



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:29 pm BST

PDB ID : 4I4W  
Title : Peptide length determines the outcome of T cell receptor/peptide-MHCI engagement  
Authors : Rizkallah, P.J.; Wooldridge, L.; Cole, D.K.  
Deposited on : 2012-11-28  
Resolution : 1.77 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

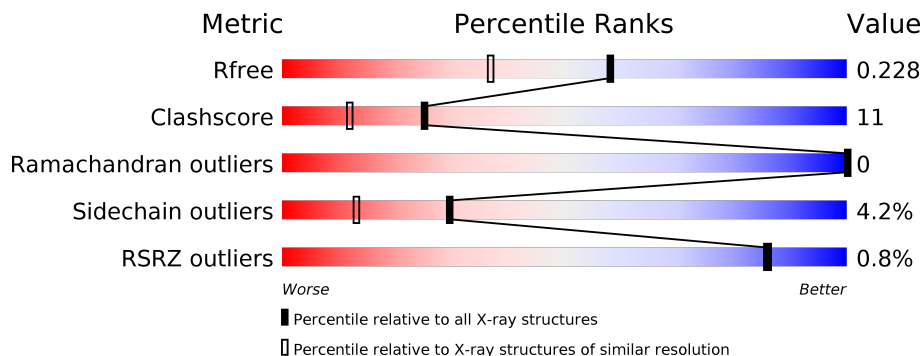
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.77 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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

Mol	Chain	Length	Quality of chain
1	A	276	
2	B	100	
3	C	9	

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	312	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3634 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	276	2260	1412	410	429	9	1	2	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	852	546	141	161	4	0	4	0

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 Immunogenic peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	86	60	16	10	0	1	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



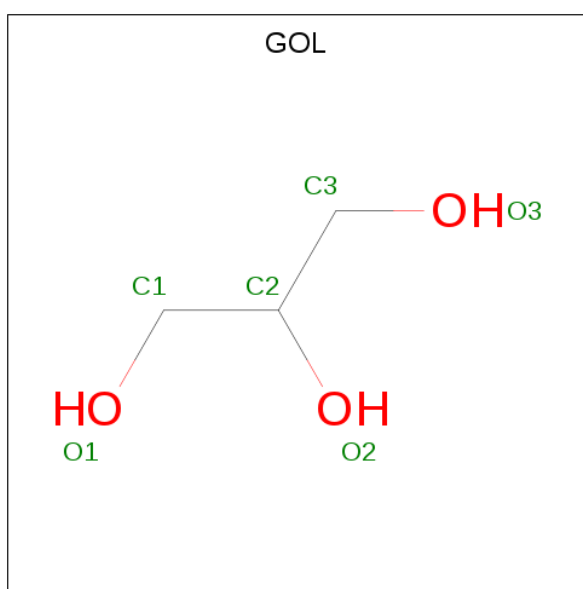
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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

- Molecule 5 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
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

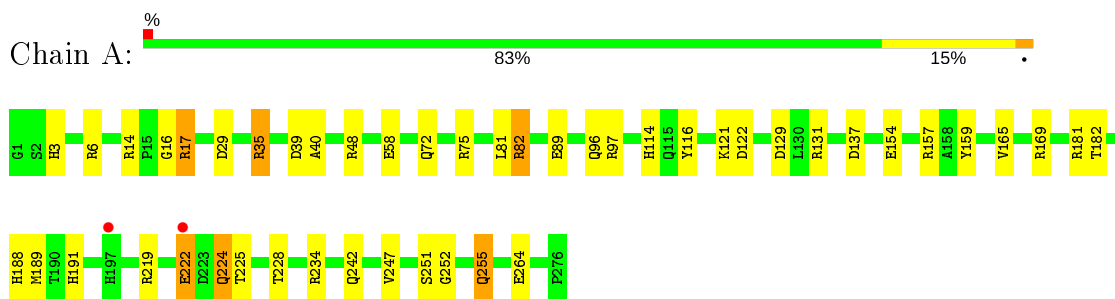
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	218	Total	O	0	0
			218	218		
7	B	107	Total	O	0	0
			107	107		
7	C	11	Total	O	0	0
			11	11		

