Full wwPDB X-ray Structure Validation Report (i)

Sep 19, 2023 – 12:04 AM EDT

PDB ID	:	5C6W
Title	:	anti-CXCL13 scFv - E10
Authors	:	Tu, C.; Bard, J.; Mosyak, L.
Deposited on	:	2015-06-23
Resolution	:	1.54 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

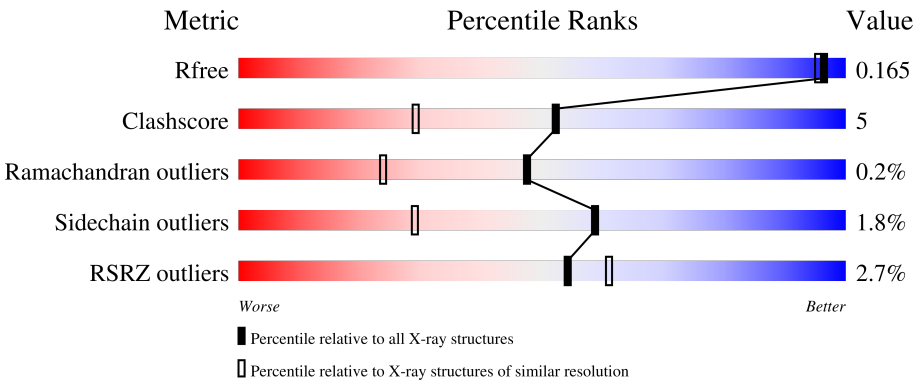
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.54 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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	H	264	3% 80% 9% • 10%
1	J	264	2% 81% 9% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	H	1223	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4436 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 Protein IGHV1-69-2,Ig lambda chain V-II region NIG-84.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	237	1867	1186	294	380	7	0	19	0
1	J	238	1849	1173	296	373	7	0	15	0

There are 148 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	99	GLU	-	linker	UNP A0A0B4J2H0
H	100	PRO	-	linker	UNP A0A0B4J2H0
H	101	ASP	-	linker	UNP A0A0B4J2H0
H	102	TYR	-	linker	UNP A0A0B4J2H0
H	103	TYR	-	linker	UNP A0A0B4J2H0
H	104	ASP	-	linker	UNP A0A0B4J2H0
H	105	SER	-	linker	UNP A0A0B4J2H0
H	106	SER	-	linker	UNP A0A0B4J2H0
H	107	GLY	-	linker	UNP A0A0B4J2H0
H	108	TYR	-	linker	UNP A0A0B4J2H0
H	109	TYR	-	linker	UNP A0A0B4J2H0
H	110	PRO	-	linker	UNP A0A0B4J2H0
H	111	ILE	-	linker	UNP A0A0B4J2H0
H	112	ASP	-	linker	UNP A0A0B4J2H0
H	113	ALA	-	linker	UNP A0A0B4J2H0
H	114	PHE	-	linker	UNP A0A0B4J2H0
H	115	ASP	-	linker	UNP A0A0B4J2H0
H	116	ILE	-	linker	UNP A0A0B4J2H0
H	117	TRP	-	linker	UNP A0A0B4J2H0
H	118	GLY	-	linker	UNP A0A0B4J2H0
H	119	GLN	-	linker	UNP A0A0B4J2H0
H	120	GLY	-	linker	UNP A0A0B4J2H0
H	121	THR	-	linker	UNP A0A0B4J2H0
H	122	THR	-	linker	UNP A0A0B4J2H0
H	123	VAL	-	linker	UNP A0A0B4J2H0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	124	THR	-	linker	UNP A0A0B4J2H0
H	125	VAL	-	linker	UNP A0A0B4J2H0
H	126	SER	-	linker	UNP A0A0B4J2H0
H	127	SER	-	linker	UNP A0A0B4J2H0
H	128	GLY	-	linker	UNP A0A0B4J2H0
H	129	GLY	-	linker	UNP A0A0B4J2H0
H	130	GLY	-	linker	UNP A0A0B4J2H0
H	131	GLY	-	linker	UNP A0A0B4J2H0
H	132	SER	-	linker	UNP A0A0B4J2H0
H	133	GLY	-	linker	UNP A0A0B4J2H0
H	134	GLY	-	linker	UNP A0A0B4J2H0
H	135	GLY	-	linker	UNP A0A0B4J2H0
H	136	GLY	-	linker	UNP A0A0B4J2H0
H	137	SER	-	linker	UNP A0A0B4J2H0
H	138	GLY	-	linker	UNP A0A0B4J2H0
H	139	GLY	-	linker	UNP A0A0B4J2H0
H	140	GLY	-	linker	UNP A0A0B4J2H0
H	141	GLY	-	linker	UNP A0A0B4J2H0
H	142	SER	-	linker	UNP A0A0B4J2H0
H	1012	ALA	GLY	conflict	UNP P04209
H	1026	SER	THR	conflict	UNP P04209
H	1031	ALA	GLY	conflict	UNP P04209
H	1034	TRP	PHE	conflict	UNP P04209
H	1051	PHE	TYR	conflict	UNP P04209
H	1055	ASN	SER	conflict	UNP P04209
H	1060	VAL	ILE	conflict	UNP P04209
H	1062	HIS	ASN	conflict	UNP P04209
H	1091	ALA	SER	conflict	UNP P04209
H	?	-	PHE	deletion	UNP P04209
H	1093	ALA	THR	conflict	UNP P04209
H	1095	LEU	THR	conflict	UNP P04209
H	1096	LEU	ASN	conflict	UNP P04209
H	1097	ASP	SER	conflict	UNP P04209
H	1098	THR	ARG	conflict	UNP P04209
H	1099	TYR	ALA	conflict	UNP P04209
H	1103	THR	GLY	conflict	UNP P04209
H	1107	VAL	LEU	conflict	UNP P04209
H	1108	THR	SER	conflict	UNP P04209
H	1112	ASP	-	expression tag	UNP P04209
H	1113	GLN	-	expression tag	UNP P04209
H	1114	GLU	-	expression tag	UNP P04209
H	1115	PRO	-	expression tag	UNP P04209

