



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:43 am BST

PDB ID : 2X4O  
Title : Crystal structure of MHC Class I HLA-A2.1 bound to HIV-1 envelope peptide env120-128  
Authors : Celie, P.H.N.; Toebes, M.; Rodenko, B.; Ovaa, H.; Perrakis, A.; Schumacher, T.N.M.  
Deposited on : 2010-02-02  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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

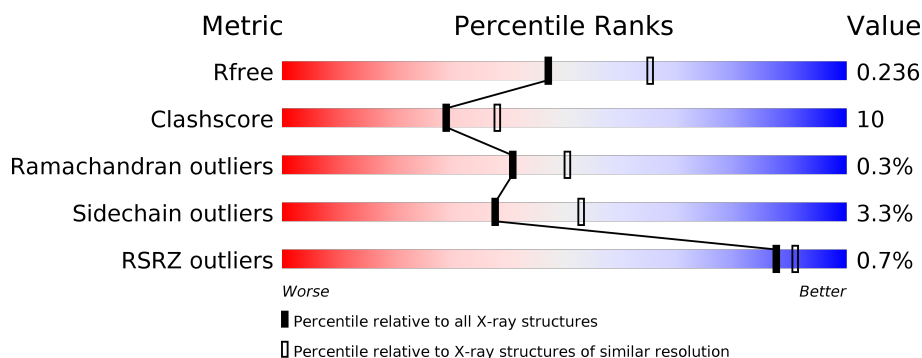
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	275	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	D	275	<div> <div>84%</div> <div>15%</div> <div>.</div> </div>
2	B	100	<div> <div>%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
2	E	100	<div> <div>81%</div> <div>17%</div> <div>.</div> </div>
3	C	9	<div> <div>22%</div> <div>44%</div> <div>33%</div> <div>22%</div> </div>
3	F	9	<div> <div>22%</div> <div>67%</div> <div>22%</div> <div>11%</div> </div>

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	E	1102[A]	-	-	X	-

## 2 Entry composition

There are 6 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-2 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	5	0
			2295	1434	420	432	9			
1	D	275	Total	C	N	O	S	0	6	0
			2295	1433	422	431	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	1	0
			842	536	141	161	4			

- Molecule 3 is a protein called ENVELOPE GLYCOPROTEIN GP160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			68	45	10	12	1			
3	F	9	Total	C	N	O	S	0	0	0
			68	45	10	12	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	D	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	1
			12	6	6		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

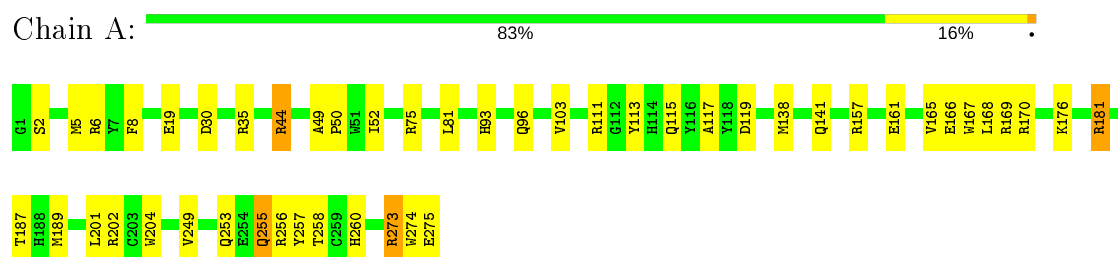
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	163	Total	O	0	0
			163	163		
6	B	80	Total	O	0	0
			80	80		
6	C	3	Total	O	0	0
			3	3		
6	D	106	Total	O	0	0
			106	106		
6	E	63	Total	O	0	0
			63	63		
6	F	2	Total	O	0	0
			2	2		

