Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 09:56 PM JST

PDB ID	:	7WT5
Title	:	Crystal structure of HLA-A*2450 complexed with 8-mer model peptide
Authors	:	Asa, M.; Morita, D.; Sugita, M.
Deposited on	:	2022-02-03
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

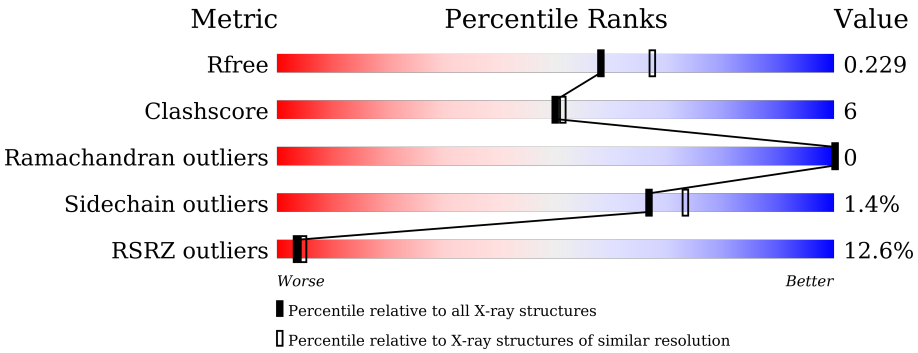
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 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 >=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% 92% 7%
1	D	277	16% 77% 11% 12%
2	B	100	92% 8%
2	E	100	40% 79% 16%
3	C	8	12% 75% 25%
3	F	8	12% 75% 25%

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
6	EDO	A	326	-	-	X	-
6	EDO	D	312	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6687 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	11	0
			2352	1463	436	443	10			
1	D	243	Total	C	N	O	S	0	4	0
			2005	1256	366	374	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	3	0
			849	541	144	161	3			
2	E	97	Total	C	N	O	S	0	0	0
			811	517	137	155	2			

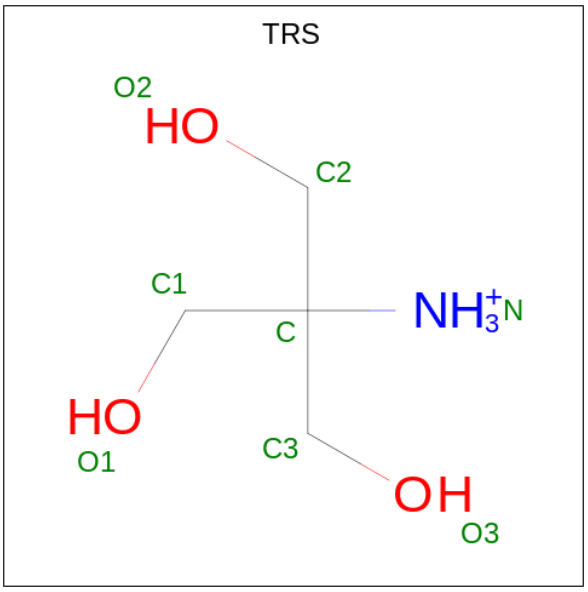
- Molecule 3 is a protein called 8-mer model peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			63	41	12	10			
3	F	8	Total	C	N	O	0	1	0
			71	49	12	10			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

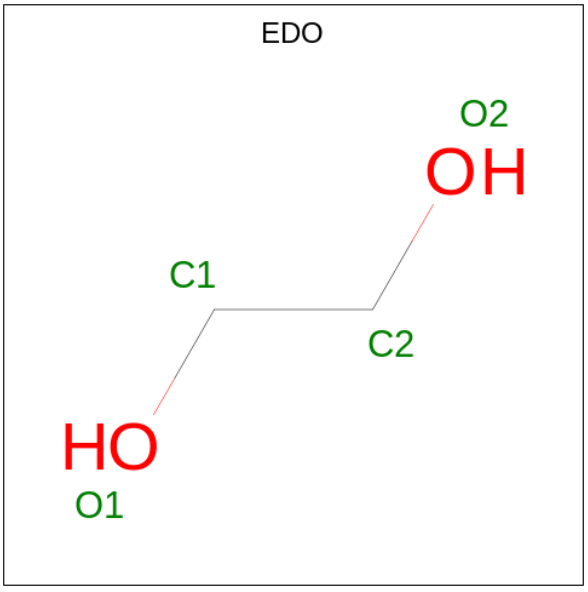
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	D	2	Total	Zn	0	0
			2	2		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 8 4 1 3	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

- Molecule 7 is water.

