wwPDB X-ray Structure Validation Summary Report (i)

Jun 2, 2016 – 05:28 AM EDT

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 wwPDB X-ray Structure Validation Summary 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:

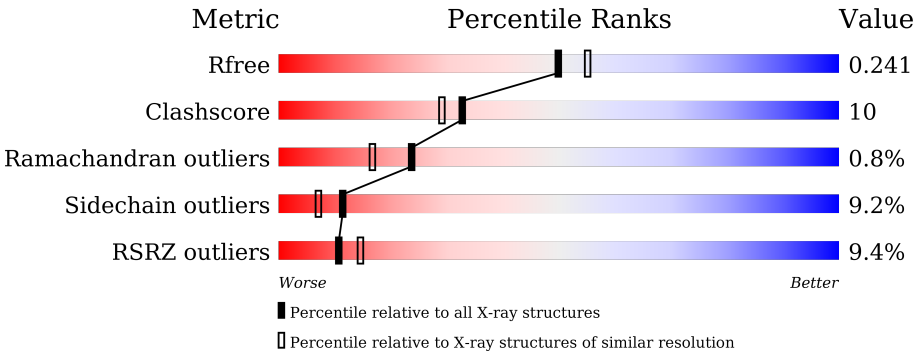
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027674
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.11 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}	91344	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (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. 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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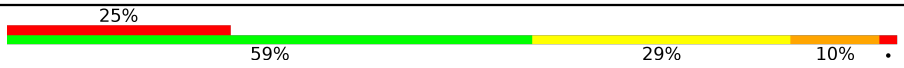
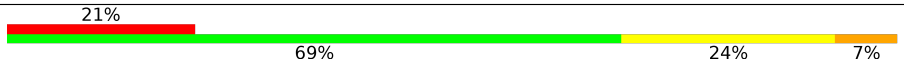
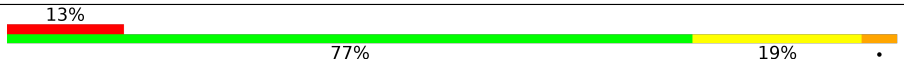
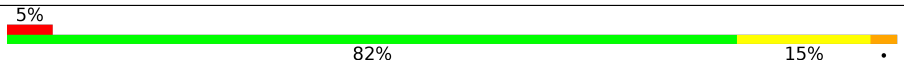
Mol	Chain	Length	Quality of chain
4	D	199	
4	I	199	
5	E	246	
5	J	246	

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	SO4	A	301	-	-	-	X
6	SO4	F	305	-	-	X	X
6	SO4	I	304	-	-	-	X
7	EDO	B	101	-	-	-	X
7	EDO	E	301	-	-	-	X
7	EDO	F	304	-	-	-	X
7	EDO	G	101	-	-	-	X
7	EDO	G	102	-	-	-	X
7	EDO	I	303	-	-	-	X
7	EDO	J	303	-	-	-	X
8	GOL	F	302	-	-	X	X
8	GOL	H	101	-	-	-	X
8	GOL	I	301	-	-	-	X
8	GOL	J	301	-	-	-	X
8	GOL	J	302	-	-	X	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			

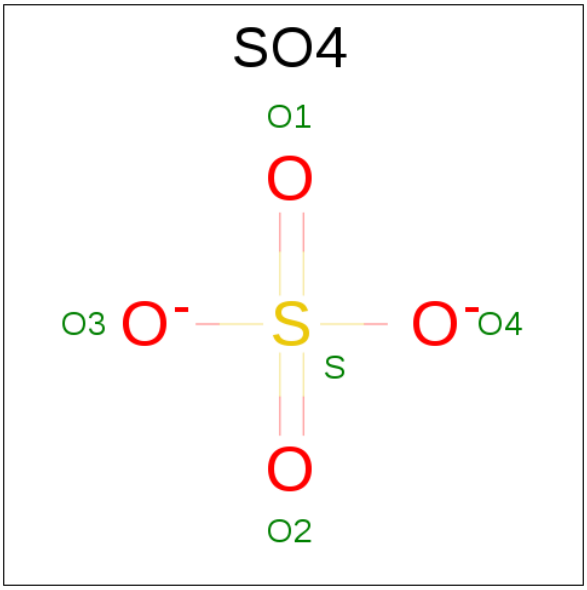
- Molecule 4 is a protein called 1E6 TCR Alpha Chain.