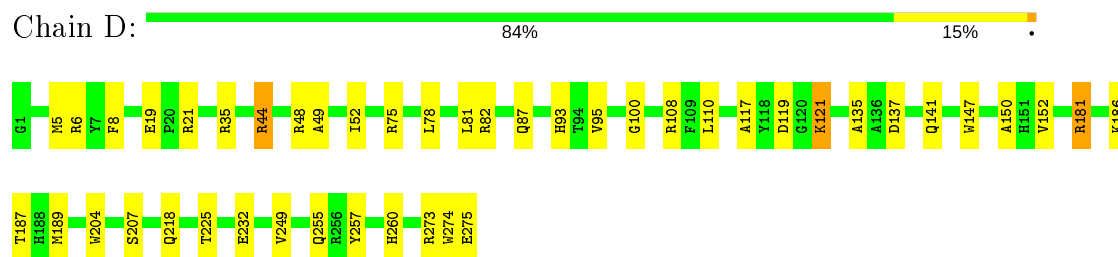
### 3 Residue-property plots

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

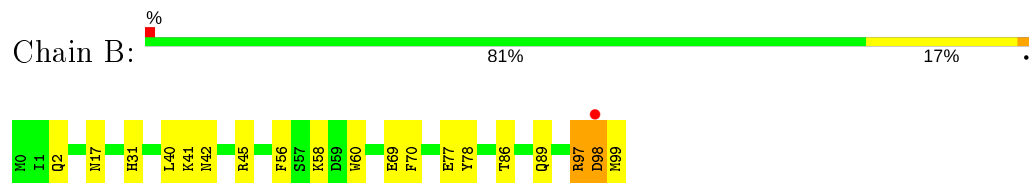
#### • Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN



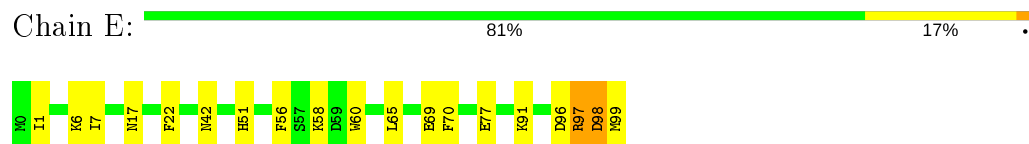
#### • Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN



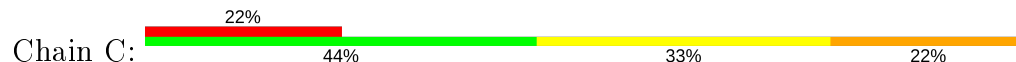
#### • Molecule 2: BETA-2-MICROGLOBULIN

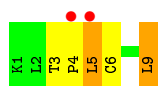


#### • Molecule 2: BETA-2-MICROGLOBULIN



#### • Molecule 3: ENVELOPE GLYCOPROTEIN GP160





● Molecule 3: ENVELOPE GLYCOPROTEIN GP160





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.99Å 81.90Å 79.75Å 90.00° 90.87° 90.00°	Depositor
Resolution (Å)	48.58 – 2.30 49.42 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.58-2.30) 99.9 (49.42-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.71 (at 2.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.175 , 0.239 0.178 , 0.236	Depositor DCC
$R_{free}$ test set	1800 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for -h,-l,-k 0.010 for -h,l,k 0.065 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6912	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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	0.31	0/2365	0.51	0/3207
1	D	0.29	0/2372	0.48	0/3214
2	B	0.35	0/860	0.50	0/1162
2	E	0.32	0/868	0.47	0/1173
3	C	0.32	0/68	0.63	0/91
3	F	0.27	0/68	0.75	0/91
All	All	0.31	0/6601	0.50	0/8938

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 [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	2295	0	2142	46	0
1	D	2295	0	2160	41	0
2	B	837	0	803	18	0
2	E	842	0	807	23	0
3	C	68	0	83	4	0
3	F	68	0	83	2	0
4	A	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	18	0	24	2	0
4	E	18	0	24	7	0
5	B	12	0	12	0	0
5	D	24	0	24	6	0
5	E	12	0	12	2	0
6	A	163	0	0	2	0
6	B	80	0	0	4	0
6	C	3	0	0	0	0
6	D	106	0	0	1	0
6	E	63	0	0	1	0
6	F	2	0	0	0	0
All	All	6912	0	6182	122	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 10.