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1116	LYS	-	expression tag	UNP P04209
H	1117	SER	-	expression tag	UNP P04209
H	1118	SER	-	expression tag	UNP P04209
H	1119	ASP	-	expression tag	UNP P04209
H	1120	LYS	-	expression tag	UNP P04209
H	1121	THR	-	expression tag	UNP P04209
H	1122	HIS	-	expression tag	UNP P04209
J	99	GLU	-	linker	UNP A0A0B4J2H0
J	100	PRO	-	linker	UNP A0A0B4J2H0
J	101	ASP	-	linker	UNP A0A0B4J2H0
J	102	TYR	-	linker	UNP A0A0B4J2H0
J	103	TYR	-	linker	UNP A0A0B4J2H0
J	104	ASP	-	linker	UNP A0A0B4J2H0
J	105	SER	-	linker	UNP A0A0B4J2H0
J	106	SER	-	linker	UNP A0A0B4J2H0
J	107	GLY	-	linker	UNP A0A0B4J2H0
J	108	TYR	-	linker	UNP A0A0B4J2H0
J	109	TYR	-	linker	UNP A0A0B4J2H0
J	110	PRO	-	linker	UNP A0A0B4J2H0
J	111	ILE	-	linker	UNP A0A0B4J2H0
J	112	ASP	-	linker	UNP A0A0B4J2H0
J	113	ALA	-	linker	UNP A0A0B4J2H0
J	114	PHE	-	linker	UNP A0A0B4J2H0
J	115	ASP	-	linker	UNP A0A0B4J2H0
J	116	ILE	-	linker	UNP A0A0B4J2H0
J	117	TRP	-	linker	UNP A0A0B4J2H0
J	118	GLY	-	linker	UNP A0A0B4J2H0
J	119	GLN	-	linker	UNP A0A0B4J2H0
J	120	GLY	-	linker	UNP A0A0B4J2H0
J	121	THR	-	linker	UNP A0A0B4J2H0
J	122	THR	-	linker	UNP A0A0B4J2H0
J	123	VAL	-	linker	UNP A0A0B4J2H0
J	124	THR	-	linker	UNP A0A0B4J2H0
J	125	VAL	-	linker	UNP A0A0B4J2H0
J	126	SER	-	linker	UNP A0A0B4J2H0
J	127	SER	-	linker	UNP A0A0B4J2H0
J	128	GLY	-	linker	UNP A0A0B4J2H0
J	129	GLY	-	linker	UNP A0A0B4J2H0
J	130	GLY	-	linker	UNP A0A0B4J2H0
J	131	GLY	-	linker	UNP A0A0B4J2H0
J	132	SER	-	linker	UNP A0A0B4J2H0
J	133	GLY	-	linker	UNP A0A0B4J2H0

