



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:36 AM UTC

PDB ID : 5WI9 / pdb_00005wi9
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 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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

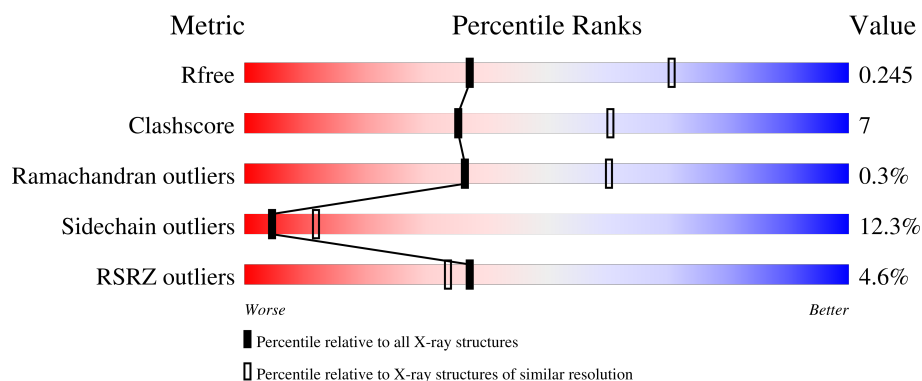
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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	
1	B	470	
2	E	215	
2	L	215	
3	F	225	

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Mol	Chain	Length	Quality of chain
3	H	225	73% 20% 2%

2 Entry composition

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
1	A	425	Total	C	N	O	S	0	0	0
			3493	2274	588	619	12			
1	B	425	Total	C	N	O	S	0	0	0
			3493	2274	588	619	12			

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

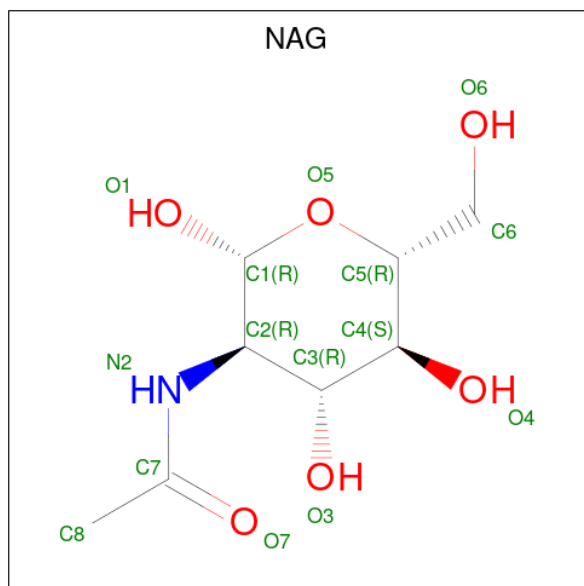
- Molecule 2 is a protein called 39F7 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 (CCD ID: EDO) (formula: C₂H₆O₂).



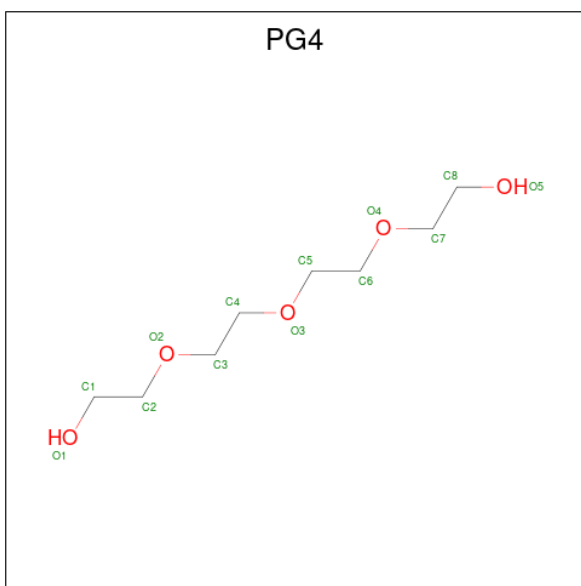
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is SULFATE ION (CCD ID: 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 (CCD ID: 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.

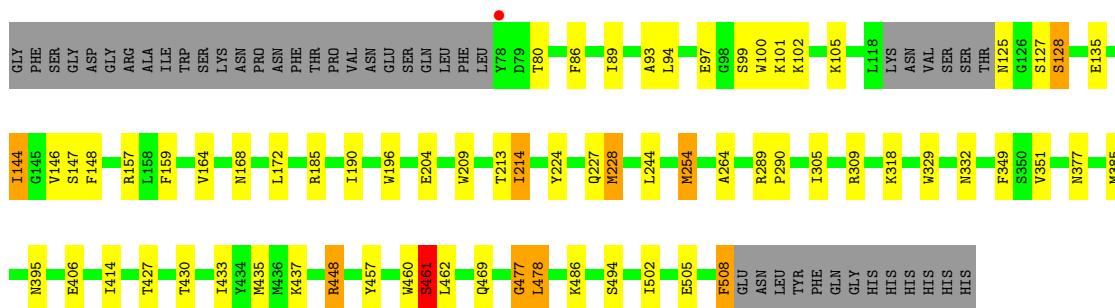
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	67	Total 67	O 67	0	0
8	B	50	Total 50	O 50	0	0
8	L	18	Total 18	O 18	0	0
8	H	11	Total 11	O 11	0	0
8	E	5	Total 5	O 5	0	0
8	F	5	Total 5	O 5	0	0

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.

