Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:05 pm BST

PDB ID	:	5C07
Title	:	1E6 TCR in complex with HLA-A02 carrying YQFGPDFPIA
Authors	:	Rizkallah, P.J.; Bulek, A.M.; Cole, D.K.; Sewell, A.K.
Deposited on	:	2015-06-12
Resolution	:	2.11 Å(reported)

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

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

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

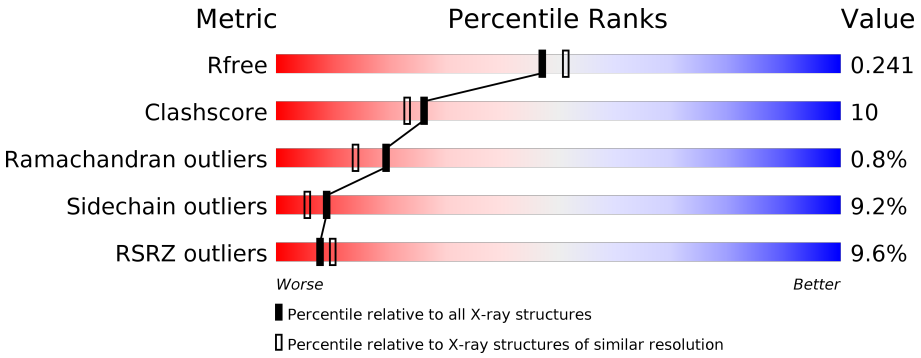
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	277	3% 82% 15%
1	F	277	4% 81% 17%
2	B	100	83% 16%
2	G	100	79% 20%
3	C	10	100%
3	H	10	90% 10%

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Mol	Chain	Length	Quality of chain
4	D	199	26% 59% 29% 10%
4	I	199	21% 69% 24% 7%
5	E	246	14% 77% 19%
5	J	246	5% 82% 15%

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	SO4	F	305	-	-	X	-
8	GOL	F	302	-	X	X	-
8	GOL	H	101	-	X	-	-
8	GOL	J	302	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14183 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	277	Total	C	N	O	S	0	5	0
			2303	1438	419	436	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01892
F	0	MET	-	initiating methionine	UNP P01892

- 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	0	0	0
			83	57	11	15			
3	H	10	Total	C	N	O	0	0	0
			83	57	11	15			

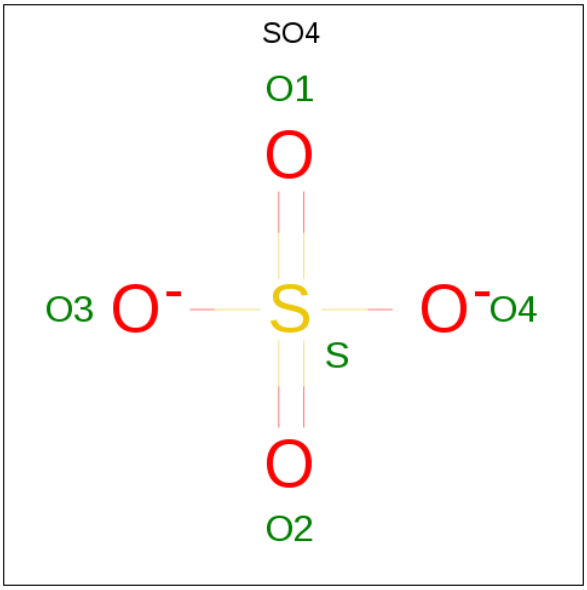
- Molecule 4 is a protein called 1E6 TCR Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	199	Total	C	N	O	S	0	1	0
			1579	989	260	320	10			
4	I	199	Total	C	N	O	S	0	1	0
			1579	989	260	320	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	1	0
			1985	1255	345	375	10			
5	J	246	Total	C	N	O	S	0	1	0
			1985	1255	345	375	10			

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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			
6	D	1	Total	O	S		0	0
			5	4	1			
6	F	1	Total	O	S		0	0
			5	4	1			
6	I	1	Total	O	S		0	0
			5	4	1			

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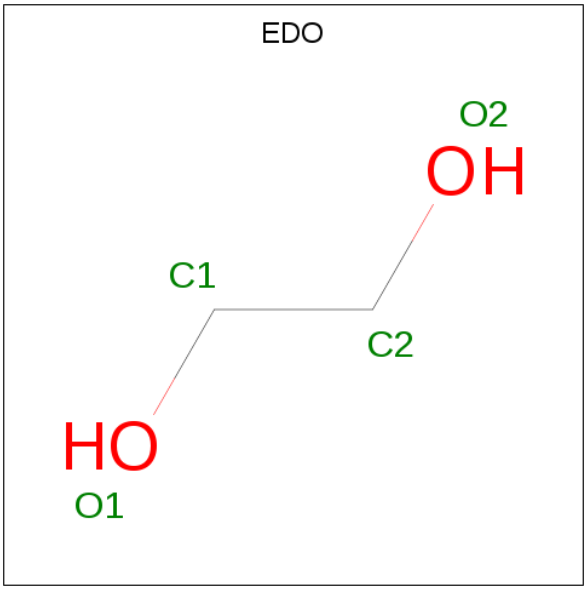
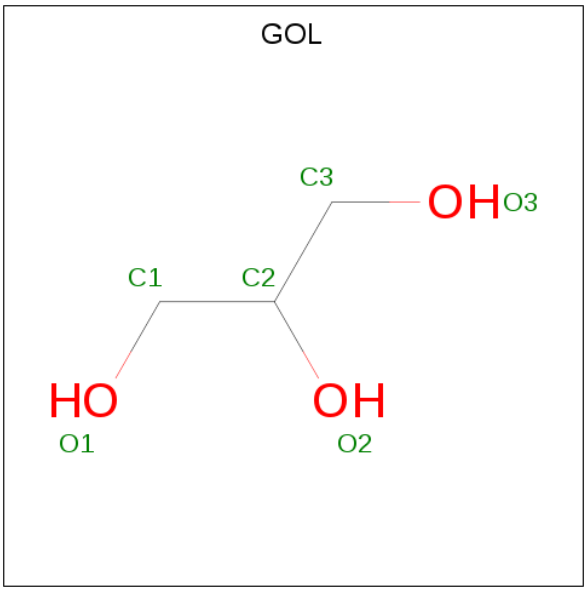
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total O S 5 4 1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	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
7	F	1	Total C O 4 2 2	0	0
7	G	1	Total C O 4 2 2	0	0
7	G	1	Total C O 4 2 2	0	0
7	I	1	Total C O 4 2 2	0	0
7	I	1	Total C O 4 2 2	0	0
7	J	1	Total C O 4 2 2	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	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	H	1	Total C O 6 3 3	0	0
8	I	1	Total C O 6 3 3	0	0
8	J	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	90	Total O 90 90	0	0
9	B	42	Total O 42 42	0	0
9	C	6	Total O 6 6	0	0
9	D	51	Total O 51 51	0	0
9	E	73	Total O 73 73	0	0

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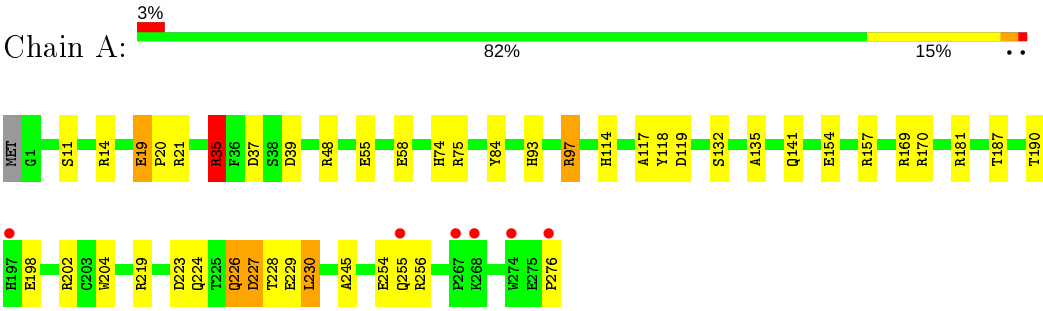
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	103	Total O 103 103	0	0
9	G	49	Total O 49 49	0	0
9	H	7	Total O 7 7	0	0
9	I	46	Total O 46 46	0	0
9	J	83	Total O 83 83	0	0

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 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.