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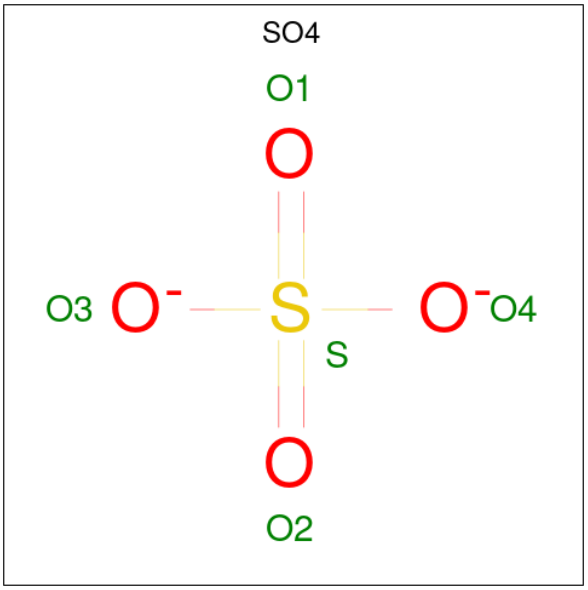
Chain	Residue	Modelled	Actual	Comment	Reference
J	134	GLY	-	linker	UNP A0A0B4J2H0
J	135	GLY	-	linker	UNP A0A0B4J2H0
J	136	GLY	-	linker	UNP A0A0B4J2H0
J	137	SER	-	linker	UNP A0A0B4J2H0
J	138	GLY	-	linker	UNP A0A0B4J2H0
J	139	GLY	-	linker	UNP A0A0B4J2H0
J	140	GLY	-	linker	UNP A0A0B4J2H0
J	141	GLY	-	linker	UNP A0A0B4J2H0
J	142	SER	-	linker	UNP A0A0B4J2H0
J	1012	ALA	GLY	conflict	UNP P04209
J	1026	SER	THR	conflict	UNP P04209
J	1031	ALA	GLY	conflict	UNP P04209
J	1034	TRP	PHE	conflict	UNP P04209
J	1051	PHE	TYR	conflict	UNP P04209
J	1055	ASN	SER	conflict	UNP P04209
J	1060	VAL	ILE	conflict	UNP P04209
J	1062	HIS	ASN	conflict	UNP P04209
J	1091	ALA	SER	conflict	UNP P04209
J	?	-	PHE	deletion	UNP P04209
J	1093	ALA	THR	conflict	UNP P04209
J	1095	LEU	THR	conflict	UNP P04209
J	1096	LEU	ASN	conflict	UNP P04209
J	1097	ASP	SER	conflict	UNP P04209
J	1098	THR	ARG	conflict	UNP P04209
J	1099	TYR	ALA	conflict	UNP P04209
J	1103	THR	GLY	conflict	UNP P04209
J	1107	VAL	LEU	conflict	UNP P04209
J	1108	THR	SER	conflict	UNP P04209
J	1112	ASP	-	expression tag	UNP P04209
J	1113	GLN	-	expression tag	UNP P04209
J	1114	GLU	-	expression tag	UNP P04209
J	1115	PRO	-	expression tag	UNP P04209
J	1116	LYS	-	expression tag	UNP P04209
J	1117	SER	-	expression tag	UNP P04209
J	1118	SER	-	expression tag	UNP P04209
J	1119	ASP	-	expression tag	UNP P04209
J	1120	LYS	-	expression tag	UNP P04209
J	1121	THR	-	expression tag	UNP P04209
J	1122	HIS	-	expression tag	UNP P04209