All (122) 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:98:ASP:CB	2:B:99:MET:HA	1.67	1.25
1:A:273:ARG:HG2	1:A:273:ARG:HH11	0.98	1.15
2:B:98:ASP:HB3	2:B:99:MET:HA	1.16	1.08
1:A:44:ARG:HG3	1:A:44:ARG:HH11	1.17	1.06
2:E:91:LYS:HD2	4:E:1102[A]:GOL:H32	1.50	0.90
1:D:44:ARG:HG3	1:D:44:ARG:HH11	1.38	0.89
1:A:273:ARG:HG2	1:A:273:ARG:NH1	1.79	0.88
2:B:98:ASP:HB3	2:B:99:MET:CA	2.02	0.88
1:A:157[B]:ARG:HH22	1:D:218:GLN:HE22	1.20	0.86
1:D:44:ARG:CG	1:D:44:ARG:HH11	1.87	0.86
2:B:98:ASP:CB	2:B:99:MET:CA	2.54	0.86
1:A:273:ARG:HH11	1:A:273:ARG:CG	1.86	0.86
1:A:30:ASP:HA	4:A:1276:GOL:H11	1.59	0.84
3:C:5:LEU:HD13	3:C:6:CYS:H	1.42	0.84
2:E:91:LYS:HE2	4:E:1102[A]:GOL:H11	1.58	0.84
2:B:98:ASP:HB2	2:B:99:MET:HA	1.62	0.80
1:D:273[A]:ARG:HB3	1:D:273[A]:ARG:HH11	1.48	0.78
1:A:44:ARG:CG	1:A:44:ARG:HH11	1.97	0.74
2:E:58:LYS:HA	4:E:1101:GOL:C3	2.19	0.72
1:A:202:ARG:NH1	2:B:99:MET:HB3	2.06	0.71
2:E:58:LYS:HA	4:E:1101:GOL:H32	1.73	0.70
2:B:42:ASN:HD21	2:B:77:GLU:H	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:HG3	1:A:44:ARG:NH1	1.98	0.69
1:A:157[B]:ARG:HH22	1:D:218:GLN:NE2	1.90	0.68
2:B:42:ASN:ND2	2:B:77:GLU:H	1.91	0.68
1:D:273[A]:ARG:NH1	1:D:273[A]:ARG:HB3	2.08	0.67
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.30	0.67
2:E:91:LYS:CE	4:E:1102[A]:GOL:H11	2.26	0.65
1:A:157[B]:ARG:NH2	1:D:218:GLN:HE22	1.91	0.65
1:D:147:TRP:CD1	1:D:152:VAL:HG21	2.32	0.65
1:D:44:ARG:CB	1:D:44:ARG:HH11	2.09	0.64
1:D:93:HIS:HD2	1:D:119:ASP:OD2	1.79	0.64
1:A:258:THR:OG1	1:A:260[A]:HIS:HE1	1.81	0.63
5:D:1276:MES:H31	2:E:98:ASP:CB	2.29	0.63
1:D:44:ARG:HG3	1:D:44:ARG:NH1	2.13	0.61
1:A:255:GLN:O	1:A:255:GLN:HG2	2.00	0.60
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.36	0.60
1:A:176:LYS:HD3	1:D:110:LEU:HD12	1.85	0.59
1:D:137:ASP:O	1:D:141:GLN:HG2	2.03	0.59
1:A:161:GLU:OE1	1:D:260:HIS:NE2	2.36	0.56
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.41	0.56
1:A:258:THR:OG1	1:A:260[A]:HIS:CE1	2.59	0.55
1:D:249:VAL:HG22	1:D:257:TYR:CZ	2.42	0.54
1:A:274:TRP:O	1:A:275:GLU:HB2	2.07	0.54
1:A:6:ARG:NE	1:A:113[B]:TYR:OH	2.42	0.53
3:C:5:LEU:HD13	3:C:6:CYS:N	2.20	0.53
1:A:44:ARG:CG	1:A:44:ARG:NH1	2.64	0.53
1:A:189:MET:HE2	1:A:274:TRP:HE3	1.74	0.52
1:A:138:MET:O	1:A:141:GLN:HB2	2.07	0.52
5:D:1276:MES:H31	2:E:98:ASP:HB2	1.92	0.52
2:B:69:GLU:HG3	6:B:2057:HOH:O	2.10	0.51
5:D:1276:MES:C3	2:E:98:ASP:HB2	2.41	0.51
1:A:111:ARG:HD2	1:A:113[B]:TYR:OH	2.11	0.51
1:D:93:HIS:CD2	1:D:119:ASP:OD2	2.62	0.51
1:D:44:ARG:HB3	1:D:44:ARG:NH1	2.27	0.50
1:A:165:VAL:O	1:A:169:ARG:HG3	2.10	0.50
2:E:22:PHE:CE1	2:E:69:GLU:HG3	2.46	0.50
1:A:81:LEU:HD11	3:C:9:LEU:HD23	1.94	0.50
1:D:189:MET:HE2	1:D:274:TRP:HE3	1.77	0.50
1:A:275:GLU:HB3	6:A:2162:HOH:O	2.12	0.50
1:D:44:ARG:CB	1:D:44:ARG:NH1	2.75	0.49
1:D:135:ALA:HB3	1:D:141:GLN:HE21	1.77	0.49
1:A:253:GLN:NE2	1:A:256:ARG:HH11	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:SER:HB2	1:A:103:VAL:O	2.12	0.49