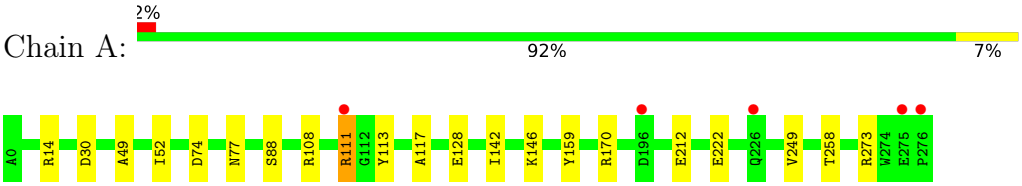
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	180	Total O 182 182	0	2
7	B	48	Total O 48 48	0	0
7	C	6	Total O 6 6	0	0
7	D	88	Total O 89 89	0	1
7	E	11	Total O 11 11	0	0
7	F	1	Total O 1 1	0	0

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.

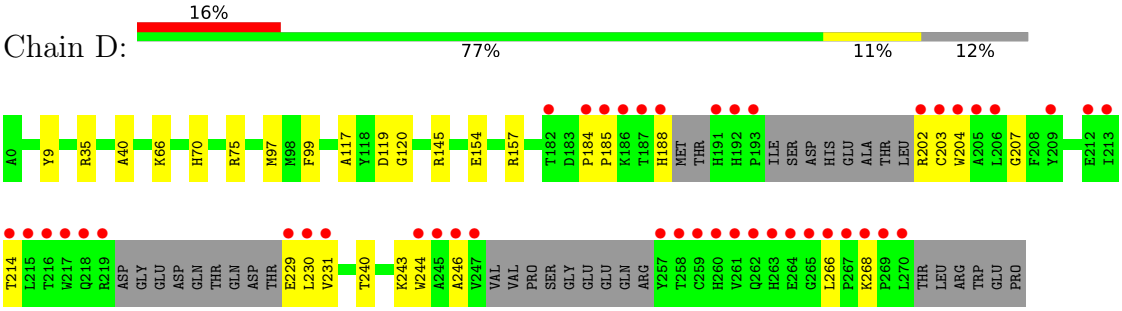
• Molecule 1: MHC class I antigen

Chain A:



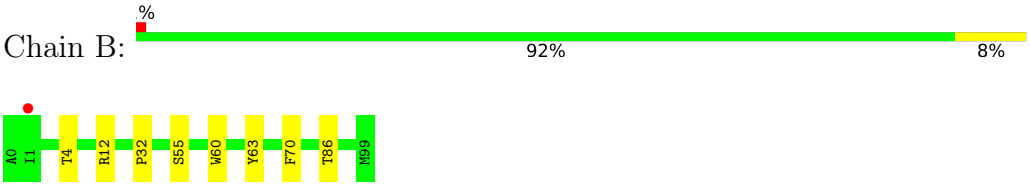
• Molecule 1: MHC class I antigen

Chain D:



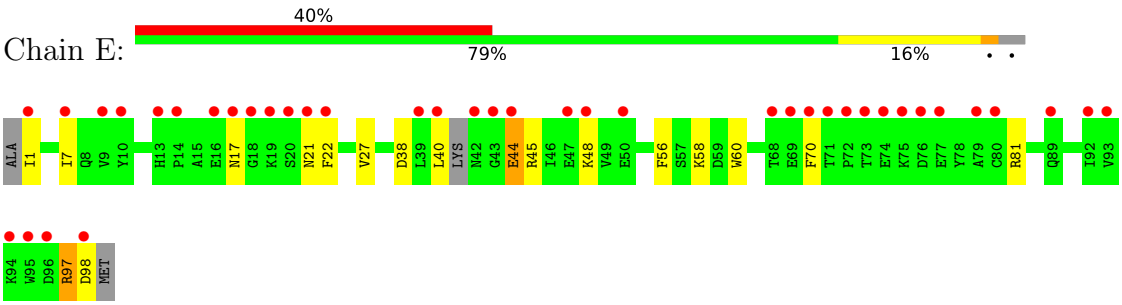
• Molecule 2: Beta-2-microglobulin

Chain B:



• Molecule 2: Beta-2-microglobulin

Chain E:

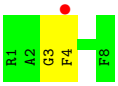


• Molecule 3: 8-mer model peptide

Chain C:

• Molecule 3: 8-mer model peptide

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.24Å 46.46Å 141.65Å 90.00° 104.01° 90.00°	Depositor
Resolution (Å)	45.81 – 2.10 45.81 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.81-2.10) 99.5 (45.81-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.9_1692+SVN	Depositor
R, R_{free}	0.186 , 0.228 0.188 , 0.229	Depositor DCC
R_{free} test set	3225 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.4	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	0.94	EDS
Total number of atoms	6687	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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.*

[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: EDO, ZN, TRS

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	0.50	0/2438	0.59	0/3300
1	D	0.48	0/2064	0.54	0/2789
2	B	0.49	0/881	0.58	0/1192
2	E	0.34	0/833	0.49	0/1128
3	C	0.53	0/64	0.54	0/83
3	F	0.40	0/76	0.39	0/99
All	All	0.47	0/6356	0.56	0/8591

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

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	2352	0	2235	23	0
1	D	2005	0	1887	30	0
2	B	849	0	824	5	0
2	E	811	0	771	20	0
3	C	63	0	61	4	0
3	F	71	0	70	3	0
4	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2	0	0	0	0
5	A	8	0	12	0	0
6	A	100	0	150	13	0
6	B	32	0	48	1	0
6	C	8	0	12	1	0
6	D	40	0	60	8	0
6	E	8	0	12	3	0
7	A	182	0	0	0	0
7	B	48	0	0	1	0
7	C	6	0	0	0	0
7	D	89	0	0	1	0
7	E	11	0	0	2	0
7	F	1	0	0	0	0
All	All	6687	0	6142	72	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 6.

