



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 10:39 pm GMT

PDB ID : 2X4U  
Title : Crystal structure of MHC CLass I HLA-A2.1 bound to HIV-1 Peptide RT468-476  
Authors : Celie, P.H.N.; Toebes, M.; Rodenko, B.; Ovaa, H.; Perrakis, A.; Schumacher, T.N.M.  
Deposited on : 2010-02-02  
Resolution : 2.10 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

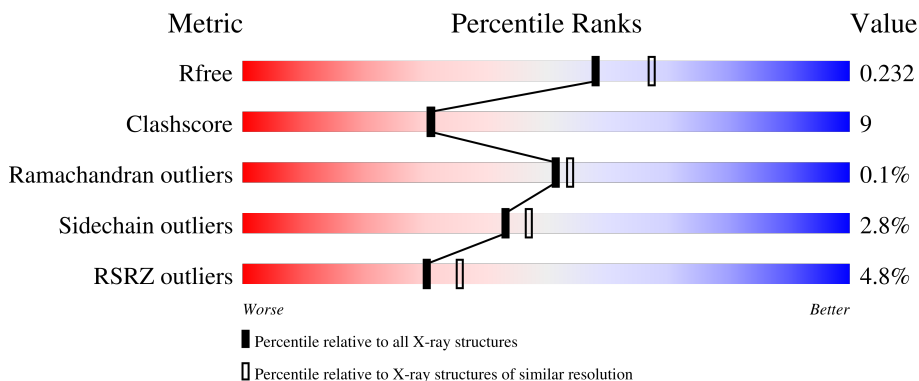
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 3% 87% 12%
1	D	275	 5% 83% 16%
2	B	100	 2% 85% 14%
2	E	100	 5% 83% 15%
3	C	9	 33% 44% 56%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	F	9	<p>44% 56% 44%</p>

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	1280	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7087 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 2405	C 1494	N 447	O 454	S 10	0	17	0
1	D	275	Total 2273	C 1418	N 416	O 430	S 9	0	3	0

- 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 865	C 548	N 148	O 165	S 4	0	3	0
2	E	100	Total 850	C 541	N 142	O 162	S 5	0	2	0

- Molecule 3 is a protein called REVERSE TRANSCRIPTASE/RIBONUCLEASE H.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	Total 79	C 52	N 14	O 13	0	1	0
3	F	9	Total 70	C 46	N 12	O 12	0	0	0

- 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	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
4	E	1	Total C O 6 3 3	0	0
4	E	1	Total C O 12 6 6	0	1

- 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
			Total	C	N	O	S		
5	A	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		

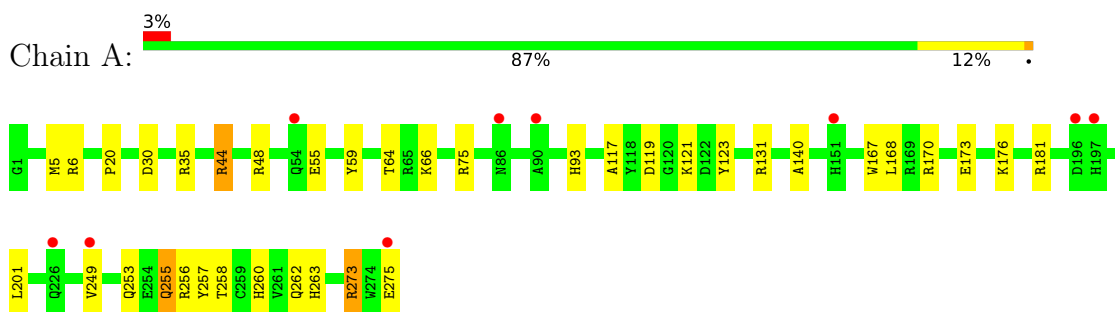
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	175	Total	O	0	0
			175	175		
6	B	87	Total	O	0	0
			87	87		
6	C	6	Total	O	0	0
			6	6		
6	D	101	Total	O	0	0
			101	101		
6	E	53	Total	O	0	0
			53	53		
6	F	3	Total	O	0	0
			3	3		