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

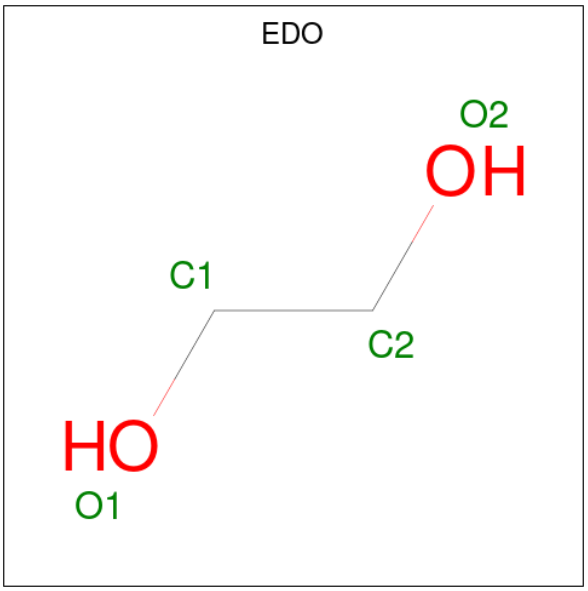
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	4	Total Cl 4 4	0	0
2	J	2	Total Cl 2 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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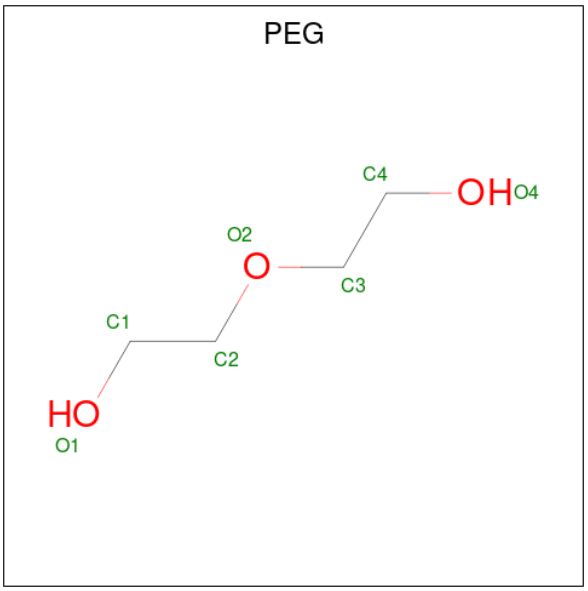
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	H	1	4	2	2		0	0
			Total	C	O			
4	H	1	4	2	2		0	0
			Total	C	O			
4	H	1	4	2	2		0	0
			Total	C	O			
4	J	1	4	2	2		0	0
			Total	C	O			
4	J	1	4	2	2		0	0
			Total	C	O			
4	J	1	4	2	2		0	0
			Total	C	O			
4	J	1	4	2	2		0	0
			Total	C	O			
4	J	1	4	2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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	H	1	7	4	3	0	0
			Total	C	O		
5	J	1	7	4	3	0	0

- Molecule 6 is water.

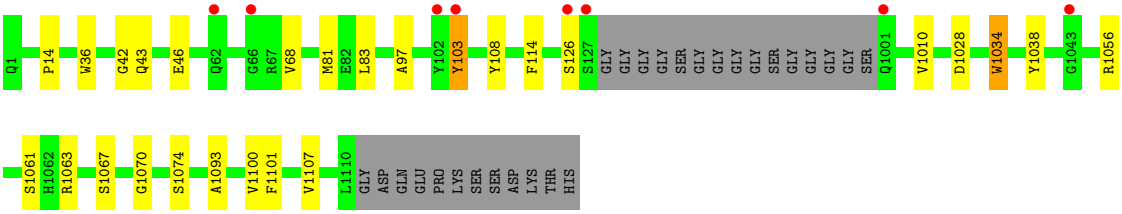
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	H	285	285	285	0	0
			Total	O		
6	J	274	274	274	0	0

