Full wwPDB X-ray Structure Validation Report (i)

Jun 2, 2016 – 04:34 AM EDT

PDB ID	:	5C0A
Title	:	1E6 TCR in complex with HLA-A02 carrying MVW peptide
Authors	:	Rizkallah, P.J.; Bulek, A.M.; Cole, D.K.; Sewell, A.K.
Deposited on	:	2015-06-12
Resolution	:	2.46 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

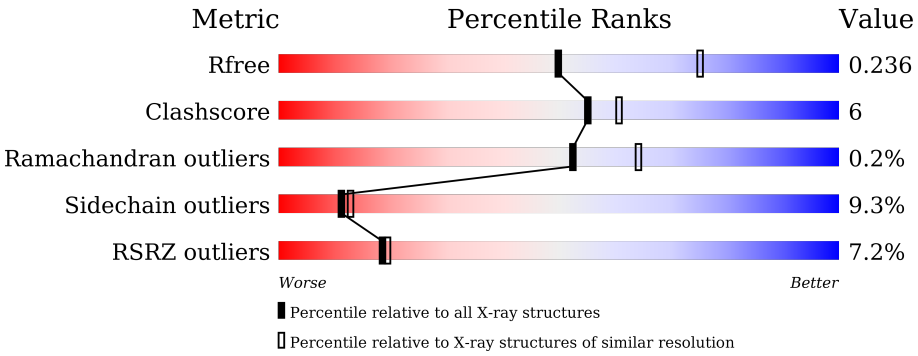
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027674
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027674

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 2.46 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}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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 >=3, 2, 1 and 0 types of geometric quality criteria. 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	276	4% 80% 17% •
1	F	276	5% 86% 11% •
2	B	100	2% 83% 14% •
2	G	100	% 88% 10% •
3	C	10	70% 30%
3	H	10	40% 80% 20%

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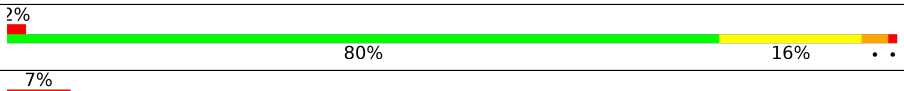
Mol	Chain	Length	Quality of chain
4	D	197	
4	I	197	
5	E	246	
5	J	246	

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	301	-	-	-	X
6	EDO	A	302	-	-	X	X
6	EDO	E	301	-	-	-	X
6	EDO	F	303	-	-	-	X
6	EDO	F	304	-	-	-	X
6	EDO	F	305	-	-	-	X
6	EDO	J	302	-	-	-	X
6	EDO	J	303	-	-	X	X
7	SO4	A	303	-	-	-	X
7	SO4	D	203	-	-	-	X
7	SO4	F	306	-	-	-	X
7	SO4	G	102	-	-	-	X
7	SO4	J	304	-	-	-	X
8	GOL	F	302	-	-	-	X
8	GOL	G	101	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13708 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
1	A	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	F	276	Total	C	N	O	S	0	2	0
			2273	1419	415	430	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	0	0
			837	533	141	159	4			
2	G	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called Marker peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	S	0	0	0
			83	57	11	14	1			
3	H	10	Total	C	N	O	S	0	0	0
			83	57	11	14	1			

- Molecule 4 is a protein called 1E6 TCR Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	197	Total	C	N	O	S	0	0	0
			1557	975	256	316	10			

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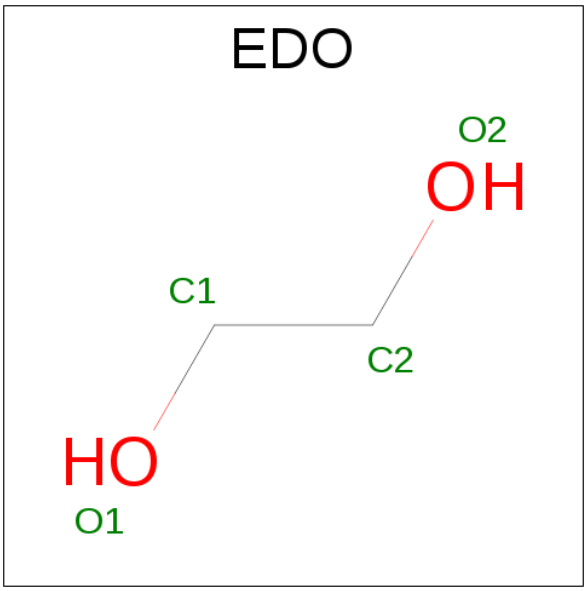
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	197	Total	C	N	O	S	0	0	0
			1557	975	256	316	10			

- Molecule 5 is a protein called 1E6 TCR Beta Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	246	Total	C	N	O	S	0	0	0
			1974	1249	341	374	10			
5	J	244	Total	C	N	O	S	0	0	0
			1961	1242	339	370	10			

- 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	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		

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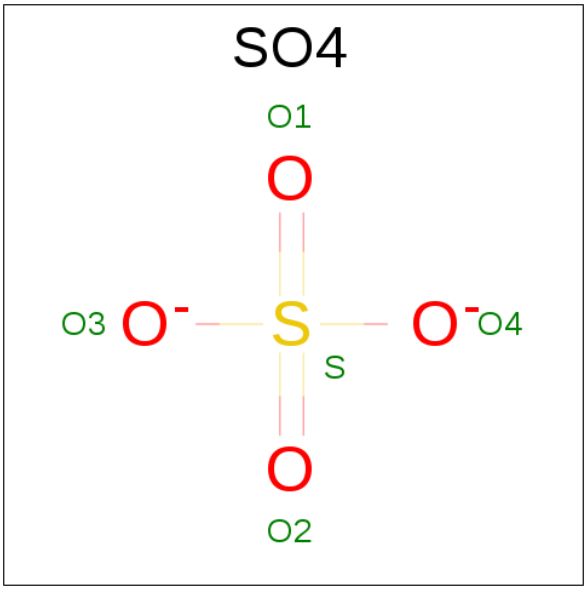
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total C O 4 2 2	0	0
6	F	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	I	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0

