



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:12 PM UTC

PDB ID : 7WT3 / pdb\_00007wt3  
Title : Crystal structure of HLA-A\*2402 complexed with 4-mer lipopeptide  
Authors : Asa, M.; Morita, D.; Sugita, M.  
Deposited on : 2022-02-03  
Resolution : 1.89 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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

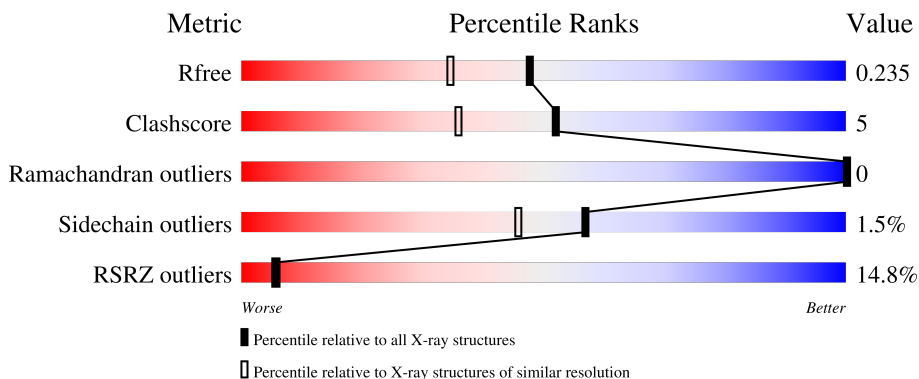
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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))
$R_{free}$	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	277	
1	D	277	
2	B	100	
2	E	100	
3	C	5	

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Mol	Chain	Length	Quality of chain
3	F	5	 80% 20%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6236 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
			Total	C	N	O	S			
1	A	277	Total 2300	C 1434	N 414	O 439	S 13	0	10	0
1	D	210	Total 1742	C 1082	N 314	O 336	S 10	0	7	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 838	C 535	N 141	O 159	S 3	0	1	0
2	E	82	Total 690	C 447	N 116	O 125	S 2	0	0	0

- Molecule 3 is a protein called 4-mer lipopeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	5	Total 44	C 32	N 5	O 7	0	0	0
3	F	5	Total 44	C 32	N 5	O 7	0	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



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

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub><sup>-</sup>).

