Full wwPDB X-ray Structure Validation Report (i)

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 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 (1)) were used in the production of this report:

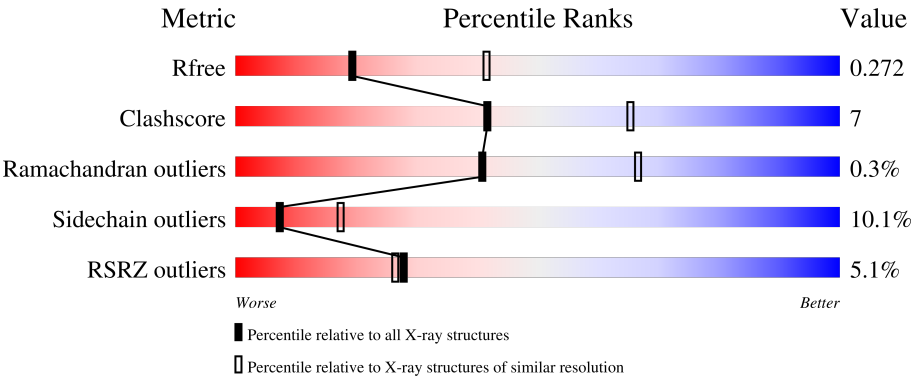
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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 <=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	7% 73% 24% ••
2	L	215	7% 67% 18% • 13%
3	F	225	14% 67% 25% • 5%

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Mol	Chain	Length	Quality of chain
3	H	225	

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
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

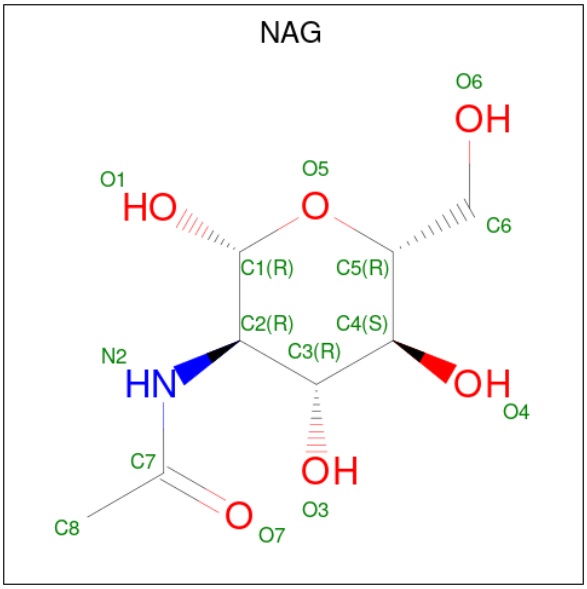
- Molecule 2 is a protein called 39F7 Fab light chain.

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 (three-letter code: 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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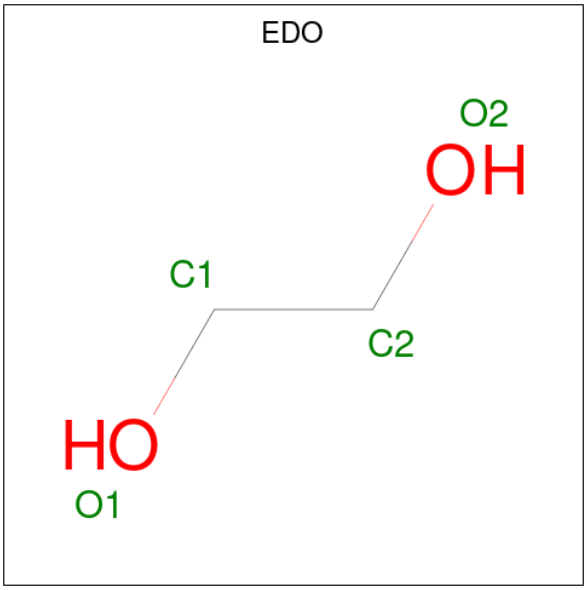
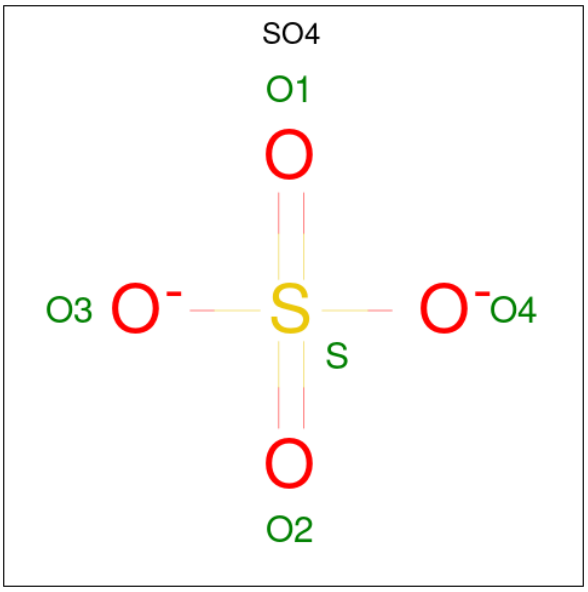
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



