Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 07:23 am GMT

PDB ID	:	4U1M
Title	:	HLA class I micropolymorphisms determine peptide-HLA landscape and dictate differential HIV-1 escape through identical epitopes
Authors	:	Rizkallah, P.J.; Cole, D.K.; Fuller, A.; Sewell, A.K.
Deposited on	:	2014-07-15
Resolution	:	1.18 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

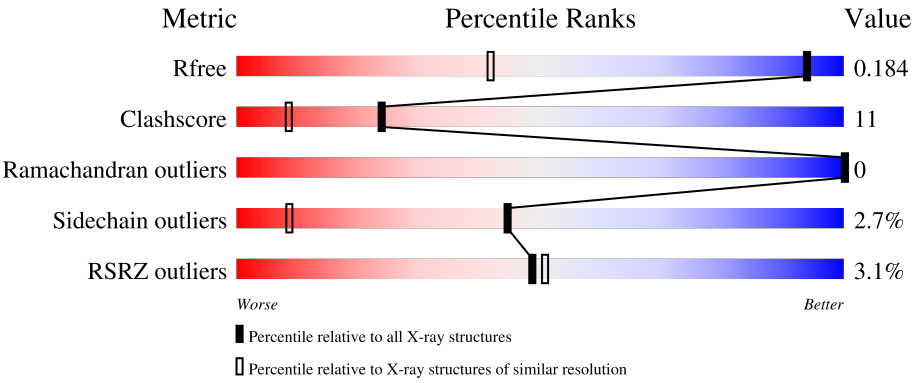
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.18 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	1123 (1.20-1.16)
Clashscore	141614	1182 (1.20-1.16)
Ramachandran outliers	138981	1134 (1.20-1.16)
Sidechain outliers	138945	1134 (1.20-1.16)
RSRZ outliers	127900	1102 (1.20-1.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	277	2% 81% 17%
2	B	100	5% 82% 16%
3	C	9	11% 33% 44% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	309	-	-	X	-
5	GOL	A	319	-	-	X	-
5	GOL	B	310	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3973 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, B-42 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	14	0
			2350	1461	422	460	7			

- 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	3	0
			855	544	142	164	5			

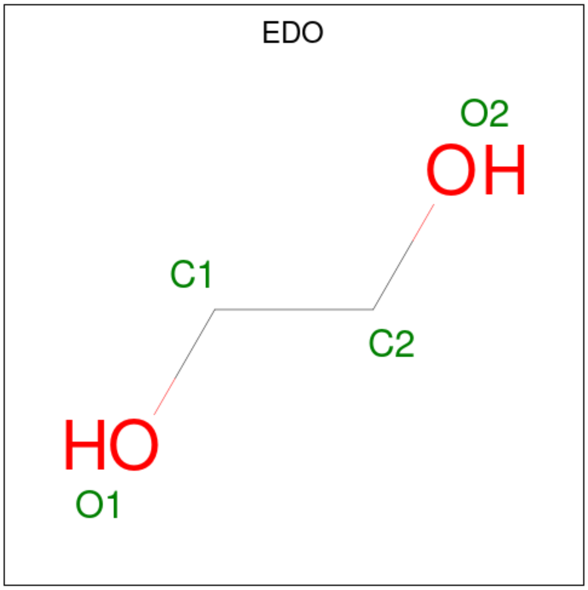
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called Protein Nef.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	1	0
			85	53	17	13	2			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

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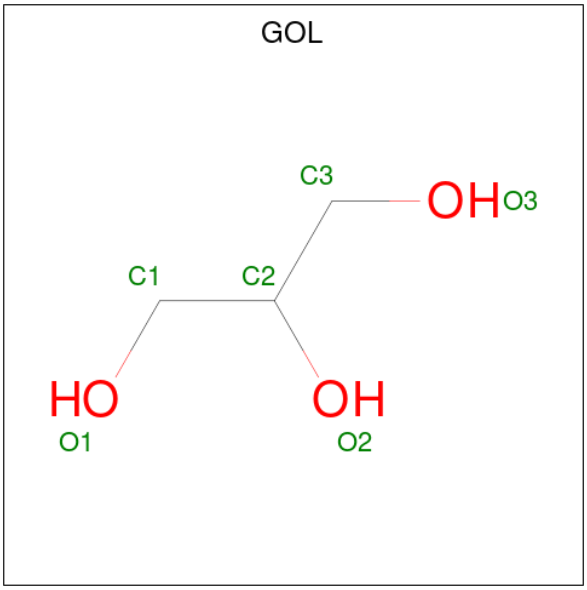
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

