



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:02 am BST

PDB ID : 6PE9
Title : Crystal Structure of CD40 complexed to FAB516
Authors : Argiriadi, M.A.
Deposited on : 2019-06-20
Resolution : 3.13 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 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 : 2.11
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) : 2.11

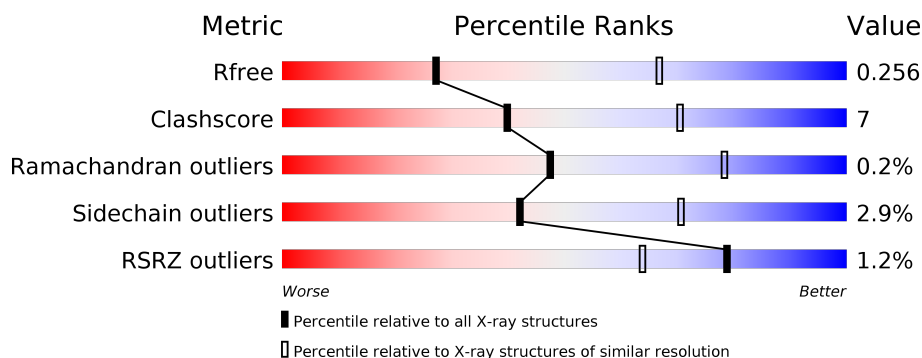
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	223	<div> <div style="width: 84%;"></div> <div style="width: 11%;"></div> <div style="width: 5%;"></div> <div style="width: 5%;"></div> </div>
1	C	223	<div> <div style="width: 2%;"></div> <div style="width: 77%;"></div> <div style="width: 17%;"></div> <div style="width: 4%;"></div> </div>
1	E	223	<div> <div style="width: 76%;"></div> <div style="width: 17%;"></div> <div style="width: 6%;"></div> </div>
1	H	223	<div> <div style="width: 2%;"></div> <div style="width: 86%;"></div> <div style="width: 10%;"></div> <div style="width: 2%;"></div> </div>
1	K	223	<div> <div style="width: 2%;"></div> <div style="width: 41%;"></div> <div style="width: 11%;"></div> <div style="width: 48%;"></div> </div>
2	B	220	<div> <div style="width: 80%;"></div> <div style="width: 19%;"></div> </div>

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Mol	Chain	Length	Quality of chain
2	D	220	 81% 18%
2	F	220	 81% 18% •
2	L	220	 86% 13%
2	M	220	 % 41% 10% 49%
3	G	173	 3% 48% 21% • 30%
3	I	173	 % 49% 7% • 44%
3	J	173	 2% 39% 8% 53%
3	U	173	 51% 16% • 31%
3	V	173	 3% 35% 10% 55%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18618 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 FAB Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1594	1009	266	312	7			
1	C	213	Total	C	N	O	S	0	0	0
			1581	1000	263	312	6			
1	E	210	Total	C	N	O	S	0	0	0
			1571	994	263	308	6			
1	H	214	Total	C	N	O	S	0	0	0
			1596	1009	266	314	7			
1	K	116	Total	C	N	O	S	0	0	0
			855	536	145	170	4			

- Molecule 2 is a protein called FAB Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	0
			1690	1059	281	345	5			
2	D	220	Total	C	N	O	S	0	0	0
			1690	1059	279	346	6			
2	F	220	Total	C	N	O	S	0	0	0
			1682	1054	277	345	6			
2	L	220	Total	C	N	O	S	0	0	0
			1700	1065	283	346	6			
2	M	113	Total	C	N	O	S	0	0	0
			872	552	141	176	3			

- Molecule 3 is a protein called Tumor necrosis factor receptor superfamily member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	121	Total	C	N	O	S	0	0	0
			873	524	149	184	16			
3	I	97	Total	C	N	O	S	0	0	0
			736	445	124	153	14			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	81	Total	C	N	O	S	0	0	0
			595	356	100	128	11			
3	U	119	Total	C	N	O	S	0	0	0
			891	537	151	187	16			
3	V	78	Total	C	N	O	S	0	0	0
			580	348	98	123	11			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		