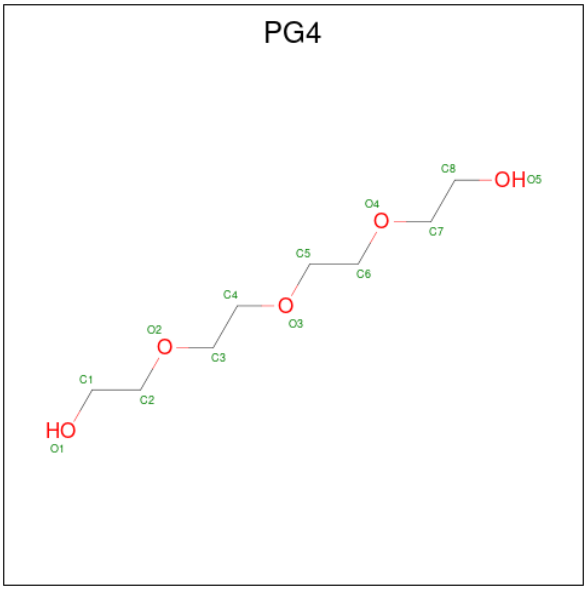
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0

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



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

- 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 13 8 5	0	0
7	L	1	Total C O 13 8 5	0	0

- Molecule 8 is water.

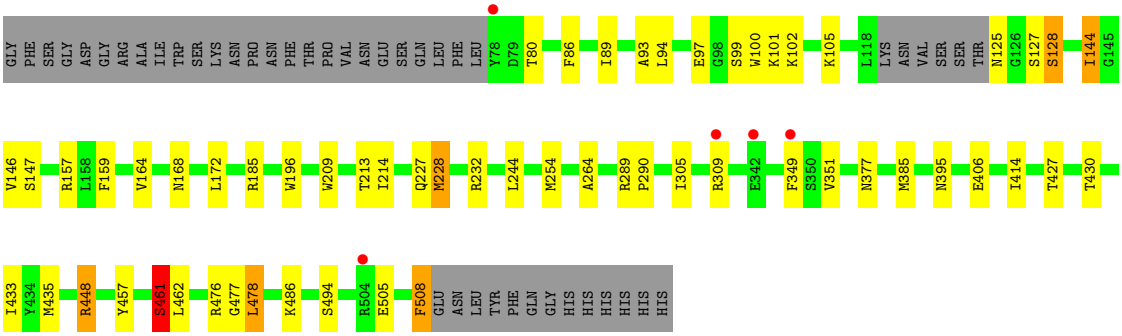
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	67	Total O 67 67	0	0
8	B	50	Total O 50 50	0	0
8	L	18	Total O 18 18	0	0
8	H	11	Total O 11 11	0	0
8	E	5	Total O 5 5	0	0
8	F	5	Total O 5 5	0	0

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.

