



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 12:19 PM EDT

PDB ID : 5WI9
Title : Crystal structure of KL with an agonist Fab
Authors : Johnstone, S.; Min, X.; Wang, Z.
Deposited on : 2017-07-18
Resolution : 2.70 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

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

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) 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 : 2.37.1
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) : 2.37.1

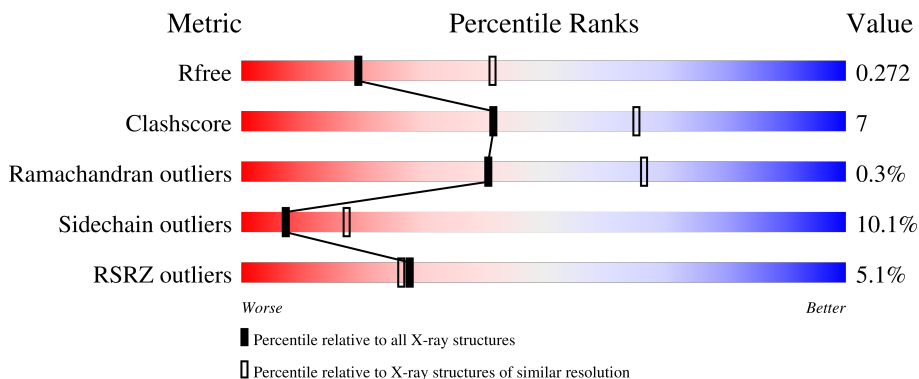
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



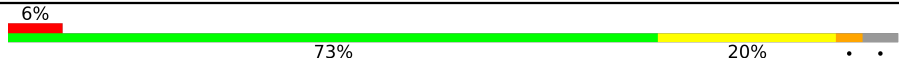
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	470	 78% 11% • 10%
1	B	470	 72% 17% • 10%
2	E	215	 73% 24% ••
2	L	215	 67% 18% • 13%
3	F	225	 67% 25% • 5%

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Mol	Chain	Length	Quality of chain
3	H	225	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into segments: a small red segment at the beginning labeled '6%', a large green segment labeled '73%', and a yellow segment at the end labeled '20%'. There are two small black dots at the far right end of the bar.</p>

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 13556 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 Beta-klotho.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	425	3493	2274	588	619	12	0	0	0
1	B	425	3493	2274	588	619	12	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	509	GLU	-	expression tag	UNP Q86Z14
A	510	ASN	-	expression tag	UNP Q86Z14
A	511	LEU	-	expression tag	UNP Q86Z14
A	512	TYR	-	expression tag	UNP Q86Z14
A	513	PHE	-	expression tag	UNP Q86Z14
A	514	GLN	-	expression tag	UNP Q86Z14
A	515	GLY	-	expression tag	UNP Q86Z14
A	516	HIS	-	expression tag	UNP Q86Z14
A	517	HIS	-	expression tag	UNP Q86Z14
A	518	HIS	-	expression tag	UNP Q86Z14
A	519	HIS	-	expression tag	UNP Q86Z14
A	520	HIS	-	expression tag	UNP Q86Z14
A	521	HIS	-	expression tag	UNP Q86Z14
B	509	GLU	-	expression tag	UNP Q86Z14
B	510	ASN	-	expression tag	UNP Q86Z14
B	511	LEU	-	expression tag	UNP Q86Z14
B	512	TYR	-	expression tag	UNP Q86Z14
B	513	PHE	-	expression tag	UNP Q86Z14
B	514	GLN	-	expression tag	UNP Q86Z14
B	515	GLY	-	expression tag	UNP Q86Z14
B	516	HIS	-	expression tag	UNP Q86Z14
B	517	HIS	-	expression tag	UNP Q86Z14
B	518	HIS	-	expression tag	UNP Q86Z14
B	519	HIS	-	expression tag	UNP Q86Z14
B	520	HIS	-	expression tag	UNP Q86Z14

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Chain	Residue	Modelled	Actual	Comment	Reference
B	521	HIS	-	expression tag	UNP Q86Z14