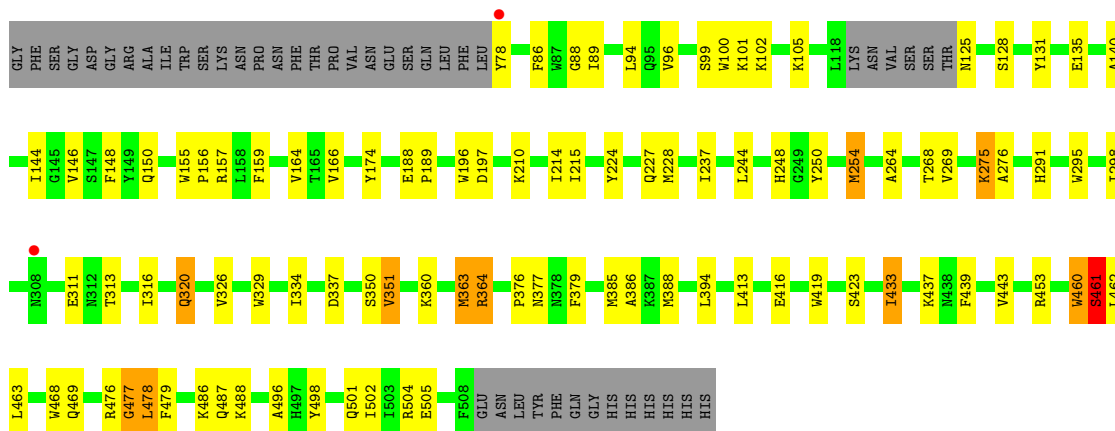
• Molecule 1: Beta-klotho

Chain A: 



• Molecule 1: Beta-klotho

Chain B: 



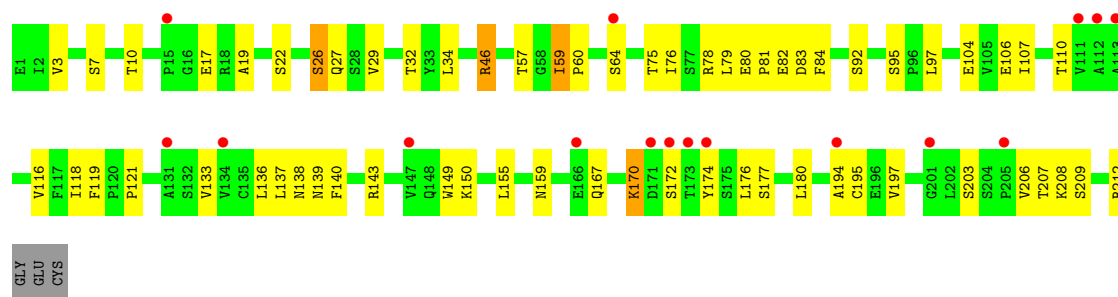
• Molecule 2: 39F7 Fab light chain

Chain L: 

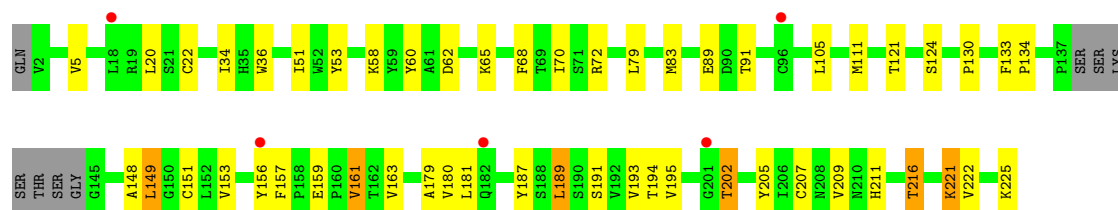




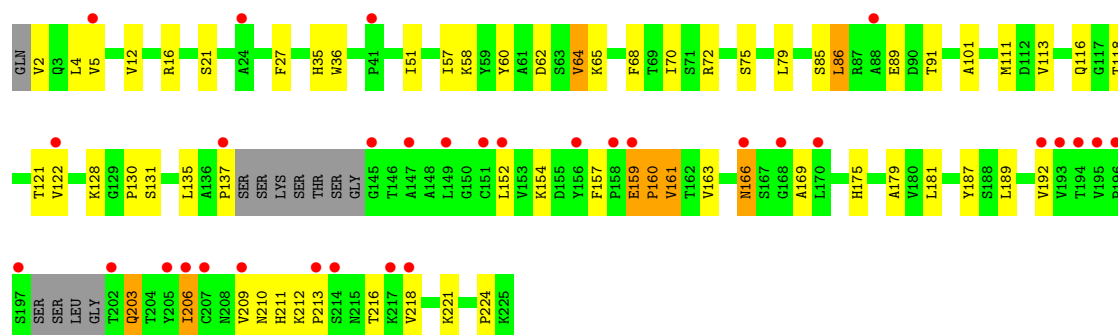
• Molecule 2: 39F7 Fab light chain



• Molecule 3: 39F7 Fab heavy chain



• Molecule 3: 39F7 Fab heavy chain



4 Data and refinement statistics

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 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.70) 99.3 (30.00-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.216 , 0.270 (Not available) , 0.245	Depositor DCC
R_{free} test set	2979 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
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

Xtriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, SO4, NAG, 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	0.63	0/3607	0.88	4/4893 (0.1%)
1	B	0.63	0/3607	0.88	5/4893 (0.1%)
2	E	0.52	0/1648	0.86	3/2239 (0.1%)
2	L	0.53	0/1441	0.84	0/1958
3	F	0.50	0/1662	0.84	2/2264 (0.1%)
3	H	0.54	0/1687	0.83	3/2299 (0.1%)
All	All	0.58	0/13652	0.86	17/18546 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	477	GLY	N-CA-C	7.31	121.90	112.54
3	H	159	GLU	N-CA-C	6.49	122.37	113.16
1	B	477	GLY	N-CA-C	6.35	120.33	112.14
2	E	83	ASP	N-CA-C	6.30	119.13	111.82
1	A	460	TRP	CA-C-N	5.81	132.64	121.54
1	A	460	TRP	C-N-CA	5.81	132.64	121.54
3	H	53	TYR	N-CA-C	5.69	117.16	111.07
3	H	202	THR	N-CA-C	-5.55	106.86	113.97
3	F	159	GLU	N-CA-C	5.49	120.96	113.16
2	E	59	ILE	N-CA-C	5.48	113.86	107.89
1	B	460	TRP	CA-C-N	5.31	131.68	121.54
1	B	460	TRP	C-N-CA	5.31	131.68	121.54
2	E	138	ASN	N-CA-C	5.27	117.50	108.90
3	F	157	PHE	C-N-CD	-5.23	109.09	120.60
1	B	462	LEU	N-CA-C	-5.20	105.51	111.07
1	B	96	VAL	N-CA-C	5.18	118.14	112.96
1	A	148	PHE	N-CA-C	5.01	116.81	109.24

There are no chirality outliers.

There are no planarity outliers.

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	3493	0	3357	28	0
1	B	3493	0	3357	52	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	42	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	194	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.