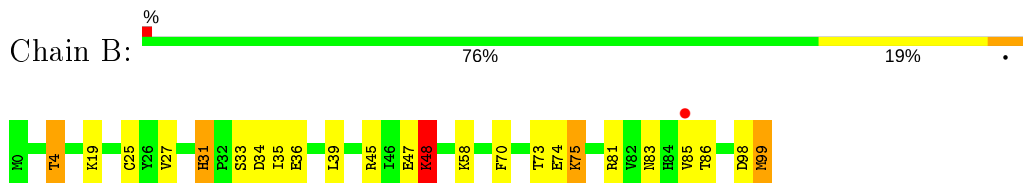
### 3 Residue-property plots [i](#)

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

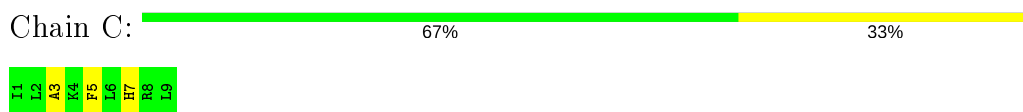
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 3: Immunogenic peptide





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.20Å 74.87Å 125.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.16 – 1.77 48.16 – 1.77	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.16-1.77) 99.9 (48.16-1.77)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 1.77Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.178 , 0.222 0.186 , 0.228	Depositor DCC
$R_{free}$ test set	2319 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.5	Xtrriage
Anisotropy	0.198	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3634	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, 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	1.09	2/2332 (0.1%)	1.16	19/3165 (0.6%)
2	B	1.06	2/887 (0.2%)	1.11	4/1201 (0.3%)
3	C	1.03	0/86	1.18	0/112
All	All	1.08	4/3305 (0.1%)	1.14	23/4478 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	GLN	CB-CG	-20.52	0.97	1.52
2	B	33	SER	CB-OG	-8.59	1.31	1.42
1	A	154	GLU	CD-OE2	5.90	1.32	1.25
2	B	34	ASP	CB-CG	-5.57	1.40	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLN	CA-CB-CG	13.27	142.59	113.40
1	A	17	ARG	NE-CZ-NH1	11.21	125.91	120.30
1	A	6	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	A	129	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	A	39	ASP	CB-CG-OD1	7.48	125.03	118.30
1	A	35	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	17	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	A	129	ASP	CB-CG-OD1	7.10	124.69	118.30
1	A	39	ASP	CB-CG-OD2	-6.85	112.14	118.30
2	B	48	LYS	CD-CE-NZ	6.65	127.00	111.70
1	A	82	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	A	35	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	B	45	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	A	48	ARG	NE-CZ-NH2	-6.02	117.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLN	N-CA-CB	-5.90	99.98	110.60
2	B	81	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	A	81	LEU	CB-CG-CD2	5.57	120.47	111.00
1	A	75	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	181	ARG	NE-CZ-NH1	5.31	122.96	120.30
2	B	45	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	A	17	ARG	CD-NE-CZ	5.21	130.90	123.60
1	A	189	MET	CG-SD-CE	-5.13	91.98	100.20
1	A	224	GLN	CB-CA-C	-5.01	100.39	110.40