1:D:232:GLU:CD	2:E:6:LYS:HE3	2.33	0.49
1:D:81:LEU:HD11	3:F:9:LEU:HD23	1.94	0.49
2:E:17:ASN:OD1	2:E:97:ARG:NH2	2.47	0.48
2:B:89:GLN:HB3	6:B:2070:HOH:O	2.13	0.48
5:D:1276:MES:H32	2:E:96:ASP:OD1	2.13	0.48
2:B:41:LYS:HG3	2:B:78:TYR:CE1	2.49	0.48
1:D:274:TRP:O	1:D:275:GLU:HB2	2.12	0.48
1:D:49:ALA:O	1:D:52:ILE:HG22	2.14	0.48
2:E:91:LYS:CD	4:E:1102[A]:GOL:H11	2.43	0.48
1:D:255:GLN:HG2	1:D:255:GLN:O	2.13	0.47
2:E:22:PHE:CZ	2:E:69:GLU:HG3	2.49	0.47
2:E:42:ASN:ND2	2:E:77:GLU:H	2.13	0.47
1:A:49:ALA:O	1:A:52:ILE:HG22	2.15	0.47
1:D:78:LEU:HD23	1:D:95:VAL:HG23	1.97	0.46
1:D:189:MET:HE2	1:D:274:TRP:CE3	2.51	0.46
1:D:232:GLU:OE2	2:E:6:LYS:HE3	2.16	0.46
4:D:1279:GOL:H12	5:E:1100:MES:H72	1.97	0.46
1:A:187:THR:HA	1:A:204:TRP:O	2.16	0.46
1:A:181:ARG:NH2	6:A:2104:HOH:O	2.47	0.45
5:D:1277:MES:H52	5:E:1100:MES:O1S	2.16	0.45
2:E:7:ILE:HD12	2:E:91:LYS:HD3	1.98	0.45
4:A:1276:GOL:H2	6:B:2054:HOH:O	2.16	0.45
1:A:273:ARG:CG	1:A:273:ARG:NH1	2.56	0.45
1:D:186[B]:LYS:HB2	1:D:186[B]:LYS:HE3	1.55	0.45
1:D:121:LYS:HB3	2:E:1:ILE:HD12	1.98	0.45
1:A:167:TRP:CD2	1:A:170:ARG:HD3	2.53	0.44
2:B:17:ASN:OD1	2:B:97:ARG:NH1	2.47	0.44
1:D:8:PHE:HD1	2:E:56:PHE:CE1	2.36	0.44
1:A:96:GLN:NE2	2:B:31:HIS:NE2	2.65	0.44
1:D:5:MET:O	1:D:100:GLY:HA3	2.17	0.44
2:E:98:ASP:O	2:E:99:MET:HB2	2.18	0.43
3:C:3:THR:HA	3:C:4:PRO:HD3	1.68	0.43
1:A:167:TRP:CE3	1:A:170:ARG:HD3	2.53	0.43
4:E:1102[B]:GOL:H12	6:E:2063:HOH:O	2.19	0.43
1:A:93:HIS:HD2	1:A:119:ASP:OD2	2.02	0.43
5:D:1276:MES:H31	2:E:98:ASP:HB3	2.01	0.43
1:A:5:MET:HB2	1:A:168:LEU:HD13	2.00	0.43
2:B:40:LEU:HD23	2:B:45:ARG:HA	2.00	0.43
3:F:3:THR:HA	3:F:4:PRO:HD3	1.81	0.43
1:A:8:PHE:HD1	2:B:56:PHE:CE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:GLU:OE1	1:D:75:ARG:HD3	2.19	0.42
1:A:166:GLU:O	1:A:170:ARG:HG3	2.19	0.42
2:B:58:LYS:HA	6:B:2045:HOH:O	2.19	0.42
1:A:189:MET:CE	1:A:274:TRP:HB2	2.50	0.42
1:D:150:ALA:HB3	1:D:152:VAL:HG23	2.01	0.42
1:D:48:ARG:HA	1:D:48:ARG:HD2	1.95	0.42
1:A:189:MET:HE3	1:A:189:MET:HB3	1.67	0.41
1:A:49:ALA:HA	1:A:50:PRO:HD3	1.95	0.41
1:A:141:GLN:HE21	1:A:141:GLN:HA	1.85	0.41
1:D:135:ALA:HB3	1:D:141:GLN:NE2	2.35	0.40
1:D:82:ARG:HG3	1:D:87:GLN:HB2	2.03	0.40
1:A:19:GLU:OE1	1:A:75:ARG:HD3	2.21	0.40
2:B:2:GLN:HB3	2:B:86:THR:HG22	2.04	0.40
1:D:6:ARG:HD2	4:D:1279:GOL:O3	2.20	0.40
2:E:51:HIS:HA	2:E:65:LEU:O	2.21	0.40
1:A:258:THR:HG22	1:A:273:ARG:HG2	2.03	0.40
1:D:187:THR:HA	1:D:204:TRP:O	2.21	0.40
1:D:181:ARG:NH2	6:D:2066:HOH:O	2.54	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	278/275 (101%)	272 (98%)	6 (2%)	0	100	100
1	D	279/275 (102%)	272 (98%)	7 (2%)	0	100	100
2	B	98/100 (98%)	95 (97%)	2 (2%)	1 (1%)	15	17
2	E	99/100 (99%)	94 (95%)	4 (4%)	1 (1%)	15	17
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	5 (71%)	2 (29%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	768/768 (100%)	745 (97%)	21 (3%)	2 (0%)	41 50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	98	ASP
2	E	98	ASP