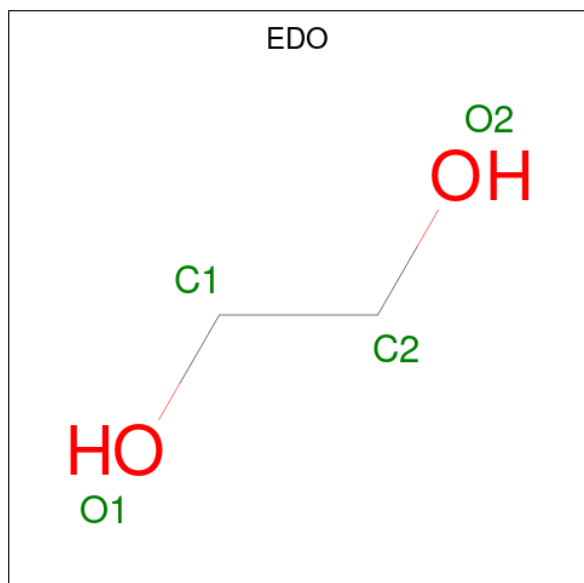


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	D	1	4	2	2	0	0

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

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

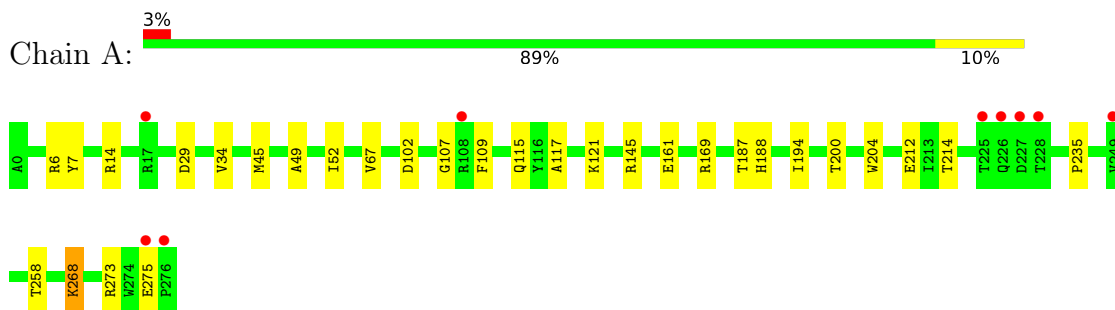
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	226	Total O 228 228	0	2
8	B	58	Total O 59 59	0	1
8	C	2	Total O 2 2	0	0
8	D	103	Total O 103 103	0	0
8	E	13	Total O 14 14	0	1
8	F	1	Total O 1 1	0	0

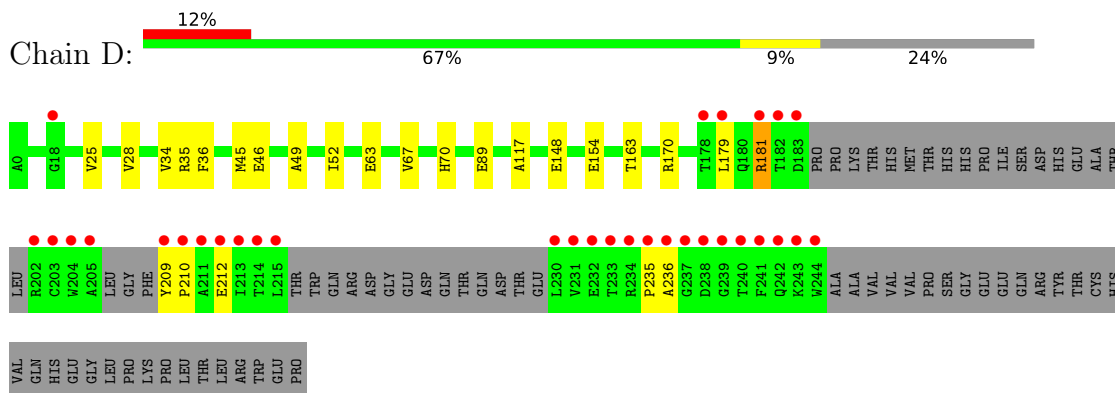
### 3 Residue-property plots [i](#)

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.