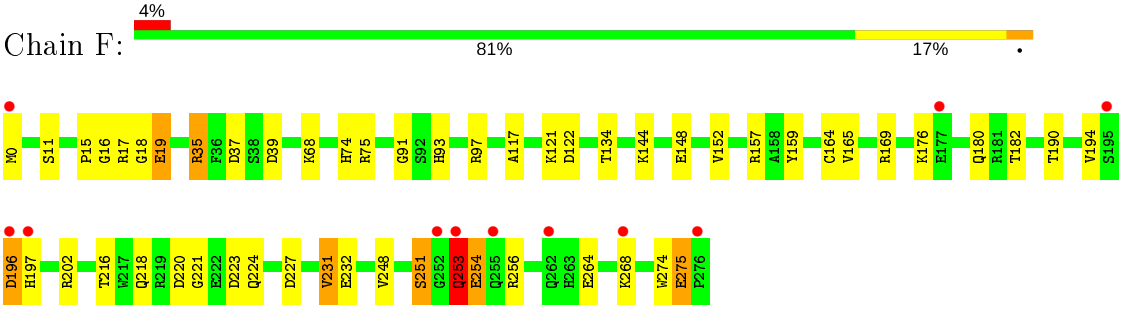
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain A:



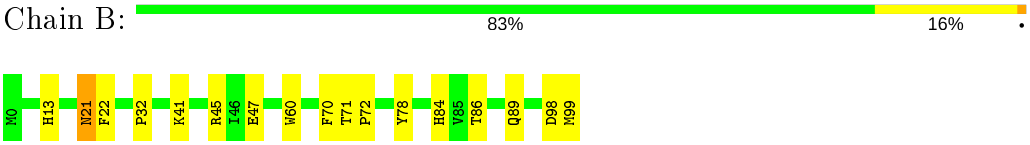
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain F:



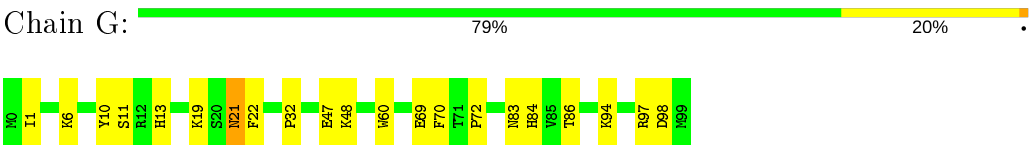
- Molecule 2: Beta-2-microglobulin

Chain B:



- Molecule 2: Beta-2-microglobulin

Chain G:



- Molecule 3: Marker peptide

Chain C:

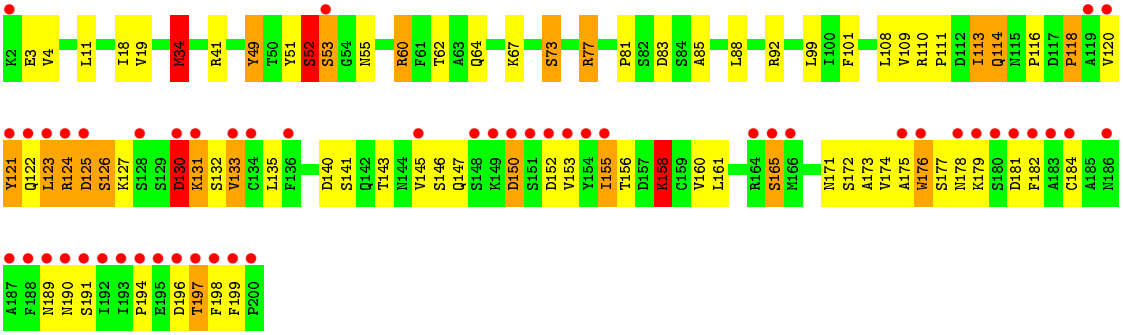
There are no outlier residues recorded for this chain.

- Molecule 3: Marker peptide

Chain H:

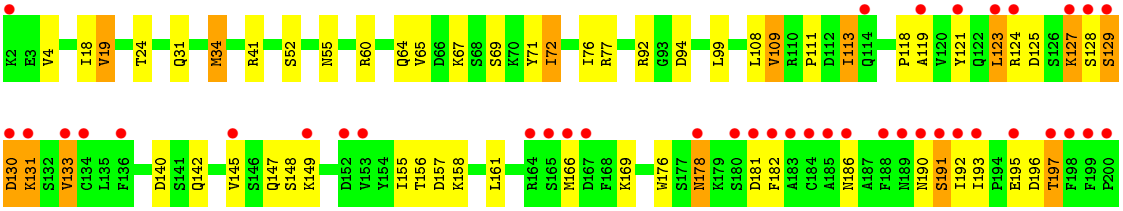
- Molecule 4: 1E6 TCR Alpha Chain

Chain D:



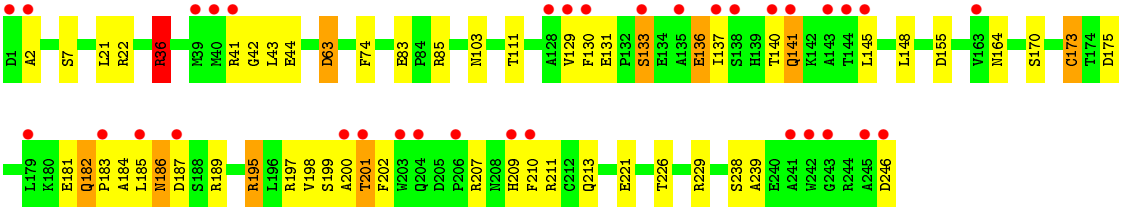
- Molecule 4: 1E6 TCR Alpha Chain

Chain I:



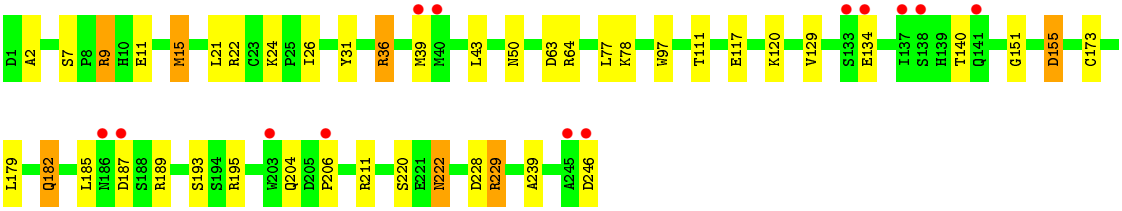
- Molecule 5: 1E6 TCR Beta Chain

Chain E:



- Molecule 5: 1E6 TCR Beta Chain

Chain J:


D1
A2
S7
P8
R9
H10
E11
M15
L21
R22
C23
K24
P25
I26
Y31
R36
M39
M40
L43
N50
D63
R64
L77
K78
W97
T111
E117
K120
V129
S133
E134
I137
S138
H139
T140
Q141
G151
D155
C173
L179
Q182
L185
N186
D187
S188
R189
S193
S194
R195
W203
Q204
D205
P206
R211
S220
E221
N222
D228
R229
A239
A245
D246

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	43.70Å 100.47Å 122.10Å 96.95° 98.11° 96.61°	Depositor
Resolution (Å)	49.41 – 2.11 49.41 – 2.11	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.41-2.11) 97.0 (49.41-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.191 , 0.237 0.197 , 0.241	Depositor DCC
R_{free} test set	5674 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14183	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.90	4/2320 (0.2%)	0.99	10/3149 (0.3%)
1	F	0.89	1/2369 (0.0%)	1.02	13/3215 (0.4%)
2	B	0.86	0/860	0.93	2/1162 (0.2%)
2	G	0.89	0/860	0.88	0/1162
3	C	1.03	0/87	0.86	0/117
3	H	1.01	0/87	0.81	0/117
4	D	0.86	2/1615 (0.1%)	1.11	9/2185 (0.4%)
4	I	0.88	0/1615	1.04	9/2185 (0.4%)
5	E	0.87	0/2040	1.00	4/2773 (0.1%)
5	J	0.92	2/2040 (0.1%)	0.99	9/2773 (0.3%)
All	All	0.89	9/13893 (0.1%)	1.00	56/18838 (0.3%)