3 Residue-property plots (i)

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

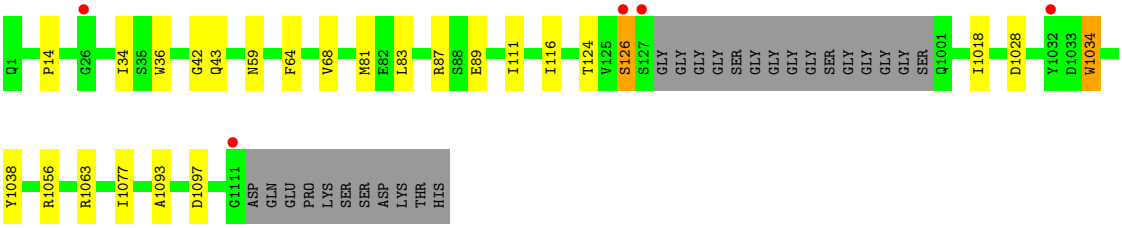
• Molecule 1: Protein IGHV1-69-2,Ig lambda chain V-II region NIG-84

Chain H:



• Molecule 1: Protein IGHV1-69-2,Ig lambda chain V-II region NIG-84

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.98Å 80.36Å 119.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.54 48.26 – 1.54	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-1.54) 98.8 (48.26-1.54)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 1.55Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.154 , 0.164 0.153 , 0.165	Depositor DCC
R_{free} test set	4903 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	19.6	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4436	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, CL, EDO, SO4

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	H	0.49	0/1965	0.67	0/2675
1	J	0.51	0/1936	0.66	0/2636
All	All	0.50	0/3901	0.66	0/5311

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	H	0	1
1	J	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	1038	TYR	Sidechain
1	J	1038	TYR	Sidechain

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	H	1867	0	1826	24	0
1	J	1849	0	1814	20	0
2	H	4	0	0	0	0
2	J	2	0	0	0	0
3	H	10	0	0	0	0
3	J	15	0	0	1	0
4	H	68	0	102	6	0
4	J	48	0	72	2	0
5	H	7	0	10	0	0
5	J	7	0	10	0	0
6	H	285	0	0	0	0
6	J	274	0	0	3	0
All	All	4436	0	3834	42	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (42) 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:H:103:TYR:CZ	1:H:108[B]:TYR:HE1	1.88	0.92
1:H:1070:GLY:H	4:H:1212:EDO:H21	1.35	0.92
1:H:103:TYR:CE1	1:H:108[B]:TYR:HE1	1.93	0.85
1:H:103:TYR:CE1	1:H:108[B]:TYR:CE1	2.69	0.81
1:H:103:TYR:CZ	1:H:108[B]:TYR:CE1	2.70	0.80
1:J:1018[A]:ILE:HD11	1:J:1077:ILE:HD12	1.68	0.75
1:H:1100:VAL:HG23	4:H:1223:EDO:H21	1.70	0.73
1:H:46:GLU:HA	4:H:1223:EDO:H11	1.69	0.73
1:J:124[A]:THR:HG22	6:J:1502:HOH:O	1.90	0.71
1:H:1101:PHE:H	4:H:1223:EDO:H12	1.57	0.69
1:H:68[B]:VAL:HG22	1:H:83:LEU:HD13	1.76	0.67
1:J:68[B]:VAL:HG12	1:J:83:LEU:HD13	1.77	0.66
1:J:87[B]:ARG:HG3	1:J:89:GLU:HG2	1.78	0.66
1:J:68[A]:VAL:HG22	1:J:83:LEU:HD13	1.80	0.63
1:J:116[B]:ILE:HD11	3:J:1204:SO4:O2	1.98	0.63
1:J:14:PRO:HD3	1:J:126:SER:HB2	1.81	0.62
1:J:124[A]:THR:CG2	6:J:1502:HOH:O	2.52	0.56
1:J:59[B]:ASN:ND2	1:J:1097:ASP:OD2	2.41	0.53
1:H:14:PRO:HD3	1:H:126:SER:HB2	1.92	0.52
1:H:1101:PHE:H	4:H:1223:EDO:C1	2.24	0.51
1:H:42:GLY:HA2	1:J:43:GLN:O	2.15	0.47
1:J:64:PHE:HB3	1:J:68[A]:VAL:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:111:ILE:HD11	6:J:1568:HOH:O	2.15	0.46
1:H:1010[A]:VAL:CG2	1:H:1107:VAL:HG22	2.46	0.46
1:H:103:TYR:CE1	1:H:108[B]:TYR:CD1	3.04	0.45
1:H:1101:PHE:N	4:H:1223:EDO:H12	2.27	0.45
1:J:1063:ARG:HE	4:J:1215:EDO:C2	2.30	0.45
1:H:81[B]:MET:O	1:H:81[B]:MET:HG3	2.18	0.44
1:H:1061[A]:SER:OG	1:H:1063:ARG:HG3	2.17	0.44
1:H:36:TRP:CE2	1:H:81[A]:MET:HB2	2.53	0.44
1:H:43:GLN:O	1:J:42:GLY:HA2	2.18	0.44
1:H:1067[B]:SER:OG	1:H:1074:SER:OG	2.37	0.42
1:J:34:ILE:HG13	4:J:1209:EDO:H22	2.01	0.42
1:J:64:PHE:HB3	1:J:68[A]:VAL:HG23	2.01	0.42
1:H:97:ALA:HB1	1:H:114:PHE:HB3	2.02	0.42
1:J:36:TRP:CE2	1:J:81[A]:MET:HB2	2.55	0.41
1:H:1010[A]:VAL:HG23	1:H:1107:VAL:HG22	2.03	0.41
1:J:68[B]:VAL:CG1	1:J:83:LEU:HD13	2.44	0.41
1:H:103:TYR:HH	1:H:108[B]:TYR:HE1	1.67	0.41
1:H:1034:TRP:CD2	1:H:1093:ALA:HB3	2.56	0.40
1:J:36:TRP:CE2	1:J:81[B]:MET:HB2	2.56	0.40
1:J:1034:TRP:CD2	1:J:1093:ALA:HB3	2.55	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	H	252/264 (96%)	248 (98%)	4 (2%)	0	100	100
1	J	249/264 (94%)	243 (98%)	5 (2%)	1 (0%)	34	13
All	All	501/528 (95%)	491 (98%)	9 (2%)	1 (0%)	47	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	126	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	H	212/207 (102%)	208 (98%)	4 (2%)	57	26
1	J	208/207 (100%)	205 (99%)	3 (1%)	67	39
All	All	420/414 (101%)	413 (98%)	7 (2%)	59	31