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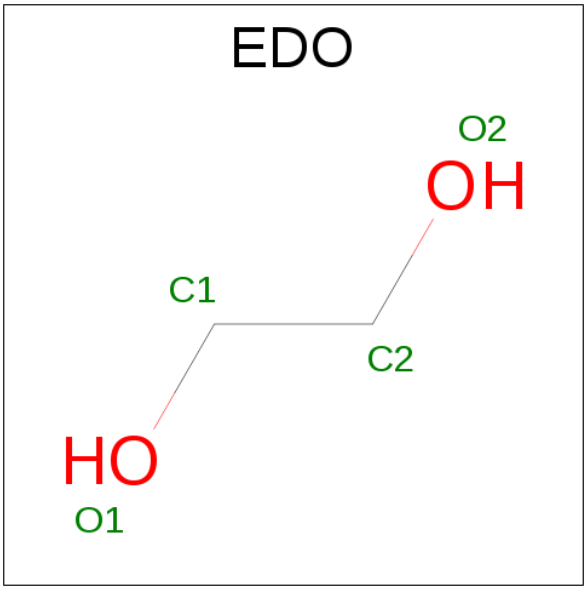
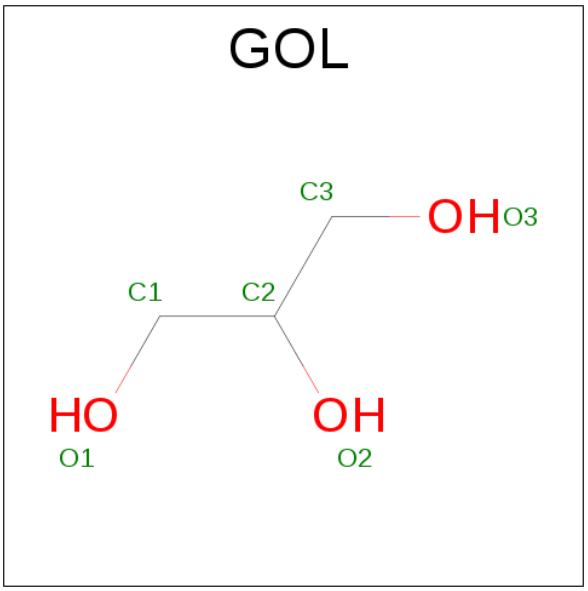
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total O S 5 4 1	0	0

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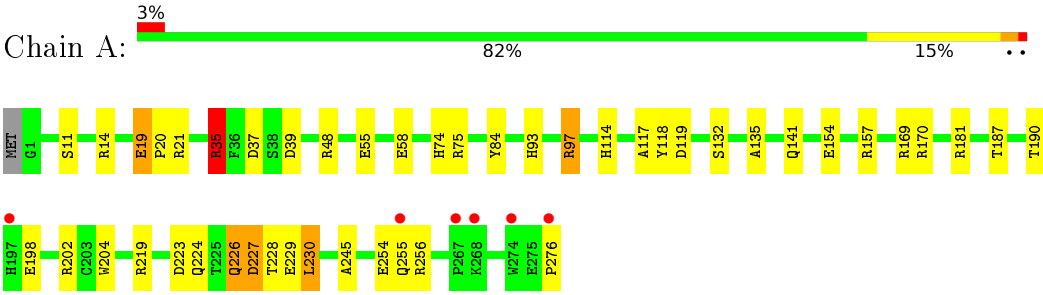
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	103	Total O 103 103	0	0
9	G	49	Total O 49 49	0	0
9	H	7	Total O 7 7	0	0
9	I	46	Total O 46 46	0	0
9	J	83	Total O 83 83	0	0

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 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.