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
1	A	0	1
1	F	0	2
4	D	0	4
4	I	0	1
5	E	0	2
All	All	0	10

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	64	ARG	N-CA	6.03	1.58	1.46
1	A	97	ARG	CZ-NH2	-5.49	1.25	1.33
1	A	84	TYR	CE1-CZ	5.34	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	31	TYR	CE1-CZ	-5.27	1.31	1.38
4	D	73	SER	CB-OG	-5.22	1.35	1.42
1	F	16	GLY	N-CA	5.20	1.53	1.46
1	A	14	ARG	C-O	5.12	1.33	1.23
4	D	158	LYS	N-CA	5.10	1.56	1.46
1	A	118	TYR	CB-CG	5.09	1.59	1.51

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	35	ARG	NE-CZ-NH1	12.63	126.61	120.30
4	D	60	ARG	NE-CZ-NH1	11.01	125.80	120.30
1	F	35	ARG	NE-CZ-NH2	-10.99	114.81	120.30
4	D	60	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	A	97	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	A	97	ARG	NE-CZ-NH2	-8.96	115.82	120.30
4	I	60	ARG	NE-CZ-NH2	-7.98	116.31	120.30
5	E	229	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	37	ASP	CB-CG-OD1	7.68	125.21	118.30
5	E	36	ARG	NE-CZ-NH1	7.44	124.02	120.30
4	D	92	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	F	97	ARG	NE-CZ-NH1	-7.21	116.70	120.30
4	D	92	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	F	97	ARG	NE-CZ-NH2	7.14	123.87	120.30
5	E	229	ARG	NE-CZ-NH1	7.12	123.86	120.30
4	D	77	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	37	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	F	202	ARG	NE-CZ-NH2	-6.58	117.01	120.30
4	I	77	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	F	39	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	75	ARG	NE-CZ-NH1	6.57	123.58	120.30
4	D	77	ARG	NE-CZ-NH2	-6.51	117.04	120.30
5	J	63	ASP	C-N-CA	-6.51	105.42	121.70
4	I	92	ARG	NE-CZ-NH1	6.32	123.46	120.30
4	I	60	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	181	ARG	NE-CZ-NH2	6.13	123.36	120.30
4	I	123	LEU	CA-CB-CG	6.07	129.25	115.30
1	A	35	ARG	NE-CZ-NH1	6.01	123.30	120.30
4	D	34	MET	CG-SD-CE	-6.00	90.60	100.20
5	J	36	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	F	15	PRO	C-N-CA	-5.88	109.95	122.30
5	J	63	ASP	O-C-N	-5.82	113.39	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	75	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	F	39	ASP	CB-CG-OD1	5.74	123.46	118.30
5	E	63	ASP	N-CA-C	5.72	126.45	111.00
5	J	211	ARG	NE-CZ-NH1	-5.71	117.45	120.30
5	J	15	MET	CG-SD-CE	5.69	109.30	100.20
5	J	155	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	A	35	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	F	37	ASP	CB-CG-OD1	5.48	123.23	118.30
5	J	229	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	39	ASP	CB-CG-OD1	5.41	123.17	118.30
1	F	35	ARG	CD-NE-CZ	5.38	131.13	123.60
4	I	34	MET	CA-CB-CG	5.37	122.43	113.30
4	D	41	ARG	NE-CZ-NH1	5.33	122.97	120.30
5	J	22[A]	ARG	NE-CZ-NH1	-5.32	117.64	120.30
5	J	22[B]	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	F	157	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	157	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	B	99	MET	N-CA-C	5.22	125.08	111.00
4	I	34	MET	CB-CG-SD	5.21	128.04	112.40
4	D	83	ASP	CB-CG-OD1	5.19	122.97	118.30
4	I	94	ASP	CB-CG-OD1	5.17	122.96	118.30
1	F	231	VAL	CB-CA-C	-5.09	101.72	111.40
4	I	77	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	B	45	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	ASP	Peptide
4	D	130	ASP	Peptide
4	D	152	ASP	Peptide
4	D	165	SER	Peptide
4	D	52	SER	Peptide
5	E	182	GLN	Peptide
5	E	201	THR	Peptide
1	F	194	VAL	Peptide
1	F	196	ASP	Peptide
4	I	196	ASP	Peptide

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	2254	0	2103	26	0
1	F	2303	0	2151	38	0
2	B	837	0	803	9	0
2	G	837	0	803	16	0
3	C	83	0	74	0	0
3	H	83	0	74	2	0
4	D	1579	0	1493	87	0
4	I	1579	0	1493	43	0
5	E	1985	0	1899	55	0
5	J	1985	0	1899	32	0
6	A	10	0	0	0	0
6	D	5	0	0	1	0
6	F	5	0	0	2	0
6	I	5	0	0	0	0
6	J	5	0	0	0	0
7	B	4	0	6	0	0
7	D	4	0	6	0	0
7	E	4	0	6	0	0
7	F	4	0	6	0	0
7	G	8	0	12	2	0
7	I	8	0	12	0	0
7	J	4	0	6	0	0
8	F	18	0	24	10	0
8	H	6	0	7	0	0
8	I	6	0	8	2	0
8	J	12	0	16	7	0
9	A	90	0	0	4	0
9	B	42	0	0	0	0
9	C	6	0	0	0	0
9	D	51	0	0	5	0
9	E	73	0	0	6	0
9	F	103	0	0	2	0
9	G	49	0	0	1	0
9	H	7	0	0	0	0
9	I	46	0	0	0	0
9	J	83	0	0	2	0
All	All	14183	0	12901	275	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 10.