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	103	TYR
1	H	1028	ASP
1	H	1034	TRP
1	H	1056	ARG
1	J	1028	ASP
1	J	1034	TRP
1	J	1056	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 6 are monoatomic - leaving 36 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	H	1209	-	3,3,3	0.28	0	2,2,2	0.62	0
4	EDO	H	1212	-	3,3,3	0.40	0	2,2,2	0.39	0
3	SO4	J	1203	-	4,4,4	0.26	0	6,6,6	0.15	0
3	SO4	H	1206	-	4,4,4	0.26	0	6,6,6	0.10	0
4	EDO	H	1210	-	3,3,3	0.46	0	2,2,2	0.38	0
4	EDO	H	1211	-	3,3,3	0.42	0	2,2,2	0.28	0
4	EDO	J	1210	-	3,3,3	0.44	0	2,2,2	0.28	0
4	EDO	J	1216	-	3,3,3	0.43	0	2,2,2	0.34	0
4	EDO	H	1219	-	3,3,3	0.49	0	2,2,2	0.26	0
4	EDO	J	1206	-	3,3,3	0.42	0	2,2,2	0.45	0
4	EDO	H	1218	-	3,3,3	0.43	0	2,2,2	0.34	0
4	EDO	H	1216	-	3,3,3	0.65	0	2,2,2	0.27	0
4	EDO	H	1208	-	3,3,3	0.46	0	2,2,2	0.31	0
3	SO4	H	1205	-	4,4,4	0.26	0	6,6,6	0.65	0
4	EDO	H	1217	-	3,3,3	0.43	0	2,2,2	0.34	0
4	EDO	H	1213	-	3,3,3	0.43	0	2,2,2	0.34	0
4	EDO	J	1209	-	3,3,3	0.40	0	2,2,2	0.36	0
5	PEG	H	1224	-	6,6,6	0.31	0	5,5,5	0.88	0
4	EDO	H	1223	-	3,3,3	0.41	0	2,2,2	0.59	0
4	EDO	H	1220	-	3,3,3	0.48	0	2,2,2	0.30	0
4	EDO	J	1214	-	3,3,3	0.42	0	2,2,2	0.21	0
4	EDO	H	1222	-	3,3,3	0.54	0	2,2,2	0.35	0
4	EDO	J	1208	-	3,3,3	0.47	0	2,2,2	0.24	0
3	SO4	J	1204	-	4,4,4	0.31	0	6,6,6	0.16	0
4	EDO	J	1215	-	3,3,3	0.40	0	2,2,2	0.30	0
5	PEG	J	1218	-	6,6,6	0.15	0	5,5,5	0.32	0
4	EDO	J	1211	-	3,3,3	0.44	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	J	1213	-	3,3,3	0.45	0	2,2,2	0.33	0
4	EDO	J	1212	-	3,3,3	0.43	0	2,2,2	0.37	0
4	EDO	H	1221	-	3,3,3	0.50	0	2,2,2	0.22	0
4	EDO	J	1207	-	3,3,3	0.44	0	2,2,2	0.32	0
4	EDO	H	1207	-	3,3,3	0.47	0	2,2,2	0.27	0
3	SO4	J	1205	-	4,4,4	0.20	0	6,6,6	0.22	0
4	EDO	H	1214	-	3,3,3	0.46	0	2,2,2	0.23	0
4	EDO	J	1217	-	3,3,3	0.49	0	2,2,2	0.33	0
4	EDO	H	1215	-	3,3,3	0.42	0	2,2,2	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	H	1209	-	-	1/1/1/1	-
4	EDO	H	1212	-	-	1/1/1/1	-