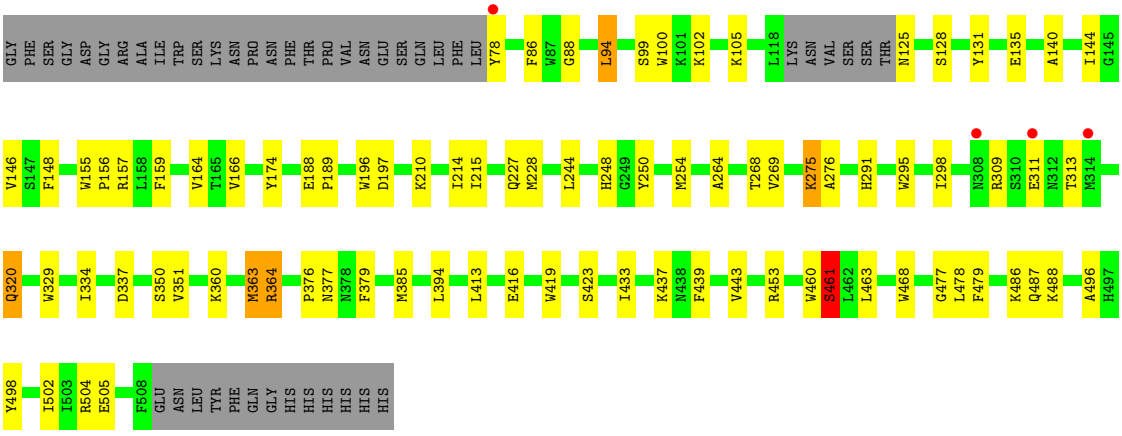
• Molecule 1: Beta-klotho

Chain A:



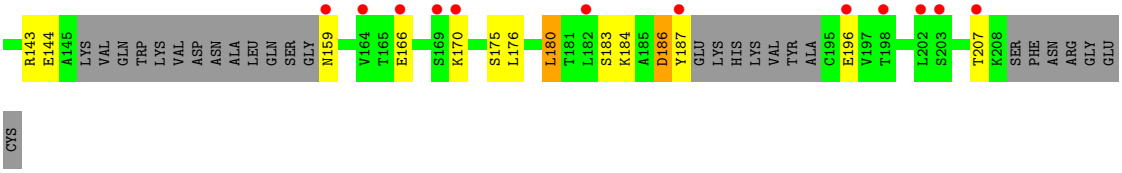
• Molecule 1: Beta-klotho

Chain B:

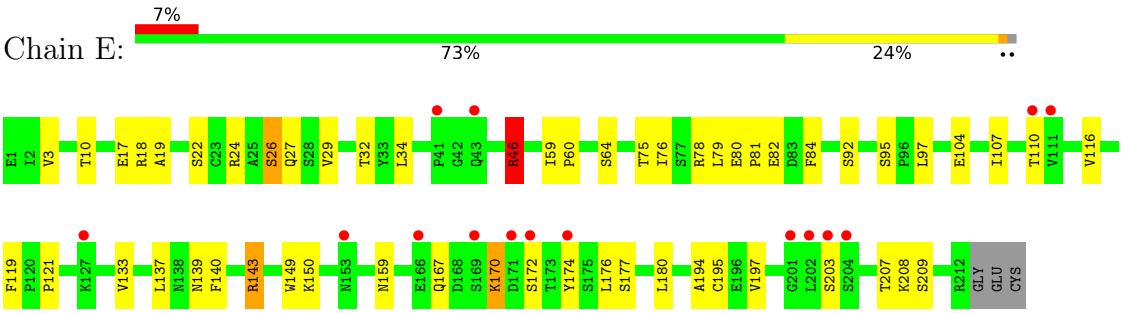


• Molecule 2: 39F7 Fab light chain

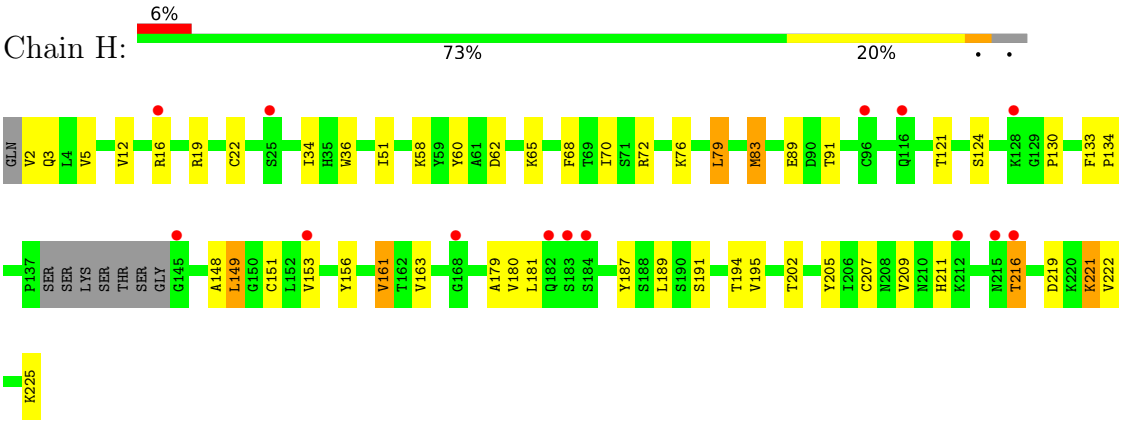
Chain L:



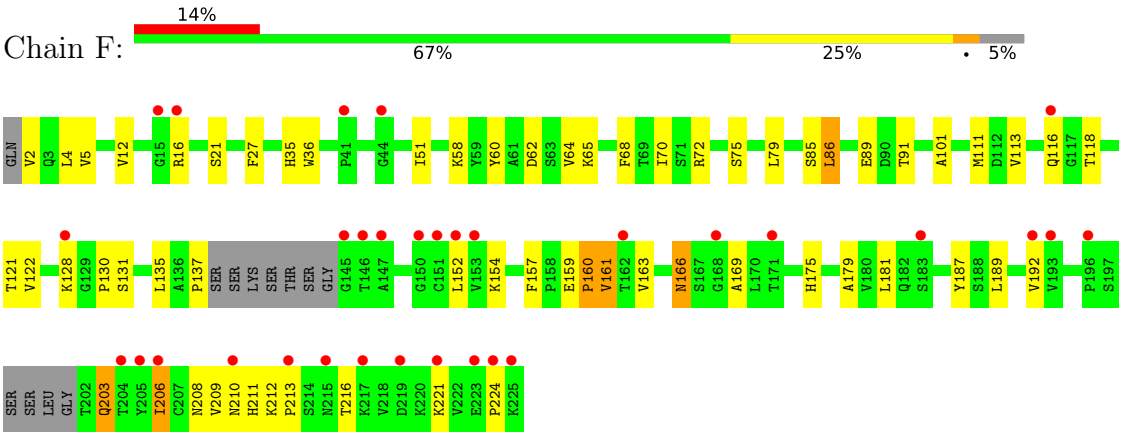
• Molecule 2: 39F7 Fab light chain



• Molecule 3: 39F7 Fab heavy chain



• Molecule 3: 39F7 Fab heavy chain



4 Data and refinement statistics (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
$< I/\sigma(I) >$ [1]	1.76 (at 2.71Å)	Xtriage
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	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	A	476	ARG	NE-CZ-NH2	5.02	122.81	120.30

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	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.