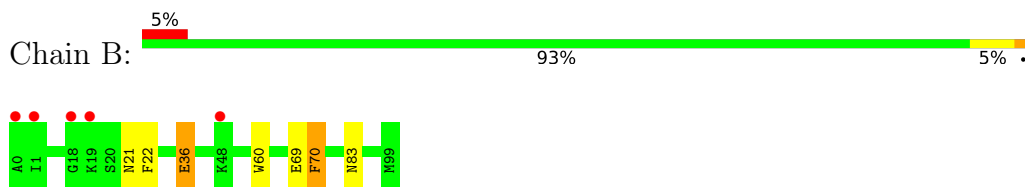
- Molecule 1: MHC class I antigen



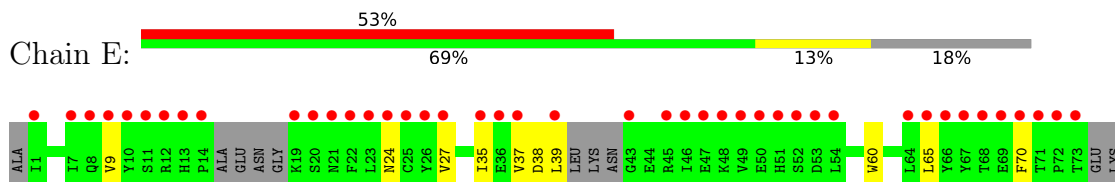
- Molecule 1: MHC class I antigen

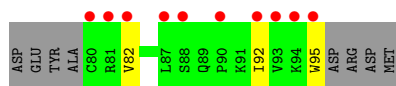


- Molecule 2: Beta-2-microglobulin

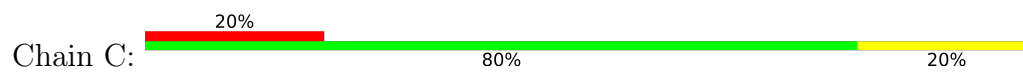


- Molecule 2: Beta-2-microglobulin

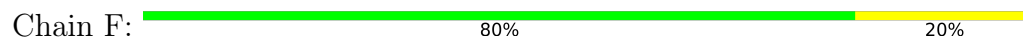




- Molecule 3: 4-mer lipopeptide



- Molecule 3: 4-mer lipopeptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.07Å 46.41Å 142.67Å 90.00° 104.87° 90.00°	Depositor
Resolution (Å)	42.08 – 1.89 42.08 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.08-1.89) 99.7 (42.08-1.89)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 1.88Å)	Xtrriage
Refinement program	PHENIX 1.9_1692+SVN	Depositor
R, $R_{free}$	0.199 , 0.235 (Not available) , 0.235	Depositor DCC
$R_{free}$ test set	4457 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.1	Xtrriage
Anisotropy	0.402	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: TRS, ZN, EDO, MYR, ACT

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	0.51	2/2386 (0.1%)	0.57	1/3234 (0.0%)
1	D	0.35	0/1790	0.52	1/2413 (0.0%)
2	B	0.25	0/864	0.47	0/1169
2	E	0.21	0/709	0.38	0/958
3	C	0.24	0/29	0.39	0/36
3	F	0.21	0/29	0.28	0/36
All	All	0.40	2/5807 (0.0%)	0.52	2/7846 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145[A]	ARG	CA-C	6.69	1.62	1.52
1	A	145[B]	ARG	CA-C	6.69	1.62	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	28	VAL	N-CA-C	-6.56	98.17	107.75
1	A	115	GLN	N-CA-C	5.18	117.07	109.24

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	2300	0	2174	23	0
1	D	1742	0	1634	21	0
2	B	838	0	808	6	0
2	E	690	0	668	10	0
3	C	44	0	49	3	0
3	F	44	0	49	2	0
4	A	8	0	12	0	0
5	A	8	0	6	0	0
5	D	4	0	3	0	0
6	A	2	0	0	0	0
6	D	1	0	0	0	0
7	A	72	0	106	7	0
7	B	32	0	48	3	0
7	D	40	0	60	8	0
7	E	4	0	6	0	0
8	A	228	0	0	2	0
8	B	59	0	0	0	0
8	C	2	0	0	0	0
8	D	103	0	0	2	0
8	E	14	0	0	0	0
8	F	1	0	0	0	0
All	All	6236	0	5623	58	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 5.