All (194) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:99:SER:HB3	1:B:102:LYS:HB3	1.66	0.77
3:H:36:TRP:HD1	3:H:70:ILE:HD12	1.50	0.77
2:E:92:SER:HA	2:E:97:LEU:HD22	1.69	0.75
1:B:100:TRP:O	1:B:105:LYS:HD3	1.87	0.75
1:B:210:LYS:HE2	1:B:250:TYR:HE2	1.53	0.74
2:E:80:GLU:HB3	2:E:81:PRO:CD	2.19	0.73
1:A:433:ILE:HD11	1:A:494:SER:HB2	1.72	0.72
1:B:125:ASN:O	1:B:125:ASN:ND2	2.24	0.70
3:H:91:THR:HG23	3:H:121:THR:HA	1.72	0.70
2:E:194:ALA:HB2	2:E:209:SER:HB3	1.74	0.70
1:B:227:GLN:HG3	1:B:228:MET:HE2	1.74	0.69
3:F:62:ASP:HA	3:F:65:LYS:HD3	1.73	0.69
3:H:34:ILE:HG21	3:H:79:LEU:HD22	1.77	0.67
3:F:211:HIS:HB3	3:F:216:THR:HG22	1.74	0.67
3:F:203:GLN:HA	3:F:203:GLN:OE1	1.93	0.67
1:A:105:LYS:HG3	1:A:157:ARG:HA	1.77	0.66
3:H:161:VAL:CG1	3:H:189:LEU:HD21	2.26	0.65
2:E:17:GLU:O	2:E:79:LEU:HD12	1.96	0.65
3:H:62:ASP:HA	3:H:65:LYS:HE2	1.77	0.65
2:L:139:ASN:HD22	2:L:139:ASN:N	1.94	0.64
1:B:275:LYS:HG3	1:B:363:MET:HE1	1.81	0.63
3:F:159:GLU:OE1	3:F:179:ALA:HB3	1.98	0.62
2:E:3:VAL:H	2:E:26:SER:HB3	1.64	0.62
3:H:89:GLU:N	3:H:89:GLU:OE1	2.32	0.62
1:A:144:ILE:HG23	1:A:146:VAL:HG13	1.81	0.62
1:B:275:LYS:HA	1:B:363:MET:HE1	1.82	0.62
2:L:186:ASP:N	2:L:186:ASP:OD1	2.32	0.61
1:B:461:SER:HB3	1:B:477:GLY:HA2	1.82	0.61
1:B:210:LYS:HE2	1:B:250:TYR:CE2	2.35	0.61
3:H:161:VAL:HG11	3:H:189:LEU:HD21	1.83	0.60
3:H:211:HIS:HB3	3:H:216:THR:HG23	1.82	0.60
2:E:84:PHE:CD2	2:E:107:ILE:HG13	2.37	0.60
3:F:166:ASN:OD1	3:F:169:ALA:HB3	2.02	0.59
3:H:134:PRO:HB2	3:H:222:VAL:HG13	1.84	0.59
1:B:244:LEU:HD11	1:B:377:ASN:HB3	1.85	0.58
3:H:181:LEU:HD13	3:H:187:TYR:CE1	2.39	0.57
2:E:46:ARG:HG2	2:E:46:ARG:HH11	1.70	0.57
3:H:36:TRP:CD1	3:H:70:ILE:HD12	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:137:LEU:HD11	2:E:197:VAL:HG21	1.87	0.57
3:F:51:ILE:HD13	3:F:72:ARG:HD2	1.87	0.56
3:F:4:LEU:HD12	3:F:113:VAL:HG12	1.86	0.56
2:L:16:GLY:HA2	2:L:78:ARG:HG3	1.87	0.56
3:F:116:GLN:HA	3:F:116:GLN:OE1	2.05	0.56
3:H:148:ALA:HB2	3:H:194:THR:HG22	1.87	0.56
2:L:21:LEU:HD22	2:L:74:LEU:HD23	1.87	0.56
3:F:137:PRO:HD2	3:F:224:PRO:HA	1.87	0.56
3:H:20:LEU:HG	3:H:83:MET:HE2	1.86	0.56
3:H:221:LYS:N	3:H:221:LYS:HD2	2.22	0.55
1:A:209:TRP:CD2	1:A:214:ILE:HD11	2.41	0.55
1:A:244:LEU:HD11	1:A:377:ASN:HB3	1.88	0.55
2:E:116:VAL:O	2:E:208:LYS:HE2	2.07	0.55
2:E:10:THR:HG22	2:E:104:GLU:HB3	1.89	0.54
1:B:224:TYR:CE2	1:B:228:MET:HE3	2.41	0.54
3:H:189:LEU:C	3:H:189:LEU:HD12	2.33	0.54
2:L:133:VAL:HB	2:L:180:LEU:HD12	1.88	0.54
1:A:224:TYR:CE1	1:A:228:MET:HE3	2.42	0.54
3:H:130:PRO:HD2	3:H:216:THR:HG21	1.89	0.54
3:F:166:ASN:CG	3:F:169:ALA:HB3	2.34	0.53
1:B:215:ILE:HG23	1:B:276:ALA:HA	1.91	0.53
1:B:94:LEU:HD22	1:B:468:TRP:CZ3	2.43	0.53
1:B:264:ALA:HB2	1:B:351:VAL:HG22	1.90	0.53
3:F:130:PRO:HD2	3:F:216:THR:HG21	1.91	0.52
1:B:105:LYS:HG3	1:B:157:ARG:HA	1.92	0.52
1:B:320:GLN:HA	1:B:320:GLN:OE1	2.09	0.52
2:E:19:ALA:HB2	2:E:79:LEU:HD11	1.91	0.52
1:B:215:ILE:HD13	1:B:275:LYS:HB3	1.92	0.52
1:B:487:GLN:OE1	1:B:487:GLN:N	2.35	0.52
3:H:195:VAL:HG11	3:H:205:TYR:CE2	2.45	0.52
3:H:130:PRO:HB3	3:H:156:TYR:HB3	1.92	0.52
3:F:2:VAL:HG13	3:F:27:PHE:CD2	2.44	0.52
3:F:36:TRP:HD1	3:F:70:ILE:HD12	1.73	0.52
2:E:119:PHE:CD2	3:F:135:LEU:HB3	2.45	0.52
3:H:51:ILE:HG13	3:H:58:LYS:HG2	1.93	0.51
1:B:416:GLU:HG3	1:B:460:TRP:CD2	2.46	0.51
2:L:48:LEU:HD23	2:L:59:ILE:HD12	1.93	0.51
1:B:159:PHE:CZ	1:B:164:VAL:HG13	2.46	0.50
2:L:90:GLN:NE2	3:H:111:MET:HE3	2.26	0.50
2:L:97:LEU:HD12	2:L:97:LEU:C	2.37	0.50
2:E:84:PHE:CE2	2:E:107:ILE:HG13	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ALA:HA	1:A:351:VAL:HG13	1.94	0.49
3:H:149:LEU:HD12	3:H:222:VAL:HB	1.93	0.49
3:H:163:VAL:HG22	3:H:209:VAL:HG22	1.94	0.49
3:H:34:ILE:HB	3:H:79:LEU:HD13	1.95	0.49
3:F:68:PHE:CD1	3:F:68:PHE:N	2.81	0.49
3:F:64:VAL:HB	3:F:68:PHE:CG	2.47	0.49
3:F:86:LEU:HD12	3:F:122:VAL:HG22	1.95	0.49
3:F:163:VAL:CG2	3:F:209:VAL:HG22	2.37	0.49
1:B:298:ILE:HG21	1:B:334:ILE:HD13	1.95	0.49
3:H:51:ILE:HD13	3:H:72:ARG:HD2	1.94	0.49
1:A:172:LEU:HD11	1:A:228:MET:HG3	1.94	0.48
1:B:144:ILE:HD12	1:B:146:VAL:HG13	1.95	0.48
1:B:250:TYR:CE1	1:B:269:VAL:HG21	2.47	0.48
1:B:329:TRP:C	1:B:329:TRP:CD1	2.90	0.48
1:B:487:GLN:H	1:B:487:GLN:CD	2.21	0.48
3:F:60:TYR:CE1	3:F:70:ILE:HG22	2.48	0.48
3:H:68:PHE:N	3:H:68:PHE:CD1	2.81	0.48
1:B:88:GLY:HA3	1:B:148:PHE:CE1	2.49	0.48
2:L:139:ASN:HD22	2:L:139:ASN:H	1.60	0.48