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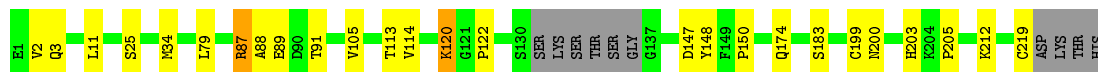
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	16	Total 16	O 16	0	0
5	C	2	Total 2	O 2	0	0
5	D	9	Total 9	O 9	0	0
5	E	7	Total 7	O 7	0	0
5	F	4	Total 4	O 4	0	0
5	G	1	Total 1	O 1	0	0
5	H	12	Total 12	O 12	0	0
5	I	2	Total 2	O 2	0	0
5	L	12	Total 12	O 12	0	0
5	U	8	Total 8	O 8	0	0
5	V	3	Total 3	O 3	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

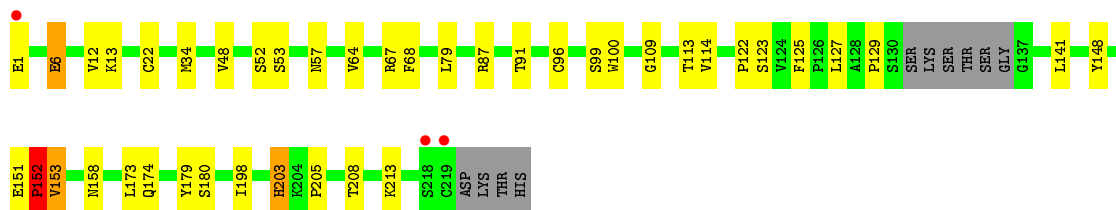
• Molecule 1: FAB Heavy chain

Chain A: 




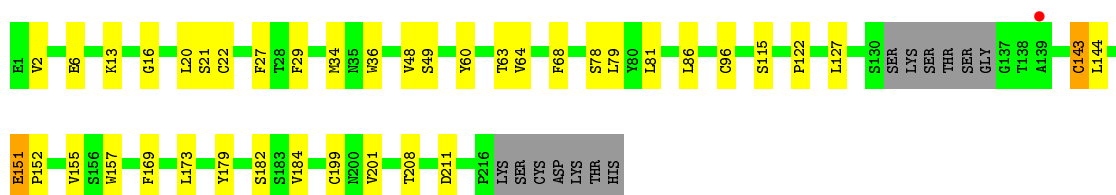
• Molecule 1: FAB Heavy chain

Chain C: 




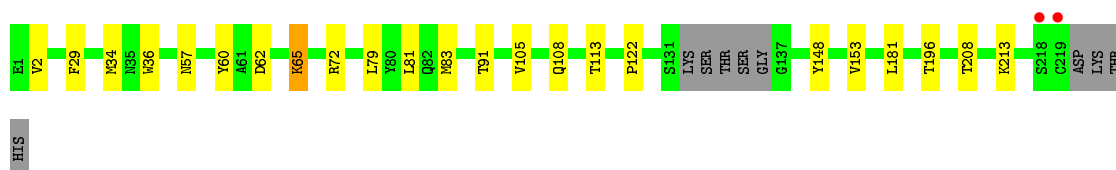
• Molecule 1: FAB Heavy chain

Chain E: 