All (275) 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)
5:J:97:TRP:HB2	8:J:301:GOL:H11	1.29	1.13
4:D:18:ILE:H	4:I:64:GLN:HE22	1.06	1.00
4:D:113:ILE:H	4:D:113:ILE:HD13	1.26	1.00
4:D:121:TYR:HD2	5:E:136:GLU:HB3	1.34	0.92
4:I:55:ASN:HD21	4:I:64:GLN:HE21	1.19	0.90
4:D:121:TYR:CD2	5:E:133:SER:HB3	2.07	0.90
5:J:97:TRP:HB2	8:J:301:GOL:C1	2.02	0.88
1:A:194:VAL:O	1:A:196:ASP:N	2.08	0.86
1:F:93:HIS:HB2	8:F:302:GOL:C3	2.06	0.85
4:I:113:ILE:HD13	4:I:113:ILE:H	1.38	0.85
4:D:126:SER:HB3	9:D:410:HOH:O	1.76	0.84
4:I:55:ASN:HD21	4:I:64:GLN:NE2	1.74	0.84
4:D:64:GLN:HE22	4:I:18:ILE:H	1.26	0.83
2:G:21:ASN:HD22	2:G:22:PHE:H	1.24	0.82
5:E:43:LEU:C	5:E:43:LEU:HD23	2.00	0.82
4:I:52:SER:O	4:I:67:LYS:HD2	1.80	0.81
5:J:15:MET:CE	5:J:117:GLU:HA	2.11	0.81
5:J:97:TRP:CB	8:J:301:GOL:H11	2.09	0.80
4:D:62:THR:OG1	4:D:77:ARG:NH2	2.16	0.79
5:E:202:PHE:HD1	9:E:408:HOH:O	1.64	0.78
4:I:113:ILE:CD1	4:I:113:ILE:H	1.95	0.78
4:D:113:ILE:H	4:D:113:ILE:CD1	1.96	0.78
1:F:251:SER:OG	1:F:254:GLU:OE1	2.01	0.78
5:E:43:LEU:HD23	5:E:44:GLU:N	2.00	0.76
5:J:15:MET:HE2	5:J:117:GLU:HA	1.66	0.76
1:F:197:HIS:CD2	1:F:251:SER:HA	2.21	0.75
5:J:222:ASN:H	5:J:222:ASN:HD22	1.34	0.75
4:I:55:ASN:ND2	4:I:64:GLN:HE21	1.83	0.75
2:B:13:HIS:H	2:B:21:ASN:HD21	1.33	0.75
2:B:21:ASN:HD22	2:B:22:PHE:H	1.33	0.75
4:D:121:TYR:CE1	4:D:123:LEU:HG	2.21	0.74
4:D:121:TYR:HD2	5:E:136:GLU:CB	2.00	0.74
1:F:93:HIS:CD2	8:F:302:GOL:H31	2.23	0.73
1:F:93:HIS:HB2	8:F:302:GOL:H31	1.69	0.73
5:E:83:GLU:OE1	5:E:85:ARG:NH1	2.23	0.72
4:I:65:VAL:HG13	4:I:72:ILE:HD11	1.71	0.72
1:F:220:ASP:OD2	1:F:256:ARG:NH1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:52:SER:O	4:I:67:LYS:CD	2.37	0.72
5:E:181:GLU:O	5:E:183:PRO:CD	2.39	0.71
1:A:55:GLU:OE2	1:A:170:ARG:NH2	2.23	0.71
4:D:121:TYR:CD2	5:E:136:GLU:HB3	2.22	0.71
5:E:186:ASN:HD22	5:E:186:ASN:N	1.89	0.70
2:G:13:HIS:H	2:G:21:ASN:HD21	1.39	0.70
4:D:113:ILE:N	4:D:113:ILE:HD13	2.05	0.70
5:J:26:ILE:HA	8:J:302:GOL:H2	1.73	0.69
1:A:187:THR:HA	1:A:204:TRP:O	1.94	0.68
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.76	0.68
4:D:113:ILE:N	4:D:113:ILE:CD1	2.54	0.68
4:D:133:VAL:HG12	4:D:175:ALA:O	1.93	0.67
1:A:224:GLN:O	1:A:228:THR:HG21	1.94	0.67
1:A:230:LEU:HD12	1:A:245:ALA:HB2	1.77	0.67
4:I:178:ASN:HD22	4:I:178:ASN:H	1.40	0.67
5:J:15:MET:CE	5:J:117:GLU:HG2	2.25	0.66
5:J:222:ASN:N	5:J:222:ASN:HD22	1.94	0.66
5:E:181:GLU:O	5:E:183:PRO:HD3	1.96	0.66
1:F:93:HIS:HB2	8:F:302:GOL:H32	1.76	0.66
4:I:133:VAL:HG22	4:I:176:TRP:HB3	1.77	0.66
5:J:2:ALA:HB3	8:J:302:GOL:H31	1.76	0.66
1:F:134:THR:HG23	6:F:305:SO4:O3	1.96	0.66
4:D:121:TYR:CD2	5:E:136:GLU:CB	2.79	0.65
4:D:110:ARG:HB3	4:D:141:SER:HB3	1.77	0.65
1:F:91:GLY:O	8:F:302:GOL:H11	1.95	0.65
4:D:153:VAL:HG13	4:D:155:ILE:HD12	1.76	0.65
4:I:113:ILE:N	4:I:113:ILE:CD1	2.59	0.65
1:F:93:HIS:CG	8:F:302:GOL:H31	2.31	0.65
4:D:120:VAL:O	4:D:121:TYR:HB3	1.96	0.65
1:F:227:ASP:HB3	1:F:248:VAL:HG12	1.78	0.65
4:D:122:GLN:O	5:E:133:SER:HB2	1.98	0.64
1:F:251:SER:O	1:F:251:SER:OG	2.16	0.64
4:D:121:TYR:OH	4:D:123:LEU:HD23	1.98	0.64
4:D:121:TYR:CE1	4:D:135:LEU:HB3	2.33	0.64
4:D:51:TYR:O	4:D:53:SER:CB	2.45	0.63
1:F:253:GLN:HB2	1:F:274:TRP:CD1	2.34	0.63
4:D:158:LYS:CD	4:D:158:LYS:N	2.62	0.62
4:D:158:LYS:HD2	4:D:158:LYS:N	2.15	0.62
4:D:52:SER:HA	4:D:67:LYS:HD2	1.80	0.62
4:D:101:PHE:CE1	5:E:43:LEU:HD22	2.35	0.62
4:D:150:ASP:N	4:D:150:ASP:OD1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:133:VAL:HG13	4:D:176:TRP:HB3	1.82	0.61
1:F:227:ASP:HB3	1:F:248:VAL:CG1	2.31	0.61
5:E:22[B]:ARG:HD3	5:E:74:PHE:HZ	1.66	0.61
2:G:10:TYR:HB2	7:G:102:EDO:H22	1.83	0.61
4:D:34:MET:HE1	5:E:103:ASN:HB2	1.84	0.60
1:A:230:LEU:CD1	1:A:245:ALA:HB2	2.30	0.60
4:D:179:LYS:O	4:D:181:ASP:N	2.34	0.60
5:E:202:PHE:CD1	9:E:408:HOH:O	2.46	0.60
5:E:145:LEU:HD11	5:E:210:PHE:CE2	2.38	0.59
5:E:129:VAL:HG23	5:E:239:ALA:HB3	1.83	0.59
4:I:161:LEU:HB3	5:J:173:CYS:HB2	1.84	0.59
1:F:91:GLY:O	8:F:302:GOL:C1	2.51	0.59
5:J:15:MET:HE3	5:J:117:GLU:HA	1.83	0.59
4:D:196:ASP:OD1	4:D:197:THR:N	2.36	0.59
2:G:84:HIS:HD2	2:G:86:THR:OG1	1.86	0.59
4:I:118:PRO:HB2	4:I:197:THR:HG22	1.85	0.59
1:F:93:HIS:CB	8:F:302:GOL:H31	2.33	0.58
4:D:51:TYR:O	4:D:53:SER:HB3	2.03	0.58
5:J:129:VAL:HG23	5:J:239:ALA:HB3	1.86	0.58
4:D:18:ILE:H	4:I:64:GLN:NE2	1.90	0.58
4:D:123:LEU:HD11	4:D:133:VAL:HB	1.84	0.58
4:D:113:ILE:HG12	4:D:140:ASP:HB2	1.86	0.57
4:D:125:ASP:N	4:D:125:ASP:OD1	2.29	0.57
4:D:120:VAL:CG1	4:D:121:TYR:N	2.68	0.57
4:D:34:MET:HE1	4:D:49:TYR:CD1	2.40	0.57
4:D:114:GLN:HA	9:D:450:HOH:O	2.04	0.57
4:D:113:ILE:CG1	4:D:140:ASP:HB2	2.35	0.56
5:E:43:LEU:C	5:E:43:LEU:CD2	2.73	0.56
2:G:11:SER:O	7:G:102:EDO:H21	2.06	0.56
4:D:18:ILE:N	4:I:64:GLN:HE22	1.90	0.56
4:D:121:TYR:CD1	4:D:135:LEU:HB3	2.41	0.55
1:F:197:HIS:O	1:F:251:SER:N	2.39	0.55
5:E:141:GLN:HE21	5:E:141:GLN:HA	1.71	0.55
4:I:145:VAL:HA	4:I:191:SER:OG	2.06	0.55
4:I:148:SER:HB2	4:I:155:ILE:CD1	2.37	0.55
4:I:127:LYS:O	4:I:129:SER:N	2.37	0.55
4:D:51:TYR:O	4:D:53:SER:HB2	2.06	0.55
4:D:60:ARG:HD3	6:D:302:SO4:O1	2.07	0.55
4:D:133:VAL:HG23	5:E:130:PHE:CD2	2.42	0.55
4:D:123:LEU:HD13	4:D:133:VAL:HG23	1.89	0.54
1:F:144:LYS:HE3	1:F:148:GLU:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:211:ARG:HH12	5:E:213:GLN:NE2	2.05	0.54
4:D:124:ARG:CZ	4:D:124:ARG:HB2	2.37	0.54
1:A:97:ARG:NH2	9:A:404:HOH:O	2.40	0.54
2:B:84:HIS:HD2	2:B:86:THR:OG1	1.90	0.54
1:A:35:ARG:CD	1:A:48:ARG:HD2	2.38	0.53
1:A:226:GLN:HE21	1:A:226:GLN:C	2.12	0.53
4:D:34:MET:HE1	5:E:103:ASN:CB	2.37	0.53
4:D:111:PRO:HG2	4:D:160:VAL:HG11	1.91	0.53
5:E:145:LEU:HD11	5:E:210:PHE:CD2	2.44	0.53
5:E:42:GLY:HA3	9:E:403:HOH:O	2.09	0.52
5:E:211:ARG:HH12	5:E:213:GLN:HE21	1.56	0.52
5:J:2:ALA:O	8:J:302:GOL:O3	2.22	0.52
4:D:133:VAL:HG11	4:D:174:VAL:HG13	1.90	0.52
1:A:226:GLN:NE2	1:A:227:ASP:OD1	2.42	0.51
4:D:101:PHE:CD1	5:E:43:LEU:HD22	2.44	0.51
1:A:93:HIS:HE1	9:A:409:HOH:O	1.92	0.51
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.45	0.51
5:J:21:LEU:HD22	5:J:111:THR:HG21	1.92	0.51
1:F:182:THR:HG21	1:F:264:GLU:HG2	1.93	0.51
2:G:21:ASN:HD22	2:G:22:PHE:N	2.02	0.51
1:A:195:SER:O	1:A:196:ASP:HB3	2.10	0.51
5:E:181:GLU:O	5:E:183:PRO:HD2	2.11	0.51
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.46	0.51