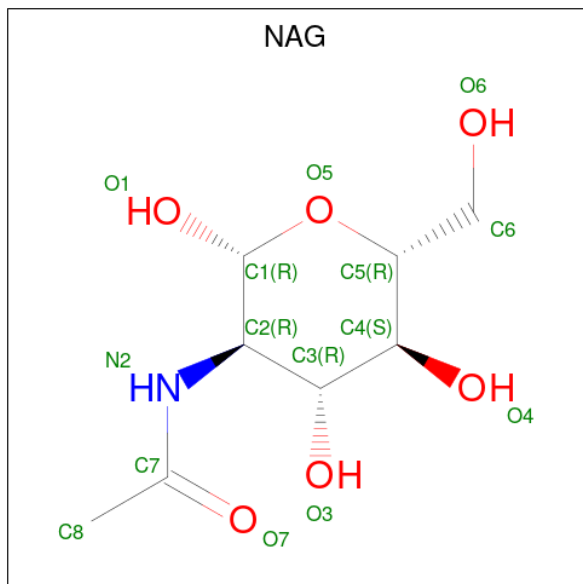
- Molecule 2 is a protein called 39F7 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	188	Total	C	N	O	S	0	0	0
			1414	880	235	295	4			
2	E	212	Total	C	N	O	S	0	0	0
			1614	1007	273	330	4			

- Molecule 3 is a protein called 39F7 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	217	Total	C	N	O	S	0	0	0
			1645	1046	280	313	6			
3	F	213	Total	C	N	O	S	0	0	0
			1621	1032	276	307	6			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



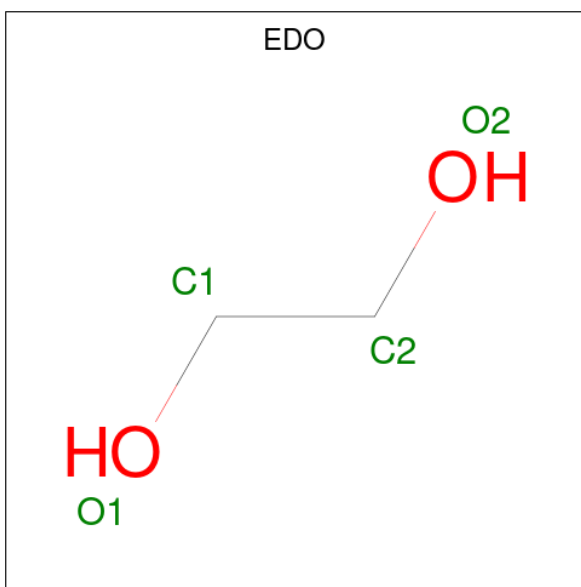
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



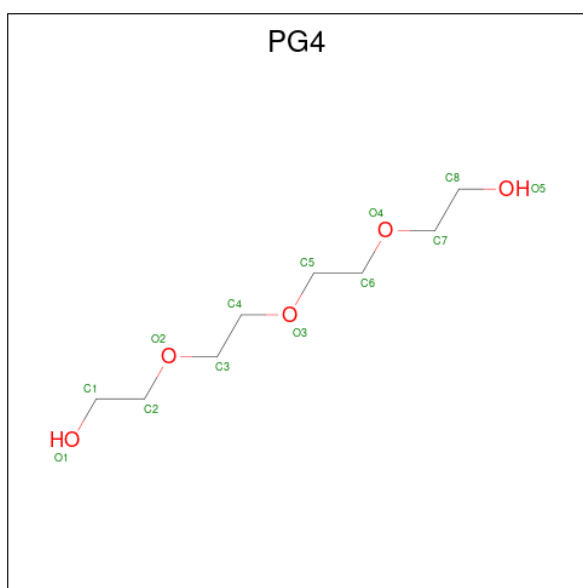
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		
7	L	1	Total	C	O	0	0
			13	8	5		