All (58) 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:35:ARG:HH21	7:D:309:EDO:H22	1.48	0.77
1:D:235:PRO:HG2	2:E:65:LEU:HD12	1.65	0.75
1:A:235:PRO:HD3	7:B:108:EDO:H21	1.77	0.66
1:A:7:TYR:HD1	3:C:1:MYR:H131	1.61	0.65
1:D:181:ARG:O	1:D:181:ARG:HG2	1.99	0.61
7:A:306:EDO:H22	7:A:314:EDO:H11	1.83	0.60
1:A:258:THR:HG22	1:A:273[A]:ARG:HG2	1.83	0.60
1:A:212:GLU:HG3	7:A:307:EDO:H21	1.85	0.58
2:E:9:VAL:HG22	2:E:95:TRP:HB2	1.85	0.57
1:D:46:GLU:HG3	7:D:307:EDO:H11	1.86	0.57
2:E:39:LEU:HD12	2:E:39:LEU:N	2.22	0.54
2:B:36:GLU:HG3	2:B:83:ASN:HB3	1.91	0.52
2:E:37:VAL:HG22	2:E:82:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:PHE:HE2	7:A:320:EDO:H21	1.75	0.51
1:D:148:GLU:HA	7:D:312:EDO:H11	1.91	0.51
2:E:38:ASP:C	2:E:39:LEU:HD12	2.36	0.50
1:D:163:THR:HG22	7:D:308:EDO:H21	1.94	0.49
1:D:170:ARG:NH2	8:D:406:HOH:O	2.45	0.49
2:B:22:PHE:CE2	2:B:69:GLU:HG2	2.47	0.49
1:A:45[B]:MET:HG2	1:A:67:VAL:HG11	1.95	0.48
1:A:107:GLY:O	1:A:169:ARG:NH2	2.44	0.48
1:D:210:PRO:HG2	1:D:212:GLU:HB3	1.96	0.48
1:D:70:HIS:HB2	3:F:1:MYR:H71	1.97	0.47
1:A:214:THR:OG1	7:A:307:EDO:O2	2.25	0.47
1:A:49:ALA:O	1:A:52:ILE:HG22	2.15	0.46
1:D:36:PHE:HA	7:D:307:EDO:H12	1.97	0.46
1:A:7:TYR:CD1	3:C:1:MYR:H131	2.47	0.46
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.51	0.46
1:D:70:HIS:CD2	3:F:1:MYR:H91	2.51	0.46
1:A:188:HIS:NE2	7:A:316:EDO:H12	2.31	0.45
1:D:25:VAL:HG12	1:D:35:ARG:HG3	1.98	0.45
1:A:14:ARG:NH2	8:A:421:HOH:O	2.43	0.45
7:D:312:EDO:H12	8:D:480:HOH:O	2.17	0.45
1:A:258:THR:HG22	1:A:273[B]:ARG:HG2	1.98	0.44
1:A:45[B]:MET:SD	3:C:1:MYR:H143	2.56	0.44
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.52	0.44
1:D:34:VAL:HG11	1:D:45:MET:HE3	2.00	0.44
1:D:35:ARG:NH2	7:D:309:EDO:H22	2.25	0.43
1:A:161:GLU:OE2	7:A:320:EDO:O1	2.32	0.43
1:A:194:ILE:HD11	1:A:200:THR:OG1	2.19	0.43
1:A:268:LYS:HB3	1:A:268:LYS:HE3	1.69	0.42
1:D:236:ALA:O	2:E:24:ASN:ND2	2.51	0.42
2:B:60:TRP:CZ2	7:B:102:EDO:H22	2.54	0.42
1:A:121:LYS:HE3	8:A:595:HOH:O	2.19	0.42
1:D:49:ALA:O	1:D:52:ILE:HG22	2.20	0.41
2:E:39:LEU:N	2:E:39:LEU:CD1	2.83	0.41
1:D:35:ARG:HE	7:D:309:EDO:C2	2.33	0.41
1:D:209:TYR:HA	1:D:210:PRO:HA	1.88	0.41
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.49	0.41
1:A:29:ASP:OD1	7:A:310:EDO:O1	2.38	0.41
1:D:63:GLU:O	1:D:67:VAL:HG23	2.20	0.41
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.56	0.41
1:D:179:LEU:HD23	1:D:179:LEU:HA	1.81	0.41
1:A:34:VAL:HG11	1:A:45[A]:MET:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:VAL:HG11	2:E:35:ILE:CD1	2.52	0.40
1:A:187:THR:HA	1:A:204:TRP:O	2.21	0.40
2:B:60:TRP:CE2	7:B:102:EDO:H22	2.56	0.40
2:E:27:VAL:HG11	2:E:35:ILE:HD13	2.03	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	285/277 (103%)	281 (99%)	4 (1%)	0	100	100
1	D	209/277 (76%)	205 (98%)	4 (2%)	0	100	100
2	B	99/100 (99%)	99 (100%)	0	0	100	100
2	E	74/100 (74%)	71 (96%)	3 (4%)	0	100	100
3	C	2/5 (40%)	2 (100%)	0	0	100	100
3	F	2/5 (40%)	2 (100%)	0	0	100	100
All	All	671/764 (88%)	660 (98%)	11 (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	241/232 (104%)	239 (99%)	2 (1%)	73	68
1	D	178/232 (77%)	174 (98%)	4 (2%)	45	30
2	B	95/94 (101%)	93 (98%)	2 (2%)	47	32
2	E	80/94 (85%)	78 (98%)	2 (2%)	42	26
3	C	2/2 (100%)	2 (100%)	0	100	100
3	F	2/2 (100%)	2 (100%)	0	100	100
All	All	598/656 (91%)	588 (98%)	10 (2%)	57	40