1:F:218:GLN:HG2	1:F:223:ASP:HA	1.93	0.50
5:J:222:ASN:ND2	5:J:222:ASN:H	2.06	0.50
4:I:125:ASP:HB3	5:J:129:VAL:O	2.10	0.50
1:F:93:HIS:HD2	8:F:302:GOL:H11	1.75	0.50
4:I:113:ILE:CG1	4:I:140:ASP:HA	2.41	0.50
4:D:126:SER:CB	9:D:410:HOH:O	2.46	0.50
1:F:220:ASP:OD1	1:F:256:ARG:NE	2.44	0.50
4:D:52:SER:CA	4:D:67:LYS:HD2	2.42	0.50
5:E:129:VAL:CG2	5:E:239:ALA:HB3	2.41	0.50
1:A:224:GLN:O	1:A:228:THR:CG2	2.60	0.50
5:E:186:ASN:ND2	5:E:186:ASN:N	2.58	0.49
1:F:121:LYS:HD3	2:G:1:ILE:HG12	1.94	0.49
5:E:211:ARG:NH1	5:E:213:GLN:HE21	2.09	0.49
4:D:116:PRO:HB3	4:D:140:ASP:HB3	1.94	0.49
4:D:160:VAL:HG22	4:D:171:ASN:ND2	2.27	0.49
4:D:161:LEU:HB3	5:E:173:CYS:HB3	1.95	0.49
4:D:113:ILE:HG13	4:D:140:ASP:HA	1.95	0.49
4:D:81:PRO:HD2	9:D:424:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:21:ASN:ND2	2:G:22:PHE:H	2.03	0.49
4:D:34:MET:CE	5:E:103:ASN:CB	2.92	0.48
5:E:141:GLN:HE21	5:E:141:GLN:CA	2.26	0.48
4:I:69:SER:CB	8:I:301:GOL:H32	2.43	0.48
1:F:165[B]:VAL:HG12	1:F:169:ARG:CZ	2.44	0.48
4:D:198:PHE:O	4:D:199:PHE:HB2	2.13	0.48
1:A:254:GLU:OE2	1:A:254:GLU:N	2.45	0.48
1:F:68:LYS:HD3	8:F:301:GOL:H11	1.95	0.48
4:I:108:LEU:HD13	4:I:108:LEU:C	2.34	0.48
5:J:21:LEU:HD12	5:J:77:LEU:HD23	1.95	0.48
4:D:52:SER:HB2	4:D:67:LYS:CD	2.43	0.48
5:E:155:ASP:N	5:E:155:ASP:OD1	2.44	0.48
1:F:18:GLY:C	1:F:19:GLU:HG2	2.34	0.48
4:I:119:ALA:HB1	4:I:121:TYR:CZ	2.49	0.48
5:J:50:ASN:ND2	9:J:404:HOH:O	2.45	0.48
4:D:143:THR:HG21	4:D:194:PRO:HD3	1.95	0.48
1:F:122:ASP:HB3	6:F:305:SO4:O2	2.14	0.47
1:A:194:VAL:HG12	1:A:195:SER:N	2.29	0.47
1:A:190:THR:OG1	1:A:202:ARG:HB3	2.13	0.47
4:D:122:GLN:O	5:E:133:SER:CB	2.61	0.47
4:I:149:LYS:HG3	4:I:190:ASN:HD21	1.78	0.47
5:J:179:LEU:HD12	5:J:179:LEU:C	2.35	0.47
4:D:122:GLN:NE2	4:D:184:CYS:SG	2.88	0.47
5:E:21:LEU:HD22	5:E:111:THR:HG21	1.96	0.47
5:E:2:ALA:HA	9:E:471:HOH:O	2.14	0.47
1:F:152:VAL:CG2	3:H:8:PRO:HG3	2.44	0.47
4:I:130:ASP:O	4:I:131:LYS:HG3	2.15	0.47
4:D:120:VAL:HG12	4:D:121:TYR:N	2.30	0.47
4:I:24:THR:HG22	4:I:71:TYR:CD1	2.50	0.47
4:I:19:VAL:HG13	4:I:76:ILE:HB	1.97	0.47
4:D:125:ASP:OD1	4:D:130:ASP:HA	2.13	0.47
4:D:34:MET:CE	4:D:49:TYR:CD1	2.98	0.47
2:B:32:PRO:O	2:B:84:HIS:HE1	1.97	0.46
4:I:24:THR:HG22	4:I:71:TYR:HD1	1.80	0.46
5:J:24:LYS:HE3	8:J:302:GOL:H12	1.97	0.46
5:E:164:ASN:HD21	5:E:207:ARG:HH22	1.63	0.46
4:D:155:ILE:HG22	4:D:176:TRP:CE3	2.50	0.46
4:D:121:TYR:CG	5:E:133:SER:HB3	2.49	0.46
4:D:123:LEU:HB2	5:E:131:GLU:O	2.15	0.46
2:G:32:PRO:O	2:G:84:HIS:HE1	1.99	0.46
4:D:67:LYS:HE2	9:D:407:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:164:ASN:HD22	5:E:209:HIS:HB3	1.81	0.45
1:F:159:TYR:CE2	1:F:164:CYS:HB2	2.52	0.45
4:I:108:LEU:HD13	4:I:109:VAL:N	2.32	0.45
1:A:97:ARG:HD3	1:A:114:HIS:NE2	2.31	0.45
4:D:131:LYS:HG2	4:D:132:SER:N	2.32	0.45
4:D:147:GLN:HB3	4:D:156:THR:CG2	2.46	0.45
1:F:190:THR:HG21	2:G:98:ASP:OD1	2.16	0.45
4:D:147:GLN:HB3	4:D:156:THR:HG23	1.99	0.45
4:D:123:LEU:CB	5:E:131:GLU:O	2.65	0.45
4:I:113:ILE:HG13	4:I:140:ASP:HA	1.99	0.45
5:E:183:PRO:O	5:E:185:LEU:N	2.50	0.45
4:D:153:VAL:HG12	4:D:177:SER:HA	1.99	0.44
5:J:9:ARG:HA	5:J:9:ARG:HD3	1.70	0.44
1:A:35:ARG:HD3	1:A:48:ARG:HD2	1.99	0.44
4:I:124:ARG:O	4:I:125:ASP:HB2	2.17	0.44
1:F:218:GLN:OE1	1:F:221:GLY:C	2.55	0.44
5:J:187:ASP:O	5:J:187:ASP:OD1	2.36	0.44
5:E:175:ASP:OD1	5:E:195:ARG:NH1	2.51	0.44
5:J:220:SER:HB2	9:J:478:HOH:O	2.18	0.44
1:A:141:GLN:NE2	9:A:402:HOH:O	2.34	0.44
4:D:133:VAL:HG11	4:D:174:VAL:CG1	2.47	0.44
1:A:135:ALA:HB3	9:A:402:HOH:O	2.17	0.43
5:J:204:GLN:O	5:J:206:PRO:HD3	2.17	0.43
2:G:22:PHE:CZ	2:G:69:GLU:HG2	2.53	0.43
4:I:111:PRO:O	4:I:113:ILE:HD12	2.18	0.43
4:D:113:ILE:HG12	4:D:140:ASP:CB	2.48	0.43
2:G:97:ARG:NH1	9:G:205:HOH:O	2.50	0.43
4:I:156:THR:HG21	5:J:193:SER:HB3	2.00	0.43
4:I:192:ILE:HD12	4:I:192:ILE:H	1.83	0.43
4:D:118:PRO:O	4:D:196:ASP:CB	2.67	0.43
1:F:152:VAL:HG22	3:H:8:PRO:HG3	2.00	0.43
1:A:195:SER:OG	1:A:198:GLU:HB2	2.19	0.42
4:D:64:GLN:NE2	4:I:18:ILE:H	2.05	0.42
4:D:135:LEU:HD12	4:D:173:ALA:O	2.19	0.42
1:F:253:GLN:HB2	1:F:274:TRP:NE1	2.34	0.42
5:J:185:LEU:N	5:J:185:LEU:HD12	2.35	0.42
4:I:113:ILE:HG12	4:I:140:ASP:HA	2.00	0.42
5:E:211:ARG:NH2	5:E:213:GLN:HB2	2.35	0.42
4:I:71:TYR:HB3	8:I:301:GOL:H31	2.01	0.42
4:I:130:ASP:C	4:I:131:LYS:HG3	2.40	0.42
5:J:228:ASP:O	5:J:229:ARG:C	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:153:VAL:CG1	4:D:177:SER:HA	2.50	0.42
1:A:19:GLU:HA	1:A:20:PRO:HD3	1.89	0.42
1:F:180:GLN:HA	9:F:498:HOH:O	2.19	0.42
5:J:182:GLN:HB3	5:J:185:LEU:HD13	2.02	0.42
4:D:118:PRO:O	4:D:196:ASP:HB3	2.20	0.41
5:E:211:ARG:HH22	5:E:213:GLN:HE21	1.67	0.41
5:E:211:ARG:NH2	5:E:213:GLN:HE21	2.17	0.41
4:D:124:ARG:HB3	4:D:130:ASP:HB3	2.01	0.41
2:B:71:THR:HA	2:B:72:PRO:HD2	1.82	0.41
4:D:147:GLN:HB2	4:D:156:THR:HG22	2.03	0.41
4:D:155:ILE:HG22	4:D:176:TRP:CD2	2.55	0.41
5:E:83:GLU:OE1	5:E:85:ARG:CZ	2.68	0.41
2:G:19:LYS:O	2:G:72:PRO:HD2	2.20	0.41
1:F:232[A]:GLU:CD	2:G:6:LYS:HZ3	2.23	0.41
4:D:124:ARG:NH1	4:D:124:ARG:HB2	2.36	0.41
1:F:196:ASP:CG	1:F:196:ASP:O	2.59	0.41
1:A:169:ARG:HD2	4:I:195:GLU:OE1	2.20	0.41
1:A:11:SER:HA	1:A:21:ARG:O	2.21	0.41
2:B:21:ASN:ND2	2:B:22:PHE:H	2.10	0.41
4:I:157:ASP:OD1	4:I:158:LYS:N	2.52	0.41
2:B:21:ASN:HD22	2:B:22:PHE:N	2.08	0.41
2:G:48:LYS:HG3	2:G:48:LYS:O	2.20	0.41
5:E:22[B]:ARG:HD3	5:E:74:PHE:CZ	2.50	0.40
4:I:181:ASP:OD1	4:I:182:PHE:N	2.53	0.40
1:F:19:GLU:N	9:F:401:HOH:O	2.55	0.40
5:E:36:ARG:NH2	9:E:402:HOH:O	2.49	0.40
5:E:63:ASP:HA	9:E:409:HOH:O	2.22	0.40
2:B:41:LYS:HG3	2:B:78:TYR:CE1	2.57	0.40
5:E:201:THR:HG22	5:E:201:THR:O	2.21	0.40
5:J:15:MET:HE2	5:J:117:GLU:HG2	2.01	0.40
5:E:246:ASP:N	5:E:246:ASP:OD1	2.55	0.40
5:J:140:THR:O	5:J:140:THR:HG22	2.21	0.40
5:J:151:GLY:O	5:J:189:ARG:HD3	2.22	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	274/277 (99%)	261 (95%)	11 (4%)	2 (1%)	22 17
1	F	280/277 (101%)	273 (98%)	5 (2%)	2 (1%)	22 17
2	B	98/100 (98%)	94 (96%)	4 (4%)	0	100 100
2	G	98/100 (98%)	95 (97%)	3 (3%)	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
4	D	198/199 (100%)	177 (89%)	18 (9%)	3 (2%)	10 5
4	I	198/199 (100%)	185 (93%)	11 (6%)	2 (1%)	15 10
5	E	245/246 (100%)	234 (96%)	7 (3%)	4 (2%)	9 4
5	J	245/246 (100%)	238 (97%)	7 (3%)	0	100 100
All	All	1652/1664 (99%)	1573 (95%)	66 (4%)	13 (1%)	19 14