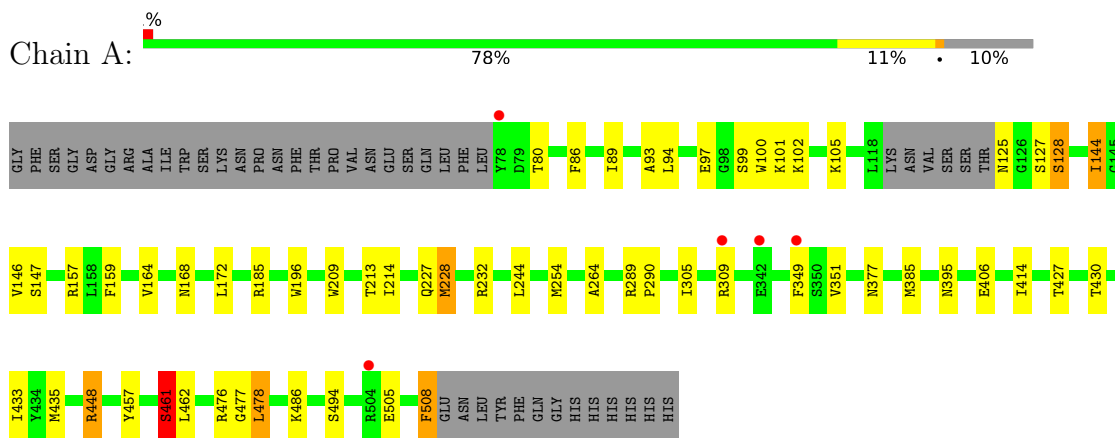
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	67	Total 67	O 67	0	0
8	B	50	Total 50	O 50	0	0
8	L	18	Total 18	O 18	0	0
8	H	11	Total 11	O 11	0	0
8	E	5	Total 5	O 5	0	0
8	F	5	Total 5	O 5	0	0

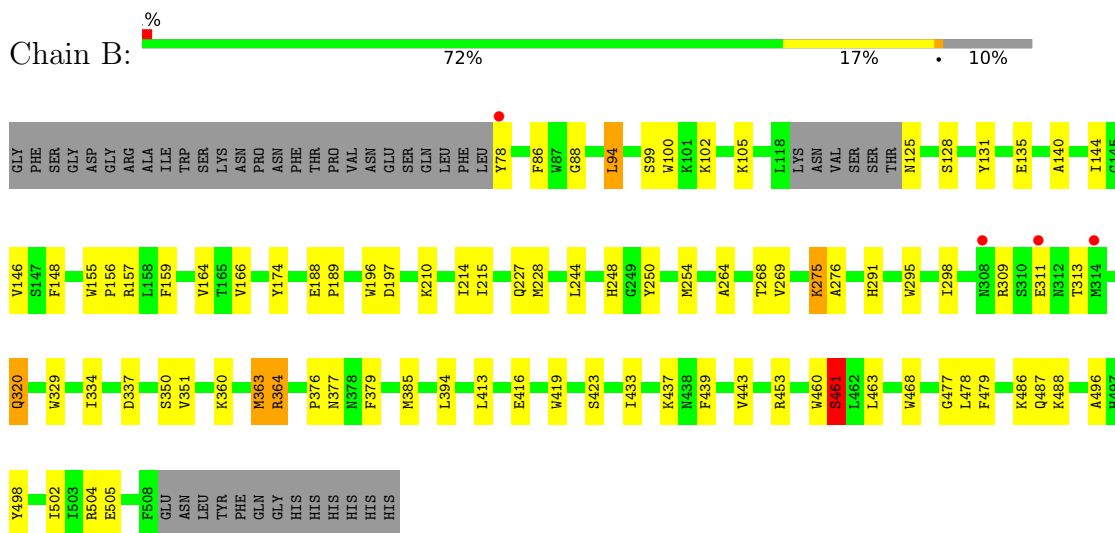
3 Residue-property plots [i](#)

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.