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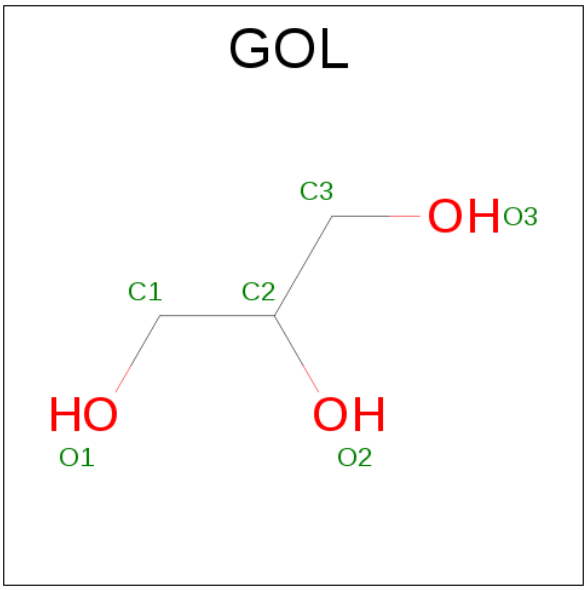
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total O S 5 4 1	0	0
7	F	1	Total O S 5 4 1	0	0
7	G	1	Total O S 5 4 1	0	0
7	J	1	Total O S 5 4 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 6 3 3	0	0
8	F	1	Total C O 6 3 3	0	0
8	F	1	Total C O 6 3 3	0	0
8	G	1	Total C O 6 3 3	0	0
8	J	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

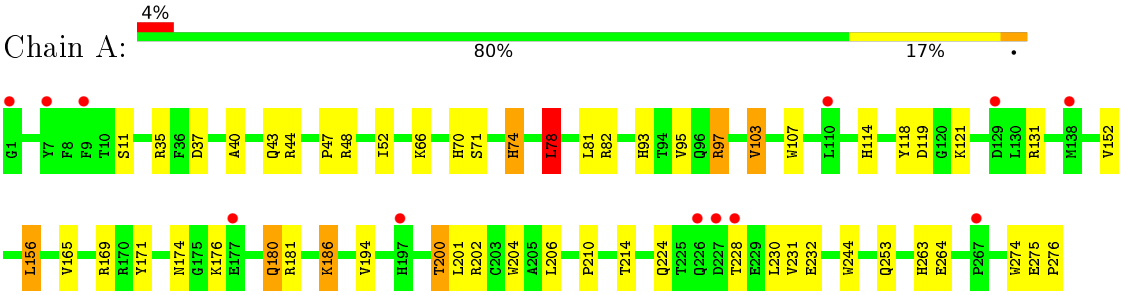
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	18	Total O 18 18	0	0
9	B	6	Total O 6 6	0	0
9	C	4	Total O 4 4	0	0
9	D	8	Total O 8 8	0	0
9	E	32	Total O 32 32	0	0
9	F	48	Total O 48 48	0	0
9	G	12	Total O 12 12	0	0
9	H	8	Total O 8 8	0	0
9	I	16	Total O 16 16	0	0
9	J	18	Total O 18 18	0	0

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 errors 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.

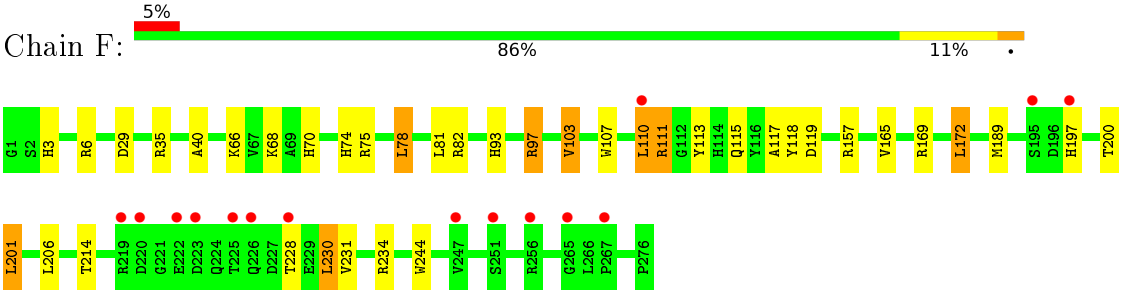
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain A:



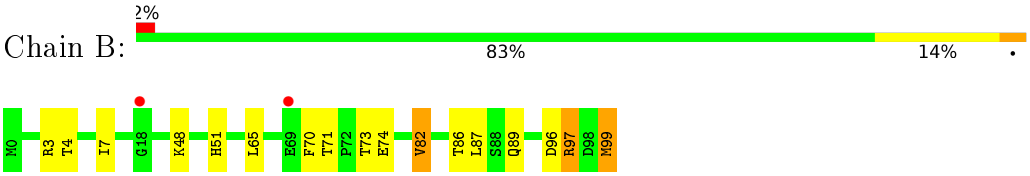
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain F:



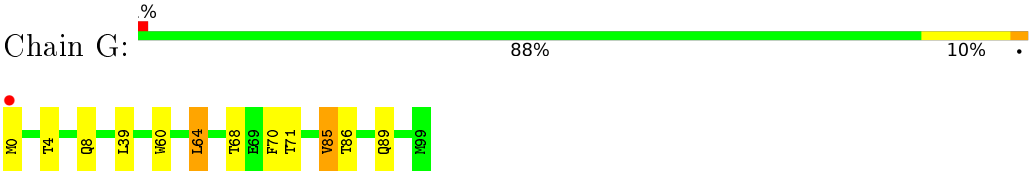
- Molecule 2: Beta-2-microglobulin

Chain B:



- Molecule 2: Beta-2-microglobulin

Chain G:

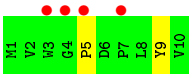


- Molecule 3: Marker peptide

Chain C:

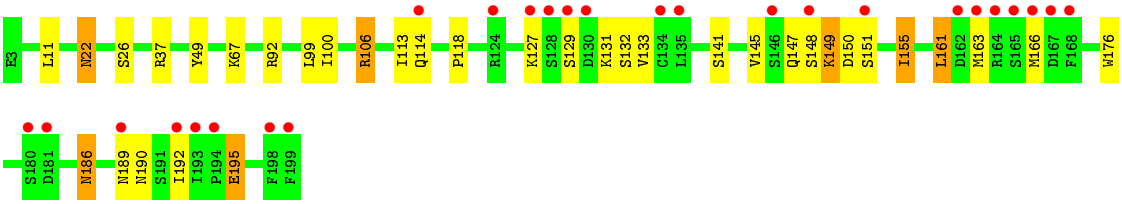
• Molecule 3: Marker peptide

Chain H:



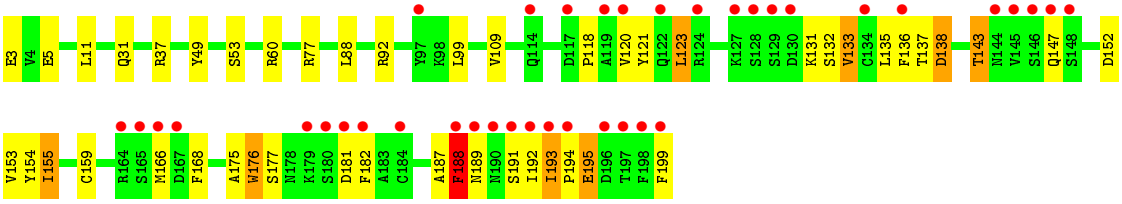
• Molecule 4: 1E6 TCR Alpha Chain

Chain D:



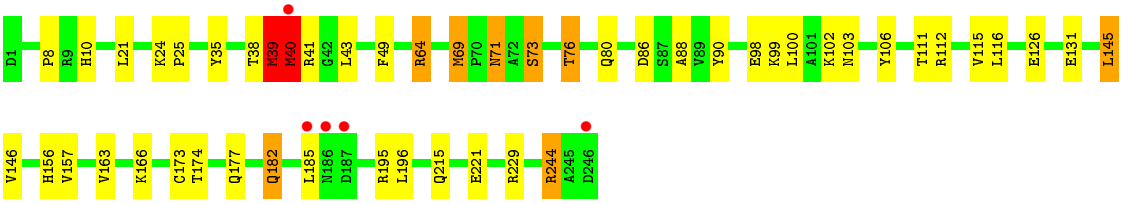
• Molecule 4: 1E6 TCR Alpha Chain

Chain I:



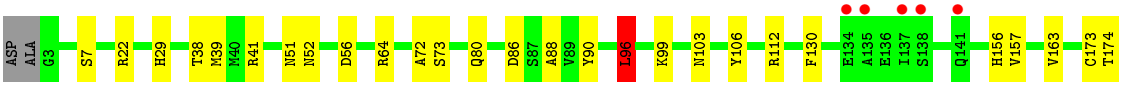
• Molecule 5: 1E6 TCR Beta Chain

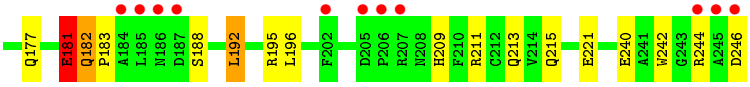
Chain E:



• Molecule 5: 1E6 TCR Beta Chain

Chain J:




Q177
E181
Q182
P183
A184
L185
N186
D187
S188
L192
R195
L196
F202
D205
P206
R207
N208
H209
F210
R211
C212
Q213
V214
Q215
E221
E240
A241
W242
G243
R244
A245
D246

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	43.88Å 100.02Å 123.28Å 96.67° 98.58° 95.80°	Depositor
Resolution (Å)	31.24 – 2.46 31.24 – 2.46	Depositor EDS
% Data completeness (in resolution range)	97.7 (31.24-2.46) 93.6 (31.24-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 2.45Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.232 0.196 , 0.236	Depositor DCC
R_{free} test set	3655 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13708	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, 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	0.67	1/2320 (0.0%)	0.86	6/3149 (0.2%)
1	F	0.73	0/2340	0.87	7/3176 (0.2%)
2	B	0.66	0/860	0.84	1/1162 (0.1%)
2	G	0.68	0/860	0.81	2/1162 (0.2%)
3	C	0.99	0/87	0.86	0/119
3	H	1.01	0/87	1.05	0/119
4	D	0.66	0/1592	0.85	3/2154 (0.1%)
4	I	0.67	0/1592	0.89	3/2154 (0.1%)
5	E	0.78	1/2029 (0.0%)	0.91	6/2759 (0.2%)
5	J	0.73	1/2016 (0.0%)	0.87	5/2741 (0.2%)
All	All	0.71	3/13783 (0.0%)	0.87	33/18695 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	I	0	5
5	E	0	2
5	J	0	1
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	73	SER	CB-OG	-6.91	1.33	1.42
5	E	98	GLU	CD-OE1	5.33	1.31	1.25
1	A	204	TRP	CB-CG	-5.31	1.40	1.50

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	97	ARG	NE-CZ-NH2	9.96	125.28	120.30
1	A	97	ARG	NE-CZ-NH1	-8.45	116.08	120.30
5	J	96	LEU	CA-CB-CG	7.77	133.16	115.30
5	E	173	CYS	CA-CB-SG	7.67	127.81	114.00
4	I	60	ARG	NE-CZ-NH2	7.66	124.13	120.30
2	G	64	LEU	CA-CB-CG	6.83	131.01	115.30
1	F	157	ARG	NE-CZ-NH1	6.42	123.51	120.30
4	I	37	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	131	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	F	157	ARG	NE-CZ-NH2	-5.85	117.37	120.30
2	B	3	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	82	ARG	NE-CZ-NH2	5.76	123.18	120.30
4	D	37	ARG	NE-CZ-NH2	-5.68	117.46	120.30
4	I	77	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	78	LEU	CB-CG-CD1	5.56	120.45	111.00
5	J	56	ASP	CB-CG-OD2	-5.52	113.34	118.30
1	F	75	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	G	85	VAL	CB-CA-C	-5.48	100.98	111.40
5	E	229	ARG	NE-CZ-NH1	5.37	122.99	120.30
5	E	64	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	F	230	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	156	LEU	CA-CB-CG	5.24	127.35	115.30
5	J	22	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	F	78	LEU	CB-CG-CD1	5.15	119.76	111.00
5	E	145	LEU	CA-CB-CG	5.13	127.11	115.30
5	E	76	THR	N-CA-CB	-5.09	100.63	110.30
5	J	56	ASP	CB-CG-OD1	5.08	122.88	118.30
5	J	192	LEU	CA-CB-CG	5.08	126.99	115.30
1	F	110	LEU	CA-CB-CG	5.08	126.98	115.30
4	D	100	ILE	CG1-CB-CG2	-5.08	100.23	111.40
5	E	64	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	F	97	ARG	NE-CZ-NH2	-5.02	117.79	120.30
4	D	161	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	39	MET	Peptide
5	E	40	MET	Peptide
4	I	137	THR	Peptide
4	I	152	ASP	Peptide
4	I	176	TRP	Peptide

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Mol	Chain	Res	Type	Group
4	I	181	ASP	Peptide
4	I	188	PHE	Peptide
5	J	181	GLU	Peptide

