
5	D	1278	MES	C7-N4-C3	3.38	119.93	111.27
5	B	1102	MES	O3S-S-O1S	3.40	119.52	111.61
5	B	1101	MES	O3S-S-O1S	3.40	119.53	111.61
5	B	1102	MES	C7-N4-C3	3.42	120.04	111.27
5	B	1101	MES	C7-N4-C3	3.43	120.06	111.27
5	D	1276	MES	O3S-S-O1S	3.47	119.68	111.61
5	D	1276	MES	C7-N4-C5	3.49	120.22	111.27
5	B	1101	MES	O3S-S-O2S	3.50	119.76	111.61
5	D	1276	MES	C7-N4-C3	3.61	120.54	111.27
5	D	1278	MES	C7-N4-C5	3.63	120.58	111.27
5	B	1102	MES	O3S-S-O2S	3.67	120.16	111.61
5	E	1100	MES	O3S-S-O1S	3.69	120.21	111.61
5	E	1100	MES	O3S-S-O2S	3.75	120.34	111.61
5	B	1101	MES	C7-N4-C5	3.93	121.34	111.27
5	D	1278	MES	O3S-S-O1S	3.94	120.78	111.61
5	B	1102	MES	C7-N4-C5	3.94	121.38	111.27
5	E	1100	MES	C7-N4-C5	4.00	121.52	111.27
5	B	1102	MES	C5-N4-C3	4.47	118.57	108.90
5	B	1101	MES	C5-N4-C3	4.48	118.60	108.90
5	D	1276	MES	C5-N4-C3	4.78	119.24	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1100	MES	C5-N4-C3	4.78	119.25	108.90
5	D	1278	MES	C5-N4-C3	4.89	119.48	108.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1276	GOL	3	0
4	B	1100	GOL	3	0
5	B	1101	MES	1	0
5	B	1102	MES	3	0
5	D	1276	MES	3	0
4	D	1277	GOL	1	0
5	D	1278	MES	3	0
5	E	1100	MES	1	0
4	E	1102	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	275/275 (100%)	-0.09	0 <span>100</span> <span>100</span>	21, 42, 73, 112	0
1	D	275/275 (100%)	0.01	1 (0%) <span>93</span> <span>95</span>	15, 46, 73, 89	0
2	B	100/100 (100%)	-0.24	0 <span>100</span> <span>100</span>	21, 35, 61, 86	0
2	E	100/100 (100%)	-0.29	0 <span>100</span> <span>100</span>	21, 37, 63, 74	0
3	C	6/9 (66%)	1.54	1 (16%) <span>2</span> <span>4</span>	37, 71, 91, 119	0
3	F	6/9 (66%)	0.85	1 (16%) <span>2</span> <span>4</span>	40, 58, 77, 103	0
All	All	762/768 (99%)	-0.08	3 (0%) <span>93</span> <span>95</span>	15, 42, 73, 119	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	7	PHE	5.2
3	F	7	PHE	4.3
1	D	130	LEU	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PRQ	F	8	14/15	0.90	0.20	-	46,94,106,106	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	C	8	14/15	0.72	0.36	-	93,128,142,146	0



### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	E	1102	6/6	0.91	0.24	3.53	35,48,56,59	0
4	GOL	D	1279	6/6	0.89	0.16	2.90	48,52,56,59	0
5	MES	B	1102	12/12	0.88	0.18	1.77	48,64,150,151	0
4	GOL	B	1100	6/6	0.88	0.17	1.76	56,63,65,65	0
5	MES	E	1100	12/12	0.92	0.15	1.16	61,65,68,68	0
4	GOL	A	1276	6/6	0.90	0.14	1.00	44,49,50,55	0
5	MES	B	1101	12/12	0.93	0.13	0.57	62,71,91,95	0
5	MES	D	1278	12/12	0.96	0.15	0.48	25,30,38,40	0
4	GOL	E	1101	6/6	0.94	0.12	0.21	27,32,39,50	0
5	MES	D	1276	12/12	0.97	0.14	-0.07	27,44,47,48	0
4	GOL	D	1277	6/6	0.92	0.17	-	46,47,50,51	0

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

There are no such residues in this entry.