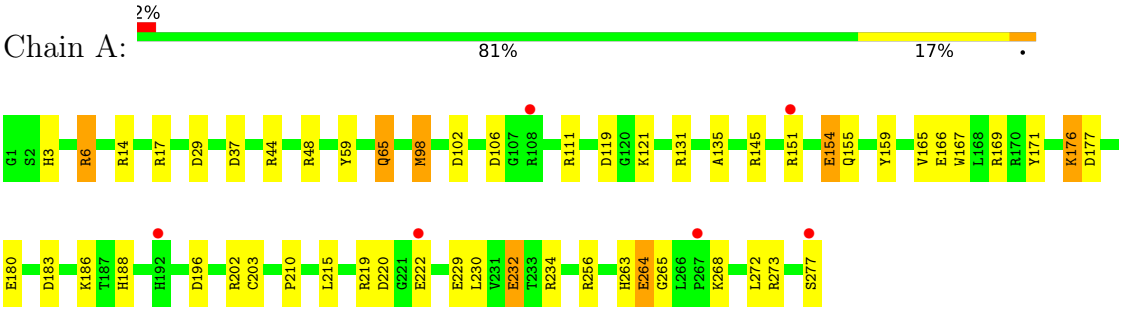
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	407	Total O 407 407	0	0
6	B	134	Total O 134 134	0	0
6	C	14	Total O 14 14	0	0

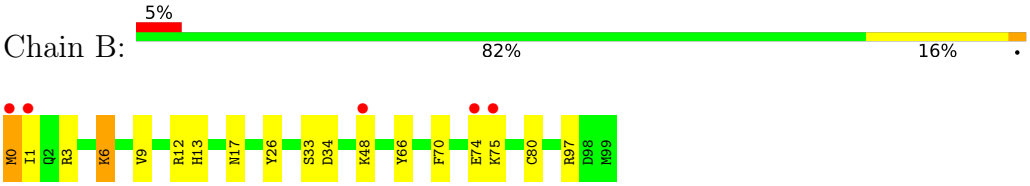
3 Residue-property plots (i)

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

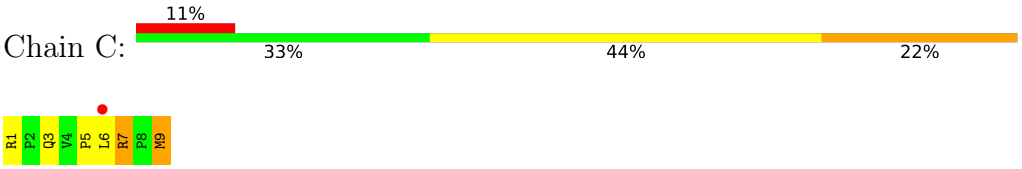
• Molecule 1: HLA class I histocompatibility antigen, B-42 alpha chain



• Molecule 2: Beta-2-microglobulin



• Molecule 3: Protein Nef



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.06Å 81.34Å 110.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.47 – 1.18 55.47 – 1.18	Depositor EDS
% Data completeness (in resolution range)	99.0 (55.47-1.18) 99.0 (55.47-1.18)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 1.18Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.162 , 0.180 0.168 , 0.184	Depositor DCC
R_{free} test set	7561 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	12.5	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3973	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.24	8/2434 (0.3%)	1.26	31/3307 (0.9%)
2	B	1.09	5/884 (0.6%)	1.07	2/1194 (0.2%)
3	C	2.35	5/86 (5.8%)	2.97	9/111 (8.1%)
All	All	1.25	18/3404 (0.5%)	1.28	42/4612 (0.9%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	33	SER	CB-OG	-8.20	1.31	1.42
3	C	9[A]	MET	CG-SD	-8.03	1.60	1.81
3	C	9[B]	MET	CG-SD	-8.03	1.60	1.81
3	C	9[A]	MET	CB-CG	7.57	1.75	1.51
3	C	9[B]	MET	CB-CG	7.57	1.75	1.51
2	B	26	TYR	CE2-CZ	-7.01	1.29	1.38
1	A	232[A]	GLU	CD-OE2	-6.30	1.18	1.25
1	A	232[B]	GLU	CD-OE2	-6.30	1.18	1.25
3	C	7	ARG	CZ-NH1	6.09	1.41	1.33
2	B	26	TYR	CE1-CZ	-5.79	1.31	1.38
1	A	65	GLN	CD-OE1	5.75	1.36	1.24
1	A	159	TYR	CE1-CZ	-5.73	1.31	1.38
1	A	65	GLN	CG-CD	5.51	1.63	1.51
2	B	34	ASP	CB-CG	5.50	1.63	1.51
2	B	66	TYR	CE1-CZ	-5.20	1.31	1.38
1	A	6	ARG	CB-CG	-5.15	1.38	1.52
1	A	234	ARG	CZ-NH2	5.05	1.39	1.33
1	A	203	CYS	CB-SG	-5.04	1.73	1.81