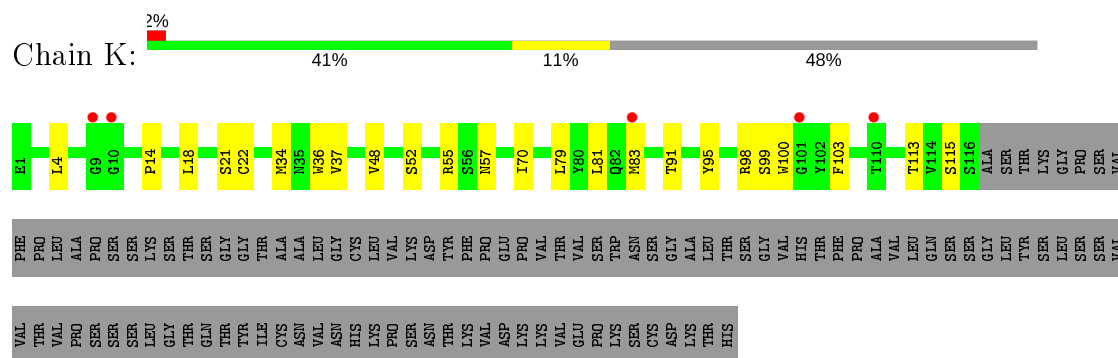


• Molecule 1: FAB Heavy chain

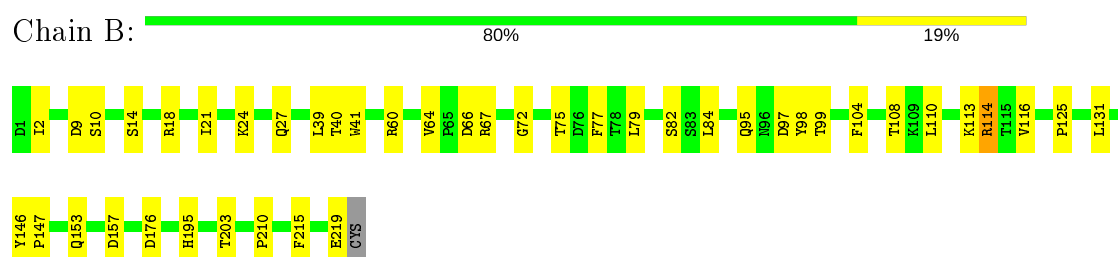
Chain H: 