All (72) 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)
1:D:120:GLY:HA3	2:E:1:ILE:HD11	1.52	0.90
1:A:142:ILE:HG23	6:A:321:EDO:H22	1.57	0.86
1:A:170[C]:ARG:HH22	3:C:1:ARG:HE	1.37	0.72
2:E:38:ASP:HB2	2:E:81:ARG:HB3	1.68	0.72
1:D:202:ARG:HG3	1:D:246:ALA:HB2	1.73	0.71
6:D:312:EDO:H22	3:F:4[A]:PHE:HA	1.72	0.70
1:D:154:GLU:HG3	1:D:157:ARG:HH12	1.57	0.68
6:D:312:EDO:H22	3:F:4[B]:PHE:HA	1.76	0.67
1:D:145:ARG:HH11	1:D:145:ARG:HG3	1.60	0.66
1:A:146:LYS:HA	6:A:314:EDO:H11	1.77	0.66
1:D:120:GLY:CA	2:E:1:ILE:HD11	2.24	0.66
1:D:188:HIS:O	1:D:204:TRP:HB2	1.97	0.65
1:A:212:GLU:HG3	6:A:307:EDO:H21	1.78	0.64
1:A:14:ARG:HH21	6:A:320:EDO:H12	1.65	0.61
1:A:14:ARG:NH2	6:A:320:EDO:H12	2.17	0.59
1:D:70:HIS:HB2	6:D:312:EDO:H21	1.83	0.59
1:D:120:GLY:HA3	2:E:1:ILE:CD1	2.31	0.58
1:D:231:VAL:O	1:D:243:LYS:NZ	2.30	0.58
1:D:120:GLY:O	2:E:1:ILE:HG12	2.07	0.55
2:B:12:ARG:HH12	6:B:105:EDO:H21	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:58:LYS:O	6:E:101:EDO:O2	2.21	0.54
1:A:170[C]:ARG:NH2	3:C:1:ARG:HE	2.04	0.53
2:E:40:LEU:HD23	2:E:45:ARG:HA	1.91	0.53
2:B:4[B]:THR:HG22	2:B:86:THR:HB	1.90	0.52
2:E:17:ASN:OD1	2:E:97:ARG:NH2	2.33	0.51
1:D:35:ARG:NE	6:D:304:EDO:O1	2.44	0.51
1:D:203:CYS:O	1:D:244:TRP:HB2	2.11	0.50
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.45	0.50
1:A:170[C]:ARG:HH22	3:C:1:ARG:NE	2.08	0.49
1:A:273[B]:ARG:H	6:A:326:EDO:H11	1.77	0.49
3:C:4:PHE:CD1	6:C:102:EDO:H22	2.49	0.48
1:A:30:ASP:O	6:A:322:EDO:H22	2.14	0.48
1:A:273[A]:ARG:H	6:A:326:EDO:H11	1.77	0.48
2:E:56:PHE:HE1	6:E:101:EDO:H11	1.77	0.48
1:D:70:HIS:CB	6:D:312:EDO:H21	2.44	0.48
1:D:120:GLY:C	2:E:1:ILE:HG12	2.34	0.48
1:D:229:GLU:N	1:D:246:ALA:O	2.48	0.47
1:D:145:ARG:HG3	1:D:145:ARG:NH1	2.28	0.47
1:A:258:THR:HG22	1:A:273[B]:ARG:HG2	1.96	0.47
1:D:185:PRO:HD2	1:D:266:LEU:HD13	1.97	0.47
1:D:119:ASP:O	2:E:1:ILE:HG13	2.14	0.47
1:A:273[A]:ARG:H	6:A:326:EDO:C1	2.27	0.46
1:A:273[B]:ARG:H	6:A:326:EDO:C1	2.28	0.46
2:E:60:TRP:CZ2	6:E:101:EDO:H22	2.51	0.46
1:D:9:TYR:HE1	1:D:99:PHE:CE2	2.33	0.46
1:A:88:SER:HA	6:A:325:EDO:H21	1.98	0.46
1:D:207:GLY:HA2	1:D:240:THR:HB	1.98	0.46
1:A:258:THR:HG22	1:A:273[A]:ARG:HG3	1.99	0.45
1:D:202:ARG:NH2	2:E:98:ASP:O	2.50	0.45
1:A:49:ALA:O	1:A:52:ILE:HG22	2.17	0.45
1:D:75:ARG:HD3	7:D:469:HOH:O	2.17	0.45
1:A:111[B]:ARG:NH1	1:A:128:GLU:HA	2.32	0.45
1:A:222:GLU:OE2	6:A:308:EDO:H11	2.17	0.45
6:D:312:EDO:H11	3:F:3:GLY:O	2.16	0.44
1:A:111[A]:ARG:HD2	1:A:113:TYR:CZ	2.52	0.44
2:B:55[B]:SER:HB2	2:B:63:TYR:CZ	2.53	0.44
1:D:268:LYS:HD3	1:D:268:LYS:HA	1.78	0.44
2:E:7:ILE:HA	7:E:206:HOH:O	2.18	0.43
1:D:230:LEU:HD11	1:D:243:LYS:HE3	2.00	0.43
1:D:66:LYS:O	6:D:312:EDO:H12	2.19	0.43
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:TYR:HA	6:A:323:EDO:H11	2.00	0.42
1:D:184:PRO:HA	1:D:185:PRO:HD3	1.87	0.42
2:E:48:LYS:HB3	2:E:48:LYS:HE2	1.77	0.42
2:E:44:GLU:H	2:E:44:GLU:HG3	1.75	0.41
2:B:32:PRO:HB2	7:B:201:HOH:O	2.19	0.41
1:A:74:ASP:HA	1:A:77:ASN:HB2	2.02	0.41
1:D:40:ALA:CB	6:D:304:EDO:H12	2.50	0.41
1:D:229:GLU:HB3	1:D:246:ALA:HB3	2.03	0.41
2:E:27:VAL:HA	7:E:206:HOH:O	2.19	0.41
1:D:120:GLY:O	2:E:1:ILE:CD1	2.69	0.41
2:E:21:ASN:OD1	2:E:22:PHE:N	2.50	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	288/277 (104%)	283 (98%)	5 (2%)	0	100	100
1	D	237/277 (86%)	231 (98%)	6 (2%)	0	100	100
2	B	101/100 (101%)	100 (99%)	1 (1%)	0	100	100
2	E	93/100 (93%)	90 (97%)	3 (3%)	0	100	100
3	C	6/8 (75%)	6 (100%)	0	0	100	100
3	F	7/8 (88%)	7 (100%)	0	0	100	100
All	All	732/770 (95%)	717 (98%)	15 (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	244/232 (105%)	239 (98%)	5 (2%)	55 60
1	D	204/232 (88%)	202 (99%)	2 (1%)	76 82
2	B	97/94 (103%)	96 (99%)	1 (1%)	76 82
2	E	92/94 (98%)	89 (97%)	3 (3%)	38 40
3	C	5/5 (100%)	5 (100%)	0	100 100
3	F	6/5 (120%)	6 (100%)	0	100 100
All	All	648/662 (98%)	637 (98%)	11 (2%)	67 67