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	7	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	A	219	ARG	NE-CZ-NH2	10.48	125.54	120.30
3	C	9[A]	MET	CG-SD-CE	-10.10	84.03	100.20
3	C	9[B]	MET	CG-SD-CE	-10.10	84.03	100.20
3	C	7	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	A	111	ARG	NE-CZ-NH1	-9.86	115.37	120.30
1	A	131	ARG	NE-CZ-NH2	9.27	124.94	120.30
1	A	44	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	A	202	ARG	NE-CZ-NH2	8.90	124.75	120.30
1	A	177	ASP	CB-CG-OD1	8.87	126.28	118.30
3	C	9[A]	MET	CB-CG-SD	-8.82	85.93	112.40
3	C	9[B]	MET	CB-CG-SD	-8.82	85.93	112.40
3	C	7	ARG	CG-CD-NE	8.42	129.47	111.80
3	C	9[A]	MET	CA-CB-CG	8.35	127.50	113.30
3	C	9[B]	MET	CA-CB-CG	8.35	127.50	113.30
1	A	37	ASP	CB-CG-OD1	7.93	125.44	118.30
1	A	220	ASP	CB-CG-OD1	7.88	125.39	118.30
1	A	44	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	145	ARG	CG-CD-NE	7.42	127.38	111.80
1	A	48	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	234	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	234	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	17	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	196	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	264[A]	GLU	CB-CA-C	-6.26	97.89	110.40
1	A	264[B]	GLU	CB-CA-C	-6.26	97.89	110.40
2	B	6	LYS	CD-CE-NZ	6.12	125.78	111.70
1	A	14	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	171	TYR	CB-CG-CD1	5.93	124.56	121.00
1	A	154	GLU	OE1-CD-OE2	5.88	130.36	123.30
1	A	256	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	102	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	37	ASP	CB-CG-OD2	-5.46	113.39	118.30
2	B	34	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	48	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	106	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	176	LYS	CA-CB-CG	5.34	125.14	113.40
1	A	131	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	A	183	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	A	215	LEU	CB-CA-C	-5.20	100.32	110.20
1	A	98[A]	MET	CG-SD-CE	5.14	108.42	100.20
1	A	98[B]	MET	CG-SD-CE	5.14	108.42	100.20

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	2350	0	2200	44	0
2	B	855	0	818	22	0
3	C	85	0	95	10	0
4	A	68	0	102	17	0
4	B	32	0	48	3	0
4	C	4	0	6	2	0
5	A	12	0	16	5	0
5	B	12	0	16	5	0
6	A	407	0	0	24	1
6	B	134	0	0	2	0
6	C	14	0	0	1	0
All	All	3973	0	3301	75	1

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 11.