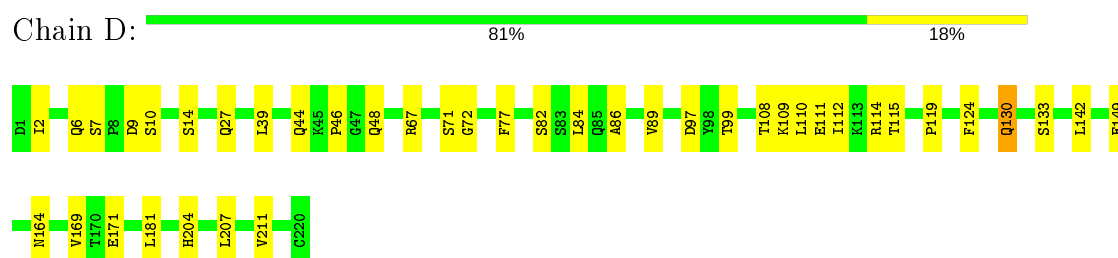
- Molecule 1: FAB Heavy chain



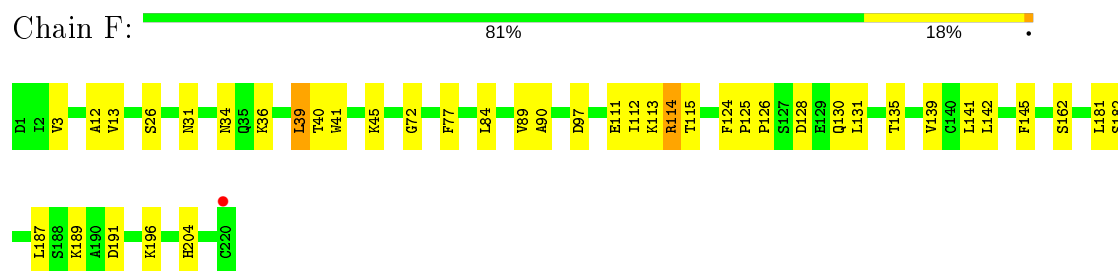
- Molecule 2: FAB Light chain



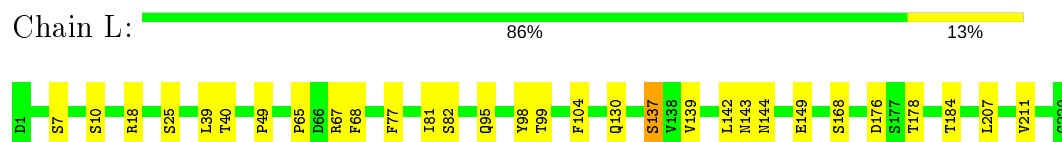
- Molecule 2: FAB Light chain



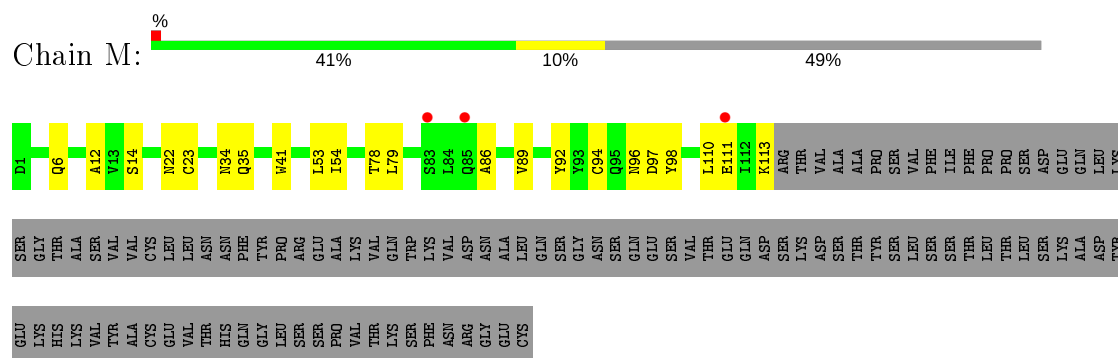
- Molecule 2: FAB Light chain



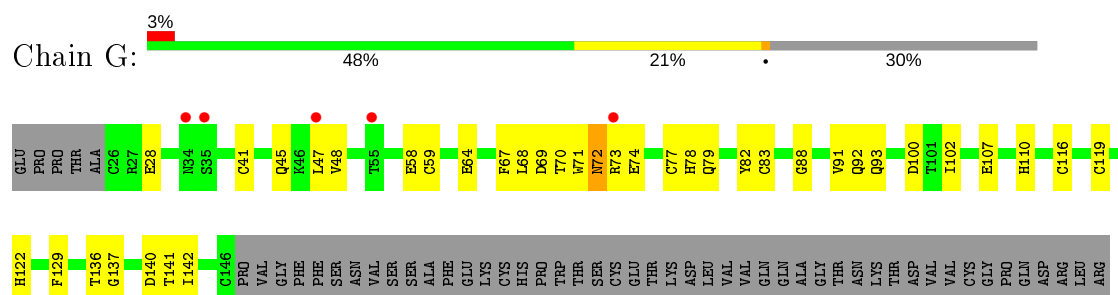
- Molecule 2: FAB Light chain



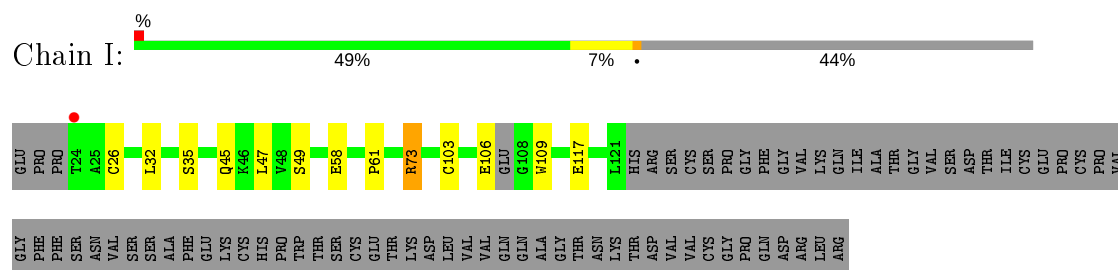