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	2254	0	2103	39	0
1	F	2273	0	2116	29	0
2	B	837	0	803	7	0
2	G	837	0	803	10	0
3	C	83	0	80	2	0
3	H	83	0	80	2	0
4	D	1557	0	1469	21	0
4	I	1557	0	1469	17	0
5	E	1974	0	1887	29	0
5	J	1961	0	1875	23	0
6	A	8	0	12	9	0
6	D	8	0	12	1	0
6	E	4	0	6	2	0
6	F	12	0	18	2	0
6	H	8	0	12	2	0
6	I	4	0	6	0	0
6	J	8	0	12	6	0
7	A	5	0	0	0	0
7	D	5	0	0	1	0
7	E	15	0	0	0	0
7	F	5	0	0	0	0
7	G	5	0	0	0	0
7	J	5	0	0	0	0
8	B	6	0	8	0	0
8	F	12	0	16	2	0
8	G	6	0	8	0	0
8	J	6	0	8	1	0
9	A	18	0	0	0	0
9	B	6	0	0	0	0
9	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	8	0	0	0	0
9	E	32	0	0	0	0
9	F	48	0	0	2	0
9	G	12	0	0	0	0
9	H	8	0	0	0	0
9	I	16	0	0	0	0
9	J	18	0	0	0	0
All	All	13708	0	12803	167	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 (167) 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:A:40:ALA:HB3	6:A:302:EDO:H11	1.53	0.90
1:A:40:ALA:HB3	6:A:302:EDO:C1	2.03	0.88
5:E:49:PHE:HB2	5:E:69:MET:HE1	1.63	0.81
3:H:5:PRO:HD2	6:H:102:EDO:H11	1.67	0.77
1:A:78:LEU:HD13	1:A:95:VAL:HG13	1.66	0.76
4:D:150:ASP:O	4:D:151:SER:OG	2.03	0.74
4:I:133:VAL:HG12	4:I:176:TRP:HB3	1.68	0.73
1:A:74:HIS:HE1	1:A:97:ARG:HH21	1.38	0.72
1:A:103:VAL:HG13	1:A:107:TRP:HA	1.72	0.71
1:F:82:ARG:HB2	8:F:302:GOL:H12	1.70	0.71
5:E:71:ASN:HD22	5:E:73:SER:H	1.39	0.71
1:F:103:VAL:HG13	1:F:107:TRP:HA	1.73	0.71
1:F:189:MET:CE	1:F:201:LEU:HG	2.21	0.70
5:J:211:ARG:HH12	5:J:213:GLN:HE21	1.39	0.69
4:D:106:ARG:HH11	4:D:106:ARG:HG3	1.58	0.69
4:I:123:LEU:HD12	4:I:133:VAL:O	1.91	0.69
1:A:107:TRP:O	1:A:169:ARG:NH1	2.26	0.69
5:J:181:GLU:O	5:J:188:SER:HB2	1.93	0.69
8:J:301:GOL:HO1	8:J:301:GOL:HO3	1.08	0.69
5:E:25:PRO:O	6:E:301:EDO:H12	1.95	0.67
4:I:3:GLU:HA	4:I:3:GLU:OE1	1.94	0.67
1:F:189:MET:HE3	1:F:201:LEU:HG	1.77	0.67
4:I:138:ASP:OD1	4:I:138:ASP:N	2.28	0.66
5:J:64:ARG:NH1	5:J:86:ASP:OD2	2.29	0.65
1:A:275:GLU:HG3	1:A:276:PRO:HD3	1.79	0.65
5:E:49:PHE:CG	5:E:69:MET:CE	2.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLU:CG	1:A:276:PRO:HD3	2.28	0.64
5:E:64:ARG:NH2	5:E:86:ASP:OD2	2.31	0.64
1:A:40:ALA:HB3	6:A:302:EDO:H12	1.78	0.64
1:A:165:VAL:CG1	1:A:169:ARG:NH2	2.61	0.63
1:A:43:GLN:HA	6:A:302:EDO:O1	1.99	0.63
1:F:3:HIS:HD2	1:F:29:ASP:OD2	1.81	0.62
5:E:35:TYR:HB3	5:E:43:LEU:HD22	1.82	0.62
2:G:4:THR:HG22	2:G:86:THR:CB	2.31	0.61
5:E:49:PHE:CB	5:E:69:MET:CE	2.78	0.61
1:A:37:ASP:O	6:A:302:EDO:H11	1.99	0.61
1:F:40:ALA:HB3	6:F:303:EDO:H12	1.83	0.61
5:J:51:ASN:HA	6:J:303:EDO:H11	1.83	0.61
1:A:171:TYR:O	1:A:174:ASN:O	2.20	0.60
5:E:49:PHE:CB	5:E:69:MET:HE1	2.31	0.59
5:J:188:SER:O	5:J:188:SER:OG	2.15	0.59
2:B:4:THR:HG22	2:B:86:THR:CB	2.32	0.59
1:A:74:HIS:CE1	1:A:97:ARG:HH21	2.20	0.59
4:D:149:LYS:HG3	4:D:150:ASP:O	2.02	0.59
5:E:49:PHE:CG	5:E:69:MET:HE3	2.39	0.58
1:A:165:VAL:HG12	1:A:169:ARG:NH2	2.19	0.57
2:B:73:THR:HG22	2:B:74:GLU:N	2.20	0.57
4:D:92:ARG:HE	5:E:103:ASN:HD21	1.52	0.57
1:F:6:ARG:NH2	1:F:113:TYR:OH	2.35	0.56
1:F:115[B]:GLN:HG3	2:G:60:TRP:CZ2	2.40	0.56
4:D:149:LYS:HE3	4:D:149:LYS:HA	1.87	0.56
1:F:74:HIS:HE1	1:F:97:ARG:HE	1.52	0.56
1:A:78:LEU:CD1	1:A:95:VAL:HG13	2.35	0.55
2:B:96:ASP:HB3	2:B:99:MET:HA	1.89	0.55
5:E:49:PHE:HB2	5:E:69:MET:CE	2.35	0.55
1:F:115[B]:GLN:CG	2:G:60:TRP:CZ2	2.91	0.54
1:A:43:GLN:N	6:A:302:EDO:O1	2.40	0.54
1:A:47:PRO:HB3	1:A:52:ILE:HD13	1.89	0.54
1:F:93:HIS:HE1	9:F:405:HOH:O	1.91	0.54
2:B:4:THR:HG22	2:B:86:THR:HB	1.89	0.54
4:D:186:ASN:C	4:D:186:ASN:HD22	2.11	0.53
2:G:4:THR:HG22	2:G:86:THR:HB	1.89	0.53
1:A:47:PRO:CB	1:A:52:ILE:CD1	2.86	0.53
1:F:115[B]:GLN:CG	2:G:60:TRP:HZ2	2.21	0.53
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.92	0.52
5:J:72:ALA:HB2	6:J:303:EDO:H12	1.90	0.52
5:J:29:HIS:HA	5:J:96:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:SER:HB2	6:A:301:EDO:H22	1.92	0.52
5:E:39:MET:N	5:E:39:MET:SD	2.83	0.51
1:A:253:GLN:OE1	1:A:253:GLN:N	2.43	0.51
1:F:234:ARG:HH11	2:G:8:GLN:NE2	2.08	0.51
1:A:210:PRO:O	1:A:263:HIS:HE1	1.94	0.51
5:E:24:LYS:HE3	6:E:301:EDO:H11	1.92	0.50
1:F:40:ALA:HB3	6:F:303:EDO:C1	2.40	0.50
1:F:231:VAL:CG1	1:F:244:TRP:CZ2	2.95	0.50
1:A:11:SER:HB2	1:A:95:VAL:HG22	1.93	0.50
1:A:66:LYS:O	1:A:70:HIS:HD2	1.95	0.49
4:D:147:GLN:HB3	4:D:155:ILE:HG12	1.94	0.49
5:E:38:THR:O	5:E:40:MET:O	2.30	0.49
1:F:66:LYS:O	1:F:70:HIS:HD2	1.96	0.49
5:J:240:GLU:OE1	5:J:242:TRP:CZ3	2.65	0.49
4:D:106:ARG:CG	4:D:106:ARG:HH11	2.24	0.49