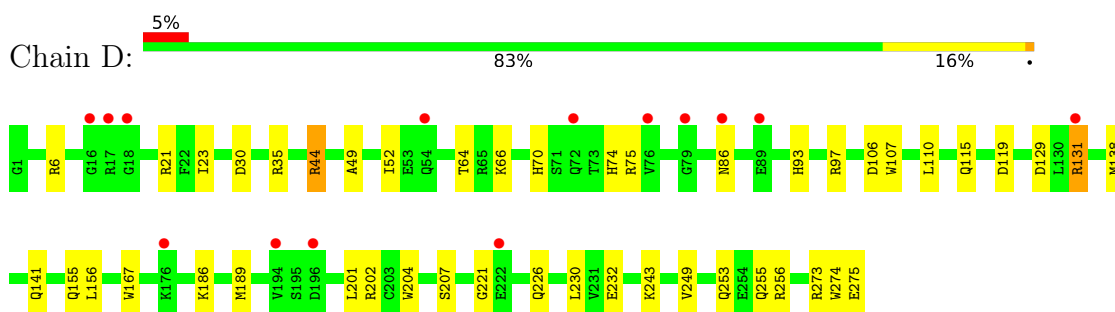
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

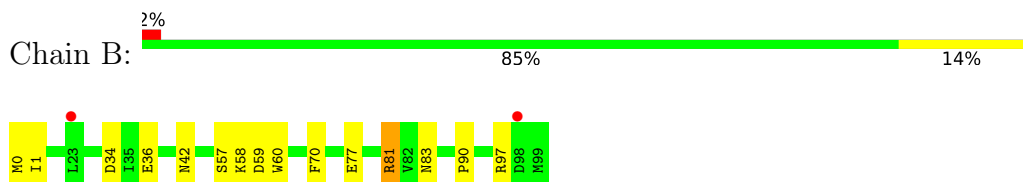
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN



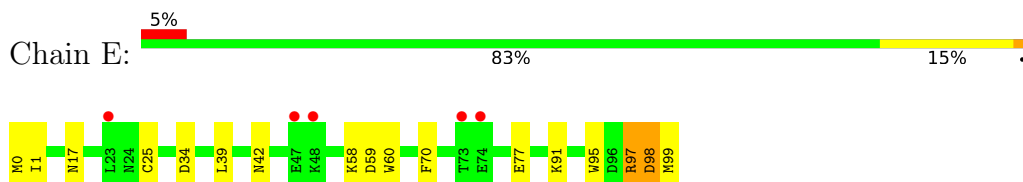
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN



- Molecule 2: BETA-2-MICROGLOBULIN



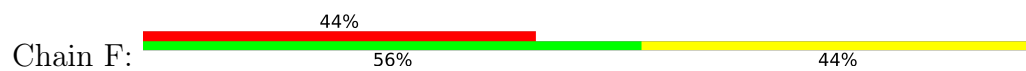
- Molecule 2: BETA-2-MICROGLOBULIN



- Molecule 3: REVERSE TRANSCRIPTASE/RIBONUCLEASE H



• Molecule 3: REVERSE TRANSCRIPTASE/RIBONUCLEASE H





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.22Å 82.77Å 79.66Å 90.00° 90.76° 90.00°	Depositor
Resolution (Å)	19.95 – 2.10 19.94 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.3 (19.95-2.10) 97.2 (19.94-2.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.96 (at 2.09Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.176 , 0.234 0.182 , 0.232	Depositor DCC
$R_{free}$ test set	2336 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h,-l,-k 0.008 for -h,l,k 0.060 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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: MES, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/2470	0.46	0/3340
1	D	0.25	0/2341	0.43	0/3175
2	B	0.28	0/888	0.45	0/1200
2	E	0.27	0/876	0.46	0/1183
3	C	0.27	0/80	0.72	0/105
3	F	0.27	0/71	0.70	0/94
All	All	0.26	0/6726	0.46	0/9097