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ARG
1	A	111[A]	ARG
1	A	111[B]	ARG
1	A	111[C]	ARG
1	A	249	VAL
2	B	70	PHE
1	D	97	MET
1	D	214	THR
2	E	44	GLU
2	E	70	PHE
2	E	97	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	188	HIS

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)

Of 51 ligands modelled in this entry, 3 are monoatomic - leaving 48 for Mogul analysis.

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	$\#\|Z\| > 2$
6	EDO	A	326	-	3,3,3	0.49	0	2,2,2	0.25	0
6	EDO	A	305	-	3,3,3	0.47	0	2,2,2	0.45	0
6	EDO	A	325	-	3,3,3	0.48	0	2,2,2	0.37	0
6	EDO	A	311	-	3,3,3	0.43	0	2,2,2	0.48	0
6	EDO	D	303	-	3,3,3	0.51	0	2,2,2	0.51	0
6	EDO	A	309	-	3,3,3	0.51	0	2,2,2	0.28	0
6	EDO	A	312	-	3,3,3	0.46	0	2,2,2	0.41	0
6	EDO	A	313	-	3,3,3	0.62	0	2,2,2	0.34	0
6	EDO	D	306	-	3,3,3	0.59	0	2,2,2	0.14	0
6	EDO	D	309	-	3,3,3	0.53	0	2,2,2	0.32	0
6	EDO	D	310	-	3,3,3	0.47	0	2,2,2	0.29	0
6	EDO	A	318	-	3,3,3	0.49	0	2,2,2	0.26	0
6	EDO	D	308	-	3,3,3	0.51	0	2,2,2	0.24	0
6	EDO	B	104	-	3,3,3	0.51	0	2,2,2	0.25	0
6	EDO	A	316	-	3,3,3	0.49	0	2,2,2	0.23	0
6	EDO	D	305	-	3,3,3	0.45	0	2,2,2	0.36	0
6	EDO	A	306	-	3,3,3	0.47	0	2,2,2	0.31	0
6	EDO	B	107	-	3,3,3	0.50	0	2,2,2	0.38	0
6	EDO	B	103	-	3,3,3	0.45	0	2,2,2	0.33	0
6	EDO	A	324	-	3,3,3	0.52	0	2,2,2	0.31	0
6	EDO	B	101	-	3,3,3	0.56	0	2,2,2	0.29	0
6	EDO	B	105	-	3,3,3	0.50	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	A	323	-	3,3,3	0.50	0	2,2,2	0.25	0
6	EDO	A	317	-	3,3,3	0.44	0	2,2,2	0.42	0
6	EDO	B	102	-	3,3,3	0.56	0	2,2,2	0.03	0
6	EDO	A	319	-	3,3,3	0.61	0	2,2,2	0.27	0
6	EDO	D	307	-	3,3,3	0.51	0	2,2,2	0.26	0
6	EDO	C	101	-	3,3,3	0.51	0	2,2,2	0.49	0
6	EDO	A	314	-	3,3,3	0.48	0	2,2,2	0.26	0
6	EDO	A	320	-	3,3,3	0.54	0	2,2,2	0.16	0
6	EDO	A	304	-	3,3,3	0.44	0	2,2,2	0.48	0
6	EDO	B	108	-	3,3,3	0.47	0	2,2,2	0.35	0
6	EDO	E	101	-	3,3,3	0.44	0	2,2,2	0.35	0
6	EDO	E	102	-	3,3,3	0.46	0	2,2,2	0.44	0
6	EDO	A	315	-	3,3,3	0.53	0	2,2,2	0.05	0
6	EDO	C	102	-	3,3,3	0.51	0	2,2,2	0.15	0
6	EDO	A	321	-	3,3,3	0.49	0	2,2,2	0.48	0
6	EDO	A	327	-	3,3,3	0.52	0	2,2,2	0.21	0
6	EDO	A	308	-	3,3,3	0.52	0	2,2,2	0.36	0
6	EDO	B	106	-	3,3,3	0.47	0	2,2,2	0.44	0