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	SER
5	E	184	ALA
5	E	182	GLN
5	E	187	ASP
4	I	128	SER
1	A	227	ASP
5	E	200	ALA
4	I	129	SER
4	D	118	PRO
4	D	52	SER
4	D	85	ALA
1	F	253	GLN
1	F	275	GLU

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	232/233 (100%)	217 (94%)	15 (6%)	17 14
1	F	238/233 (102%)	222 (93%)	16 (7%)	16 13
2	B	95/95 (100%)	90 (95%)	5 (5%)	22 20
2	G	95/95 (100%)	90 (95%)	5 (5%)	22 20
3	C	8/8 (100%)	8 (100%)	0	100 100
3	H	8/8 (100%)	8 (100%)	0	100 100
4	D	181/180 (101%)	143 (79%)	38 (21%)	1 0
4	I	181/180 (101%)	158 (87%)	23 (13%)	4 2
5	E	217/216 (100%)	197 (91%)	20 (9%)	9 5
5	J	217/216 (100%)	203 (94%)	14 (6%)	17 14
All	All	1472/1464 (100%)	1336 (91%)	136 (9%)	9 5

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	35	ARG
1	A	58	GLU
1	A	74	HIS
1	A	132	SER
1	A	154	GLU
1	A	195	SER
1	A	219	ARG
1	A	223	ASP
1	A	226	GLN
1	A	229	GLU
1	A	230	LEU
1	A	255	GLN
1	A	256	ARG
1	A	276	PRO
2	B	21	ASN

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Mol	Chain	Res	Type
2	B	47	GLU
2	B	70	PHE
2	B	89	GLN
2	B	98	ASP
4	D	3	GLU
4	D	4	VAL
4	D	11	LEU
4	D	19	VAL
4	D	34	MET
4	D	49	TYR
4	D	53	SER
4	D	55	ASN
4	D	73	SER
4	D	88	LEU
4	D	99	LEU
4	D	108	LEU
4	D	109	VAL
4	D	113	ILE
4	D	114	GLN
4	D	121	TYR
4	D	123	LEU
4	D	124	ARG
4	D	125	ASP
4	D	126	SER
4	D	127	LYS
4	D	130	ASP
4	D	131	LYS
4	D	133	VAL
4	D	145	VAL
4	D	146	SER
4	D	150	ASP
4	D	155	ILE
4	D	158	LYS
4	D	165	SER
4	D	172	SER
4	D	176	TRP
4	D	178	ASN
4	D	182	PHE
4	D	189	ASN
4	D	190	ASN
4	D	191	SER
4	D	197	THR