4	EDO	H	1210	-	-	0/1/1/1	-
4	EDO	H	1211	-	-	0/1/1/1	-
4	EDO	J	1210	-	-	0/1/1/1	-
4	EDO	J	1216	-	-	0/1/1/1	-
4	EDO	H	1219	-	-	1/1/1/1	-
4	EDO	J	1206	-	-	0/1/1/1	-
4	EDO	H	1218	-	-	0/1/1/1	-
4	EDO	H	1216	-	-	0/1/1/1	-
4	EDO	H	1208	-	-	0/1/1/1	-
4	EDO	H	1217	-	-	1/1/1/1	-
4	EDO	H	1213	-	-	0/1/1/1	-
4	EDO	J	1209	-	-	0/1/1/1	-
5	PEG	H	1224	-	-	3/4/4/4	-
4	EDO	H	1223	-	-	0/1/1/1	-
4	EDO	H	1220	-	-	1/1/1/1	-
4	EDO	J	1214	-	-	0/1/1/1	-
4	EDO	H	1222	-	-	0/1/1/1	-
4	EDO	J	1208	-	-	1/1/1/1	-
4	EDO	J	1215	-	-	1/1/1/1	-
5	PEG	J	1218	-	-	4/4/4/4	-
4	EDO	J	1211	-	-	0/1/1/1	-
4	EDO	J	1213	-	-	0/1/1/1	-
4	EDO	J	1212	-	-	0/1/1/1	-
4	EDO	H	1221	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	J	1207	-	-	0/1/1/1	-
4	EDO	H	1207	-	-	1/1/1/1	-
4	EDO	H	1214	-	-	0/1/1/1	-
4	EDO	J	1217	-	-	1/1/1/1	-
4	EDO	H	1215	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	1218	PEG	O2-C3-C4-O4
5	H	1224	PEG	O2-C3-C4-O4
4	H	1207	EDO	O1-C1-C2-O2
4	H	1220	EDO	O1-C1-C2-O2
5	J	1218	PEG	O1-C1-C2-O2
4	H	1217	EDO	O1-C1-C2-O2
4	J	1208	EDO	O1-C1-C2-O2
4	J	1215	EDO	O1-C1-C2-O2
4	J	1217	EDO	O1-C1-C2-O2
5	H	1224	PEG	C1-C2-O2-C3
5	J	1218	PEG	C4-C3-O2-C2
5	J	1218	PEG	C1-C2-O2-C3
5	H	1224	PEG	C4-C3-O2-C2
4	H	1209	EDO	O1-C1-C2-O2
4	H	1212	EDO	O1-C1-C2-O2
4	H	1219	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1212	EDO	1	0
4	J	1209	EDO	1	0
4	H	1223	EDO	5	0
3	J	1204	SO4	1	0
4	J	1215	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	H	237/264 (89%)	-0.06	8 (3%)	45	51	14, 22, 38, 69	4 (1%)
1	J	238/264 (90%)	-0.07	5 (2%)	63	69	14, 20, 38, 60	7 (2%)
All	All	475/528 (89%)	-0.06	13 (2%)	54	61	14, 21, 38, 69	11 (2%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	102[A]	TYR	4.8
1	J	26	GLY	4.5
1	H	1001	GLN	4.2
1	H	66	GLY	4.1
1	J	127	SER	4.1
1	H	126	SER	3.8
1	H	127	SER	3.7
1	J	1111	GLY	3.4
1	J	126	SER	3.2
1	H	62	GLN	2.3
1	J	1032[A]	TYR	2.3
1	H	1043	GLY	2.1
1	H	103	TYR	2.1