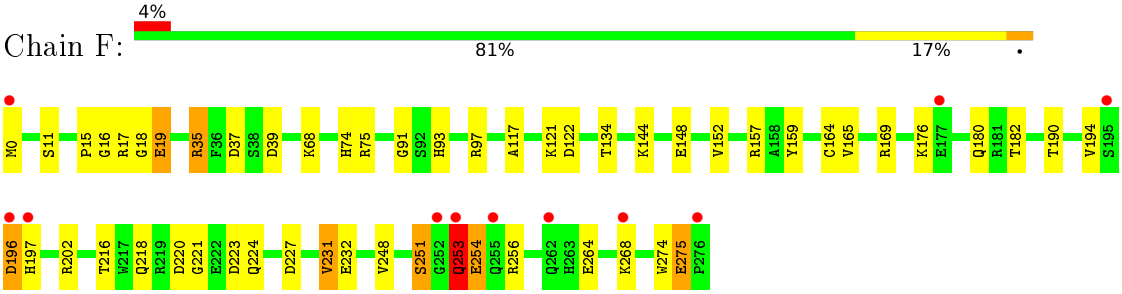
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain A:



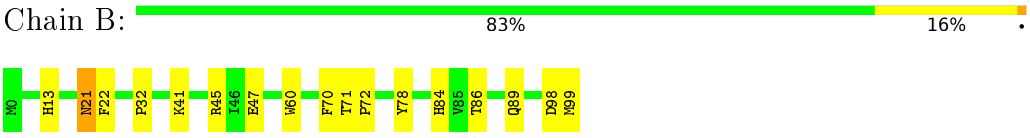
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain F:



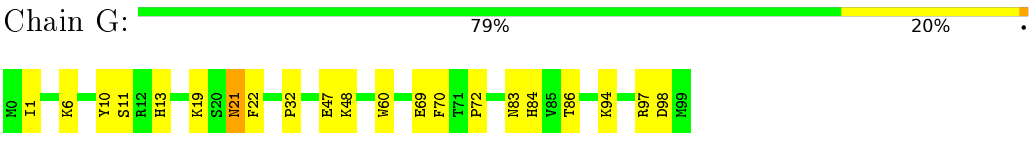
- Molecule 2: Beta-2-microglobulin

Chain B:



- Molecule 2: Beta-2-microglobulin

Chain G:



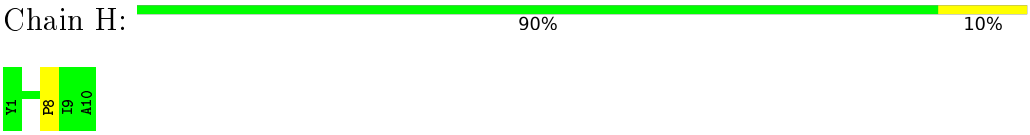
- Molecule 3: Marker peptide

Chain C:

There are no outlier residues recorded for this chain.

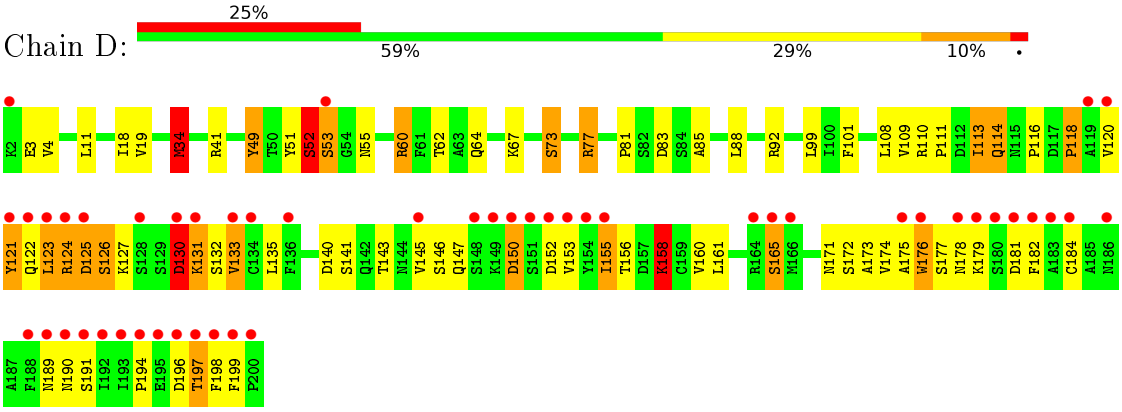
- Molecule 3: Marker peptide

Chain H:



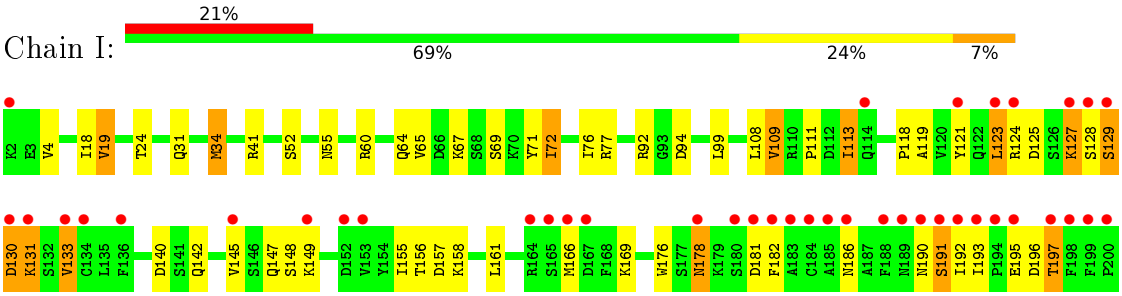
- Molecule 4: 1E6 TCR Alpha Chain

Chain D:



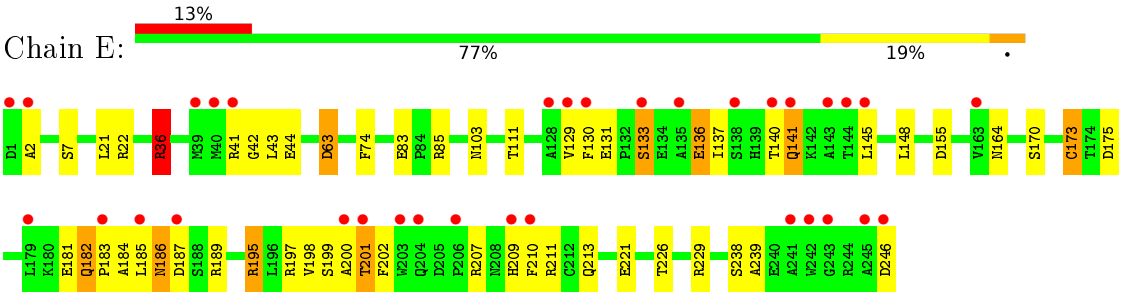
- Molecule 4: 1E6 TCR Alpha Chain

Chain I:



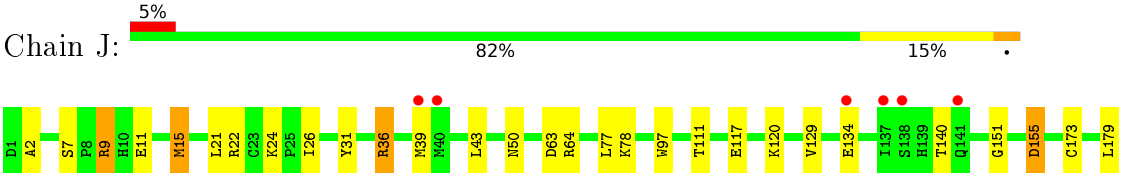
- Molecule 5: 1E6 TCR Beta Chain

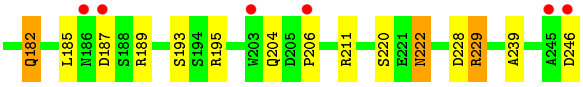
Chain E:



- Molecule 5: 1E6 TCR Beta Chain

Chain J:




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) 92.6 (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	Depositor
R, R_{free}	0.191 , 0.237 0.197 , 0.241	Depositor DCC
R_{free} test set	5659 reflections (5.27%)	DCC
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 , 45.6	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, 0.375 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	0.90	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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 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

5.2 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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

The worst 5 of 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

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%)	26 20
1	F	280/277 (101%)	273 (98%)	5 (2%)	2 (1%)	26 20
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%)	13 6
4	I	198/199 (100%)	185 (93%)	11 (6%)	2 (1%)	19 12
5	E	245/246 (100%)	234 (96%)	7 (3%)	4 (2%)	12 5
5	J	245/246 (100%)	238 (97%)	7 (3%)	0	100 100
All	All	1652/1664 (99%)	1573 (95%)	66 (4%)	13 (1%)	24 17