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Mol	Chain	Res	Type
5	E	7	SER
5	E	36	ARG
5	E	41	ARG
5	E	133	SER
5	E	136	GLU
5	E	137	ILE
5	E	140	THR
5	E	141	GLN
5	E	148	LEU
5	E	170	SER
5	E	173	CYS
5	E	186	ASN
5	E	189	ARG
5	E	195	ARG
5	E	197	ARG
5	E	198	VAL
5	E	199	SER
5	E	221	GLU
5	E	226	THR
5	E	238	SER
1	F	0	MET
1	F	11	SER
1	F	17	ARG
1	F	19	GLU
1	F	35	ARG
1	F	74	HIS
1	F	176	LYS
1	F	216[A]	THR
1	F	216[B]	THR
1	F	224	GLN
1	F	231	VAL
1	F	251	SER
1	F	253	GLN
1	F	254	GLU
1	F	268	LYS
1	F	275	GLU
2	G	21	ASN
2	G	47	GLU
2	G	70	PHE
2	G	83	ASN
2	G	94	LYS
4	I	4	VAL

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Mol	Chain	Res	Type
4	I	19	VAL
4	I	31	GLN
4	I	34	MET
4	I	41	ARG
4	I	72	ILE
4	I	99	LEU
4	I	109	VAL
4	I	113	ILE
4	I	123	LEU
4	I	127	LYS
4	I	130	ASP
4	I	131	LYS
4	I	133	VAL
4	I	142	GLN
4	I	147	GLN
4	I	166	MET
4	I	169	LYS
4	I	178	ASN
4	I	186	ASN
4	I	191	SER
4	I	193	ILE
4	I	197	THR
5	J	7	SER
5	J	9	ARG
5	J	11	GLU
5	J	36	ARG
5	J	39	MET
5	J	43	LEU
5	J	78	LYS
5	J	120	LYS
5	J	134	GLU
5	J	155	ASP
5	J	182	GLN
5	J	195	ARG
5	J	222	ASN
5	J	246	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	180	GLN

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Mol	Chain	Res	Type
1	A	226	GLN
2	B	21	ASN
2	B	24	ASN
2	B	51	HIS
2	B	83	ASN
2	B	84	HIS
4	D	64	GLN
4	D	122	GLN
4	D	171	ASN
4	D	189	ASN
4	D	190	ASN
5	E	18	GLN
5	E	80	GLN
5	E	141	GLN
5	E	164	ASN
5	E	182	GLN
5	E	186	ASN
5	E	208	ASN
5	E	213	GLN
5	E	235	GLN
1	F	86	ASN
1	F	180	GLN
1	F	191	HIS
1	F	197	HIS
2	G	21	ASN
2	G	24	ASN
2	G	83	ASN
2	G	84	HIS
4	I	31	GLN
4	I	64	GLN
4	I	122	GLN
4	I	144	ASN
4	I	171	ASN
4	I	178	ASN
4	I	186	ASN
4	I	189	ASN
5	J	18	GLN
5	J	50	ASN
5	J	141	GLN
5	J	182	GLN
5	J	222	ASN
5	J	235	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

22 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	$\#\|Z\| > 2$
8	GOL	F	303	-	5,5,5	1.33	0	5,5,5	1.18	0
6	SO4	F	305	-	4,4,4	0.53	0	6,6,6	0.81	0
8	GOL	J	302	-	5,5,5	0.62	0	5,5,5	0.77	0
8	GOL	H	101	-	5,5,5	1.34	1 (20%)	5,5,5	2.51	3 (60%)
6	SO4	I	304	-	4,4,4	0.43	0	6,6,6	0.87	0
6	SO4	A	302	-	4,4,4	0.42	0	6,6,6	0.24	0
8	GOL	F	302	-	5,5,5	1.47	2 (40%)	5,5,5	1.93	2 (40%)
7	EDO	G	101	-	3,3,3	1.36	0	2,2,2	0.88	0
7	EDO	I	303	-	3,3,3	1.07	0	2,2,2	0.72	0
6	SO4	D	302	-	4,4,4	0.49	0	6,6,6	0.58	0
6	SO4	A	301	-	4,4,4	0.60	0	6,6,6	0.91	0
6	SO4	J	304	-	4,4,4	0.73	0	6,6,6	0.87	0
7	EDO	D	301	-	3,3,3	0.56	0	2,2,2	0.50	0
8	GOL	J	301	-	5,5,5	1.16	0	5,5,5	2.01	1 (20%)
8	GOL	F	301	-	5,5,5	0.82	0	5,5,5	0.82	0
7	EDO	E	301	-	3,3,3	0.66	0	2,2,2	0.77	0
7	EDO	G	102	-	3,3,3	0.85	0	2,2,2	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	EDO	J	303	-	3,3,3	1.06	0	2,2,2	0.21	0
7	EDO	I	302	-	3,3,3	0.59	0	2,2,2	0.50	0
8	GOL	I	301	-	5,5,5	0.80	0	5,5,5	1.52	1 (20%)
7	EDO	B	101	-	3,3,3	0.52	0	2,2,2	0.35	0
7	EDO	F	304	-	3,3,3	0.41	0	2,2,2	0.25	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	G	101	-	-	0/1/1/1	-
7	EDO	G	102	-	-	0/1/1/1	-
8	GOL	F	303	-	-	4/4/4/4	-
8	GOL	J	302	-	-	3/4/4/4	-
7	EDO	J	303	-	-	1/1/1/1	-
8	GOL	H	101	-	-	2/4/4/4	-
7	EDO	I	303	-	-	1/1/1/1	-
7	EDO	D	301	-	-	1/1/1/1	-
7	EDO	I	302	-	-	0/1/1/1	-
8	GOL	I	301	-	-	2/4/4/4	-
7	EDO	B	101	-	-	0/1/1/1	-
8	GOL	J	301	-	-	2/4/4/4	-
8	GOL	F	302	-	-	3/4/4/4	-
8	GOL	F	301	-	-	2/4/4/4	-
7	EDO	E	301	-	-	0/1/1/1	-
7	EDO	F	304	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	101	GOL	O2-C2	-2.63	1.35	1.43
8	F	302	GOL	O3-C3	2.38	1.52	1.42
8	F	302	GOL	O1-C1	2.16	1.51	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	101	GOL	C3-C2-C1	4.07	127.53	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	301	GOL	O1-C1-C2	3.92	129.01	110.20
8	F	302	GOL	O3-C3-C2	3.09	125.00	110.20
8	H	101	GOL	O2-C2-C3	-2.74	97.04	109.12
8	I	301	GOL	O3-C3-C2	2.61	122.70	110.20
8	H	101	GOL	O2-C2-C1	-2.43	98.42	109.12
8	F	302	GOL	C3-C2-C1	2.09	119.82	111.70

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	303	GOL	C1-C2-C3-O3
8	J	302	GOL	O2-C2-C3-O3
8	F	302	GOL	O1-C1-C2-O2
8	F	302	GOL	O1-C1-C2-C3
8	F	302	GOL	C1-C2-C3-O3
8	F	303	GOL	O1-C1-C2-O2
8	H	101	GOL	O2-C2-C3-O3
8	F	303	GOL	O1-C1-C2-C3
8	J	302	GOL	C1-C2-C3-O3
8	H	101	GOL	C1-C2-C3-O3
8	J	301	GOL	C1-C2-C3-O3
8	I	301	GOL	O1-C1-C2-C3
8	F	303	GOL	O2-C2-C3-O3
8	J	301	GOL	O2-C2-C3-O3
7	I	303	EDO	O1-C1-C2-O2
7	J	303	EDO	O1-C1-C2-O2
7	D	301	EDO	O1-C1-C2-O2
8	F	301	GOL	O1-C1-C2-C3
8	F	301	GOL	O1-C1-C2-O2
8	I	301	GOL	O1-C1-C2-O2
8	J	302	GOL	O1-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	305	SO4	2	0
8	J	302	GOL	4	0
8	F	302	GOL	9	0
6	D	302	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	J	301	GOL	3	0
8	F	301	GOL	1	0
7	G	102	EDO	2	0
8	I	301	GOL	2	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	276/277 (99%)	0.12	9 (3%) 46 53	23, 44, 86, 112	0
1	F	277/277 (100%)	0.11	11 (3%) 38 44	22, 40, 81, 102	0
2	B	100/100 (100%)	-0.27	0 100 100	27, 41, 68, 73	0
2	G	100/100 (100%)	-0.16	0 100 100	26, 40, 56, 66	0
3	C	10/10 (100%)	-0.11	0 100 100	26, 27, 30, 31	0
3	H	10/10 (100%)	-0.22	0 100 100	24, 26, 28, 31	0
4	D	199/199 (100%)	1.26	51 (25%) 0 0	25, 55, 125, 151	0
4	I	199/199 (100%)	0.87	41 (20%) 1 1	24, 52, 113, 126	0
5	E	246/246 (100%)	0.54	34 (13%) 2 4	21, 47, 102, 126	0
5	J	246/246 (100%)	0.15	13 (5%) 26 31	20, 43, 85, 119	0
All	All	1663/1664 (99%)	0.37	159 (9%) 8 10	20, 43, 106, 151	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	151	SER	16.4
1	F	252	GLY	11.9
4	D	197	THR	11.6
4	D	199	PHE	10.0
5	J	246	ASP	9.4
4	D	200	PRO	9.4
4	D	149	LYS	9.0
4	D	182	PHE	7.9
4	I	128	SER	7.5
4	I	130	ASP	7.1
4	D	134	CYS	7.1
4	I	129	SER	7.1
4	I	166	MET	7.1