- Molecule 2: FAB Light chain



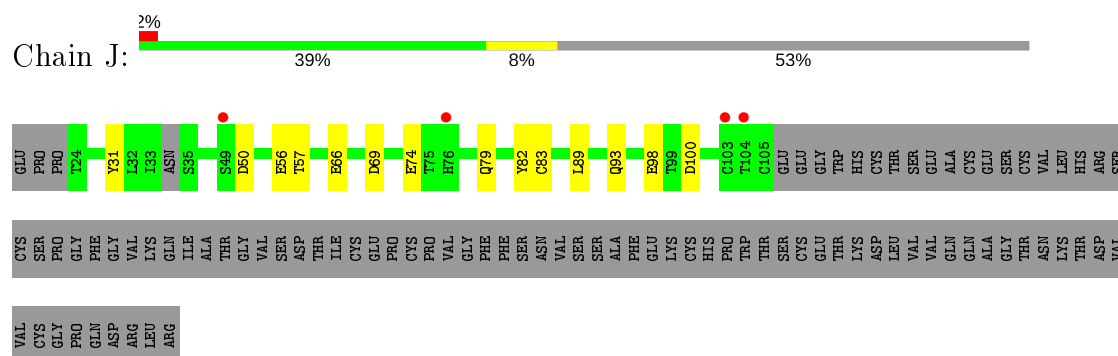
- Molecule 3: Tumor necrosis factor receptor superfamily member 5



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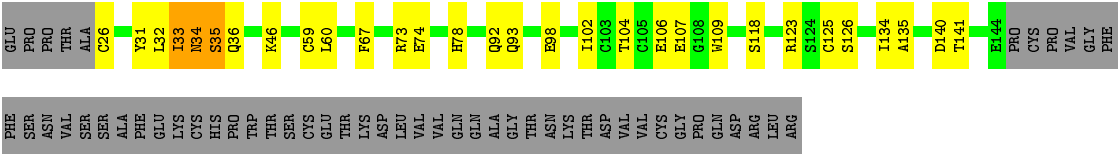


- Molecule 3: Tumor necrosis factor receptor superfamily member 5

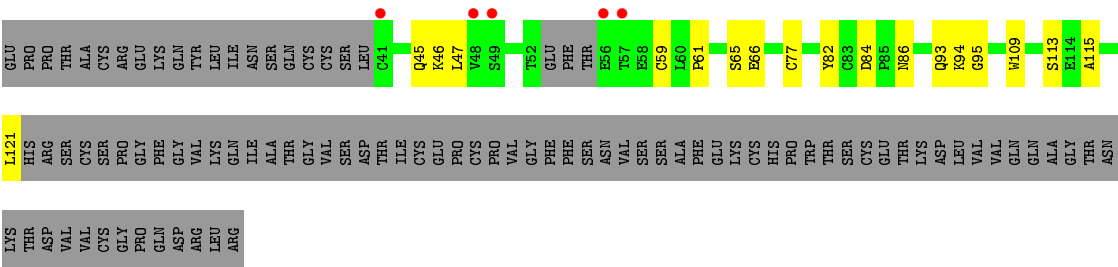
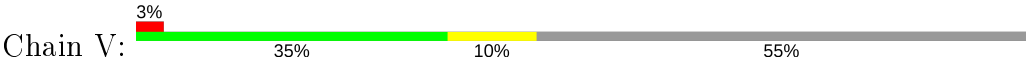