5 of 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

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%)	21 17
1	F	238/233 (102%)	222 (93%)	16 (7%)	20 16
2	B	95/95 (100%)	90 (95%)	5 (5%)	28 25
2	G	95/95 (100%)	90 (95%)	5 (5%)	28 25
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%)	5 3
5	E	217/216 (100%)	197 (91%)	20 (9%)	11 7
5	J	217/216 (100%)	203 (94%)	14 (6%)	21 17
All	All	1472/1464 (100%)	1336 (91%)	136 (9%)	11 7

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	133	SER
5	E	226	THR
5	J	36	ARG
5	E	137	ILE
5	E	186	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	208	ASN
1	F	191	HIS
5	J	141	GLN
5	E	213	GLN
1	F	86	ASN

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)

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	$\#\|Z\| > 2$
6	SO4	A	301	-	4,4,4	0.79	0	6,6,6	0.74	0
6	SO4	A	302	-	4,4,4	0.66	0	6,6,6	0.20	0
7	EDO	B	101	-	3,3,3	0.50	0	2,2,2	0.42	0
7	EDO	D	301	-	3,3,3	0.54	0	2,2,2	0.57	0
6	SO4	D	302	-	4,4,4	0.59	0	6,6,6	0.44	0
7	EDO	E	301	-	3,3,3	0.64	0	2,2,2	0.78	0
8	GOL	F	301	-	5,5,5	0.78	0	5,5,5	0.83	0
8	GOL	F	302	-	5,5,5	1.43	2 (40%)	5,5,5	1.88	2 (40%)
8	GOL	F	303	-	5,5,5	1.30	0	5,5,5	1.15	0
7	EDO	F	304	-	3,3,3	0.40	0	2,2,2	0.31	0
6	SO4	F	305	-	4,4,4	0.75	0	6,6,6	0.55	0
7	EDO	G	101	-	3,3,3	1.30	0	2,2,2	0.88	0
7	EDO	G	102	-	3,3,3	0.81	0	2,2,2	1.11	0
8	GOL	H	101	-	5,5,5	1.35	1 (20%)	5,5,5	2.32	3 (60%)
8	GOL	I	301	-	5,5,5	0.77	0	5,5,5	1.44	1 (20%)
7	EDO	I	302	-	3,3,3	0.57	0	2,2,2	0.58	0
7	EDO	I	303	-	3,3,3	1.03	0	2,2,2	0.71	0
6	SO4	I	304	-	4,4,4	0.58	0	6,6,6	0.89	0
8	GOL	J	301	-	5,5,5	1.16	0	5,5,5	1.91	1 (20%)
8	GOL	J	302	-	5,5,5	0.59	0	5,5,5	0.78	0
7	EDO	J	303	-	3,3,3	1.01	0	2,2,2	0.19	0
6	SO4	J	304	-	4,4,4	0.98	0	6,6,6	0.74	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	SO4	A	301	-	-	0/0/0/0	0/0/0/0
6	SO4	A	302	-	-	0/0/0/0	0/0/0/0
7	EDO	B	101	-	-	0/1/1/1	0/0/0/0
7	EDO	D	301	-	-	0/1/1/1	0/0/0/0
6	SO4	D	302	-	-	0/0/0/0	0/0/0/0
7	EDO	E	301	-	-	0/1/1/1	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
8	GOL	F	303	-	-	0/4/4/4	0/0/0/0
7	EDO	F	304	-	-	0/1/1/1	0/0/0/0
6	SO4	F	305	-	-	0/0/0/0	0/0/0/0
7	EDO	G	101	-	-	0/1/1/1	0/0/0/0
7	EDO	G	102	-	-	0/1/1/1	0/0/0/0
8	GOL	H	101	-	-	0/4/4/4	0/0/0/0
8	GOL	I	301	-	-	0/4/4/4	0/0/0/0
7	EDO	I	302	-	-	0/1/1/1	0/0/0/0
7	EDO	I	303	-	-	0/1/1/1	0/0/0/0
6	SO4	I	304	-	-	0/0/0/0	0/0/0/0
8	GOL	J	301	-	-	0/4/4/4	0/0/0/0
8	GOL	J	302	-	-	0/4/4/4	0/0/0/0
7	EDO	J	303	-	-	0/1/1/1	0/0/0/0
6	SO4	J	304	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	101	GOL	O2-C2	-2.71	1.35	1.43
8	F	302	GOL	O1-C1	2.12	1.51	1.42
8	F	302	GOL	O3-C3	2.33	1.52	1.42