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	LYS
1	A	275	GLU
2	B	36	GLU
2	B	70	PHE
1	D	89	GLU
1	D	154[A]	GLU
1	D	154[B]	GLU
1	D	181	ARG
2	E	70	PHE
2	E	92	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	GLN
1	A	224	GLN
1	D	43	GLN
1	D	156	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 3 are monoatomic - leaving 41 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
7	EDO	A	322	-	3,3,3	0.40	0	2,2,2	0.45	0
7	EDO	D	310	-	3,3,3	0.47	0	2,2,2	0.43	0
4	TRS	A	301	-	7,7,7	0.27	0	9,9,9	0.44	0
7	EDO	A	320	-	3,3,3	0.42	0	2,2,2	0.38	0
7	EDO	D	307	-	3,3,3	0.42	0	2,2,2	0.34	0
7	EDO	D	305	-	3,3,3	0.46	0	2,2,2	0.40	0
7	EDO	A	317	-	3,3,3	0.47	0	2,2,2	0.36	0
7	EDO	B	101	-	3,3,3	0.46	0	2,2,2	0.40	0
7	EDO	A	311	-	3,3,3	0.50	0	2,2,2	0.47	0
7	EDO	D	303	-	3,3,3	0.47	0	2,2,2	0.32	0
7	EDO	A	312	-	3,3,3	0.45	0	2,2,2	0.53	0
7	EDO	A	310	-	3,3,3	0.37	0	2,2,2	0.17	0
7	EDO	B	106	-	3,3,3	0.50	0	2,2,2	0.17	0
7	EDO	B	108	-	3,3,3	0.34	0	2,2,2	0.40	0
7	EDO	A	307	-	3,3,3	0.32	0	2,2,2	0.55	0
7	EDO	A	319	-	3,3,3	0.46	0	2,2,2	0.27	0
7	EDO	B	103	-	3,3,3	0.55	0	2,2,2	0.32	0
7	EDO	D	311	-	3,3,3	0.48	0	2,2,2	0.31	0
7	EDO	D	308	-	3,3,3	0.45	0	2,2,2	0.58	0
7	EDO	A	318	-	3,3,3	0.46	0	2,2,2	0.50	0
7	EDO	A	314	-	3,3,3	0.35	0	2,2,2	0.50	0
7	EDO	B	105	-	3,3,3	0.44	0	2,2,2	0.34	0
7	EDO	D	312	-	3,3,3	0.43	0	2,2,2	0.36	0
7	EDO	A	323	-	3,3,3	0.45	0	2,2,2	0.41	0
5	ACT	A	303	-	3,3,3	1.75	1 (33%)	3,3,3	1.32	0
7	EDO	A	308	-	3,3,3	0.46	0	2,2,2	0.53	0
7	EDO	A	306	-	3,3,3	0.46	0	2,2,2	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	EDO	A	315	-	3,3,3	0.37	0	2,2,2	0.49	0
5	ACT	A	302	-	3,3,3	1.29	0	3,3,3	1.46	0
7	EDO	B	104	-	3,3,3	0.42	0	2,2,2	0.45	0
7	EDO	B	107	-	3,3,3	0.43	0	2,2,2	0.46	0
7	EDO	D	309	-	3,3,3	0.41	0	2,2,2	0.46	0
7	EDO	D	304	-	3,3,3	0.43	0	2,2,2	0.60	0
7	EDO	B	102	-	3,3,3	0.41	0	2,2,2	0.27	0
7	EDO	A	321	-	3,3,3	0.50	0	2,2,2	0.38	0
7	EDO	A	313	-	3,3,3	0.38	0	2,2,2	0.54	0
5	ACT	D	301	-	3,3,3	1.47	1 (33%)	3,3,3	1.54	0
7	EDO	D	306	-	3,3,3	0.41	0	2,2,2	0.44	0
7	EDO	A	316	-	3,3,3	0.46	0	2,2,2	0.31	0
7	EDO	A	309	6	3,3,3	0.39	0	2,2,2	0.64	0