4:D:133:VAL:HG23	4:D:176:TRP:HB3	1.94	0.49
5:E:10:HIS:HD2	5:E:156:HIS:ND1	2.11	0.49
1:A:97:ARG:HE	1:A:114:HIS:CE1	2.30	0.49
1:A:43:GLN:CA	6:A:302:EDO:O1	2.61	0.48
5:E:131:GLU:OE1	5:E:244:ARG:NH1	2.46	0.48
5:J:52:ASN:OD1	6:J:303:EDO:H22	2.13	0.48
4:I:187:ALA:O	4:I:189:ASN:N	2.45	0.48
5:E:88:ALA:HB3	5:E:90:TYR:CE1	2.48	0.48
1:F:93:HIS:HD2	1:F:119:ASP:OD2	1.97	0.48
1:F:68:LYS:NZ	9:F:403:HOH:O	2.41	0.47
4:D:113:ILE:HG23	4:D:113:ILE:O	2.14	0.47
1:A:274:TRP:CE2	1:A:276:PRO:HD2	2.50	0.47
1:A:232:GLU:N	1:A:232:GLU:OE1	2.45	0.47
1:F:165:VAL:CG1	1:F:169:ARG:NH2	2.78	0.47
1:A:44:ARG:O	6:A:302:EDO:H21	2.13	0.47
4:I:118:PRO:HB2	4:I:195:GLU:HB3	1.97	0.47
5:J:51:ASN:HA	6:J:303:EDO:C1	2.45	0.46
4:I:92:ARG:HE	5:J:103:ASN:HD21	1.64	0.46
4:D:147:GLN:OE1	4:D:148:SER:N	2.48	0.46
1:A:194:VAL:HG13	1:A:200:THR:OG1	2.15	0.46
4:D:147:GLN:CD	4:D:149:LYS:HB2	2.36	0.46
5:E:112:ARG:HG2	5:E:156:HIS:CE1	2.50	0.46
5:E:157:VAL:HA	5:E:215:GLN:O	2.16	0.46
5:J:99:LYS:HE3	5:J:106:TYR:OH	2.15	0.46
4:D:147:GLN:OE1	4:D:149:LYS:HB2	2.16	0.46
1:F:81:LEU:HD13	1:F:118:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:153:VAL:HA	4:I:176:TRP:O	2.15	0.46
5:J:88:ALA:HB3	5:J:90:TYR:CE1	2.51	0.46
5:E:49:PHE:CD2	5:E:69:MET:CE	2.99	0.45
4:I:133:VAL:HG22	5:J:130:PHE:CD2	2.52	0.45
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.52	0.45
5:E:99:LYS:HE3	5:E:106:TYR:OH	2.17	0.45
4:I:193:ILE:HB	4:I:194:PRO:HD3	1.98	0.45
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.52	0.44
1:F:115[B]:GLN:HG3	2:G:60:TRP:CH2	2.52	0.44
5:E:182:GLN:HG3	5:E:185:LEU:HD12	1.99	0.44
2:B:73:THR:CG2	2:B:74:GLU:N	2.81	0.44
1:A:47:PRO:CB	1:A:52:ILE:HD13	2.46	0.44
5:J:157:VAL:HA	5:J:215:GLN:O	2.18	0.44
2:B:7:ILE:HD13	2:B:82:VAL:CG1	2.48	0.44
4:D:147:GLN:OE1	4:D:149:LYS:N	2.50	0.44
1:F:231:VAL:HG11	1:F:244:TRP:CZ2	2.53	0.43
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.53	0.43
5:J:182:GLN:O	5:J:182:GLN:HG3	2.18	0.43
2:B:51:HIS:HA	2:B:65:LEU:O	2.19	0.43
4:D:11:LEU:HD22	7:D:203:SO4:O1	2.19	0.43
5:J:112:ARG:HG2	5:J:156:HIS:CE1	2.53	0.43
1:F:110:LEU:HD13	1:F:111:ARG:NH2	2.34	0.43
5:J:51:ASN:HA	6:J:303:EDO:C2	2.49	0.43
1:A:180:GLN:HB3	1:A:180:GLN:HE21	1.68	0.42
1:F:107:TRP:CH2	1:F:172:LEU:HB3	2.54	0.42
4:I:123:LEU:CD1	4:I:133:VAL:HG23	2.49	0.42
5:J:72:ALA:CB	6:J:303:EDO:H12	2.49	0.42
1:F:82:ARG:HB2	8:F:302:GOL:C1	2.44	0.42
1:F:74:HIS:CE1	1:F:97:ARG:HE	2.36	0.42
5:J:64:ARG:HH12	5:J:86:ASP:CG	2.23	0.42
5:E:64:ARG:HH22	5:E:86:ASP:CG	2.23	0.42
2:G:39:LEU:HD23	2:G:68:THR:HG22	2.02	0.42
1:A:47:PRO:HB3	1:A:52:ILE:CD1	2.49	0.42
1:A:156:LEU:HD13	3:C:3:TRP:CZ2	2.55	0.42
1:F:231:VAL:HG13	1:F:244:TRP:CZ2	2.55	0.42
5:E:49:PHE:CB	5:E:69:MET:HE3	2.50	0.42
1:A:176:LYS:HA	1:A:180:GLN:HG3	2.01	0.42
5:E:49:PHE:CD2	5:E:69:MET:HE2	2.54	0.41
5:J:211:ARG:HH12	5:J:213:GLN:NE2	2.13	0.41
1:A:186:LYS:N	1:A:186:LYS:HD2	2.35	0.41
1:F:115[B]:GLN:HG3	2:G:60:TRP:HZ2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:155:ILE:O	4:I:155:ILE:HD12	2.21	0.41
4:I:154:TYR:O	4:I:175:ALA:HA	2.20	0.41
4:D:22:ASN:C	4:D:22:ASN:HD22	2.24	0.41
4:D:163:MET:O	4:D:166:MET:O	2.38	0.41
5:E:8:PRO:O	5:E:111:THR:HG23	2.21	0.41
4:D:145:VAL:HG13	4:D:190:ASN:ND2	2.36	0.41
4:D:92:ARG:NE	5:E:103:ASN:HD21	2.17	0.41
6:D:201:EDO:HO2	5:E:103:ASN:HD22	1.65	0.41
4:I:123:LEU:HD12	4:I:133:VAL:HG23	2.03	0.41
4:D:118:PRO:HB2	4:D:195:GLU:HB3	2.03	0.41
4:I:166:MET:HG3	4:I:168:PHE:HB2	2.02	0.41
4:I:143:THR:HG22	4:I:192:ILE:HD11	2.03	0.41
3:C:4:GLY:HA2	3:C:5:PRO:C	2.41	0.40
3:H:9:TYR:CZ	6:H:101:EDO:H22	2.56	0.40
5:J:181:GLU:O	5:J:183:PRO:HD2	2.21	0.40
4:D:92:ARG:HE	5:E:103:ASN:ND2	2.17	0.40
4:I:188:PHE:HB3	4:I:189:ASN:ND2	2.36	0.40
5:J:240:GLU:OE1	5:J:242:TRP:CH2	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	274/276 (99%)	267 (97%)	7 (3%)	0	100	100
1	F	276/276 (100%)	270 (98%)	6 (2%)	0	100	100
2	B	98/100 (98%)	97 (99%)	0	1 (1%)	19	21
2	G	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
3	H	8/10 (80%)	8 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	195/197 (99%)	181 (93%)	14 (7%)	0	100 100
4	I	195/197 (99%)	174 (89%)	20 (10%)	1 (0%)	34 41
5	E	244/246 (99%)	235 (96%)	9 (4%)	0	100 100
5	J	242/246 (98%)	230 (95%)	11 (4%)	1 (0%)	39 49
All	All	1638/1658 (99%)	1567 (96%)	68 (4%)	3 (0%)	52 64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	188	PHE
2	B	97	ARG
5	J	39	MET