3:H:149:LEU:CD1	3:H:222:VAL:HB	2.44	0.48
3:F:130:PRO:CD	3:F:216:THR:HG21	2.44	0.48
1:A:99:SER:HB3	1:A:102:LYS:CB	2.44	0.47
1:B:140:ALA:HB1	1:B:479:PHE:CE2	2.49	0.47
3:F:206:ILE:HD13	3:F:221:LYS:HA	1.96	0.47
1:B:416:GLU:HG3	1:B:460:TRP:CG	2.50	0.47
2:E:159:ASN:HB2	2:E:180:LEU:HD12	1.96	0.47
1:A:254:MET:HE3	1:A:469:GLN:CD	2.39	0.47
1:A:159:PHE:CZ	1:A:164:VAL:HG13	2.50	0.47
1:B:128:SER:HB3	1:B:463:LEU:HD11	1.95	0.47
3:F:166:ASN:ND2	3:F:169:ALA:HB3	2.30	0.47
1:B:295:TRP:CZ3	2:E:32:THR:HG21	2.49	0.47
1:B:439:PHE:O	1:B:443:VAL:HG23	2.15	0.47
1:B:88:GLY:HA3	1:B:148:PHE:CZ	2.50	0.46
3:H:68:PHE:N	3:H:68:PHE:HD1	2.13	0.46
1:B:196:TRP:CD1	1:B:196:TRP:N	2.84	0.46
1:B:148:PHE:C	1:B:148:PHE:CD1	2.94	0.46
1:B:254:MET:HE3	1:B:469:GLN:HG3	1.97	0.46
1:A:196:TRP:N	1:A:196:TRP:CD1	2.83	0.46
3:F:175:HIS:HB2	3:F:192:VAL:HG23	1.97	0.46
1:A:209:TRP:CE3	1:A:214:ILE:HD11	2.50	0.46
2:E:121:PRO:HD3	2:E:133:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:51:ILE:HB	3:H:70:ILE:HG12	1.97	0.46
3:F:68:PHE:N	3:F:68:PHE:HD1	2.14	0.46
1:A:172:LEU:HD11	1:A:228:MET:CG	2.46	0.46
2:E:140:PHE:CE1	2:E:174:TYR:O	2.69	0.46
3:F:159:GLU:N	3:F:160:PRO:HD2	2.31	0.45
3:H:130:PRO:HB2	3:H:153:VAL:HG13	1.98	0.45
2:L:63:PHE:CE2	2:L:76:ILE:HD13	2.52	0.45
1:B:155:TRP:HB3	1:B:156:PRO:CD	2.47	0.44
2:E:116:VAL:O	2:E:208:LYS:CE	2.64	0.44
2:E:137:LEU:HD11	2:E:197:VAL:CG2	2.46	0.44
1:A:461:SER:HB3	1:A:477:GLY:HA2	1.99	0.44
2:E:140:PHE:N	2:E:140:PHE:CD1	2.85	0.44
1:A:93:ALA:O	1:A:97:GLU:HB2	2.17	0.44
1:B:99:SER:HB3	1:B:102:LYS:CB	2.43	0.44
1:B:376:PRO:HG3	1:B:419:TRP:HA	1.99	0.44
3:F:2:VAL:HG13	3:F:27:PHE:HD2	1.82	0.44
1:B:244:LEU:HD22	1:B:248:HIS:HD2	1.83	0.44
2:L:114:PRO:CB	2:L:137:LEU:HD23	2.47	0.43
3:F:35:HIS:CD2	3:F:111:MET:HG2	2.53	0.43
1:A:414:ILE:HB	1:A:457:TYR:HA	2.00	0.43
1:A:100:TRP:CE2	1:A:101:LYS:HG3	2.53	0.43
3:H:65:LYS:HE2	3:H:65:LYS:HB2	1.77	0.43
2:E:167:GLN:HG2	2:E:172:SER:HA	1.99	0.43
3:H:163:VAL:HG11	3:H:191:SER:CB	2.48	0.43
1:A:508:PHE:N	1:A:508:PHE:CD1	2.85	0.43
3:H:68:PHE:CE1	3:H:83:MET:HB3	2.53	0.43
1:B:188:GLU:HA	1:B:189:PRO:HD3	1.87	0.43
1:B:329:TRP:O	1:B:329:TRP:HD1	2.01	0.43
2:L:129:GLY:HA2	2:L:184:LYS:HE3	2.00	0.43
3:F:181:LEU:HD13	3:F:187:TYR:CE1	2.54	0.43
1:A:127:SER:OG	1:A:128:SER:N	2.51	0.42
1:B:360:LYS:O	1:B:364:ARG:HG2	2.18	0.42
1:A:254:MET:HB3	1:A:254:MET:HE2	1.68	0.42
1:B:105:LYS:HG3	1:B:157:ARG:HG3	2.02	0.42
3:H:60:TYR:CZ	3:H:70:ILE:HG22	2.54	0.42
1:B:386:ALA:HB3	1:B:388:MET:HE3	2.02	0.42
2:L:140:PHE:HE1	2:L:175:SER:HA	1.84	0.42
1:B:128:SER:HB3	1:B:463:LEU:CD1	2.49	0.42
1:B:250:TYR:CD1	1:B:269:VAL:HG21	2.55	0.42
3:H:5:VAL:O	3:H:22:CYS:HA	2.19	0.42
1:A:289:ARG:N	1:A:290:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ILE:CG2	1:A:146:VAL:HG13	2.48	0.42
1:A:329:TRP:CD1	1:A:329:TRP:C	2.97	0.42
1:B:131:TYR:HA	1:B:174:TYR:CE1	2.54	0.42
2:E:170:LYS:N	2:E:170:LYS:HD2	2.35	0.42
1:A:80:THR:O	1:A:448:ARG:NH2	2.53	0.41
1:A:105:LYS:HD2	1:A:157:ARG:CZ	2.50	0.41
3:H:157:PHE:CD1	3:H:157:PHE:C	2.98	0.41
2:E:119:PHE:CD1	2:E:119:PHE:N	2.88	0.41
2:L:114:PRO:HB2	2:L:137:LEU:HD23	2.02	0.41
2:L:48:LEU:HD11	2:L:87:TYR:CE2	2.55	0.41
2:E:149:TRP:CZ3	2:E:195:CYS:HB3	2.56	0.41
3:H:134:PRO:CB	3:H:222:VAL:HG13	2.49	0.41
3:H:181:LEU:HD13	3:H:187:TYR:CD1	2.56	0.41
1:A:89:ILE:HD11	1:A:478:LEU:HG	2.02	0.41
3:F:161:VAL:HG23	3:F:211:HIS:CD2	2.56	0.41
3:F:161:VAL:CG1	3:F:189:LEU:HD22	2.51	0.41
2:L:125:GLN:HG3	3:H:133:PHE:CE2	2.55	0.41
2:E:59:ILE:HA	2:E:60:PRO:HD2	1.80	0.41
1:B:433:ILE:HG22	1:B:437:LYS:HD2	2.02	0.41
3:H:189:LEU:HD12	3:H:189:LEU:O	2.21	0.41
1:A:105:LYS:HG3	1:A:157:ARG:CA	2.47	0.40
1:B:379:PHE:CZ	1:B:394:LEU:HD23	2.57	0.40
2:E:140:PHE:CD1	2:E:174:TYR:O	2.74	0.40
1:B:264:ALA:CA	1:B:351:VAL:HG22	2.52	0.40
1:B:478:LEU:HD13	1:B:496:ALA:HA	2.04	0.40
3:F:212:LYS:N	3:F:213:PRO:CD	2.84	0.40
3:H:179:ALA:HA	3:H:189:LEU:HB3	2.04	0.40
3:H:189:LEU:C	3:H:189:LEU:CD1	2.94	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	421/470 (90%)	406 (96%)	14 (3%)	1 (0%)	43	68
1	B	421/470 (90%)	408 (97%)	12 (3%)	1 (0%)	43	68
2	E	210/215 (98%)	202 (96%)	7 (3%)	1 (0%)	24	48
2	L	150/215 (70%)	147 (98%)	3 (2%)	0	100	100
3	F	207/225 (92%)	199 (96%)	6 (3%)	2 (1%)	12	32
3	H	213/225 (95%)	205 (96%)	8 (4%)	0	100	100
All	All	1622/1820 (89%)	1567 (97%)	50 (3%)	5 (0%)	36	60