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	2260	0	2113	33	0
2	B	852	0	833	25	0
3	C	86	0	104	10	0
4	A	48	0	72	10	0
4	B	24	0	36	6	0
5	A	18	0	24	6	1
6	A	10	0	0	0	0
7	A	218	0	0	7	0
7	B	107	0	0	10	1
7	C	11	0	0	1	0
All	All	3634	0	3182	69	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 (69) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85[A]:VAL:HG13	7:B:233:HOH:O	1.60	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:THR:HG22	1:A:247:VAL:HG12	1.47	0.96
2:B:48:LYS:HD3	7:B:289:HOH:O	1.66	0.94
3:C:3:ALA:CB	3:C:5:PHE:CZ	2.62	0.82
3:C:3:ALA:HB1	3:C:5:PHE:CE1	2.17	0.80
3:C:3:ALA:HB3	3:C:5:PHE:CE2	2.21	0.76
2:B:4[B]:THR:HG22	2:B:86:THR:HB	1.70	0.73
2:B:48:LYS:HE2	7:B:295:HOH:O	1.90	0.70
1:A:40:ALA:CB	5:A:313:GOL:H31	2.21	0.69
2:B:48:LYS:HD2	2:B:48:LYS:H	1.57	0.69
1:A:191:HIS:HE1	7:A:596:HOH:O	1.74	0.69
1:A:188:HIS:HD2	7:A:439:HOH:O	1.78	0.68
2:B:48:LYS:CD	2:B:48:LYS:H	2.06	0.66
1:A:122:ASP:O	4:A:306:EDO:H11	1.96	0.65
1:A:228:THR:HG22	1:A:247:VAL:CG1	2.24	0.64
1:A:137:ASP:OD2	4:A:306:EDO:O1	2.16	0.64
1:A:3:HIS:HE1	7:A:570:HOH:O	1.82	0.63
1:A:219:ARG:O	1:A:222:GLU:HG3	2.00	0.61
1:A:72:GLN:NE2	7:A:609:HOH:O	2.33	0.61
1:A:40:ALA:HB1	5:A:313:GOL:H31	1.81	0.60
2:B:48:LYS:CE	7:B:295:HOH:O	2.45	0.60
5:A:314:GOL:H2	7:A:421:HOH:O	2.00	0.59
5:A:314:GOL:H12	7:A:594:HOH:O	2.02	0.59
2:B:47:GLU:HB2	2:B:48:LYS:HE3	1.86	0.58
4:A:301:EDO:H21	7:B:224:HOH:O	2.04	0.58
1:A:14:ARG:HG2	4:A:312:EDO:H22	1.87	0.57
3:C:3:ALA:HB1	3:C:5:PHE:CZ	2.34	0.57
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.52	0.57
4:B:103:EDO:H12	7:B:283:HOH:O	2.05	0.56
2:B:98:ASP:C	2:B:99:MET:HG2	2.24	0.56
3:C:3:ALA:CB	3:C:5:PHE:CE2	2.87	0.56
2:B:36:GLU:HG3	4:B:106:EDO:H21	1.88	0.56
2:B:4[B]:THR:HG22	2:B:86:THR:CB	2.34	0.56
2:B:31:HIS:HD2	7:B:212:HOH:O	1.90	0.54
3:C:3:ALA:HB3	3:C:5:PHE:CD2	2.42	0.54
1:A:16:GLY:HA2	5:A:315:GOL:H31	1.91	0.52
1:A:3:HIS:HD2	1:A:29:ASP:OD2	1.94	0.51
2:B:98:ASP:O	2:B:99:MET:HG2	2.11	0.51
2:B:58:LYS:HA	4:B:101:EDO:H11	1.92	0.50
1:A:96:GLN:OE1	2:B:31:HIS:HE1	1.93	0.50
1:A:165:VAL:O	1:A:169:ARG:HG3	2.12	0.50
1:A:16:GLY:HA2	5:A:315:GOL:C3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:MET:HB3	4:B:103:EDO:H11	1.94	0.49
1:A:252:GLY:O	1:A:255:GLN:NE2	2.46	0.49
1:A:40:ALA:HB3	7:A:601:HOH:O	2.12	0.49
2:B:73:THR:HB	2:B:75:LYS:HD2	1.95	0.49
2:B:4[A]:THR:HG22	7:B:244:HOH:O	2.13	0.48
1:A:17:ARG:NH1	4:A:303:EDO:O1	2.42	0.46
2:B:36:GLU:HG3	4:B:106:EDO:C2	2.44	0.46
2:B:19:LYS:NZ	7:B:278:HOH:O	2.49	0.46
1:A:131:ARG:HH21	1:A:157:ARG:HH12	1.62	0.46
3:C:3:ALA:CB	3:C:5:PHE:CE1	2.87	0.46
1:A:14:ARG:HE	4:A:312:EDO:C2	2.30	0.45
1:A:14:ARG:HG2	4:A:312:EDO:C2	2.46	0.45
1:A:182:THR:HG22	1:A:264:GLU:OE2	2.17	0.45
1:A:188:HIS:HE1	4:A:302:EDO:O1	1.99	0.44
3:C:7:HIS:HD2	7:C:105:HOH:O	2.00	0.44
1:A:97:ARG:HD3	1:A:116:TYR:CZ	2.53	0.43
1:A:82:ARG:CZ	1:A:89:GLU:HG2	2.48	0.43
2:B:74:GLU:H	2:B:75:LYS:HZ2	1.66	0.42
1:A:14:ARG:HE	4:A:312:EDO:H21	1.84	0.42
1:A:114:HIS:NE2	3:C:7:HIS:HE1	2.17	0.42
2:B:36:GLU:CG	4:B:106:EDO:C2	2.98	0.42
1:A:121:LYS:HG3	4:A:306:EDO:H22	2.02	0.41
1:A:159:TYR:CE1	3:C:3:ALA:HB2	2.55	0.41
1:A:121:LYS:HB2	1:A:121:LYS:HE2	1.78	0.41
2:B:25:CYS:HB2	2:B:39:LEU:HD21	2.02	0.41
2:B:27[B]:VAL:HG11	2:B:35:ILE:HD11	2.02	0.41
2:B:85[A]:VAL:HG11	7:B:246:HOH:O	2.21	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)
5:A:315:GOL:O1	7:B:238:HOH:O[4_545]	1.36	0.84