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	2405	0	2244	41	0
1	D	2273	0	2123	42	0
2	B	865	0	826	15	0
2	E	850	0	817	19	0
3	C	79	0	90	7	0
3	F	70	0	78	8	0
4	A	18	0	24	5	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	8	0	0
4	D	18	0	24	4	0
4	E	18	0	24	5	0
5	A	12	0	12	4	0
5	B	12	0	12	1	0
5	D	24	0	24	2	0
5	E	12	0	12	2	0
6	A	175	0	0	4	0
6	B	87	0	0	1	0
6	C	6	0	0	0	0
6	D	101	0	0	1	0
6	E	53	0	0	0	0
6	F	3	0	0	0	0
All	All	7087	0	6318	118	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 9.

All (118) 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:98:ASP:CB	2:E:99:MET:HA	1.74	1.14
1:A:44:ARG:HH11	1:A:44:ARG:HG3	0.99	1.10
1:D:44:ARG:HG3	1:D:44:ARG:HH11	1.16	1.08
2:E:98:ASP:HB3	2:E:99:MET:HA	1.27	1.08
4:A:1276:GOL:H12	2:B:58:LYS:HA	1.43	0.99
2:B:81[A]:ARG:HG2	2:B:81[A]:ARG:HH11	1.26	0.96
1:A:44:ARG:HG3	1:A:44:ARG:NH1	1.81	0.93
1:A:44:ARG:HH11	1:A:44:ARG:CG	1.81	0.92
2:B:81[A]:ARG:HG2	2:B:81[A]:ARG:NH1	1.83	0.91
1:D:75[B]:ARG:CG	1:D:75[B]:ARG:HH11	1.85	0.89
1:D:44:ARG:HH11	1:D:44:ARG:CG	1.90	0.83
3:C:3[B]:LYS:HZ1	3:C:6:VAL:HG13	1.45	0.82
2:E:58:LYS:HA	4:E:1101:GOL:H31	1.61	0.81
2:E:98:ASP:CB	2:E:99:MET:CA	2.59	0.81
2:E:98:ASP:HB2	2:E:99:MET:HA	1.63	0.80
1:D:155[B]:GLN:HG2	3:F:3:LYS:HZ1	1.46	0.80
1:D:75[B]:ARG:HH11	1:D:75[B]:ARG:HG3	1.46	0.79
4:A:1276:GOL:C1	2:B:58:LYS:HA	2.12	0.78
2:B:81[A]:ARG:HH11	2:B:81[A]:ARG:CG	1.97	0.77
1:A:273:ARG:HB2	1:A:273:ARG:HH11	1.52	0.75