All (75) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9[A]:MET:CG	3:C:9[A]:MET:CB	1.75	1.58
3:C:9[A]:MET:CB	3:C:9[A]:MET:SD	2.29	1.21
1:A:98[B]:MET:CE	6:A:688:HOH:O	2.13	0.97
1:A:121:LYS:HE2	6:A:700:HOH:O	1.68	0.94
1:A:98[B]:MET:HE3	6:A:688:HOH:O	1.71	0.89
3:C:9[A]:MET:SD	3:C:9[A]:MET:HB3	2.11	0.87
1:A:180:GLU:CG	6:A:415:HOH:O	2.24	0.86
1:A:119:ASP:HB3	2:B:0:MET:HB3	1.58	0.83
2:B:12:ARG:HH11	5:B:310:GOL:H12	1.51	0.76
1:A:180:GLU:CD	6:A:415:HOH:O	2.25	0.74
1:A:180:GLU:HG2	6:A:415:HOH:O	1.84	0.72
1:A:3:HIS:HD2	1:A:29:ASP:OD2	1.72	0.72
1:A:188:HIS:HD2	6:A:598:HOH:O	1.73	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232[A]:GLU:HG3	6:A:698:HOH:O	1.92	0.69
1:A:263:HIS:CD2	1:A:265:GLY:H	2.09	0.69
1:A:165:VAL:HG12	1:A:169:ARG:NH1	2.08	0.69
1:A:263:HIS:HD2	1:A:265:GLY:H	1.41	0.69
1:A:232[A]:GLU:OE2	2:B:6:LYS:HD2	1.93	0.68
1:A:98[B]:MET:HE2	6:A:688:HOH:O	1.83	0.66
1:A:232[A]:GLU:CG	6:A:698:HOH:O	2.43	0.65
1:A:232[A]:GLU:CD	2:B:6:LYS:HZ2	2.02	0.61
2:B:1:ILE:HD13	2:B:3:ARG:HE	1.64	0.61
1:A:59:TYR:HA	4:A:307:EDO:H11	1.82	0.59
1:A:151:ARG:HA	4:A:309:EDO:H22	1.83	0.59
1:A:135:ALA:HB3	4:A:313:EDO:H12	1.85	0.58
1:A:232[A]:GLU:OE2	2:B:6:LYS:NZ	2.37	0.57
1:A:121:LYS:CE	6:A:700:HOH:O	2.41	0.57
1:A:222:GLU:HG3	6:A:737:HOH:O	2.04	0.56
5:A:319:GOL:C3	3:C:6:LEU:HD12	2.36	0.56
2:B:6:LYS:NZ	6:B:402:HOH:O	2.33	0.56
5:A:319:GOL:H31	3:C:6:LEU:HD12	1.90	0.54
2:B:9:VAL:HG22	2:B:80[B]:CYS:SG	2.50	0.52
1:A:155:GLN:NE2	6:A:402:HOH:O	2.31	0.52
5:A:319:GOL:H31	4:C:101:EDO:O2	2.10	0.52
1:A:166:GLU:OE1	4:A:305:EDO:O1	2.23	0.51
1:A:273:ARG:O	4:A:316:EDO:H11	2.12	0.50
1:A:272:LEU:HD23	4:A:316:EDO:H12	1.94	0.50
1:A:165:VAL:CG1	1:A:169:ARG:NH1	2.74	0.50
1:A:232[A]:GLU:OE2	2:B:6:LYS:CE	2.59	0.50
1:A:229:GLU:HB2	4:A:306:EDO:H21	1.94	0.49
4:A:309:EDO:C2	6:A:586:HOH:O	2.60	0.49
4:A:309:EDO:H22	6:A:586:HOH:O	2.12	0.49
1:A:232[A]:GLU:OE2	2:B:6:LYS:CD	2.59	0.48
1:A:3:HIS:HE1	6:A:415:HOH:O	1.94	0.48
1:A:186:LYS:HD2	6:A:418:HOH:O	2.14	0.48
2:B:13:HIS:NE2	5:B:310:GOL:H11	2.29	0.47
4:A:311:EDO:H12	3:C:5:PRO:HB2	1.97	0.47
6:A:757:HOH:O	2:B:0:MET:CE	2.62	0.47
1:A:176:LYS:HG2	6:A:637:HOH:O	2.13	0.47
2:B:17:ASN:ND2	2:B:97:ARG:HH12	2.13	0.47
2:B:12:ARG:HH11	5:B:310:GOL:C1	2.25	0.47
1:A:119:ASP:O	2:B:1:ILE:HG13	2.15	0.47
1:A:176:LYS:HE3	6:A:433:HOH:O	2.15	0.46
5:A:319:GOL:O3	4:C:101:EDO:C2	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLU:HG3	4:A:309:EDO:O2	2.16	0.46
1:A:230[B]:LEU:HD21	6:A:452:HOH:O	2.16	0.46
2:B:1:ILE:HD13	2:B:3:ARG:NE	2.31	0.45
3:C:3:GLN:NE2	6:C:201:HOH:O	2.39	0.45
2:B:1:ILE:CD1	2:B:3:ARG:HE	2.29	0.45
4:A:307:EDO:C2	3:C:1:ARG:HH22	2.29	0.45
1:A:264[B]:GLU:OE2	5:A:318:GOL:H31	2.16	0.44
1:A:188:HIS:HE1	6:A:747:HOH:O	2.01	0.44
2:B:17:ASN:HB3	4:B:305:EDO:H12	2.00	0.44
1:A:6:ARG:HD2	1:A:98[A]:MET:SD	2.57	0.43
1:A:229:GLU:CB	4:A:306:EDO:H21	2.48	0.43
4:A:307:EDO:H22	3:C:1:ARG:HH22	1.84	0.42
1:A:210:PRO:O	1:A:263:HIS:HE1	2.01	0.42
4:A:309:EDO:H12	6:A:603:HOH:O	2.19	0.42
4:B:308:EDO:O2	6:B:401:HOH:O	2.22	0.42
2:B:12:ARG:CD	5:B:310:GOL:H12	2.50	0.42
2:B:12:ARG:HD2	5:B:310:GOL:H12	2.02	0.41
2:B:17:ASN:HB3	4:B:305:EDO:C1	2.50	0.41
6:A:757:HOH:O	2:B:0:MET:HE3	2.20	0.41
1:A:167:TRP:HE1	4:A:305:EDO:H12	1.86	0.41
4:A:315:EDO:H11	3:C:9[A]:MET:HG2	2.02	0.41