## 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	276/276 (100%)	271 (98%)	5 (2%)	0	100	100
2	B	102/100 (102%)	101 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
All	All	385/385 (100%)	379 (98%)	6 (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	234/232 (101%)	227 (97%)	7 (3%)	41	24
2	B	99/95 (104%)	91 (92%)	8 (8%)	11	3
3	C	9/8 (112%)	9 (100%)	0	100	100
All	All	342/335 (102%)	327 (96%)	15 (4%)	30	12

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	58	GLU
1	A	222	GLU
1	A	224	GLN
1	A	225	THR
1	A	251	SER
1	A	255	GLN
2	B	4[A]	THR
2	B	4[B]	THR
2	B	31	HIS
2	B	48	LYS

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Mol	Chain	Res	Type
2	B	70	PHE
2	B	75	LYS
2	B	83	ASN
2	B	99	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	43	GLN
1	A	72	GLN
1	A	86	ASN
1	A	141	GLN
1	A	174	ASN
1	A	188	HIS
1	A	191	HIS
1	A	226	GLN
1	A	242	GLN
1	A	253	GLN
1	A	255	GLN
2	B	31	HIS
2	B	83	ASN
3	C	7	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 carbohydrates in this entry.

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

23 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	310	-	3,3,3	0.53	0	2,2,2	0.24	0
5	GOL	A	313	-	5,5,5	0.60	0	5,5,5	1.60	1 (20%)
4	EDO	A	306	-	3,3,3	0.73	0	2,2,2	0.45	0
4	EDO	B	102	-	3,3,3	0.48	0	2,2,2	0.73	0
4	EDO	A	311	-	3,3,3	0.59	0	2,2,2	0.30	0
4	EDO	A	308	-	3,3,3	0.72	0	2,2,2	0.11	0
4	EDO	A	304	-	3,3,3	0.73	0	2,2,2	0.51	0
5	GOL	A	315	-	5,5,5	0.69	0	5,5,5	0.98	0
4	EDO	B	105	-	3,3,3	0.55	0	2,2,2	0.15	0
4	EDO	A	309	-	3,3,3	0.59	0	2,2,2	0.15	0
4	EDO	A	307	-	3,3,3	0.50	0	2,2,2	0.49	0
4	EDO	A	305	-	3,3,3	0.62	0	2,2,2	0.06	0
4	EDO	A	301	-	3,3,3	0.52	0	2,2,2	0.15	0
6	SO4	A	317	-	4,4,4	0.53	0	6,6,6	0.36	0
4	EDO	A	303	-	3,3,3	0.51	0	2,2,2	0.32	0
4	EDO	B	106	-	3,3,3	0.43	0	2,2,2	0.58	0
6	SO4	A	316	-	4,4,4	0.56	0	6,6,6	0.39	0
4	EDO	A	302	-	3,3,3	0.68	0	2,2,2	0.51	0
4	EDO	B	104	-	3,3,3	0.39	0	2,2,2	0.63	0
4	EDO	B	101	-	3,3,3	0.45	0	2,2,2	0.42	0
5	GOL	A	314	-	5,5,5	0.60	0	5,5,5	1.49	1 (20%)
4	EDO	A	312	-	3,3,3	0.52	0	2,2,2	0.53	0
4	EDO	B	103	-	3,3,3	0.45	0	2,2,2	0.54	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	310	-	-	0/1/1/1	-
5	GOL	A	313	-	-	0/4/4/4	-
4	EDO	A	309	-	-	1/1/1/1	-
4	EDO	B	106	-	-	1/1/1/1	-
4	EDO	A	306	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	102	-	-	1/1/1/1	-
4	EDO	A	303	-	-	1/1/1/1	-
4	EDO	A	302	-	-	1/1/1/1	-
4	EDO	A	311	-	-	1/1/1/1	-
4	EDO	A	305	-	-	0/1/1/1	-
4	EDO	A	308	-	-	1/1/1/1	-
4	EDO	A	304	-	-	0/1/1/1	-
4	EDO	A	301	-	-	0/1/1/1	-
4	EDO	B	103	-	-	1/1/1/1	-
4	EDO	B	104	-	-	0/1/1/1	-
4	EDO	A	312	-	-	1/1/1/1	-
4	EDO	B	105	-	-	1/1/1/1	-
5	GOL	A	315	-	-	4/4/4/4	-
5	GOL	A	314	-	-	4/4/4/4	-
4	EDO	A	307	-	-	0/1/1/1	-
4	EDO	B	101	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	313	GOL	O1-C1-C2	-2.45	98.46	110.20
5	A	314	GOL	O1-C1-C2	2.41	121.76	110.20