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:TRP:CE2	3:C:1:ILE:HD12	2.23	0.73
1:D:21:ARG:NH1	1:D:23:ILE:HD11	2.06	0.71
1:A:273:ARG:HB2	1:A:273:ARG:NH1	2.06	0.71
2:E:91:LYS:HD2	4:E:1102[A]:GOL:H2	1.76	0.68
1:D:204:TRP:CZ3	4:D:1278:GOL:H31	2.30	0.67
2:E:98:ASP:HB3	2:E:99:MET:CA	2.15	0.67
2:B:42:ASN:ND2	2:B:77:GLU:H	1.94	0.64
1:A:30:ASP:HA	4:A:1278:GOL:H12	1.81	0.63
1:A:201[B]:LEU:HD12	1:A:249:VAL:HG21	1.79	0.63
1:D:44:ARG:HG3	1:D:44:ARG:NH1	1.98	0.63
1:D:93:HIS:HD2	1:D:119:ASP:OD2	1.81	0.63
1:D:66:LYS:NZ	3:F:1:ILE:HG23	2.14	0.62
2:B:42:ASN:HD21	2:B:77:GLU:H	1.47	0.62
1:A:93:HIS:HE1	6:A:2071:HOH:O	1.82	0.62
2:B:57:SER:HB3	5:B:1100:MES:O2S	1.99	0.62
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.84	0.61
2:E:42:ASN:ND2	2:E:77:GLU:H	1.97	0.60
1:D:156:LEU:HD23	3:F:3:LYS:HE2	1.84	0.59
2:E:42:ASN:HD21	2:E:77:GLU:H	1.50	0.59
3:C:3[A]:LYS:HG3	3:C:4:GLU:N	2.17	0.59
1:D:44:ARG:HD2	1:D:64:THR:HG21	1.84	0.59
1:A:55:GLU:HG2	1:A:59:TYR:CG	2.38	0.59
1:D:75[B]:ARG:CG	1:D:75[B]:ARG:NH1	2.54	0.58
1:A:66:LYS:NZ	3:C:1:ILE:HG23	2.18	0.58
5:A:1277:MES:H22	6:A:2134:HOH:O	2.04	0.57
1:D:106:ASP:O	1:D:107:TRP:HB2	2.05	0.56
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.40	0.56
1:A:131[B]:ARG:HE	1:D:221:GLY:HA3	1.71	0.55
1:A:167:TRP:CE3	1:A:170[B]:ARG:HD3	2.40	0.55
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.42	0.55
3:C:3[A]:LYS:CG	3:C:4:GLU:N	2.70	0.54
1:A:121[B]:LYS:HE3	2:B:1:ILE:HG13	1.89	0.54
1:D:202:ARG:NH1	2:E:99:MET:HB3	2.22	0.54
1:A:6:ARG:HD2	4:A:1278:GOL:O3	2.08	0.54
1:D:75[B]:ARG:HH11	1:D:75[B]:ARG:HG2	1.68	0.54
1:A:173:GLU:HG2	1:D:110:LEU:HD21	1.90	0.54
1:D:274:TRP:O	1:D:275:GLU:HB2	2.07	0.53
1:A:273:ARG:NH1	1:A:273:ARG:CB	2.72	0.53
1:D:232:GLU:OE2	5:D:1277:MES:H32	2.08	0.53
1:D:138:MET:O	1:D:141:GLN:HB2	2.09	0.53
1:D:44:ARG:CG	1:D:44:ARG:NH1	2.59	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLN:NE2	1:A:256:ARG:HH11	2.08	0.51
2:E:0[A]:MET:HG2	2:E:1:ILE:N	2.24	0.51
2:E:17:ASN:OD1	2:E:97:ARG:NH2	2.43	0.51
1:A:30:ASP:OD1	4:A:1278:GOL:H11	2.11	0.50
1:D:75[B]:ARG:NH1	1:D:75[B]:ARG:HG2	2.25	0.50
1:D:186:LYS:HE2	1:D:207:SER:HB3	1.92	0.50
5:D:1277:MES:H52	5:E:1100:MES:O1S	2.12	0.49
2:E:91:LYS:HE2	4:E:1102[A]:GOL:H12	1.94	0.49
1:D:30:ASP:OD1	4:D:1279:GOL:H12	2.13	0.48
1:A:255:GLN:H	1:A:255:GLN:NE2	2.11	0.48
1:A:44:ARG:NH1	1:A:44:ARG:CG	2.51	0.48