All (1) 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)
6:A:474:HOH:O	6:A:503:HOH:O[3_554]	0.75	1.45

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	289/277 (104%)	283 (98%)	6 (2%)	0	100 100
2	B	101/100 (101%)	100 (99%)	1 (1%)	0	100 100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100 100
All	All	397/386 (103%)	389 (98%)	8 (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	249/235 (106%)	246 (99%)	3 (1%)	71 36
2	B	98/95 (103%)	93 (95%)	5 (5%)	24 2
3	C	10/9 (111%)	9 (90%)	1 (10%)	7 0
All	All	357/339 (105%)	348 (98%)	9 (2%)	44 10

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	268	LYS
1	A	277	SER
2	B	0	MET
2	B	48	LYS
2	B	70	PHE
2	B	74	GLU
2	B	75	LYS
3	C	7	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	3	HIS

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Mol	Chain	Res	Type
1	A	65	GLN
1	A	174	ASN
1	A	188	HIS
1	A	192	HIS
1	A	224	GLN
1	A	255	GLN
1	A	263	HIS
2	B	17	ASN
2	B	24	ASN
2	B	89	GLN
3	C	3	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

30 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	EDO	A	317	-	3,3,3	0.86	0	2,2,2	0.81	0
4	EDO	A	301	-	3,3,3	0.88	0	2,2,2	1.85	1 (50%)
4	EDO	A	303	-	3,3,3	0.71	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GOL	A	319	-	5,5,5	0.94	0	5,5,5	0.97	0
4	EDO	A	307	-	3,3,3	0.39	0	2,2,2	0.76	0
4	EDO	A	316	-	3,3,3	0.46	0	2,2,2	0.39	0
5	GOL	A	318	-	5,5,5	1.19	1 (20%)	5,5,5	0.81	0
4	EDO	A	313	-	3,3,3	0.66	0	2,2,2	1.05	0
4	EDO	A	304	-	3,3,3	0.38	0	2,2,2	0.69	0
4	EDO	A	309	-	3,3,3	1.05	0	2,2,2	2.28	1 (50%)
4	EDO	A	306	-	3,3,3	0.42	0	2,2,2	0.55	0
4	EDO	A	314	-	3,3,3	0.59	0	2,2,2	0.21	0
4	EDO	B	301	-	3,3,3	0.24	0	2,2,2	0.50	0
4	EDO	A	305	-	3,3,3	0.39	0	2,2,2	0.60	0
5	GOL	B	309	-	5,5,5	0.43	0	5,5,5	1.29	0
4	EDO	A	315	-	3,3,3	0.94	0	2,2,2	0.38	0
4	EDO	B	305	-	3,3,3	0.73	0	2,2,2	0.40	0
4	EDO	B	304	-	3,3,3	0.53	0	2,2,2	0.31	0
4	EDO	B	303	-	3,3,3	0.44	0	2,2,2	1.17	0
4	EDO	A	302	-	3,3,3	0.53	0	2,2,2	0.27	0
4	EDO	B	306	-	3,3,3	0.79	0	2,2,2	0.59	0
4	EDO	B	302	-	3,3,3	0.42	0	2,2,2	0.40	0
5	GOL	B	310	-	5,5,5	1.23	0	5,5,5	3.45	2 (40%)
4	EDO	A	312	-	3,3,3	0.40	0	2,2,2	0.62	0