All (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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:275:LYS:HG3	1:B:363:MET:HE1	1.79	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
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
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
1:B:227:GLN:HG3	1:B:228:MET:HE1	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:10:THR:HG22	2:E:104:GLU:HB3	1.89	0.54
2:L:133:VAL:HB	2:L:180:LEU:HD12	1.88	0.54
3:H:130:PRO:HD2	3:H:216:THR:HG21	1.89	0.54
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:E:84:PHE:CE2	2:E:107:ILE:HG13	2.46	0.50
3:H:189:LEU:C	3:H:189:LEU:HD12	2.33	0.49
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
3:F:166:ASN:CG	3:F:169:ALA:HB3	2.34	0.48
1:B:250:TYR:CE1	1:B:269:VAL:HG21	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:97:LEU:HD12	2:L:97:LEU:C	2.37	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
1:B:329:TRP:C	1:B:329:TRP:CD1	2.90	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:275:LYS:HA	1:B:363:MET:HE1	2.00	0.44
1:B:244:LEU:HD22	1:B:248:HIS:HD2	1.83	0.44
1:B:487:GLN:H	1:B:487:GLN:CD	2.21	0.43
2:L:114:PRO:CB	2:L:137:LEU:HD23	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:L:139:ASN:N	2:L:139:ASN:ND2	2.66	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
1:A:144:ILE:CG2	1:A:146:VAL:HG13	2.48	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
1:B:148:PHE:CD1	1:B:148:PHE:C	2.94	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
1:B:254:MET:HE3	1:B:254:MET:HB3	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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
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

All (145) 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	144	ILE
1	A	147	SER
1	A	168	ASN
1	A	185	ARG
1	A	213	THR
1	A	227	GLN
1	A	228	MET
1	A	232	ARG
1	A	254	MET
1	A	305	ILE
1	A	309	ARG
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

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Mol	Chain	Res	Type
1	A	448	ARG
1	A	461	SER
1	A	462	LEU
1	A	478	LEU
1	A	486	LYS
1	A	505	GLU
1	A	508	PHE
1	B	78	TYR
1	B	86	PHE
1	B	94	LEU
1	B	135	GLU
1	B	166	VAL
1	B	197	ASP
1	B	214	ILE
1	B	268	THR
1	B	275	LYS
1	B	291	HIS
1	B	309	ARG
1	B	311	GLU
1	B	313	THR
1	B	320	GLN
1	B	337	ASP
1	B	350	SER
1	B	363	MET
1	B	364	ARG
1	B	385	MET
1	B	413	LEU
1	B	423	SER
1	B	453	ARG
1	B	461	SER
1	B	486	LYS
1	B	488	LYS
1	B	504	ARG
1	B	505	GLU
2	L	7	SER
2	L	11	LEU
2	L	14	SER
2	L	32	THR
2	L	34	LEU
2	L	57	THR
2	L	64	SER
2	L	76	ILE

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Mol	Chain	Res	Type
2	L	82	GLU
2	L	90	GLN
2	L	95	SER
2	L	97	LEU
2	L	118	ILE
2	L	124	GLU
2	L	130	THR
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	196	GLU
2	L	207	THR
3	H	2	VAL
3	H	3	GLN
3	H	12	VAL
3	H	16	ARG
3	H	19	ARG
3	H	76	LYS
3	H	79	LEU
3	H	83	MET
3	H	124	SER
3	H	149	LEU
3	H	151	CYS
3	H	161	VAL
3	H	180	VAL
3	H	202	THR
3	H	207	CYS
3	H	216	THR
3	H	219	ASP
3	H	221	LYS
3	H	225	LYS
2	E	22	SER
2	E	24	ARG
2	E	26	SER

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Mol	Chain	Res	Type
2	E	27	GLN
2	E	29	VAL
2	E	34	LEU
2	E	46	ARG
2	E	64	SER
2	E	75	THR
2	E	76	ILE
2	E	78	ARG
2	E	82	GLU
2	E	95	SER
2	E	110	THR
2	E	143	ARG
2	E	150	LYS
2	E	170	LYS
2	E	176	LEU
2	E	177	SER
2	E	203	SER
2	E	207	THR
3	F	5	VAL
3	F	12	VAL
3	F	16	ARG
3	F	21	SER
3	F	58	LYS
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	208	ASN
3	F	210	ASN

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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	-
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