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	232/232 (100%)	213 (92%)	19 (8%)	14 18
1	F	234/232 (101%)	222 (95%)	12 (5%)	29 41
2	B	95/95 (100%)	87 (92%)	8 (8%)	14 17
2	G	95/95 (100%)	89 (94%)	6 (6%)	22 30
3	C	9/9 (100%)	9 (100%)	0	100 100
3	H	9/9 (100%)	9 (100%)	0	100 100
4	D	178/178 (100%)	159 (89%)	19 (11%)	8 8
4	I	178/178 (100%)	150 (84%)	28 (16%)	3 2
5	E	216/216 (100%)	191 (88%)	25 (12%)	7 7
5	J	215/216 (100%)	197 (92%)	18 (8%)	14 17
All	All	1461/1460 (100%)	1326 (91%)	135 (9%)	11 13

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	48	ARG
1	A	74	HIS
1	A	78	LEU
1	A	103	VAL
1	A	121	LYS
1	A	152	VAL
1	A	180	GLN
1	A	181	ARG
1	A	186	LYS
1	A	200	THR
1	A	201	LEU
1	A	206	LEU
1	A	214	THR
1	A	224	GLN
1	A	228	THR
1	A	230	LEU
1	A	231	VAL
1	A	264	GLU
2	B	48	LYS
2	B	70	PHE
2	B	71	THR
2	B	82	VAL
2	B	87	LEU
2	B	89	GLN
2	B	97	ARG
2	B	99	MET
4	D	22	ASN
4	D	26	SER
4	D	49	TYR
4	D	67	LYS
4	D	99	LEU
4	D	106	ARG
4	D	114	GLN
4	D	127	LYS
4	D	129	SER
4	D	131	LYS
4	D	132	SER
4	D	141	SER
4	D	149	LYS
4	D	155	ILE
4	D	161	LEU
4	D	186	ASN

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Mol	Chain	Res	Type
4	D	189	ASN
4	D	192	ILE
4	D	195	GLU
5	E	21	LEU
5	E	39	MET
5	E	40	MET
5	E	41	ARG
5	E	69	MET
5	E	71	ASN
5	E	73	SER
5	E	76	THR
5	E	80	GLN
5	E	100	LEU
5	E	102	LYS
5	E	115	VAL
5	E	116	LEU
5	E	126	GLU
5	E	145	LEU
5	E	146	VAL
5	E	163	VAL
5	E	166	LYS
5	E	174	THR
5	E	177	GLN
5	E	182	GLN
5	E	195	ARG
5	E	196	LEU
5	E	221	GLU
5	E	244	ARG
1	F	35	ARG
1	F	78	LEU
1	F	103	VAL
1	F	111	ARG
1	F	172	LEU
1	F	197	HIS
1	F	200	THR
1	F	201	LEU
1	F	206	LEU
1	F	214	THR
1	F	228	THR
1	F	230	LEU
2	G	0	MET
2	G	64	LEU

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Mol	Chain	Res	Type
2	G	70	PHE
2	G	71	THR
2	G	85	VAL
2	G	89	GLN
4	I	5	GLU
4	I	11	LEU
4	I	31	GLN
4	I	49	TYR
4	I	53	SER
4	I	88	LEU
4	I	99	LEU
4	I	109	VAL
4	I	120	VAL
4	I	121	TYR
4	I	123	LEU
4	I	131	LYS
4	I	132	SER
4	I	133	VAL
4	I	135	LEU
4	I	136	PHE
4	I	138	ASP
4	I	143	THR
4	I	147	GLN
4	I	155	ILE
4	I	159	CYS
4	I	177	SER
4	I	182	PHE
4	I	188	PHE
4	I	191	SER
4	I	193	ILE
4	I	195	GLU
4	I	199	PHE
5	J	7	SER
5	J	38	THR
5	J	41	ARG
5	J	80	GLN
5	J	96	LEU
5	J	163	VAL
5	J	173	CYS
5	J	174	THR
5	J	177	GLN
5	J	181	GLU

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Mol	Chain	Res	Type
5	J	182	GLN
5	J	192	LEU
5	J	195	ARG
5	J	196	LEU
5	J	209	HIS
5	J	221	GLU
5	J	244	ARG
5	J	246	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	70	HIS
1	A	74	HIS
1	A	86	ASN
1	A	87	GLN
1	A	93	HIS
1	A	114	HIS
1	A	174	ASN
1	A	180	GLN
1	A	226	GLN
1	A	242	GLN
1	A	255	GLN
1	A	263	HIS
2	B	8	GLN
2	B	17	ASN
2	B	24	ASN
2	B	42	ASN
2	B	84	HIS
2	B	89	GLN
4	D	22	ASN
4	D	186	ASN
5	E	10	HIS
5	E	51	ASN
5	E	71	ASN
5	E	103	ASN
5	E	141	GLN
5	E	208	ASN
5	E	235	GLN
1	F	3	HIS
1	F	70	HIS

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Mol	Chain	Res	Type
1	F	74	HIS
1	F	174	ASN
1	F	255	GLN
2	G	8	GLN
2	G	42	ASN
2	G	84	HIS
2	G	89	GLN
4	I	147	GLN
4	I	189	ASN
5	J	80	GLN
5	J	141	GLN
5	J	182	GLN
5	J	213	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 carbohydrates in this entry.