4	EDO	B	307	-	3,3,3	0.88	0	2,2,2	0.77	0
4	EDO	A	308	-	3,3,3	0.31	0	2,2,2	0.81	0
4	EDO	A	310	-	3,3,3	1.17	0	2,2,2	1.15	0
4	EDO	C	101	-	3,3,3	0.59	0	2,2,2	2.30	1 (50%)
4	EDO	B	308	-	3,3,3	0.41	0	2,2,2	0.33	0
4	EDO	A	311	-	3,3,3	0.66	0	2,2,2	0.18	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	EDO	A	317	-	-	1/1/1/1	-
4	EDO	A	301	-	-	0/1/1/1	-
4	EDO	A	303	-	-	0/1/1/1	-
5	GOL	A	319	-	-	2/4/4/4	-
4	EDO	A	307	-	-	1/1/1/1	-
4	EDO	A	316	-	-	1/1/1/1	-
5	GOL	A	318	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	313	-	-	1/1/1/1	-
4	EDO	A	304	-	-	0/1/1/1	-
4	EDO	A	309	-	-	0/1/1/1	-
4	EDO	A	306	-	-	0/1/1/1	-
4	EDO	A	314	-	-	0/1/1/1	-
4	EDO	B	301	-	-	0/1/1/1	-
4	EDO	A	305	-	-	1/1/1/1	-
5	GOL	B	309	-	-	2/4/4/4	-
4	EDO	A	315	-	-	0/1/1/1	-
4	EDO	B	305	-	-	1/1/1/1	-
4	EDO	B	304	-	-	1/1/1/1	-
4	EDO	B	303	-	-	1/1/1/1	-
4	EDO	A	302	-	-	0/1/1/1	-
4	EDO	B	306	-	-	1/1/1/1	-
4	EDO	B	302	-	-	1/1/1/1	-
5	GOL	B	310	-	-	3/4/4/4	-
4	EDO	A	312	-	-	1/1/1/1	-
4	EDO	B	307	-	-	0/1/1/1	-
4	EDO	A	308	-	-	0/1/1/1	-
4	EDO	A	310	-	-	0/1/1/1	-
4	EDO	C	101	-	-	1/1/1/1	-
4	EDO	B	308	-	-	1/1/1/1	-
4	EDO	A	311	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	318	GOL	O1-C1	2.17	1.51	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	310	GOL	O3-C3-C2	6.57	141.68	110.20
5	B	310	GOL	C3-C2-C1	3.75	126.28	111.70
4	C	101	EDO	O1-C1-C2	-3.25	88.52	111.91
4	A	309	EDO	O2-C2-C1	2.92	132.93	111.91
4	A	301	EDO	O2-C2-C1	2.61	130.66	111.91

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	318	GOL	O1-C1-C2-C3
5	A	319	GOL	C1-C2-C3-O3
5	B	309	GOL	O1-C1-C2-C3
5	B	310	GOL	C1-C2-C3-O3
5	B	310	GOL	O2-C2-C3-O3
5	B	309	GOL	O1-C1-C2-O2
4	A	305	EDO	O1-C1-C2-O2
4	A	307	EDO	O1-C1-C2-O2
4	A	311	EDO	O1-C1-C2-O2
4	A	313	EDO	O1-C1-C2-O2
4	A	316	EDO	O1-C1-C2-O2
4	A	317	EDO	O1-C1-C2-O2
4	B	303	EDO	O1-C1-C2-O2
4	B	305	EDO	O1-C1-C2-O2
4	C	101	EDO	O1-C1-C2-O2
4	B	302	EDO	O1-C1-C2-O2
5	B	310	GOL	O1-C1-C2-O2
4	A	312	EDO	O1-C1-C2-O2
4	B	304	EDO	O1-C1-C2-O2
4	B	306	EDO	O1-C1-C2-O2
5	A	318	GOL	O1-C1-C2-O2
4	B	308	EDO	O1-C1-C2-O2
5	A	319	GOL	O2-C2-C3-O3

There are no ring outliers.