### 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	236/231 (102%)	229 (97%)	7 (3%)	41 57
1	D	237/231 (103%)	229 (97%)	8 (3%)	37 51
2	B	95/95 (100%)	93 (98%)	2 (2%)	53 70
2	E	96/95 (101%)	94 (98%)	2 (2%)	53 70
3	C	9/9 (100%)	7 (78%)	2 (22%)	1 1
3	F	9/9 (100%)	8 (89%)	1 (11%)	6 7
All	All	682/670 (102%)	660 (97%)	22 (3%)	38 54

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	44	ARG
1	A	115	GLN
1	A	181	ARG
1	A	201	LEU
1	A	255	GLN
1	A	273	ARG
2	B	70	PHE
2	B	97	ARG
3	C	5	LEU

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Mol	Chain	Res	Type
3	C	9	LEU
1	D	21	ARG
1	D	35	ARG
1	D	44	ARG
1	D	108	ARG
1	D	121	LYS
1	D	181	ARG
1	D	207	SER
1	D	225	THR
2	E	70	PHE
2	E	97	ARG
3	F	9	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	96	GLN
1	A	141	GLN
1	A	224	GLN
1	A	253	GLN
2	B	42	ASN
1	D	93	HIS
1	D	96	GLN
1	D	141	GLN
1	D	218	GLN
1	D	253	GLN
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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