6	EDO	A	303	-	3,3,3	0.51	0	2,2,2	0.35	0
6	EDO	D	304	-	3,3,3	0.41	0	2,2,2	0.28	0
6	EDO	A	322	-	3,3,3	0.46	0	2,2,2	0.22	0
6	EDO	D	312	-	3,3,3	0.47	0	2,2,2	0.24	0
6	EDO	A	310	-	3,3,3	0.48	0	2,2,2	0.53	0
6	EDO	A	307	-	3,3,3	0.36	0	2,2,2	0.68	0
5	TRS	A	302	-	7,7,7	0.31	0	9,9,9	0.51	0
6	EDO	D	311	-	3,3,3	0.30	0	2,2,2	0.65	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
6	EDO	A	326	-	-	0/1/1/1	-
6	EDO	A	305	-	-	1/1/1/1	-
6	EDO	A	325	-	-	0/1/1/1	-
6	EDO	A	311	-	-	1/1/1/1	-
6	EDO	D	303	-	-	1/1/1/1	-
6	EDO	A	309	-	-	0/1/1/1	-
6	EDO	A	312	-	-	0/1/1/1	-
6	EDO	A	313	-	-	1/1/1/1	-
6	EDO	D	306	-	-	0/1/1/1	-
6	EDO	D	309	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	D	310	-	-	0/1/1/1	-
6	EDO	A	318	-	-	1/1/1/1	-
6	EDO	D	308	-	-	1/1/1/1	-
6	EDO	B	104	-	-	1/1/1/1	-
6	EDO	A	316	-	-	0/1/1/1	-
6	EDO	D	305	-	-	0/1/1/1	-
6	EDO	A	306	-	-	0/1/1/1	-
6	EDO	B	107	-	-	0/1/1/1	-
6	EDO	B	103	-	-	0/1/1/1	-
6	EDO	A	324	-	-	1/1/1/1	-
6	EDO	B	101	-	-	0/1/1/1	-
6	EDO	B	105	-	-	1/1/1/1	-
6	EDO	A	323	-	-	1/1/1/1	-
6	EDO	A	317	-	-	0/1/1/1	-
6	EDO	B	102	-	-	0/1/1/1	-
6	EDO	A	319	-	-	0/1/1/1	-
6	EDO	D	307	-	-	0/1/1/1	-
6	EDO	C	101	-	-	0/1/1/1	-
6	EDO	A	314	-	-	0/1/1/1	-
6	EDO	A	320	-	-	0/1/1/1	-
6	EDO	A	304	-	-	0/1/1/1	-
6	EDO	B	108	-	-	0/1/1/1	-
6	EDO	E	101	-	-	0/1/1/1	-
6	EDO	E	102	-	-	0/1/1/1	-
6	EDO	A	315	-	-	0/1/1/1	-
6	EDO	C	102	-	-	0/1/1/1	-
6	EDO	A	321	-	-	0/1/1/1	-
6	EDO	A	327	-	-	0/1/1/1	-
6	EDO	A	308	-	-	0/1/1/1	-
6	EDO	B	106	-	-	1/1/1/1	-
6	EDO	A	303	-	-	0/1/1/1	-
6	EDO	D	304	-	-	1/1/1/1	-
6	EDO	A	322	-	-	0/1/1/1	-
6	EDO	D	312	-	-	0/1/1/1	-
6	EDO	A	310	-	-	1/1/1/1	-
6	EDO	A	307	-	-	1/1/1/1	-
5	TRS	A	302	-	-	1/9/9/9	-
6	EDO	D	311	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	307	EDO	O1-C1-C2-O2
6	A	311	EDO	O1-C1-C2-O2
6	B	106	EDO	O1-C1-C2-O2
6	A	318	EDO	O1-C1-C2-O2
6	A	305	EDO	O1-C1-C2-O2
6	A	313	EDO	O1-C1-C2-O2
6	A	323	EDO	O1-C1-C2-O2
6	D	311	EDO	O1-C1-C2-O2
5	A	302	TRS	C3-C-C2-O2
6	A	324	EDO	O1-C1-C2-O2
6	B	105	EDO	O1-C1-C2-O2
6	D	308	EDO	O1-C1-C2-O2
6	A	310	EDO	O1-C1-C2-O2
6	B	104	EDO	O1-C1-C2-O2
6	D	303	EDO	O1-C1-C2-O2
6	D	304	EDO	O1-C1-C2-O2

There are no ring outliers.