1:D:155[B]:GLN:NE2	3:F:5:PRO:HD2	2.29	0.48
3:C:3[B]:LYS:HE2	3:C:5:PRO:O	2.12	0.48
1:A:176:LYS:HD3	1:D:110:LEU:HD12	1.96	0.48
1:A:255:GLN:H	1:A:255:GLN:CD	2.17	0.47
1:D:230:LEU:HD11	1:D:243:LYS:HE3	1.96	0.47
2:E:58:LYS:HG3	4:E:1101:GOL:H31	1.97	0.47
1:A:167:TRP:CZ3	1:A:170[B]:ARG:HD3	2.50	0.46
2:E:58:LYS:HA	4:E:1101:GOL:H12	1.98	0.46
1:D:201:LEU:HD22	1:D:249:VAL:HG21	1.98	0.46
1:D:6:ARG:HH11	4:D:1279:GOL:C3	2.28	0.45
1:D:253:GLN:NE2	1:D:256:ARG:HH11	2.14	0.45
1:A:258:THR:OG1	1:A:260[A]:HIS:HE1	2.00	0.45
2:B:59:ASP:O	2:B:60:TRP:HB2	2.17	0.45
6:A:2175:HOH:O	2:B:58:LYS:HE2	2.17	0.44
2:B:90:PRO:HG2	6:B:2073:HOH:O	2.17	0.44
1:D:204:TRP:HZ3	4:D:1278:GOL:H31	1.80	0.44
1:A:263:HIS:N	5:A:1277:MES:H81	2.32	0.44
2:E:95:TRP:CE2	2:E:97:ARG:HA	2.53	0.44
1:A:55:GLU:HG2	1:A:59:TYR:CD1	2.53	0.44
2:E:25:CYS:HB2	2:E:39:LEU:HD21	2.00	0.44
1:A:44:ARG:HD2	1:A:64:THR:HG21	2.00	0.44
1:D:129:ASP:O	1:D:131:ARG:HG2	2.18	0.43
1:A:48[B]:ARG:HA	1:A:48[B]:ARG:HD3	1.77	0.43
1:D:255:GLN:O	1:D:255:GLN:HG2	2.18	0.43
1:D:74:HIS:CE1	1:D:97:ARG:HH11	2.37	0.43
1:A:275[A]:GLU:OE2	1:A:275[A]:GLU:HA	2.19	0.42
2:B:36:GLU:HB2	2:B:83:ASN:HB3	2.00	0.42
1:D:66:LYS:HZ1	3:F:1:ILE:HG23	1.82	0.42
1:A:44:ARG:HD3	6:A:2032:HOH:O	2.20	0.42
1:A:20:PRO:HG2	1:A:75:ARG:HG3	2.01	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131[B]:ARG:NE	1:D:221:GLY:HA3	2.35	0.42
1:A:253:GLN:HE21	1:A:256:ARG:HD3	1.84	0.42
2:B:0:MET:HE3	2:B:0:MET:HB2	1.87	0.42
1:A:5:MET:HB2	1:A:168:LEU:HD13	2.02	0.42
1:A:262:GLN:HA	5:A:1277:MES:O3S	2.20	0.41
1:D:189:MET:CE	1:D:274:TRP:HB2	2.50	0.41
6:D:2096:HOH:O	5:E:1100:MES:H31	2.19	0.41
1:A:263:HIS:HA	5:A:1277:MES:H21	2.02	0.41
2:E:98:ASP:HB2	2:E:99:MET:HG3	2.03	0.41
1:D:49:ALA:O	1:D:52:ILE:HG22	2.21	0.41
2:E:59:ASP:O	2:E:60:TRP:HB2	2.21	0.41
1:D:156:LEU:CD2	3:F:3:LYS:HE2	2.50	0.41
1:D:70:HIS:CE1	3:F:6:VAL:CG2	3.04	0.40
1:D:167:TRP:CE2	3:F:1:ILE:HD12	2.56	0.40
1:A:123:TYR:CZ	1:A:140:ALA:HA	2.57	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	289/275 (105%)	284 (98%)	5 (2%)	0	100	100
1	D	276/275 (100%)	269 (98%)	7 (2%)	0	100	100
2	B	101/100 (101%)	99 (98%)	2 (2%)	0	100	100
2	E	99/100 (99%)	95 (96%)	3 (3%)	1 (1%)	15	11
3	C	8/9 (89%)	7 (88%)	1 (12%)	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	780/768 (102%)	761 (98%)	18 (2%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	98	ASP