7	EDO	E	101	-	3,3,3	0.48	0	2,2,2	0.43	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
7	EDO	A	322	-	-	0/1/1/1	-
7	EDO	D	310	-	-	0/1/1/1	-
4	TRS	A	301	-	-	3/9/9/9	-
7	EDO	A	320	-	-	1/1/1/1	-
7	EDO	D	307	-	-	1/1/1/1	-
7	EDO	D	305	-	-	0/1/1/1	-
7	EDO	A	317	-	-	0/1/1/1	-
7	EDO	B	101	-	-	0/1/1/1	-
7	EDO	A	311	-	-	0/1/1/1	-
7	EDO	D	303	-	-	0/1/1/1	-
7	EDO	A	312	-	-	0/1/1/1	-
7	EDO	A	310	-	-	1/1/1/1	-
7	EDO	B	106	-	-	0/1/1/1	-
7	EDO	B	108	-	-	1/1/1/1	-
7	EDO	A	307	-	-	1/1/1/1	-
7	EDO	A	319	-	-	0/1/1/1	-
7	EDO	B	103	-	-	0/1/1/1	-
7	EDO	D	311	-	-	0/1/1/1	-
7	EDO	D	308	-	-	1/1/1/1	-
7	EDO	A	318	-	-	0/1/1/1	-
7	EDO	A	314	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	105	-	-	1/1/1/1	-
7	EDO	D	312	-	-	0/1/1/1	-
7	EDO	A	323	-	-	0/1/1/1	-
7	EDO	A	308	-	-	1/1/1/1	-
7	EDO	A	306	-	-	0/1/1/1	-
7	EDO	A	315	-	-	1/1/1/1	-
7	EDO	B	104	-	-	0/1/1/1	-
7	EDO	B	107	-	-	1/1/1/1	-
7	EDO	D	309	-	-	1/1/1/1	-
7	EDO	D	304	-	-	0/1/1/1	-
7	EDO	B	102	-	-	0/1/1/1	-
7	EDO	A	321	-	-	1/1/1/1	-
7	EDO	A	313	-	-	1/1/1/1	-
7	EDO	D	306	-	-	0/1/1/1	-
7	EDO	A	316	-	-	0/1/1/1	-
7	EDO	A	309	6	-	1/1/1/1	-
7	EDO	E	101	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	303	ACT	CH3-C	2.56	1.59	1.49
5	D	301	ACT	CH3-C	2.13	1.57	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	TRS	C3-C-C1-O1
7	A	313	EDO	O1-C1-C2-O2
7	A	315	EDO	O1-C1-C2-O2
7	B	108	EDO	O1-C1-C2-O2
4	A	301	TRS	N-C-C1-O1
7	B	107	EDO	O1-C1-C2-O2
4	A	301	TRS	C2-C-C1-O1
7	B	105	EDO	O1-C1-C2-O2
7	A	314	EDO	O1-C1-C2-O2
7	D	307	EDO	O1-C1-C2-O2
7	D	309	EDO	O1-C1-C2-O2
7	A	307	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	A	308	EDO	O1-C1-C2-O2
7	A	310	EDO	O1-C1-C2-O2
7	A	320	EDO	O1-C1-C2-O2
7	A	309	EDO	O1-C1-C2-O2
7	A	321	EDO	O1-C1-C2-O2
7	D	308	EDO	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	320	EDO	2	0
7	D	307	EDO	2	0
7	A	310	EDO	1	0
7	B	108	EDO	1	0
7	A	307	EDO	2	0
7	D	308	EDO	1	0
7	A	314	EDO	1	0
7	D	312	EDO	2	0
7	A	306	EDO	1	0
7	D	309	EDO	3	0
7	B	102	EDO	2	0