14 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	319	GOL	4	0
4	A	307	EDO	3	0
4	A	316	EDO	2	0
5	A	318	GOL	1	0
4	A	313	EDO	1	0
4	A	309	EDO	5	0
4	A	306	EDO	2	0
4	A	305	EDO	2	0
4	A	315	EDO	1	0
4	B	305	EDO	2	0
5	B	310	GOL	5	0
4	C	101	EDO	2	0
4	B	308	EDO	1	0
4	A	311	EDO	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	277/277 (100%)	0.62	6 (2%) 62 62	7, 13, 26, 64	0
2	B	100/100 (100%)	0.67	5 (5%) 28 30	9, 19, 36, 40	0
3	C	9/9 (100%)	0.91	1 (11%) 5 7	9, 15, 20, 24	0
All	All	386/386 (100%)	0.64	12 (3%) 49 51	7, 14, 31, 64	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	ILE	6.6
1	A	277	SER	5.9
2	B	0	MET	5.3
2	B	48	LYS	3.2
1	A	267	PRO	3.1
3	C	6	LEU	3.0
1	A	192	HIS	2.5
2	B	75	LYS	2.3
1	A	222	GLU	2.3
1	A	108	ARG	2.2
1	A	151	ARG	2.1
2	B	74	GLU	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	306	4/4	0.65	0.33	32,35,35,40	0
4	EDO	B	303	4/4	0.69	0.23	34,36,36,41	0
4	EDO	B	305	4/4	0.70	0.26	43,44,51,51	0
4	EDO	A	309	4/4	0.72	0.29	22,27,31,33	0
5	GOL	B	310	6/6	0.75	0.26	15,27,28,35	0
5	GOL	B	309	6/6	0.77	0.25	38,43,44,45	0
4	EDO	A	305	4/4	0.78	0.22	35,43,44,47	0
4	EDO	B	308	4/4	0.79	0.19	41,41,44,46	0
5	GOL	A	318	6/6	0.80	0.21	23,25,31,42	0
5	GOL	A	319	6/6	0.81	0.26	19,22,27,34	0
4	EDO	A	312	4/4	0.81	0.24	44,44,47,49	0
4	EDO	A	317	4/4	0.81	0.16	16,26,26,36	0
4	EDO	A	304	4/4	0.83	0.19	27,32,38,44	0
4	EDO	A	311	4/4	0.86	0.12	31,35,39,40	0
4	EDO	C	101	4/4	0.86	0.26	27,28,34,38	0
4	EDO	A	303	4/4	0.87	0.19	17,20,21,21	0
4	EDO	A	301	4/4	0.88	0.18	16,16,22,32	0
4	EDO	A	313	4/4	0.88	0.23	27,33,34,38	0
4	EDO	A	307	4/4	0.88	0.21	31,35,38,41	0
4	EDO	B	302	4/4	0.88	0.21	34,40,40,44	0
4	EDO	A	316	4/4	0.89	0.20	21,32,33,41	0
4	EDO	B	304	4/4	0.90	0.29	26,27,30,38	0
4	EDO	A	308	4/4	0.90	0.19	18,21,23,36	0
4	EDO	A	310	4/4	0.91	0.17	14,17,23,26	0
4	EDO	A	314	4/4	0.92	0.22	25,25,25,26	0
4	EDO	A	315	4/4	0.94	0.11	11,12,15,21	0
4	EDO	B	306	4/4	0.94	0.19	17,25,27,32	0
4	EDO	B	301	4/4	0.95	0.09	15,16,18,21	0
4	EDO	B	307	4/4	0.95	0.10	16,21,21,23	0
4	EDO	A	302	4/4	0.96	0.09	17,17,19,20	0

6.5 Other polymers (i)

There are no such residues in this entry.