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	D	1278	-	5,5,5	0.37	0	5,5,5	0.33	0
5	MES	D	1277	-	12,12,12	2.06	1 (8%)	14,16,16	7.79	10 (71%)
5	MES	E	1100	-	12,12,12	2.02	1 (8%)	14,16,16	7.62	8 (57%)
5	MES	D	1276	-	12,12,12	2.13	1 (8%)	14,16,16	7.65	9 (64%)
4	GOL	E	1102[B]	-	5,5,5	0.39	0	5,5,5	0.29	0
4	GOL	E	1101	-	5,5,5	0.39	0	5,5,5	0.27	0
4	GOL	D	1279	-	5,5,5	0.37	0	5,5,5	0.55	0
4	GOL	E	1102[A]	-	5,5,5	0.41	0	5,5,5	0.30	0
4	GOL	A	1276	-	5,5,5	0.41	0	5,5,5	0.38	0
4	GOL	D	1280	-	5,5,5	0.37	0	5,5,5	0.26	0
5	MES	B	1100	-	12,12,12	1.90	1 (8%)	14,16,16	7.64	8 (57%)

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	D	1278	-	-	2/4/4/4	-
5	MES	D	1277	-	-	4/6/14/14	0/1/1/1
5	MES	E	1100	-	-	1/6/14/14	0/1/1/1
5	MES	D	1276	-	-	2/6/14/14	0/1/1/1
4	GOL	E	1102[B]	-	-	2/4/4/4	-
4	GOL	E	1101	-	-	2/4/4/4	-
4	GOL	D	1279	-	-	2/4/4/4	-
4	GOL	E	1102[A]	-	-	0/4/4/4	-
4	GOL	A	1276	-	-	2/4/4/4	-
4	GOL	D	1280	-	-	1/4/4/4	-
5	MES	B	1100	-	-	1/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1276	MES	C8-S	-6.93	1.67	1.77
5	D	1277	MES	C8-S	-6.72	1.68	1.77
5	E	1100	MES	C8-S	-6.54	1.68	1.77
5	B	1100	MES	C8-S	-6.13	1.68	1.77

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1277	MES	O1S-S-C8	-19.72	83.17	106.92
5	B	1100	MES	O1S-S-C8	-19.17	83.84	106.92
5	D	1276	MES	O1S-S-C8	-17.53	85.81	106.92
5	E	1100	MES	O2S-S-C8	-17.12	86.30	106.92
5	E	1100	MES	O1S-S-C8	-17.03	86.41	106.92
5	B	1100	MES	O2S-S-C8	-16.32	87.27	106.92
5	D	1277	MES	O2S-S-C8	-16.09	87.54	106.92
5	D	1276	MES	O2S-S-C8	-16.01	87.63	106.92
5	D	1276	MES	O3S-S-C8	-12.85	84.98	105.77
5	E	1100	MES	O3S-S-C8	-11.77	86.73	105.77
5	D	1277	MES	O3S-S-C8	-10.42	88.91	105.77
5	B	1100	MES	O3S-S-C8	-10.04	89.53	105.77
5	E	1100	MES	C5-N4-C3	6.58	123.63	108.83
5	B	1100	MES	C5-N4-C3	5.24	120.63	108.83
5	D	1276	MES	C5-N4-C3	4.84	119.73	108.83
5	D	1277	MES	C5-N4-C3	4.25	118.40	108.83
5	D	1276	MES	O3S-S-O1S	4.17	121.46	111.27
5	D	1277	MES	C7-N4-C5	4.07	121.65	111.23
5	D	1277	MES	O3S-S-O1S	3.91	120.83	111.27
5	D	1276	MES	C7-N4-C5	3.60	120.44	111.23
5	B	1100	MES	O3S-S-O2S	3.56	119.98	111.27
5	E	1100	MES	O3S-S-O2S	3.51	119.85	111.27
5	D	1277	MES	C2-C3-N4	-3.42	104.91	110.10
5	B	1100	MES	C7-N4-C3	3.41	119.96	111.23
5	D	1277	MES	C7-N4-C3	3.41	119.95	111.23
5	E	1100	MES	O3S-S-O1S	3.36	119.49	111.27
5	D	1276	MES	C7-N4-C3	3.36	119.83	111.23
5	D	1276	MES	O3S-S-O2S	3.20	119.09	111.27
5	B	1100	MES	C7-N4-C5	3.20	119.41	111.23
5	E	1100	MES	C7-N4-C5	3.12	119.23	111.23
5	D	1276	MES	C6-C5-N4	-3.11	105.39	110.10
5	D	1277	MES	O3S-S-O2S	2.96	118.52	111.27
5	B	1100	MES	O3S-S-O1S	2.87	118.30	111.27
5	D	1277	MES	C6-C5-N4	-2.73	105.96	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1100	MES	C7-N4-C3	2.31	117.13	111.23