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Mol	Chain	Res	Type	RSRZ
1	F	0	MET	6.9
4	D	165	SER	6.8
4	D	121	TYR	6.6
4	I	127	LYS	6.4
4	D	148	SER	6.3
4	D	176	TRP	6.3
5	E	185	LEU	6.3
4	D	136	PHE	6.3
4	D	128	SER	6.2
4	I	180	SER	5.9
4	D	198	PHE	5.9
4	I	182	PHE	5.9
4	D	119	ALA	5.8
4	I	165	SER	5.6
4	D	120	VAL	5.6
5	E	2	ALA	5.4
4	I	198	PHE	5.3
4	I	199	PHE	5.3
4	I	188	PHE	5.0
5	E	246	ASP	4.8
4	D	123	LEU	4.8
4	I	200	PRO	4.8
5	E	210	PHE	4.7
1	F	276	PRO	4.7
4	D	153	VAL	4.7
4	I	2	LYS	4.6
4	D	124	ARG	4.6
4	D	53	SER	4.5
5	E	128	ALA	4.4
4	D	152	ASP	4.4
4	D	195	GLU	4.3
5	J	138	SER	4.2
5	E	138	SER	4.2
5	E	179	LEU	4.0
4	D	150	ASP	4.0
5	E	206	PRO	4.0
1	A	194	VAL	4.0
1	F	253	GLN	4.0
5	E	144	THR	4.0
4	D	186	ASN	4.0
4	D	2	LYS	4.0
4	D	190	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
4	D	193	ILE	3.9
5	E	209	HIS	3.8
5	E	135	ALA	3.8
4	I	123	LEU	3.8
5	J	134	GLU	3.8
4	D	180	SER	3.8
5	E	203	TRP	3.7
5	E	1	ASP	3.7
5	E	243	GLY	3.7
4	I	195	GLU	3.7
4	I	190	ASN	3.7
1	A	195	SER	3.7
5	E	130	PHE	3.7
4	I	153	VAL	3.6
1	A	197	HIS	3.6
4	D	191	SER	3.6
4	I	167	ASP	3.6
4	I	185	ALA	3.6
4	D	175	ALA	3.5
4	I	192	ILE	3.5
4	D	179	LYS	3.4
5	E	140	THR	3.4
5	J	137	ILE	3.4
4	D	166	MET	3.3
4	D	188	PHE	3.3
4	D	154	TYR	3.3
1	A	267	PRO	3.3
5	E	129	VAL	3.3
4	I	197	THR	3.2
4	I	178	ASN	3.2
5	J	40	MET	3.2
5	J	203	TRP	3.2
4	D	145	VAL	3.1
5	E	245	ALA	3.0
4	D	189	ASN	3.0
4	I	189	ASN	3.0
4	D	155	ILE	3.0
4	D	194	PRO	3.0
1	A	276	PRO	3.0
5	E	201	THR	3.0
1	F	177	GLU	3.0
5	E	133	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	255	GLN	3.0
4	D	122	GLN	2.9
4	I	164	ARG	2.9
4	I	184	CYS	2.9
4	D	178	ASN	2.9
5	E	187	ASP	2.9
4	D	196	ASP	2.8
4	I	124	ARG	2.8
4	D	181	ASP	2.8
5	J	245	ALA	2.8
1	F	268	LYS	2.8
1	F	197	HIS	2.8
5	E	40	MET	2.8
4	I	186	ASN	2.7
5	E	145	LEU	2.7
1	A	196	ASP	2.7
5	E	241	ALA	2.7
5	E	39	MET	2.7
4	I	114	GLN	2.6
5	E	141	GLN	2.6
5	E	204	GLN	2.6
4	D	184	CYS	2.6
4	D	133	VAL	2.6
4	I	136	PHE	2.6
4	I	134	CYS	2.6
5	E	200	ALA	2.5
1	F	195	SER	2.5
4	I	131	LYS	2.5
4	D	192	ILE	2.5
1	A	274	TRP	2.5
4	I	191	SER	2.4
4	I	183	ALA	2.4
5	E	183	PRO	2.4
4	D	125	ASP	2.4
5	J	206	PRO	2.4
4	I	152	ASP	2.4
5	J	186	ASN	2.3
4	I	193	ILE	2.3
5	E	41	ARG	2.3
1	F	196	ASP	2.3
4	I	133	VAL	2.3
4	I	149	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	262	GLN	2.3
5	J	141	GLN	2.3
5	E	143	ALA	2.3
4	D	131	LYS	2.3
4	I	181	ASP	2.3
5	J	187	ASP	2.2
4	I	145	VAL	2.2
1	F	255	GLN	2.2
5	E	163	VAL	2.2
4	D	130	ASP	2.1
4	D	183	ALA	2.1
4	D	187	ALA	2.1
4	D	164	ARG	2.1
4	I	121	TYR	2.1
5	E	242	TRP	2.1
1	A	268	LYS	2.1
5	J	133	SER	2.1
5	E	137	ILE	2.0
5	J	39	MET	2.0
4	I	119	ALA	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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GOL	F	303	6/6	0.60	0.28	43,52,59,68	0
7	EDO	G	102	4/4	0.68	0.23	36,37,41,45	0
7	EDO	G	101	4/4	0.69	0.23	46,48,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	J	303	4/4	0.73	0.18	40,57,61,61	0
8	GOL	F	301	6/6	0.77	0.33	50,59,60,65	0
6	SO4	F	305	5/5	0.80	0.25	74,82,91,98	0
7	EDO	I	303	4/4	0.83	0.19	47,49,49,52	0
8	GOL	I	301	6/6	0.84	0.20	45,49,52,56	0
8	GOL	J	302	6/6	0.87	0.28	48,57,61,63	0
8	GOL	J	301	6/6	0.87	0.21	25,30,38,42	0
8	GOL	F	302	6/6	0.88	0.27	21,31,44,58	0
6	SO4	D	302	5/5	0.89	0.26	82,92,95,96	0
6	SO4	I	304	5/5	0.90	0.29	77,82,92,98	0
8	GOL	H	101	6/6	0.90	0.21	35,42,45,50	0
7	EDO	B	101	4/4	0.91	0.19	44,44,47,49	0
6	SO4	A	302	5/5	0.92	0.20	83,87,94,95	0
6	SO4	A	301	5/5	0.92	0.27	53,58,79,89	0
6	SO4	J	304	5/5	0.94	0.16	57,57,60,60	0
7	EDO	E	301	4/4	0.95	0.15	30,32,33,37	0
7	EDO	D	301	4/4	0.96	0.13	27,27,31,37	0
7	EDO	I	302	4/4	0.97	0.14	24,27,30,32	0
7	EDO	F	304	4/4	0.97	0.15	41,42,43,45	0

6.5 Other polymers

There are no such residues in this entry.