7	A	316	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<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	277/277 (100%)	0.05	9 (3%) 50 55	11, 26, 42, 69	10 (3%)
1	D	210/277 (75%)	0.86	32 (15%) 5 5	12, 30, 82, 92	7 (3%)
2	B	100/100 (100%)	0.43	5 (5%) 34 36	16, 35, 54, 57	1 (1%)
2	E	82/100 (82%)	2.78	53 (64%) 0 0	27, 73, 87, 99	0
3	C	4/5 (80%)	1.01	1 (25%) 2 1	23, 28, 30, 42	0
3	F	4/5 (80%)	0.54	0 100 100	30, 33, 34, 47	0
All	All	677/764 (88%)	0.70	100 (14%) 5 6	11, 30, 81, 99	18 (2%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	209	TYR	8.5
2	E	39	LEU	7.6
1	D	215	LEU	7.4
1	D	205	ALA	7.3
1	D	241	PHE	6.8
2	E	65	LEU	6.6
1	D	213	ILE	6.5
2	E	49	VAL	6.3
2	E	9	VAL	6.2
1	D	211	ALA	6.2
1	D	182	THR	6.2
1	D	210	PRO	6.0
2	E	95	TRP	5.9
1	D	204	TRP	5.8
1	D	244	TRP	5.7
2	E	46	ILE	5.7
2	E	23	LEU	5.5
1	A	275	GLU	5.5
2	E	37	VAL	5.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	E	43	GLY	5.2
2	E	92	ILE	5.0
2	E	22	PHE	4.9
2	E	68	THR	4.9
2	E	14	PRO	4.9
1	D	230	LEU	4.8
2	E	70	PHE	4.7
1	D	231	VAL	4.6
1	A	225	THR	4.5
2	B	1	ILE	4.5
1	D	183	ASP	4.4
1	D	233	THR	4.3
2	E	25	CYS	4.3
2	E	93	VAL	4.2
2	E	26	TYR	4.2
2	E	72	PRO	4.2
2	E	82	VAL	4.1
1	D	240	THR	4.1
2	E	73	THR	4.1
3	C	2	GLY	4.0
2	E	66	TYR	4.0
2	E	67	TYR	4.0
2	E	10	TYR	3.8
1	D	242	GLN	3.7
2	E	21	ASN	3.7
2	E	13	HIS	3.7
1	D	214	THR	3.7
2	E	51	HIS	3.6
1	D	232	GLU	3.6
1	D	243	LYS	3.6
2	E	80	CYS	3.5
1	A	276	PRO	3.5
1	D	181	ARG	3.5
2	E	50	GLU	3.5
2	E	19	LYS	3.5
1	D	202	ARG	3.5
2	E	12	ARG	3.3
2	E	81	ARG	3.3
1	D	212	GLU	3.3
2	E	90	PRO	3.3
1	D	203	CYS	3.2
1	D	236	ALA	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	239	GLY	3.1
2	E	48	LYS	3.0
2	E	69	GLU	3.0
2	E	8	GLN	3.0
1	A	228	THR	3.0
2	E	71	THR	2.9
2	E	7	ILE	2.8
1	A	227	ASP	2.8
2	E	45	ARG	2.7
2	E	11	SER	2.7
1	A	226	GLN	2.7
1	D	237	GLY	2.7
2	E	64	LEU	2.7
2	E	35	ILE	2.7
2	B	0	ALA	2.6
2	E	53	ASP	2.6
2	E	24	ASN	2.6
2	E	87	LEU	2.6
2	B	18	GLY	2.6
1	D	234	ARG	2.5
2	E	47	GLU	2.4
2	E	1	ILE	2.4
1	D	238	ASP	2.4
2	E	27	VAL	2.4
2	E	54	LEU	2.4
2	B	48	LYS	2.4
1	D	179	LEU	2.3
2	E	88	SER	2.3
2	E	36	GLU	2.3
2	E	94	LYS	2.3
1	A	108	ARG	2.3
2	E	20	SER	2.3
1	D	235	PRO	2.2
1	D	18	GLY	2.2
2	E	52	SER	2.1