### 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	248/231 (107%)	242 (98%)	6 (2%)	49	53
1	D	234/231 (101%)	227 (97%)	7 (3%)	41	44
2	B	98/95 (103%)	92 (94%)	6 (6%)	18	16
2	E	97/95 (102%)	93 (96%)	4 (4%)	30	31
3	C	9/8 (112%)	9 (100%)	0	100	100
3	F	8/8 (100%)	8 (100%)	0	100	100
All	All	694/668 (104%)	671 (97%)	23 (3%)	43	40

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35[A]	ARG
1	A	35[B]	ARG
1	A	44	ARG
1	A	181	ARG
1	A	255	GLN
1	A	273	ARG
2	B	34[A]	ASP
2	B	34[B]	ASP
2	B	70	PHE
2	B	81[A]	ARG
2	B	81[B]	ARG
2	B	97	ARG
1	D	35	ARG
1	D	44	ARG
1	D	86	ASN
1	D	115	GLN
1	D	131	ARG
1	D	226	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	273	ARG
2	E	34[A]	ASP
2	E	34[B]	ASP
2	E	70	PHE
2	E	97	ARG

Sometimes 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	197	HIS
1	A	253	GLN
2	B	42	ASN
1	D	74	HIS
1	D	86	ASN
1	D	93	HIS
1	D	96	GLN
1	D	197	HIS
1	D	224	GLN
1	D	253	GLN
2	E	42	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

15 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	E	1102[A]	-	5,5,5	0.40	0	5,5,5	0.19	0
5	MES	B	1100	-	12,12,12	2.10	1 (8%)	14,16,16	7.57	9 (64%)
5	MES	D	1277	-	12,12,12	2.16	1 (8%)	14,16,16	7.83	10 (71%)
5	MES	E	1100	-	12,12,12	2.13	1 (8%)	14,16,16	7.69	8 (57%)
4	GOL	E	1101	-	5,5,5	0.40	0	5,5,5	0.15	0
4	GOL	D	1279	-	5,5,5	0.34	0	5,5,5	0.34	0
4	GOL	E	1102[B]	-	5,5,5	0.51	0	5,5,5	0.15	0
5	MES	A	1277	-	12,12,12	2.26	1 (8%)	14,16,16	7.71	10 (71%)
4	GOL	B	1101	-	5,5,5	0.36	0	5,5,5	0.28	0
4	GOL	D	1278	-	5,5,5	0.39	0	5,5,5	0.16	0
4	GOL	A	1279	-	5,5,5	0.40	0	5,5,5	0.23	0
5	MES	D	1276	-	12,12,12	2.21	1 (8%)	14,16,16	7.63	9 (64%)
4	GOL	A	1276	-	5,5,5	0.36	0	5,5,5	0.17	0
4	GOL	D	1280	-	5,5,5	0.36	0	5,5,5	0.26	0
4	GOL	A	1278	-	5,5,5	0.35	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	E	1102[A]	-	-	2/4/4/4	-
5	MES	B	1100	-	-	4/6/14/14	0/1/1/1
5	MES	D	1277	-	-	4/6/14/14	0/1/1/1
5	MES	E	1100	-	-	1/6/14/14	0/1/1/1
4	GOL	E	1101	-	-	1/4/4/4	-
4	GOL	D	1279	-	-	3/4/4/4	-
4	GOL	E	1102[B]	-	-	2/4/4/4	-
5	MES	A	1277	-	-	5/6/14/14	0/1/1/1
4	GOL	B	1101	-	-	2/4/4/4	-
4	GOL	D	1278	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	1279	-	-	0/4/4/4	-
5	MES	D	1276	-	-	1/6/14/14	0/1/1/1
4	GOL	A	1276	-	-	2/4/4/4	-
4	GOL	D	1280	-	-	2/4/4/4	-
4	GOL	A	1278	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1277	MES	C8-S	-7.38	1.67	1.77
5	D	1276	MES	C8-S	-7.24	1.67	1.77
5	D	1277	MES	C8-S	-7.07	1.67	1.77
5	E	1100	MES	C8-S	-6.99	1.67	1.77
5	B	1100	MES	C8-S	-6.87	1.67	1.77