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1278	GOL	C1-C2-C3-O3
5	D	1277	MES	C8-C7-N4-C5
5	D	1277	MES	C7-C8-S-O2S
5	D	1276	MES	C8-C7-N4-C3
5	D	1276	MES	N4-C7-C8-S
4	E	1102[B]	GOL	C1-C2-C3-O3
4	D	1279	GOL	C1-C2-C3-O3
4	A	1276	GOL	C1-C2-C3-O3
5	D	1277	MES	C7-C8-S-O3S
4	E	1101	GOL	C1-C2-C3-O3
4	D	1278	GOL	O2-C2-C3-O3
4	E	1101	GOL	O2-C2-C3-O3
4	E	1102[B]	GOL	O2-C2-C3-O3
4	D	1279	GOL	O2-C2-C3-O3
4	A	1276	GOL	O2-C2-C3-O3
5	E	1100	MES	C8-C7-N4-C3
5	B	1100	MES	C8-C7-N4-C3
5	D	1277	MES	C7-C8-S-O1S
4	D	1280	GOL	O2-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1277	MES	1	0
5	E	1100	MES	2	0
5	D	1276	MES	5	0
4	E	1102[B]	GOL	1	0
4	E	1101	GOL	2	0
4	D	1279	GOL	2	0
4	E	1102[A]	GOL	4	0
4	A	1276	GOL	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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%)	-0.34	0 100 100	16, 32, 57, 73	0
1	D	275/275 (100%)	-0.27	0 100 100	17, 39, 70, 89	0
2	B	100/100 (100%)	-0.43	1 (1%) 82 86	18, 28, 50, 76	0
2	E	100/100 (100%)	-0.45	0 100 100	21, 33, 64, 78	0
3	C	9/9 (100%)	0.87	2 (22%) 0 1	32, 32, 32, 32	0
3	F	9/9 (100%)	1.33	2 (22%) 0 1	32, 32, 32, 32	0
All	All	768/768 (100%)	-0.31	5 (0%) 87 91	16, 33, 64, 89	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	6	CYS	6.8
3	C	4	PRO	2.9
2	B	98	ASP	2.9
3	C	5	LEU	2.4
3	F	7	VAL	2.3

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

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

### 6.3 Carbohydrates ⓘ

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( $\text{\AA}^2$ )	Q<0.9
4	GOL	E	1102[B]	6/6	0.83	0.29	31,31,31,31	6
4	GOL	E	1102[A]	6/6	0.83	0.29	31,31,31,31	6
4	GOL	D	1280	6/6	0.85	0.26	31,31,31,31	0
4	GOL	D	1278	6/6	0.89	0.40	31,31,31,31	0
4	GOL	E	1101	6/6	0.89	0.25	31,31,31,31	0
5	MES	D	1277	12/12	0.91	0.41	31,31,31,31	0
4	GOL	D	1279	6/6	0.91	0.16	31,31,31,31	0
5	MES	D	1276	12/12	0.93	0.34	31,31,31,31	0
5	MES	E	1100	12/12	0.93	0.29	31,31,31,31	0
5	MES	B	1100	12/12	0.93	0.15	31,31,31,31	0
4	GOL	A	1276	6/6	0.94	0.19	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.