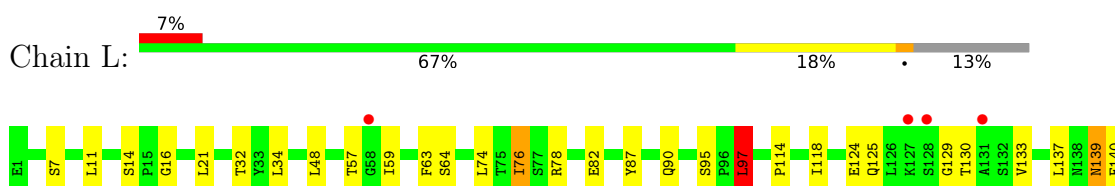
- Molecule 1: Beta-klotho

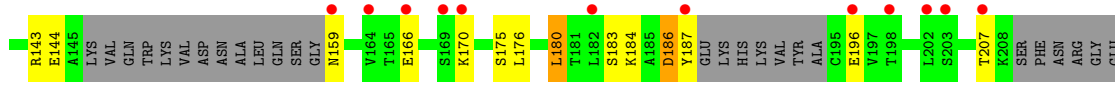


- Molecule 1: Beta-klotho



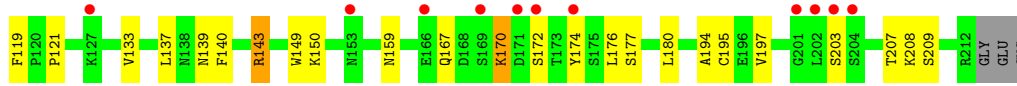
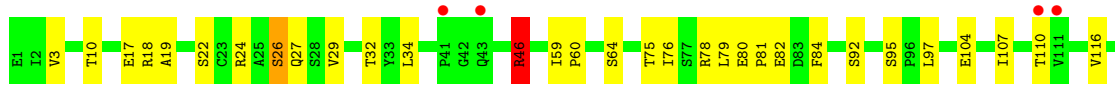
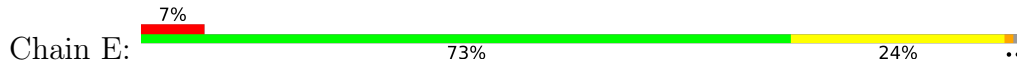
- Molecule 2: 39F7 Fab light chain



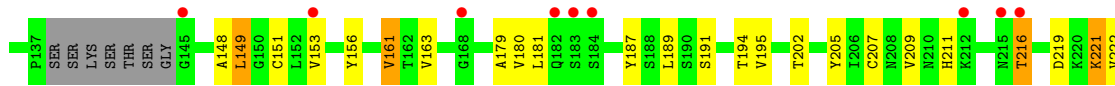
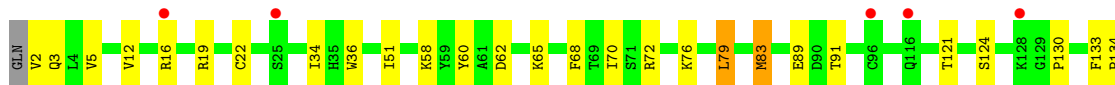
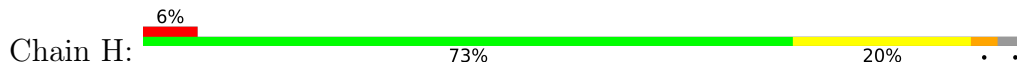


CYS

• Molecule 2: 39F7 Fab light chain

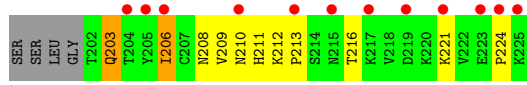
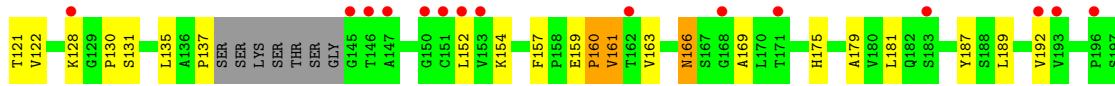
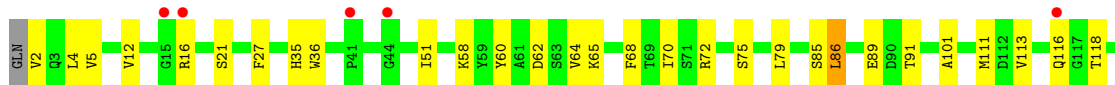


• Molecule 3: 39F7 Fab heavy chain



K225

• Molecule 3: 39F7 Fab heavy chain



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.02Å 68.47Å 147.81Å 90.00° 111.86° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 19.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.70) 99.6 (19.80-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.71Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.216 , 0.270 0.219 , 0.272	Depositor DCC
R_{free} test set	2979 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtrriage
Anisotropy	0.529	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13556	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, SO4, PG4, NAG