- Molecule 3: Tumor necrosis factor receptor superfamily member 5





● Molecule 3: Tumor necrosis factor receptor superfamily member 5



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	254.84Å 224.03Å 111.36Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	35.34 – 3.13 35.34 – 3.13	Depositor EDS
% Data completeness (in resolution range)	99.3 (35.34-3.13) 99.4 (35.34-3.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.216 , 0.255 0.217 , 0.256	Depositor DCC
R_{free} test set	5446 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18618	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: 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	A	0.55	0/1633	0.65	0/2224
1	C	0.48	0/1620	0.67	1/2211 (0.0%)
1	E	0.46	0/1610	0.62	0/2196
1	H	0.58	0/1635	0.69	0/2228
1	K	0.30	0/874	0.50	0/1189
2	B	0.56	0/1726	0.67	0/2348
2	D	0.51	0/1726	0.63	0/2349
2	F	0.42	0/1718	0.56	0/2340
2	L	0.57	0/1736	0.68	1/2360 (0.0%)
2	M	0.31	0/891	0.47	0/1212
3	G	0.38	0/890	0.59	0/1213
3	I	0.60	0/749	0.70	1/1016 (0.1%)
3	J	0.33	0/605	0.52	0/824
3	U	0.52	0/908	0.68	1/1233 (0.1%)
3	V	0.52	0/590	0.70	0/801
All	All	0.49	0/18911	0.63	4/25744 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	103	CYS	CA-CB-SG	-7.00	101.40	114.00
3	U	33	ILE	C-N-CA	5.59	135.66	121.70
2	L	142	LEU	CA-CB-CG	5.20	127.25	115.30
1	C	152	PRO	N-CA-C	5.11	125.39	112.10