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 ⓘ

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%)	332 (90%)	36 (10%)	7	19
1	B	368/408 (90%)	331 (90%)	37 (10%)	7	18
2	E	183/185 (99%)	155 (85%)	28 (15%)	3	7
2	L	155/185 (84%)	125 (81%)	30 (19%)	1	4
3	F	176/186 (95%)	153 (87%)	23 (13%)	4	10
3	H	109/186 (59%)	96 (88%)	13 (12%)	5	13
All	All	1359/1558 (87%)	1192 (88%)	167 (12%)	4	12

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	PHE
1	A	94	LEU
1	A	125	ASN
1	A	128	SER
1	A	135	GLU
1	A	144	ILE
1	A	147	SER
1	A	168	ASN
1	A	185	ARG
1	A	190	ILE
1	A	204	GLU
1	A	213	THR
1	A	214	ILE
1	A	227	GLN
1	A	228	MET
1	A	254	MET
1	A	305	ILE
1	A	309	ARG
1	A	318	LYS
1	A	332	ASN
1	A	349	PHE
1	A	385	MET
1	A	395	ASN
1	A	406	GLU
1	A	427	THR
1	A	430	THR
1	A	435	MET
1	A	437	LYS
1	A	448	ARG
1	A	461	SER
1	A	462	LEU
1	A	478	LEU
1	A	486	LYS
1	A	502	ILE
1	A	505	GLU
1	A	508	PHE
1	B	78	TYR
1	B	86	PHE
1	B	89	ILE
1	B	101	LYS
1	B	135	GLU
1	B	150	GLN
1	B	166	VAL

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Mol	Chain	Res	Type
1	B	197	ASP
1	B	214	ILE
1	B	237	ILE
1	B	254	MET
1	B	268	THR
1	B	275	LYS
1	B	291	HIS
1	B	311	GLU
1	B	313	THR
1	B	316	ILE
1	B	320	GLN
1	B	326	VAL
1	B	337	ASP
1	B	350	SER
1	B	351	VAL
1	B	363	MET
1	B	364	ARG
1	B	385	MET
1	B	413	LEU
1	B	423	SER
1	B	433	ILE
1	B	453	ARG
1	B	461	SER
1	B	476	ARG
1	B	478	LEU
1	B	486	LYS
1	B	488	LYS
1	B	501	GLN
1	B	504	ARG
1	B	505	GLU
2	L	11	LEU
2	L	14	SER
2	L	32	THR
2	L	34	LEU
2	L	40	LYS
2	L	57	THR
2	L	64	SER
2	L	76	ILE
2	L	82	GLU
2	L	90	GLN
2	L	95	SER
2	L	97	LEU