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	101	GOL	O2-C2-C3	-2.38	97.04	108.47
8	H	101	GOL	O2-C2-C1	-2.09	98.42	108.47
8	F	302	GOL	C3-C2-C1	2.08	119.82	111.06
8	I	301	GOL	O3-C3-C2	2.51	122.70	109.97
8	F	302	GOL	O3-C3-C2	2.96	125.00	109.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	302	SO4	1	0
8	F	301	GOL	1	0
8	F	302	GOL	9	0
6	F	305	SO4	2	0
7	G	102	EDO	2	0
8	I	301	GOL	2	0
8	J	301	GOL	3	0
8	J	302	GOL	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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%)	0.10	9 (3%) 50 59	23, 44, 86, 112	0
1	F	277/277 (100%)	0.09	11 (3%) 42 51	22, 40, 81, 102	0
2	B	100/100 (100%)	-0.28	0 100 100	27, 41, 68, 73	0
2	G	100/100 (100%)	-0.18	0 100 100	26, 40, 56, 66	0
3	C	10/10 (100%)	-0.13	0 100 100	26, 27, 30, 31	0
3	H	10/10 (100%)	-0.26	0 100 100	24, 26, 28, 31	0
4	D	199/199 (100%)	1.23	50 (25%) 1 1	25, 55, 125, 151	0
4	I	199/199 (100%)	0.83	41 (20%) 1 1	24, 52, 113, 126	0
5	E	246/246 (100%)	0.51	33 (13%) 4 6	21, 47, 102, 126	0
5	J	246/246 (100%)	0.12	12 (4%) 33 42	20, 43, 85, 119	0
All	All	1663/1664 (99%)	0.34	156 (9%) 11 14	20, 43, 106, 151	0

The worst 5 of 156 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	151	SER	16.6
1	F	252	GLY	11.6
4	D	197	THR	11.5
4	D	199	PHE	10.2
4	D	149	LYS	9.5

6.2 Non-standard residues in protein, DNA, RNA chains

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
8	GOL	F	302	6/6	0.88	0.26	11.88	21,31,44,58	0
6	SO4	A	301	5/5	0.93	0.27	11.69	53,58,79,89	0
6	SO4	I	304	5/5	0.91	0.29	9.72	77,82,92,98	0
8	GOL	I	301	6/6	0.85	0.20	9.62	45,49,52,56	0
6	SO4	F	305	5/5	0.80	0.24	9.13	74,82,91,98	0
7	EDO	G	102	4/4	0.67	0.23	7.99	36,37,41,45	0
7	EDO	G	101	4/4	0.70	0.22	7.43	46,48,51,51	0
7	EDO	B	101	4/4	0.91	0.19	7.14	44,44,47,49	0
8	GOL	J	301	6/6	0.86	0.20	7.05	25,30,38,42	0
8	GOL	H	101	6/6	0.90	0.21	5.94	35,42,45,50	0
7	EDO	I	303	4/4	0.83	0.18	5.32	47,49,49,52	0
8	GOL	J	302	6/6	0.87	0.27	4.79	48,57,61,63	0
7	EDO	E	301	4/4	0.95	0.15	2.95	30,32,33,37	0
7	EDO	F	304	4/4	0.97	0.15	2.28	41,42,43,45	0
7	EDO	J	303	4/4	0.73	0.18	2.25	40,57,61,61	0
8	GOL	F	303	6/6	0.60	0.28	1.53	43,52,59,68	0
7	EDO	D	301	4/4	0.96	0.13	1.41	27,27,31,37	0
7	EDO	I	302	4/4	0.97	0.14	1.36	24,27,30,32	0
6	SO4	J	304	5/5	0.94	0.16	0.99	57,57,60,60	0
6	SO4	D	302	5/5	0.90	0.25	-	82,92,95,96	0
8	GOL	F	301	6/6	0.78	0.32	-	50,59,60,65	0
6	SO4	A	302	5/5	0.92	0.20	-	83,87,94,95	0

6.5 Other polymers (i)

There are no such residues in this entry.