5.6 Ligand geometry

26 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	$\#\|Z\| > 2$
6	EDO	A	301	-	3,3,3	1.11	0	2,2,2	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	A	302	-	3,3,3	0.26	0	2,2,2	0.48	0
7	SO4	A	303	-	4,4,4	0.46	0	6,6,6	0.60	0
8	GOL	B	101	-	5,5,5	0.41	0	5,5,5	0.50	0
6	EDO	D	201	-	3,3,3	0.38	0	2,2,2	0.34	0
6	EDO	D	202	-	3,3,3	0.50	0	2,2,2	0.62	0
7	SO4	D	203	-	4,4,4	0.44	0	6,6,6	0.59	0
6	EDO	E	301	-	3,3,3	0.28	0	2,2,2	0.54	0
7	SO4	E	302	-	4,4,4	0.42	0	6,6,6	0.31	0
7	SO4	E	303	-	4,4,4	0.53	0	6,6,6	0.12	0
7	SO4	E	304	-	4,4,4	0.62	0	6,6,6	1.14	1 (16%)
8	GOL	F	301	-	5,5,5	0.45	0	5,5,5	0.32	0
8	GOL	F	302	-	5,5,5	0.86	0	5,5,5	2.04	2 (40%)
6	EDO	F	303	-	3,3,3	0.35	0	2,2,2	0.39	0
6	EDO	F	304	-	3,3,3	0.53	0	2,2,2	0.59	0
6	EDO	F	305	-	3,3,3	0.77	0	2,2,2	0.43	0
7	SO4	F	306	-	4,4,4	0.49	0	6,6,6	0.18	0
8	GOL	G	101	-	5,5,5	0.27	0	5,5,5	0.38	0
7	SO4	G	102	-	4,4,4	0.51	0	6,6,6	0.59	0
6	EDO	H	101	-	3,3,3	0.43	0	2,2,2	0.14	0
6	EDO	H	102	-	3,3,3	0.39	0	2,2,2	0.48	0
6	EDO	I	201	-	3,3,3	0.57	0	2,2,2	0.20	0
8	GOL	J	301	-	5,5,5	0.38	0	5,5,5	0.60	0
6	EDO	J	302	-	3,3,3	0.51	0	2,2,2	0.18	0
6	EDO	J	303	-	3,3,3	0.68	0	2,2,2	0.32	0
7	SO4	J	304	-	4,4,4	0.54	0	6,6,6	0.32	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	301	-	-	0/1/1/1	0/0/0/0
6	EDO	A	302	-	-	0/1/1/1	0/0/0/0
7	SO4	A	303	-	-	0/0/0/0	0/0/0/0
8	GOL	B	101	-	-	0/4/4/4	0/0/0/0
6	EDO	D	201	-	-	0/1/1/1	0/0/0/0
6	EDO	D	202	-	-	0/1/1/1	0/0/0/0
7	SO4	D	203	-	-	0/0/0/0	0/0/0/0
6	EDO	E	301	-	-	0/1/1/1	0/0/0/0
7	SO4	E	302	-	-	0/0/0/0	0/0/0/0
7	SO4	E	303	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SO4	E	304	-	-	0/0/0/0	0/0/0/0
8	GOL	F	301	-	-	0/4/4/4	0/0/0/0
8	GOL	F	302	-	-	0/4/4/4	0/0/0/0
6	EDO	F	303	-	-	0/1/1/1	0/0/0/0
6	EDO	F	304	-	-	0/1/1/1	0/0/0/0
6	EDO	F	305	-	-	0/1/1/1	0/0/0/0
7	SO4	F	306	-	-	0/0/0/0	0/0/0/0
8	GOL	G	101	-	-	0/4/4/4	0/0/0/0
7	SO4	G	102	-	-	0/0/0/0	0/0/0/0
6	EDO	H	101	-	-	0/1/1/1	0/0/0/0
6	EDO	H	102	-	-	0/1/1/1	0/0/0/0
6	EDO	I	201	-	-	0/1/1/1	0/0/0/0
8	GOL	J	301	-	-	0/4/4/4	0/0/0/0
6	EDO	J	302	-	-	0/1/1/1	0/0/0/0
6	EDO	J	303	-	-	0/1/1/1	0/0/0/0
7	SO4	J	304	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	304	SO4	O4-S-O3	-2.33	99.72	109.09
8	F	302	GOL	O1-C1-C2	2.57	123.03	109.97
8	F	302	GOL	O3-C3-C2	2.78	124.06	109.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	301	EDO	1	0
6	A	302	EDO	8	0
6	D	201	EDO	1	0
7	D	203	SO4	1	0
6	E	301	EDO	2	0
8	F	302	GOL	2	0
6	F	303	EDO	2	0
6	H	101	EDO	1	0
6	H	102	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	J	301	GOL	1	0
6	J	303	EDO	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	276/276 (100%)	0.25	12 (4%) 39 43	34, 68, 112, 124	0
1	F	276/276 (100%)	0.18	15 (5%) 29 32	32, 55, 117, 140	0
2	B	100/100 (100%)	-0.02	2 (2%) 68 71	41, 65, 89, 102	0
2	G	100/100 (100%)	-0.11	1 (1%) 84 86	34, 57, 86, 107	0
3	C	10/10 (100%)	0.71	0 100 100	36, 43, 51, 61	0
3	H	10/10 (100%)	1.25	4 (40%) 0 0	33, 37, 43, 46	0
4	D	197/197 (100%)	0.63	26 (13%) 4 4	37, 69, 133, 152	0
4	I	197/197 (100%)	1.01	38 (19%) 2 1	34, 70, 152, 179	0
5	E	246/246 (100%)	-0.01	5 (2%) 68 71	27, 57, 103, 130	0
5	J	244/246 (99%)	0.30	16 (6%) 22 23	30, 67, 132, 176	0
All	All	1656/1658 (99%)	0.31	119 (7%) 18 19	27, 62, 128, 179	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	165	SER	11.4
5	J	184	ALA	10.6
5	J	246	ASP	8.8
4	I	199	PHE	8.3
4	I	128	SER	7.6
5	E	246	ASP	7.5
4	I	166	MET	7.1
4	I	182	PHE	6.7
4	I	165	SER	6.3
4	D	128	SER	6.0
4	I	198	PHE	5.9
4	I	134	CYS	5.6
4	I	196	ASP	5.6