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
4	A	601	NAG	O5-C5-C6	2.95	111.82	107.20
4	A	601	NAG	C2-N2-C7	-2.86	118.83	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	NAG	O5-C5-C6	2.79	111.58	107.20
4	B	602	NAG	O5-C5-C6	2.62	111.31	107.20
4	B	601	NAG	C3-C4-C5	-2.53	105.73	110.24
4	A	601	NAG	O7-C7-N2	2.39	126.34	121.95
4	A	602	NAG	O5-C5-C4	-2.33	105.16	110.83
4	A	602	NAG	C1-C2-N2	-2.14	106.84	110.49
4	B	601	NAG	O5-C5-C4	-2.07	105.80	110.83
4	B	601	NAG	O7-C7-N2	2.00	125.63	121.95

There are no chirality outliers.

All (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
7	A	609	PG4	O2-C3-C4-O3
5	B	603	EDO	O1-C1-C2-O2
5	H	301	EDO	O1-C1-C2-O2
5	A	607	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
7	L	301	PG4	C3-C4-O3-C5
5	A	603	EDO	O1-C1-C2-O2
7	L	301	PG4	C4-C3-O2-C2
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, 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	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

All (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
2	E	169	SER	4.0
1	A	78	TYR	4.0
2	E	201	GLY	4.0
3	F	147	ALA	4.0
3	H	183	SER	3.9
3	F	171	THR	3.6
2	L	182	LEU	3.5
3	F	215	ASN	3.4
1	B	311	GLU	3.4
3	F	151	CYS	3.3
3	F	221	LYS	3.3
2	L	203	SER	3.3
3	F	145	GLY	3.2
2	E	111	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	L	196	GLU	3.1
3	F	150	GLY	3.1
2	L	187	TYR	3.0
2	L	207	THR	3.0
3	H	182	GLN	2.9
2	E	172	SER	2.8
2	E	174	TYR	2.8
2	E	153	ASN	2.8
2	E	166	GLU	2.8
2	E	203	SER	2.8
3	F	16	ARG	2.7
2	L	166	GLU	2.7
2	L	170	LYS	2.6
3	F	152	LEU	2.6
2	E	202	LEU	2.6
1	A	309	ARG	2.6
2	E	171	ASP	2.6
1	B	314	MET	2.5
3	F	206	ILE	2.5
2	L	202	LEU	2.5
1	A	349	PHE	2.4
2	L	159	ASN	2.4
2	L	128	SER	2.4
3	F	15	GLY	2.4
3	F	146	THR	2.4
3	F	116	GLN	2.4
2	L	198	THR	2.4
3	F	204	THR	2.4
3	H	16	ARG	2.4
3	F	219	ASP	2.4
3	H	96	CYS	2.4
3	H	116	GLN	2.3
3	H	25	SER	2.3
2	L	164	VAL	2.3
3	H	212	LYS	2.3
3	F	44	GLY	2.3
3	F	192	VAL	2.3
3	H	168	GLY	2.3
3	H	216	THR	2.2
3	F	223	GLU	2.2
3	F	162	THR	2.2
3	F	205	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	342	GLU	2.2
3	H	153	VAL	2.2
3	F	224	PRO	2.2
2	E	110	THR	2.2
2	L	58	GLY	2.1
2	E	41	PRO	2.1
3	F	183	SER	2.1
1	B	78	TYR	2.1
3	F	153	VAL	2.1
3	H	145	GLY	2.1
2	L	127	LYS	2.1
3	F	193	VAL	2.1
3	F	128	LYS	2.1
2	E	43	GLN	2.1
2	E	127	LYS	2.1
3	F	213	PRO	2.1
1	B	308	ASN	2.1
3	H	215	ASN	2.1
3	H	184	SER	2.1
2	L	131	ALA	2.0
3	F	210	ASN	2.0
3	F	41	PRO	2.0
2	L	169	SER	2.0
1	A	504	ARG	2.0
3	H	128	LYS	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 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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.