14 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	326	EDO	4	0
6	A	325	EDO	1	0
6	B	105	EDO	1	0
6	A	323	EDO	1	0
6	A	314	EDO	1	0
6	A	320	EDO	2	0
6	E	101	EDO	3	0
6	C	102	EDO	1	0
6	A	321	EDO	1	0
6	A	308	EDO	1	0
6	D	304	EDO	2	0
6	A	322	EDO	1	0
6	D	312	EDO	6	0
6	A	307	EDO	1	0

5.7 Other polymers

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%)	0.10	5 (1%) 68 72	13, 22, 44, 66	0
1	D	243/277 (87%)	0.85	44 (18%) 1 1	20, 29, 95, 103	0
2	B	100/100 (100%)	0.16	1 (1%) 82 85	13, 32, 55, 59	0
2	E	97/100 (97%)	1.86	40 (41%) 0 0	23, 66, 90, 96	0
3	C	8/8 (100%)	0.27	1 (12%) 3 5	19, 21, 37, 37	0
3	F	8/8 (100%)	0.48	1 (12%) 3 5	26, 35, 42, 51	0
All	All	733/770 (95%)	0.59	92 (12%) 3 5	13, 28, 88, 103	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	246	ALA	9.8
1	D	257	TYR	7.7
1	D	266	LEU	7.5
1	D	215	LEU	7.4
1	D	217	TRP	7.4
2	E	93	VAL	7.2
1	D	203	CYS	7.0
1	D	230	LEU	6.9
1	D	218	GLN	6.7
1	D	268	LYS	6.3
1	D	205	ALA	6.3
1	D	259	CYS	6.2
1	D	204	TRP	6.1
1	D	192	HIS	6.0
1	D	191	HIS	6.0
1	D	260	HIS	5.6
1	D	270	LEU	5.6
1	D	261	VAL	5.5
2	E	43	GLY	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	269	PRO	5.4
1	D	245	ALA	5.2
2	E	73	THR	5.2
2	E	19	LYS	5.0
1	D	182	THR	4.9
2	E	48	LYS	4.8
1	D	214	THR	4.8
2	E	98	ASP	4.8
2	E	14	PRO	4.6
1	D	258	THR	4.6
1	D	231	VAL	4.5
2	E	1	ILE	4.5
1	D	212	GLU	4.5
2	E	20	SER	4.4
1	D	187	THR	4.4
2	E	75	LYS	4.4
2	E	18	GLY	4.3
2	E	79	ALA	4.1
1	D	213	ILE	4.1
2	E	94	LYS	4.1
2	E	95	TRP	4.0
2	E	16	GLU	3.9
2	E	71	THR	3.9
1	D	202	ARG	3.8
2	E	42	ASN	3.8
2	E	92	ILE	3.7
1	D	267	PRO	3.7
1	D	206	LEU	3.6
2	E	21	ASN	3.6
2	E	40	LEU	3.6
1	D	219	ARG	3.5
1	D	244	TRP	3.5
2	E	13	HIS	3.5
1	D	185	PRO	3.4
1	D	193	PRO	3.4
2	E	74	GLU	3.3
1	D	209	TYR	3.2
1	D	188	HIS	3.2
1	A	276	PRO	3.2
1	D	247	VAL	3.2
1	D	229	GLU	3.2
1	D	262	GLN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	72	PRO	3.1
2	E	47	GLU	3.1
2	E	68	THR	3.1
2	E	80	CYS	3.1
2	E	39	LEU	3.1
2	E	69	GLU	3.1
1	D	265	GLY	3.0
2	E	96	ASP	3.0
2	E	44	GLU	2.9
1	D	216	THR	2.9
2	E	10	TYR	2.8
3	F	4[A]	PHE	2.8
1	A	226	GLN	2.7
2	E	70	PHE	2.5
1	D	186	LYS	2.5
2	E	17	ASN	2.4
2	E	50	GLU	2.4
1	D	184	PRO	2.4
2	E	22	PHE	2.4
1	A	275	GLU	2.4
2	E	9	VAL	2.4
2	E	77	GLU	2.3
2	E	76	ASP	2.3
1	A	196	ASP	2.2
2	B	1	ILE	2.2
1	D	263	HIS	2.2
2	E	89	GLN	2.1
1	D	264	GLU	2.1
3	C	4	PHE	2.1
1	A	111[A]	ARG	2.1