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1277	MES	O1S-S-C8	-18.06	85.17	106.92
5	D	1276	MES	O1S-S-C8	-17.70	85.60	106.92
5	D	1277	MES	O2S-S-C8	-17.57	85.76	106.92
5	E	1100	MES	O2S-S-C8	-17.56	85.77	106.92
5	A	1277	MES	O2S-S-C8	-17.52	85.82	106.92
5	B	1100	MES	O1S-S-C8	-17.22	86.18	106.92
5	E	1100	MES	O1S-S-C8	-17.13	86.28	106.92
5	B	1100	MES	O2S-S-C8	-16.83	86.64	106.92
5	A	1277	MES	O1S-S-C8	-16.76	86.73	106.92
5	D	1276	MES	O2S-S-C8	-16.72	86.79	106.92
5	A	1277	MES	O3S-S-C8	-12.29	85.89	105.77
5	E	1100	MES	O3S-S-C8	-11.91	86.50	105.77
5	B	1100	MES	O3S-S-C8	-11.72	86.82	105.77
5	D	1276	MES	O3S-S-C8	-11.52	87.14	105.77
5	D	1277	MES	O3S-S-C8	-11.28	87.52	105.77
5	E	1100	MES	C5-N4-C3	6.26	122.93	108.83
5	D	1276	MES	C5-N4-C3	5.14	120.41	108.83
5	B	1100	MES	C5-N4-C3	4.68	119.36	108.83
5	A	1277	MES	C5-N4-C3	4.63	119.26	108.83
5	D	1277	MES	C5-N4-C3	4.32	118.55	108.83
5	D	1277	MES	C7-N4-C5	4.24	122.07	111.23
5	D	1277	MES	C2-C3-N4	-3.71	104.48	110.10
5	A	1277	MES	C7-N4-C5	3.70	120.69	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1100	MES	C7-N4-C3	3.61	120.48	111.23
5	D	1276	MES	O3S-S-O1S	3.58	120.03	111.27
5	A	1277	MES	O3S-S-O2S	3.50	119.82	111.27
5	B	1100	MES	O3S-S-O1S	3.50	119.81	111.27
5	B	1100	MES	C7-N4-C5	3.49	120.16	111.23
5	A	1277	MES	C6-C5-N4	-3.47	104.83	110.10
5	A	1277	MES	C7-N4-C3	3.44	120.02	111.23
5	E	1100	MES	O3S-S-O2S	3.40	119.58	111.27
5	D	1276	MES	C7-N4-C3	3.38	119.89	111.23
5	D	1277	MES	O3S-S-O1S	3.35	119.46	111.27
5	B	1100	MES	O3S-S-O2S	3.35	119.45	111.27
5	E	1100	MES	O3S-S-O1S	3.34	119.42	111.27
5	D	1276	MES	C7-N4-C5	3.31	119.70	111.23
5	D	1276	MES	O3S-S-O2S	3.30	119.35	111.27
5	E	1100	MES	C7-N4-C5	3.24	119.53	111.23
5	D	1277	MES	C7-N4-C3	3.18	119.36	111.23
5	D	1277	MES	C6-C5-N4	-3.18	105.29	110.10
5	D	1277	MES	O3S-S-O2S	3.14	118.94	111.27
5	D	1276	MES	C6-C5-N4	-2.96	105.61	110.10
5	A	1277	MES	C2-C3-N4	-2.95	105.63	110.10
5	A	1277	MES	O3S-S-O1S	2.92	118.41	111.27
5	B	1100	MES	C6-C5-N4	-2.69	106.02	110.10
5	E	1100	MES	C7-N4-C3	2.46	117.52	111.23

There are no chirality outliers.

All (33) torsion outliers are listed below:

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

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	D	1278	GOL	O1-C1-C2-C3
4	B	1101	GOL	O2-C2-C3-O3
4	D	1278	GOL	O1-C1-C2-O2
4	E	1102[A]	GOL	O2-C2-C3-O3
4	E	1102[B]	GOL	O2-C2-C3-O3
4	A	1278	GOL	O2-C2-C3-O3
4	D	1280	GOL	O2-C2-C3-O3
5	B	1100	MES	C8-C7-N4-C3
5	D	1276	MES	C8-C7-N4-C3
5	D	1277	MES	C8-C7-N4-C3
5	E	1100	MES	C8-C7-N4-C3
4	D	1279	GOL	O2-C2-C3-O3
5	A	1277	MES	C7-C8-S-O2S
5	B	1100	MES	C7-C8-S-O1S
5	D	1277	MES	C7-C8-S-O1S
5	D	1277	MES	C7-C8-S-O2S
5	A	1277	MES	C8-C7-N4-C5
4	E	1101	GOL	O2-C2-C3-O3
4	D	1279	GOL	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1102[A]	GOL	2	0
5	B	1100	MES	1	0
5	D	1277	MES	2	0
5	E	1100	MES	2	0
4	E	1101	GOL	3	0
4	D	1279	GOL	2	0
5	A	1277	MES	4	0
4	D	1278	GOL	2	0
4	A	1276	GOL	2	0
4	A	1278	GOL	3	0

## 5.7 Other polymers [i](#)

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 [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	275/275 (100%)	0.10	9 (3%) 46 53	16, 35, 63, 87	0
1	D	275/275 (100%)	0.35	14 (5%) 28 33	20, 44, 77, 103	0
2	B	100/100 (100%)	-0.04	2 (2%) 65 69	19, 29, 53, 64	0
2	E	100/100 (100%)	0.17	5 (5%) 28 34	24, 37, 73, 96	1 (1%)
3	C	9/9 (100%)	1.75	3 (33%) 0 0	33, 33, 33, 33	0
3	F	9/9 (100%)	2.49	4 (44%) 0 0	33, 33, 33, 33	0
All	All	768/768 (100%)	0.23	37 (4%) 30 36	16, 37, 71, 103	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	5	PRO	6.3
3	F	5	PRO	5.1
3	C	4	GLU	4.8
1	D	86	ASN	4.7
1	D	16	GLY	4.3
3	F	7	HIS	4.2
1	D	194	VAL	4.1
3	F	4	GLU	4.0
3	F	6	VAL	3.5
1	D	17	ARG	3.4
1	D	18	GLY	3.1
2	B	98	ASP	3.1
1	D	76	VAL	2.9
1	D	196	ASP	2.8
1	D	54	GLN	2.7
2	E	73	THR	2.7
1	A	196	ASP	2.7
1	D	222	GLU	2.6
2	E	48	LYS	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	151	HIS	2.5
2	E	23	LEU	2.5
1	A	90	ALA	2.5
1	A	197	HIS	2.5
1	A	54	GLN	2.4
1	D	131	ARG	2.4
2	E	47	GLU	2.4
1	D	176	LYS	2.4
1	A	226[A]	GLN	2.3
1	A	275[A]	GLU	2.3
1	A	86	ASN	2.3
1	A	249	VAL	2.3
3	C	7	HIS	2.3
1	D	89	GLU	2.3
2	E	74	GLU	2.2
1	D	79	GLY	2.0
2	B	23	LEU	2.0
1	D	72	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	E	1102[A]	6/6	0.76	0.26	33,33,33,33	6
4	GOL	E	1102[B]	6/6	0.76	0.26	33,33,33,33	6
4	GOL	D	1280	6/6	0.78	0.40	33,33,33,33	0
4	GOL	E	1101	6/6	0.81	0.38	33,33,33,33	0
4	GOL	B	1101	6/6	0.83	0.25	33,33,33,33	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	1278	6/6	0.84	0.19	33,33,33,33	0
4	GOL	A	1276	6/6	0.85	0.24	33,33,33,33	0
4	GOL	D	1279	6/6	0.85	0.26	33,33,33,33	0
4	GOL	D	1278	6/6	0.88	0.24	33,33,33,33	0
5	MES	E	1100	12/12	0.88	0.39	33,33,33,33	0
5	MES	D	1276	12/12	0.90	0.37	33,33,33,33	0
5	MES	D	1277	12/12	0.90	0.47	33,33,33,33	0
5	MES	A	1277	12/12	0.90	0.45	33,33,33,33	0
5	MES	B	1100	12/12	0.92	0.22	33,33,33,33	0
4	GOL	A	1279	6/6	0.92	0.25	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.