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Mol	Chain	Res	Type
2	L	107	ILE
2	L	116	VAL
2	L	118	ILE
2	L	124	GLU
2	L	130	THR
2	L	133	VAL
2	L	139	ASN
2	L	143	ARG
2	L	144	GLU
2	L	159	ASN
2	L	166	GLU
2	L	170	LYS
2	L	176	LEU
2	L	180	LEU
2	L	183	SER
2	L	186	ASP
2	L	187	TYR
2	L	197	VAL
3	H	105	LEU
3	H	124	SER
3	H	149	LEU
3	H	151	CYS
3	H	161	VAL
3	H	180	VAL
3	H	189	LEU
3	H	193	VAL
3	H	202	THR
3	H	207	CYS
3	H	216	THR
3	H	221	LYS
3	H	225	LYS
2	E	7	SER
2	E	22	SER
2	E	26	SER
2	E	27	GLN
2	E	29	VAL
2	E	34	LEU
2	E	46	ARG
2	E	57	THR
2	E	64	SER
2	E	75	THR
2	E	76	ILE

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Mol	Chain	Res	Type
2	E	78	ARG
2	E	82	GLU
2	E	95	SER
2	E	106	GLU
2	E	110	THR
2	E	118	ILE
2	E	136	LEU
2	E	143	ARG
2	E	150	LYS
2	E	155	LEU
2	E	170	LYS
2	E	176	LEU
2	E	177	SER
2	E	203	SER
2	E	206	VAL
2	E	207	THR
2	E	212	ARG
3	F	5	VAL
3	F	12	VAL
3	F	16	ARG
3	F	21	SER
3	F	57	ILE
3	F	58	LYS
3	F	64	VAL
3	F	75	SER
3	F	79	LEU
3	F	85	SER
3	F	86	LEU
3	F	89	GLU
3	F	118	THR
3	F	128	LYS
3	F	131	SER
3	F	152	LEU
3	F	154	LYS
3	F	161	VAL
3	F	166	ASN
3	F	203	GLN
3	F	206	ILE
3	F	210	ASN
3	F	218	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	ASN
1	A	227	GLN
1	A	241	ASN
1	A	283	ASN
1	A	321	GLN
1	A	378	ASN
1	A	438	ASN
1	B	219	ASN
1	B	241	ASN
1	B	262	ASN
1	B	378	ASN
1	B	395	ASN
1	B	408	ASN
1	B	409	ASN
1	B	445	GLN
1	B	501	GLN
2	L	27	GLN
2	L	90	GLN
2	L	139	ASN
2	E	27	GLN
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 oligosaccharides 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	$\# Z > 2$
5	EDO	H	301	-	3,3,3	0.31	0	2,2,2	0.48	0
6	SO4	B	604	-	4,4,4	0.45	0	6,6,6	0.18	0
7	PG4	L	301	-	12,12,12	0.46	0	11,11,11	0.35	0
5	EDO	A	604	-	3,3,3	0.47	0	2,2,2	0.05	0
5	EDO	A	603	-	3,3,3	0.50	0	2,2,2	0.22	0
6	SO4	A	608	-	4,4,4	0.48	0	6,6,6	0.24	0
5	EDO	A	605	-	3,3,3	0.50	0	2,2,2	0.17	0
5	EDO	A	606	-	3,3,3	0.44	0	2,2,2	0.27	0
5	EDO	A	607	-	3,3,3	0.36	0	2,2,2	0.37	0
5	EDO	B	603	-	3,3,3	0.32	0	2,2,2	0.51	0
7	PG4	A	609	-	12,12,12	0.49	0	11,11,11	0.47	0
4	NAG	B	602	1	14,14,15	0.51	0	17,19,21	1.02	1 (5%)
4	NAG	A	602	1	14,14,15	0.58	0	17,19,21	1.47	3 (17%)
4	NAG	B	601	1	14,14,15	0.68	0	17,19,21	1.80	5 (29%)
4	NAG	A	601	1	14,14,15	0.89	1 (7%)	17,19,21	2.64	6 (35%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	C2-N2	-2.75	1.41	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	C1-C2-N2	-7.43	98.72	110.43
4	B	601	NAG	C1-C2-N2	-4.93	102.67	110.43
4	A	601	NAG	O5-C1-C2	-4.72	103.99	111.29
4	A	601	NAG	C8-C7-N2	-3.71	109.97	116.12
4	A	602	NAG	O5-C1-C2	-3.40	106.02	111.29
4	A	601	NAG	C2-N2-C7	-3.04	118.83	122.90
4	B	601	NAG	C3-C4-C5	-2.48	105.73	110.23
4	A	601	NAG	O7-C7-N2	2.47	126.34	121.98
4	A	602	NAG	O5-C5-C4	-2.33	105.16	110.83
4	A	602	NAG	C1-C2-N2	-2.28	106.84	110.43
4	A	601	NAG	O5-C5-C6	2.14	111.82	107.66
4	B	601	NAG	O7-C7-N2	2.07	125.63	121.98
4	B	601	NAG	O5-C5-C4	-2.07	105.80	110.83
4	B	601	NAG	O5-C5-C6	2.01	111.58	107.66
4	B	602	NAG	C1-C2-N2	-2.01	107.27	110.43