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Mol	Chain	Res	Type	RSRZ
4	I	148	SER	5.5
4	D	166	MET	5.4
4	D	148	SER	5.3
4	D	198	PHE	5.2
4	D	192	ILE	5.0
5	J	137	ILE	5.0
5	J	245	ALA	4.9
4	I	190	ASN	4.7
4	D	181	ASP	4.6
5	J	185	LEU	4.6
4	D	162	ASP	4.6
4	I	127	LYS	4.5
4	I	167	ASP	4.4
4	D	164	ARG	4.4
4	D	146	SER	4.4
4	D	194	PRO	4.3
5	J	138	SER	4.2
1	A	197	HIS	4.0
1	F	197	HIS	4.0
4	I	164	ARG	4.0
5	J	186	ASN	3.9
4	D	180	SER	3.8
1	F	110	LEU	3.8
1	F	265	GLY	3.7
5	E	187	ASP	3.7
5	E	186	ASN	3.7
5	J	141	GLN	3.7
4	D	193	ILE	3.6
5	J	134	GLU	3.6
4	I	130	ASP	3.6
4	I	197	THR	3.5
5	J	206	PRO	3.5
4	I	146	SER	3.4
4	D	124	ARG	3.4
4	I	124	ARG	3.4
4	I	194	PRO	3.4
4	I	181	ASP	3.4
4	D	199	PHE	3.4
4	D	129	SER	3.3
4	D	163	MET	3.3
4	I	179	LYS	3.3
4	D	167	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
4	I	145	VAL	3.2
1	F	267	PRO	3.2
4	I	188	PHE	3.1
4	D	130	ASP	3.1
4	I	191	SER	3.1
4	I	147	GLN	3.1
4	I	184	CYS	3.0
2	G	0	MET	3.0
4	I	114	GLN	3.0
4	D	168	PHE	3.0
4	D	114	GLN	3.0
4	D	151	SER	2.9
4	D	134	CYS	2.9
5	J	135	ALA	2.9
4	D	135	LEU	2.9
4	I	120	VAL	2.9
4	I	129	SER	2.9
4	D	189	ASN	2.8
1	A	177	GLU	2.7
4	I	136	PHE	2.7
1	A	228	THR	2.6
1	F	228	THR	2.6
1	F	226	GLN	2.6
1	A	7	TYR	2.6
4	I	192	ILE	2.6
1	F	223	ASP	2.6
1	F	219	ARG	2.6
1	F	222	GLU	2.6
4	I	144	ASN	2.5
5	J	202	PHE	2.5
1	A	267	PRO	2.5
1	F	256	ARG	2.5
1	F	225	THR	2.5
5	J	205	ASP	2.5
4	I	117	ASP	2.5
1	A	226	GLN	2.5
1	F	251	SER	2.5
5	J	244	ARG	2.5
4	I	122	GLN	2.4
4	I	119	ALA	2.3
1	F	247	VAL	2.3
5	E	40	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	129	ASP	2.3
4	D	127	LYS	2.3
3	H	3	TRP	2.3
1	A	1	GLY	2.2
5	E	185	LEU	2.2
1	A	227	ASP	2.2
3	H	4	GLY	2.2
1	A	9	PHE	2.2
4	I	189	ASN	2.2
1	A	110	LEU	2.2
4	I	180	SER	2.2
5	J	207	ARG	2.1
3	H	5	PRO	2.1
3	H	7	PRO	2.1
2	B	18	GLY	2.1
1	F	195	SER	2.1
5	J	187	ASP	2.1
2	B	69	GLU	2.1
1	F	220	ASP	2.1
4	I	193	ILE	2.0
1	A	138	MET	2.0
4	I	97	TYR	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
6	EDO	F	303	4/4	0.92	0.61	14.61	44,65,67,69	0
8	GOL	F	302	6/6	0.91	0.41	13.76	43,55,59,60	0
6	EDO	E	301	4/4	0.97	0.30	12.82	55,58,59,60	0
7	SO4	A	303	5/5	0.91	0.44	6.73	66,104,108,113	0
6	EDO	A	302	4/4	0.97	0.35	6.61	44,48,51,54	0
8	GOL	G	101	6/6	0.81	0.36	6.42	73,78,92,95	0
6	EDO	A	301	4/4	0.74	0.33	6.06	62,69,69,75	0
7	SO4	D	203	5/5	0.89	0.28	5.78	78,92,100,115	0
7	SO4	F	306	5/5	0.86	0.30	5.48	107,116,121,126	0
6	EDO	F	304	4/4	0.90	0.26	4.68	57,57,58,61	0
6	EDO	J	302	4/4	0.97	0.40	4.65	46,49,52,53	0
6	EDO	F	305	4/4	0.68	0.33	3.78	65,72,78,80	0
6	EDO	J	303	4/4	0.90	0.21	3.38	50,56,57,57	0
7	SO4	J	304	5/5	0.78	0.34	2.58	115,117,133,140	0
7	SO4	G	102	5/5	0.76	0.23	2.08	107,112,132,134	0
8	GOL	J	301	6/6	0.90	0.24	1.93	54,78,88,90	0
8	GOL	B	101	6/6	0.87	0.20	1.77	73,77,79,82	0
7	SO4	E	303	5/5	0.87	0.23	1.74	105,107,112,114	0
6	EDO	I	201	4/4	0.84	0.23	1.17	76,81,83,84	0
6	EDO	D	201	4/4	0.98	0.22	1.13	42,44,46,47	0
6	EDO	D	202	4/4	0.93	0.18	0.26	65,66,68,69	0
6	EDO	H	101	4/4	0.96	0.20	-0.14	44,46,51,54	0
6	EDO	H	102	4/4	0.97	0.25	-0.40	45,53,54,55	0
7	SO4	E	304	5/5	0.96	0.11	-0.73	58,59,63,66	0
8	GOL	F	301	6/6	0.69	0.34	-	62,74,81,84	0
7	SO4	E	302	5/5	0.85	0.32	-	114,115,127,129	0

6.5 Other polymers (i)

There are no such residues in this entry.