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	0.46	0/3607	0.64	1/4893 (0.0%)
1	B	0.46	0/3607	0.64	0/4893
2	E	0.40	0/1648	0.66	3/2239 (0.1%)
2	L	0.41	0/1441	0.65	1/1958 (0.1%)
3	F	0.38	0/1662	0.63	1/2264 (0.0%)
3	H	0.40	0/1687	0.61	0/2299
All	All	0.43	0/13652	0.64	6/18546 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	97	LEU	CA-CB-CG	5.47	127.87	115.30
2	E	18	ARG	NE-CZ-NH1	5.29	122.95	120.30
3	F	157	PHE	C-N-CD	-5.23	109.09	120.60
2	E	46	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	E	143	ARG	NE-CZ-NH1	5.17	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3493	0	3357	24	0
1	B	3493	0	3357	50	0
2	E	1614	0	1570	27	0
2	L	1414	0	1369	16	0
3	F	1621	0	1583	33	0
3	H	1645	0	1608	38	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0
5	A	20	0	30	0	0
5	B	4	0	6	0	0
5	H	4	0	6	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	13	0	18	0	0
7	L	13	0	18	0	0
8	A	67	0	0	0	0
8	B	50	0	0	0	0
8	E	5	0	0	0	0
8	F	5	0	0	0	0
8	H	11	0	0	0	0
8	L	18	0	0	0	0
All	All	13556	0	12974	185	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 7.

The worst 5 of 185 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)
3:F:163:VAL:HG22	3:F:209:VAL:HG22	1.58	0.86
3:F:91:THR:HG23	3:F:121:THR:HA	1.56	0.86
1:B:498:TYR:CE2	1:B:502:ILE:HD11	2.10	0.86
2:E:80:GLU:HB3	2:E:81:PRO:HD2	1.59	0.81
3:H:22:CYS:HB3	3:H:79:LEU:HD23	1.65	0.78

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	421/470 (90%)	406 (96%)	14 (3%)	1 (0%)	47	73
1	B	421/470 (90%)	408 (97%)	12 (3%)	1 (0%)	47	73
2	E	210/215 (98%)	202 (96%)	7 (3%)	1 (0%)	29	54
2	L	182/215 (85%)	177 (97%)	5 (3%)	0	100	100
3	F	207/225 (92%)	199 (96%)	6 (3%)	2 (1%)	15	37
3	H	213/225 (95%)	205 (96%)	8 (4%)	0	100	100
All	All	1654/1820 (91%)	1597 (97%)	52 (3%)	5 (0%)	41	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	461	SER
1	B	461	SER
2	E	139	ASN
3	F	101	ALA
3	F	160	PRO

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	368/408 (90%)	339 (92%)	29 (8%)	12	28
1	B	368/408 (90%)	341 (93%)	27 (7%)	14	33
2	E	183/185 (99%)	162 (88%)	21 (12%)	5	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	162/185 (88%)	134 (83%)	28 (17%)	2 5
3	F	176/186 (95%)	155 (88%)	21 (12%)	5 12
3	H	179/186 (96%)	160 (89%)	19 (11%)	6 15
All	All	1436/1558 (92%)	1291 (90%)	145 (10%)	7 17

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	95	SER
3	F	208	ASN
2	E	170	LYS
3	F	79	LEU
1	B	413	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	150	GLN
2	L	90	GLN
2	L	139	ASN
3	F	77	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 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	$\# Z > 2$
7	PG4	A	609	-	12,12,12	0.48	0	11,11,11	0.48	0
7	PG4	L	301	-	12,12,12	0.45	0	11,11,11	0.36	0
5	EDO	A	605	-	3,3,3	0.54	0	2,2,2	0.12	0
5	EDO	A	604	-	3,3,3	0.50	0	2,2,2	0.07	0
5	EDO	H	301	-	3,3,3	0.34	0	2,2,2	0.45	0
4	NAG	B	601	1	14,14,15	0.66	0	17,19,21	1.80	5 (29%)
4	NAG	A	601	1	14,14,15	0.88	1 (7%)	17,19,21	2.56	6 (35%)
6	SO4	B	604	-	4,4,4	0.35	0	6,6,6	0.18	0
5	EDO	A	606	-	3,3,3	0.47	0	2,2,2	0.22	0
5	EDO	A	603	-	3,3,3	0.53	0	2,2,2	0.28	0
4	NAG	B	602	1	14,14,15	0.49	0	17,19,21	1.10	1 (5%)
5	EDO	A	607	-	3,3,3	0.39	0	2,2,2	0.33	0
5	EDO	B	603	-	3,3,3	0.35	0	2,2,2	0.47	0
6	SO4	A	608	-	4,4,4	0.39	0	6,6,6	0.23	0
4	NAG	A	602	1	14,14,15	0.56	0	17,19,21	1.47	3 (17%)