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	315	GOL	O1-C1-C2-C3
5	A	315	GOL	C1-C2-C3-O3
5	A	314	GOL	C1-C2-C3-O3
5	A	314	GOL	O2-C2-C3-O3
5	A	315	GOL	O1-C1-C2-O2
5	A	314	GOL	O1-C1-C2-C3
5	A	315	GOL	O2-C2-C3-O3
5	A	314	GOL	O1-C1-C2-O2
4	B	105	EDO	O1-C1-C2-O2
4	A	308	EDO	O1-C1-C2-O2
4	B	106	EDO	O1-C1-C2-O2
4	A	302	EDO	O1-C1-C2-O2
4	B	103	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	309	EDO	O1-C1-C2-O2
4	A	312	EDO	O1-C1-C2-O2
4	A	311	EDO	O1-C1-C2-O2
4	B	101	EDO	O1-C1-C2-O2
4	B	102	EDO	O1-C1-C2-O2
4	A	303	EDO	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	313	GOL	2	0
4	A	306	EDO	3	0
5	A	315	GOL	2	1
4	A	301	EDO	1	0
4	A	303	EDO	1	0
4	B	106	EDO	3	0
4	A	302	EDO	1	0
4	B	101	EDO	1	0
5	A	314	GOL	2	0
4	A	312	EDO	4	0
4	B	103	EDO	2	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 [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	276/276 (100%)	0.08	2 (0%) 87 88	11, 25, 49, 66	1 (0%)
2	B	100/100 (100%)	0.02	1 (1%) 82 82	12, 23, 40, 49	0
3	C	9/9 (100%)	0.03	0 100 100	14, 19, 24, 26	0
All	All	385/385 (100%)	0.06	3 (0%) 86 86	11, 24, 46, 66	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	GLU	2.7
2	B	85[A]	VAL	2.6
1	A	197	HIS	2.2

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	A	311	4/4	0.71	0.21	49,58,62,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	106	4/4	0.74	0.19	48,53,54,59	0
5	GOL	A	315	6/6	0.75	0.21	36,40,45,47	0
4	EDO	A	304	4/4	0.77	0.26	38,38,44,46	0
4	EDO	A	308	4/4	0.78	0.29	36,40,45,48	0
4	EDO	A	310	4/4	0.79	0.14	46,52,54,58	0
5	GOL	A	314	6/6	0.82	0.20	32,34,36,47	0
6	SO4	A	317	5/5	0.84	0.29	66,75,77,80	0
4	EDO	A	307	4/4	0.85	0.15	39,48,50,53	0
5	GOL	A	313	6/6	0.87	0.16	36,36,45,50	0
4	EDO	B	101	4/4	0.87	0.18	25,32,34,42	0
4	EDO	A	309	4/4	0.88	0.30	46,47,48,50	0
4	EDO	B	105	4/4	0.89	0.15	36,38,40,45	0
4	EDO	A	302	4/4	0.89	0.19	30,35,35,36	0
4	EDO	B	104	4/4	0.89	0.25	38,41,42,46	0
4	EDO	A	301	4/4	0.90	0.11	39,42,45,50	0
4	EDO	A	312	4/4	0.91	0.12	34,39,39,40	0
4	EDO	A	303	4/4	0.92	0.11	48,48,50,51	0
4	EDO	A	306	4/4	0.94	0.14	29,30,31,42	0
4	EDO	B	102	4/4	0.94	0.11	24,24,26,32	0
6	SO4	A	316	5/5	0.96	0.14	43,50,53,59	0
4	EDO	B	103	4/4	0.96	0.23	23,25,26,29	0
4	EDO	A	305	4/4	0.98	0.08	20,22,23,24	0

## 6.5 Other polymers

There are no such residues in this entry.