1	A	17	ARG	2.1
1	D	178	THR	2.0
2	B	19	LYS	2.0
1	A	249	VAL	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 oligosaccharides 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
7	EDO	A	313	4/4	0.77	0.27	35,45,47,54	0
7	EDO	D	312	4/4	0.77	0.22	47,53,55,58	0
7	EDO	A	322	4/4	0.78	0.23	39,47,49,61	0
7	EDO	A	317	4/4	0.79	0.18	54,56,57,58	0
5	ACT	A	303	4/4	0.81	0.17	41,42,42,46	0
7	EDO	A	310	4/4	0.82	0.21	36,42,44,50	0
7	EDO	B	105	4/4	0.83	0.22	39,42,45,53	0
7	EDO	B	108	4/4	0.83	0.24	36,38,39,50	0
7	EDO	A	323	4/4	0.83	0.15	52,53,56,57	0
7	EDO	B	101	4/4	0.84	0.19	36,46,47,53	0
7	EDO	D	310	4/4	0.84	0.18	40,40,47,50	0
7	EDO	A	314	4/4	0.84	0.24	34,39,39,47	0
7	EDO	A	312	4/4	0.85	0.20	33,34,36,43	0
7	EDO	A	321	4/4	0.86	0.19	42,42,48,51	0
7	EDO	A	315	4/4	0.86	0.31	38,39,45,47	0
7	EDO	D	308	4/4	0.86	0.18	43,43,44,45	0
5	ACT	A	302	4/4	0.86	0.15	26,36,43,46	0
7	EDO	A	320	4/4	0.86	0.14	42,43,43,55	0
4	TRS	A	301	8/8	0.87	0.14	38,45,52,64	0
7	EDO	A	318	4/4	0.87	0.18	30,35,42,54	0
7	EDO	A	311	4/4	0.87	0.20	30,36,44,45	0
7	EDO	D	306	4/4	0.89	0.13	37,40,46,54	0
7	EDO	D	309	4/4	0.89	0.20	40,45,50,55	0
7	EDO	D	304	4/4	0.90	0.18	34,38,41,43	0
7	EDO	B	107	4/4	0.90	0.14	31,36,42,54	0
7	EDO	D	311	4/4	0.90	0.11	45,48,51,52	0
5	ACT	D	301	4/4	0.90	0.21	36,43,45,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	A	319	4/4	0.91	0.14	46,47,50,52	0
7	EDO	D	305	4/4	0.91	0.17	36,40,44,51	0
7	EDO	A	307	4/4	0.91	0.20	36,38,38,44	0
7	EDO	A	316	4/4	0.91	0.12	36,36,47,55	0
7	EDO	B	104	4/4	0.92	0.14	34,41,44,46	0
7	EDO	A	309	4/4	0.92	0.12	42,43,43,50	0
7	EDO	D	307	4/4	0.93	0.17	28,37,41,53	0
7	EDO	B	106	4/4	0.93	0.16	28,29,32,44	0
7	EDO	E	101	4/4	0.93	0.10	34,37,38,44	0
7	EDO	B	102	4/4	0.94	0.13	26,28,33,39	0
7	EDO	D	303	4/4	0.94	0.12	30,39,40,42	0
7	EDO	B	103	4/4	0.95	0.08	26,31,33,37	0
7	EDO	A	306	4/4	0.96	0.08	25,27,29,29	0
7	EDO	A	308	4/4	0.96	0.09	30,31,32,38	0
6	ZN	A	304	1/1	0.98	0.04	44,44,44,44	0
6	ZN	D	302	1/1	0.99	0.02	26,26,26,26	0
6	ZN	A	305	1/1	1.00	0.04	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.