2	E	7	ILE	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^{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
6	EDO	A	315	4/4	0.67	0.24	45,45,47,56	0
6	EDO	A	321	4/4	0.78	0.28	33,38,46,51	0
6	EDO	A	323	4/4	0.78	0.27	40,44,49,50	0
6	EDO	A	313	4/4	0.79	0.27	29,35,43,44	0
6	EDO	B	107	4/4	0.79	0.23	41,49,52,57	0
6	EDO	A	319	4/4	0.80	0.19	29,39,44,45	0
6	EDO	A	308	4/4	0.80	0.22	30,39,42,54	0
6	EDO	A	326	4/4	0.82	0.27	50,56,56,64	0
6	EDO	B	105	4/4	0.84	0.28	42,42,45,63	0
6	EDO	A	312	4/4	0.84	0.25	37,40,40,43	0
6	EDO	D	306	4/4	0.84	0.14	32,37,45,52	0
6	EDO	A	309	4/4	0.85	0.17	38,39,43,48	0
6	EDO	A	320	4/4	0.85	0.29	25,44,48,51	0
6	EDO	A	324	4/4	0.85	0.14	50,51,55,56	0
6	EDO	A	325	4/4	0.85	0.16	44,49,51,57	0
6	EDO	D	307	4/4	0.85	0.33	39,43,47,47	0
6	EDO	D	308	4/4	0.85	0.12	39,42,44,48	0
6	EDO	D	311	4/4	0.85	0.18	34,47,49,52	0
6	EDO	A	327	4/4	0.86	0.15	41,50,50,52	0
6	EDO	C	102	4/4	0.86	0.39	32,35,44,53	0
6	EDO	A	310	4/4	0.86	0.19	31,33,41,44	0
6	EDO	B	108	4/4	0.87	0.23	44,45,46,57	0
6	EDO	A	322	4/4	0.88	0.18	29,39,43,43	0
4	ZN	D	302	1/1	0.90	0.15	92,92,92,92	0
6	EDO	D	303	4/4	0.90	0.12	29,30,41,42	0
6	EDO	A	316	4/4	0.90	0.30	43,43,48,55	0
6	EDO	B	103	4/4	0.91	0.20	31,34,35,36	0
6	EDO	B	102	4/4	0.91	0.18	28,30,36,48	0
6	EDO	D	305	4/4	0.92	0.15	40,41,41,57	0
6	EDO	A	311	4/4	0.92	0.22	28,34,35,53	0
6	EDO	C	101	4/4	0.92	0.16	30,31,35,56	0
6	EDO	B	106	4/4	0.92	0.11	35,42,42,54	0
6	EDO	A	306	4/4	0.92	0.23	39,40,50,55	0
6	EDO	D	312	4/4	0.92	0.15	37,44,45,59	0
6	EDO	A	314	4/4	0.93	0.14	31,37,38,44	0
6	EDO	A	305	4/4	0.93	0.15	24,40,40,43	0
6	EDO	D	310	4/4	0.93	0.48	30,38,40,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	TRS	A	302	8/8	0.93	0.20	38,39,45,53	0
6	EDO	A	318	4/4	0.93	0.23	40,45,47,50	0
6	EDO	A	304	4/4	0.94	0.20	25,26,30,31	0
6	EDO	A	307	4/4	0.94	0.16	32,33,33,49	0
6	EDO	D	309	4/4	0.94	0.16	28,33,35,36	0
6	EDO	E	101	4/4	0.94	0.15	27,32,37,46	0
6	EDO	D	304	4/4	0.95	0.18	28,41,46,48	0
6	EDO	A	317	4/4	0.95	0.10	26,29,43,47	0
6	EDO	B	104	4/4	0.96	0.19	19,28,32,32	0
6	EDO	E	102	4/4	0.96	0.15	35,39,41,44	0
6	EDO	A	303	4/4	0.98	0.09	21,24,27,28	0
6	EDO	B	101	4/4	0.99	0.11	23,25,33,33	0
4	ZN	D	301	1/1	1.00	0.11	21,21,21,21	0
4	ZN	A	301	1/1	1.00	0.15	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.