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 monosaccharides 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, 95th 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
5	PEG	H	1224	7/7	0.42	0.28	60,61,63,65	0
4	EDO	J	1217	4/4	0.51	0.25	65,67,68,68	0
4	EDO	H	1220	4/4	0.51	0.28	72,74,76,77	0
4	EDO	H	1221	4/4	0.58	0.36	60,61,62,65	0
2	CL	H	1204	1/1	0.63	0.05	96,96,96,96	0
2	CL	H	1202	1/1	0.69	0.12	95,95,95,95	0
4	EDO	H	1219	4/4	0.71	0.19	53,54,55,58	0
4	EDO	H	1213	4/4	0.73	0.26	57,58,62,65	0
4	EDO	H	1212	4/4	0.73	0.14	41,45,49,52	0
4	EDO	H	1215	4/4	0.76	0.15	56,58,61,62	0
5	PEG	J	1218	7/7	0.76	0.16	66,66,67,71	0
4	EDO	J	1213	4/4	0.78	0.22	81,83,85,85	0
4	EDO	J	1206	4/4	0.79	0.17	56,57,59,64	0
3	SO4	J	1205	5/5	0.80	0.18	77,81,82,82	0
4	EDO	H	1208	4/4	0.80	0.13	59,60,61,66	0
4	EDO	J	1216	4/4	0.80	0.20	36,39,44,49	0
4	EDO	J	1210	4/4	0.81	0.15	60,62,63,64	0
4	EDO	H	1217	4/4	0.81	0.13	61,63,65,65	0
4	EDO	J	1214	4/4	0.83	0.10	41,41,43,47	0
4	EDO	H	1207	4/4	0.86	0.11	50,51,52,57	0
4	EDO	H	1222	4/4	0.86	0.22	31,40,42,48	0
4	EDO	H	1216	4/4	0.87	0.12	29,32,35,39	0
4	EDO	J	1211	4/4	0.88	0.26	47,50,51,59	0
4	EDO	H	1210	4/4	0.88	0.20	47,47,50,55	0
2	CL	H	1201	1/1	0.88	0.07	85,85,85,85	0
4	EDO	J	1215	4/4	0.88	0.11	35,37,43,48	0
4	EDO	J	1212	4/4	0.89	0.14	44,45,46,55	0
2	CL	H	1203	1/1	0.90	0.08	59,59,59,59	0
4	EDO	H	1214	4/4	0.90	0.16	38,38,38,43	0
2	CL	J	1202	1/1	0.91	0.22	84,84,84,84	0
4	EDO	J	1207	4/4	0.91	0.11	43,44,47,50	0
4	EDO	H	1218	4/4	0.91	0.12	51,52,54,56	0
4	EDO	H	1209	4/4	0.91	0.10	30,36,38,41	0
4	EDO	H	1223	4/4	0.92	0.15	24,28,28,37	0
4	EDO	J	1208	4/4	0.92	0.10	36,38,39,42	0
4	EDO	H	1211	4/4	0.92	0.09	44,45,46,47	0
4	EDO	J	1209	4/4	0.93	0.10	34,35,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	J	1201	1/1	0.95	0.19	51,51,51,51	0
3	SO4	J	1204	5/5	0.96	0.10	32,35,38,38	5
3	SO4	J	1203	5/5	0.98	0.10	32,34,38,39	5
3	SO4	H	1205	5/5	0.99	0.10	24,29,31,33	5
3	SO4	H	1206	5/5	0.99	0.07	32,35,38,38	5

6.5 Other polymers (i)

There are no such residues in this entry.