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	PG4	A	609	-	-	6/10/10/10	-
7	PG4	L	301	-	-	5/10/10/10	-
5	EDO	A	605	-	-	1/1/1/1	-
5	EDO	A	604	-	-	0/1/1/1	-
5	EDO	H	301	-	-	1/1/1/1	-
4	NAG	B	601	1	-	2/6/23/26	0/1/1/1
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1
5	EDO	A	606	-	-	1/1/1/1	-
5	EDO	A	603	-	-	1/1/1/1	-
4	NAG	B	602	1	-	0/6/23/26	0/1/1/1
5	EDO	A	607	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	603	-	-	1/1/1/1	-
4	NAG	A	602	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	C2-N2	-2.70	1.41	1.46

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	C1-C2-N2	-6.89	98.72	110.49
4	A	601	NAG	O5-C1-C2	-4.62	103.99	111.29
4	B	601	NAG	C1-C2-N2	-4.58	102.67	110.49
4	A	601	NAG	C8-C7-N2	-3.62	109.97	116.10
4	A	602	NAG	O5-C1-C2	-3.33	106.02	111.29

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	301	PG4	O1-C1-C2-O2
4	B	601	NAG	C4-C5-C6-O6
4	B	601	NAG	O5-C5-C6-O6
7	A	609	PG4	O3-C5-C6-O4
7	L	301	PG4	O4-C7-C8-O5

There are no ring outliers.

No monomer is involved in short contacts.

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	A	425/470 (90%)	-0.36	5 (1%) 79 80	19, 29, 50, 80	0
1	B	425/470 (90%)	-0.23	4 (0%) 84 85	21, 33, 53, 74	0
2	E	212/215 (98%)	0.55	15 (7%) 16 14	36, 67, 89, 106	0
2	L	188/215 (87%)	0.49	16 (8%) 10 9	23, 55, 93, 97	0
3	F	213/225 (94%)	0.84	32 (15%) 2 1	34, 71, 101, 111	0
3	H	217/225 (96%)	0.42	14 (6%) 18 17	27, 62, 87, 98	0
All	All	1680/1820 (92%)	0.14	86 (5%) 28 26	19, 42, 89, 111	0

The worst 5 of 86 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	168	GLY	5.4
3	F	196	PRO	4.6
3	F	217	LYS	4.4
2	E	204	SER	4.3
3	F	225	LYS	4.1

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	EDO	A	606	4/4	0.74	0.28	60,61,62,63	0
4	NAG	A	601	14/15	0.77	0.35	60,65,71,72	0
4	NAG	A	602	14/15	0.79	0.36	63,67,72,73	0
7	PG4	A	609	13/13	0.81	0.22	48,59,63,65	0
4	NAG	B	601	14/15	0.83	0.31	59,63,64,67	0
5	EDO	H	301	4/4	0.88	0.19	47,48,48,50	0
4	NAG	B	602	14/15	0.88	0.35	56,59,62,64	0
7	PG4	L	301	13/13	0.89	0.19	49,54,57,57	0
6	SO4	A	608	5/5	0.94	0.14	63,66,67,68	0
5	EDO	A	603	4/4	0.95	0.16	32,32,32,33	0
5	EDO	A	607	4/4	0.96	0.16	47,47,47,48	0
5	EDO	B	603	4/4	0.96	0.15	29,31,31,31	0
5	EDO	A	604	4/4	0.97	0.17	36,36,36,37	0
6	SO4	B	604	5/5	0.97	0.13	59,59,62,63	0
5	EDO	A	605	4/4	0.98	0.09	36,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.