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	NAG	C4-C5-C6-O6
4	B	601	NAG	O5-C5-C6-O6
7	L	301	PG4	O1-C1-C2-O2
7	A	609	PG4	O3-C5-C6-O4
7	L	301	PG4	O4-C7-C8-O5
7	A	609	PG4	O2-C3-C4-O3
5	H	301	EDO	O1-C1-C2-O2
5	B	603	EDO	O1-C1-C2-O2
7	A	609	PG4	C1-C2-O2-C3
7	L	301	PG4	C5-C6-O4-C7
7	A	609	PG4	C3-C4-O3-C5
7	A	609	PG4	C4-C3-O2-C2
5	A	607	EDO	O1-C1-C2-O2
7	L	301	PG4	C3-C4-O3-C5
7	L	301	PG4	C4-C3-O2-C2
5	A	603	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	A	609	PG4	O4-C7-C8-O5
4	A	602	NAG	O5-C5-C6-O6
5	A	605	EDO	O1-C1-C2-O2
5	A	606	EDO	O1-C1-C2-O2

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

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, 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%)	-0.31	1 (0%) 91 90	19, 29, 50, 80	0
1	B	425/470 (90%)	-0.17	2 (0%) 87 86	21, 33, 53, 74	0
2	E	212/215 (98%)	0.79	16 (7%) 20 17	36, 67, 89, 106	0
2	L	188/215 (87%)	0.57	21 (11%) 10 8	23, 55, 93, 97	0
3	F	213/225 (94%)	1.05	32 (15%) 5 4	34, 71, 101, 111	0
3	H	217/225 (96%)	0.63	5 (2%) 61 58	27, 62, 87, 98	0
All	All	1680/1820 (92%)	0.26	77 (4%) 37 34	19, 42, 89, 111	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	172	SER	4.9
3	F	207	CYS	4.0
2	L	187	TYR	3.8
2	E	174	TYR	3.8
2	E	201	GLY	3.4
3	F	152	LEU	3.4
3	F	158	PRO	3.3
2	L	145	ALA	3.3
3	F	206	ILE	3.3
3	F	202	THR	3.2
3	F	145	GLY	3.2
2	L	159	ASN	3.1
2	L	118	ILE	3.1
3	F	147	ALA	3.1
2	L	116	VAL	3.1
2	L	198	THR	3.1
2	L	131	ALA	3.1
3	H	201	GLY	3.0
2	L	185	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	173	THR	3.0
1	A	78	TYR	2.9
3	F	170	LEU	2.9
3	F	217	LYS	2.8
3	F	41	PRO	2.8
3	F	196	PRO	2.8
2	E	111	VAL	2.8
3	F	218	VAL	2.8
3	H	182	GLN	2.7
2	L	180	LEU	2.7
2	E	112	ALA	2.7
2	L	117	PHE	2.7
2	L	196	GLU	2.6
3	F	193	VAL	2.6
2	E	205	PRO	2.6
3	F	5	VAL	2.6
3	H	156	TYR	2.6
3	F	192	VAL	2.5
3	F	205	TYR	2.5
2	E	113	ALA	2.5
2	L	195	CYS	2.5
2	L	202	LEU	2.5
3	F	149	LEU	2.5
3	F	168	GLY	2.5
3	F	195	VAL	2.4
3	F	213	PRO	2.4
2	E	194	ALA	2.4
2	L	182	LEU	2.4
3	F	214	SER	2.4
3	F	159	GLU	2.4
2	L	179	THR	2.4
3	F	194	THR	2.4
2	L	203	SER	2.4
3	H	96	CYS	2.4
2	L	197	VAL	2.4
1	B	78	TYR	2.3
3	F	24	ALA	2.3
3	F	151	CYS	2.2
3	F	197	SER	2.2
2	E	166	GLU	2.2
2	E	15	PRO	2.2
2	L	183	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	134	VAL	2.2
3	F	122	VAL	2.2
3	F	166	ASN	2.2
3	F	88	ALA	2.1
2	E	171	ASP	2.1
2	L	130	THR	2.1
3	F	137	PRO	2.1
3	H	18	LEU	2.1
1	B	308	ASN	2.1
3	F	156	TYR	2.1
2	L	186	ASP	2.1
2	E	64	SER	2.1
2	E	131	ALA	2.1
2	L	181	THR	2.1
2	E	147	VAL	2.1
3	F	209	VAL	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 oligosaccharides 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
4	NAG	A	601	14/15	0.55	0.16	60,65,71,72	0
5	EDO	H	301	4/4	0.61	0.16	47,48,48,50	0
4	NAG	B	601	14/15	0.69	0.13	59,63,64,67	0
5	EDO	A	606	4/4	0.74	0.14	60,61,62,63	0
4	NAG	A	602	14/15	0.75	0.15	63,67,72,73	0
4	NAG	B	602	14/15	0.79	0.13	56,59,62,64	0
7	PG4	A	609	13/13	0.80	0.16	48,59,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PG4	L	301	13/13	0.88	0.11	49,54,57,57	0
6	SO4	A	608	5/5	0.90	0.10	63,66,67,68	0
5	EDO	A	605	4/4	0.92	0.09	36,39,39,39	0
6	SO4	B	604	5/5	0.93	0.11	59,59,62,63	0
5	EDO	B	603	4/4	0.95	0.14	29,31,31,31	0
5	EDO	A	603	4/4	0.95	0.07	32,32,32,33	0
5	EDO	A	604	4/4	0.95	0.12	36,36,36,37	0
5	EDO	A	607	4/4	0.96	0.09	47,47,47,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.