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	1594	0	1550	12	0
1	C	1581	0	1514	31	0
1	E	1571	0	1518	31	0
1	H	1596	0	1543	13	0
1	K	855	0	785	17	0
2	B	1690	0	1629	24	0
2	D	1690	0	1623	27	0
2	F	1682	0	1606	26	0
2	L	1700	0	1644	19	0
2	M	872	0	848	12	0
3	G	873	0	740	24	0
3	I	736	0	650	7	0
3	J	595	0	491	10	0
3	U	891	0	781	22	0
3	V	580	0	498	16	0
4	A	5	0	0	0	0
4	H	10	0	0	1	0
4	I	5	0	0	0	0
4	L	5	0	0	0	0
5	A	11	0	0	0	0
5	B	16	0	0	1	0
5	C	2	0	0	0	0
5	D	9	0	0	0	0
5	E	7	0	0	0	0
5	F	4	0	0	0	0
5	G	1	0	0	0	0
5	H	12	0	0	0	0
5	I	2	0	0	0	0
5	L	12	0	0	0	0
5	U	8	0	0	0	0
5	V	3	0	0	0	0
All	All	18618	0	17420	263	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 (263) 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:U:134:ILE:HD13	3:U:135:ALA:O	1.61	0.99
1:K:52:SER:HB3	1:K:57:ASN:H	1.34	0.89
2:B:114:ARG:NH2	1:H:208:THR:OG1	2.11	0.82
2:F:3:VAL:H	2:F:26:SER:HB3	1.43	0.82
2:D:142:LEU:HD22	2:D:181:LEU:HD22	1.67	0.77
1:E:34:MET:HB3	1:E:79:LEU:HD22	1.68	0.76
2:B:2:ILE:HG12	2:B:27:GLN:NE2	2.02	0.75
1:C:158:ASN:HA	1:C:198:ILE:HG22	1.74	0.69
2:M:53:LEU:HB3	2:M:54:ILE:HD12	1.72	0.69
1:C:91:THR:HG23	1:C:113:THR:HA	1.73	0.69
2:D:119:PRO:HD3	2:D:204:HIS:HD2	1.57	0.69
3:V:46:LYS:O	3:V:59:CYS:HB2	1.93	0.68
1:H:153:VAL:HG22	1:H:181:LEU:HD21	1.76	0.68
3:I:49:SER:HB3	3:I:58:GLU:HB2	1.75	0.67
3:U:134:ILE:O	3:U:134:ILE:HD12	1.95	0.67
3:U:134:ILE:C	3:U:134:ILE:HD12	2.17	0.66
2:D:114:ARG:HG2	2:D:115:THR:N	2.11	0.65
2:L:98:TYR:CZ	3:V:93:GLN:HG3	2.32	0.64
1:C:174:GLN:NE2	1:C:180:SER:HB2	2.13	0.64
1:E:184:VAL:HG11	2:F:141:LEU:HD22	1.78	0.64
2:B:114:ARG:NH1	2:B:176:ASP:O	2.31	0.63
3:J:83:CYS:HB3	3:J:89:LEU:HB3	1.80	0.63
1:K:36:TRP:NE1	1:K:81:LEU:HB2	2.13	0.63
1:C:52:SER:HB3	1:C:57:ASN:H	1.64	0.63
1:H:91:THR:HG23	1:H:113:THR:HA	1.81	0.62
2:F:128:ASP:HA	2:F:131:LEU:HD12	1.80	0.62
3:G:136:THR:HG22	3:G:137:GLY:H	1.65	0.62
2:D:119:PRO:HD3	2:D:204:HIS:CD2	2.33	0.61
1:A:88:ALA:HA	1:A:114:VAL:HB	1.82	0.61
1:C:123:SER:HB3	1:C:125:PHE:CZ	2.35	0.61
2:F:39:LEU:HD13	2:F:77:PHE:CD2	2.35	0.61
2:B:60:ARG:HG2	2:B:64:VAL:HB	1.82	0.59
3:U:92:GLN:HE21	3:U:104:THR:HG23	1.68	0.59
1:C:129:PRO:HG3	1:C:141:LEU:HD23	1.85	0.59
3:G:68:LEU:HG	3:G:77:CYS:SG	2.43	0.59
1:C:52:SER:HB3	1:C:57:ASN:N	2.17	0.58
1:K:91:THR:HG23	1:K:113:THR:HA	1.85	0.58
2:M:14:SER:HA	2:M:113:LYS:HB2	1.85	0.58
1:E:20:LEU:HB2	1:E:81:LEU:HB3	1.86	0.58
1:C:48:VAL:HG13	1:C:64:VAL:HG21	1.84	0.57
3:V:84:ASP:OD2	3:V:86:ASN:HB2	2.04	0.57
2:B:21:ILE:HG12	2:B:108:THR:HG21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:92:GLN:HB3	3:G:102:ILE:HG22	1.86	0.57
1:C:122:PRO:HB3	1:C:148:TYR:HB3	1.86	0.57
1:A:91:THR:HG23	1:A:113:THR:HA	1.86	0.56
2:B:84:LEU:HD11	2:B:110:LEU:HD21	1.87	0.56
3:V:66:GLU:HB3	3:V:77:CYS:HB2	1.87	0.56
2:D:89:VAL:HG23	2:D:110:LEU:O	2.06	0.55
1:K:36:TRP:O	1:K:48:VAL:HG22	2.06	0.55
1:C:198:ILE:HD12	1:C:213:LYS:HA	1.87	0.55
1:A:120:LYS:HE3	1:A:147:ASP:O	2.07	0.55
2:B:2:ILE:HG12	2:B:27:GLN:CD	2.27	0.55
1:E:143:CYS:HG	1:E:199:CYS:HG	1.53	0.55
1:E:22:CYS:HB3	1:E:79:LEU:HB3	1.87	0.55
3:J:56:GLU:HG3	3:J:57:THR:H	1.72	0.55
3:U:134:ILE:CD1	3:U:135:ALA:O	2.47	0.55
3:G:88:GLY:HA3	3:G:119:CYS:HB2	1.89	0.54
1:K:52:SER:HB3	1:K:57:ASN:N	2.13	0.54
3:I:73:ARG:NH1	3:U:74:GLU:OE2	2.34	0.54
2:F:45:LYS:HG2	2:F:90:ALA:HB2	1.89	0.54
1:A:34:MET:HB3	1:A:79:LEU:HD22	1.90	0.53
1:E:36:TRP:NE1	1:E:81:LEU:HB2	2.24	0.53
3:V:109:TRP:HA	3:V:121:LEU:HA	1.91	0.52
2:D:207:LEU:HD13	2:D:211:VAL:HG23	1.91	0.52
1:E:49:SER:HG	1:E:60:TYR:HD1	1.55	0.52
1:C:13:LYS:HB2	3:U:107:GLU:HG3	1.92	0.52
2:B:2:ILE:CG1	2:B:27:GLN:NE2	2.73	0.52
3:U:33:ILE:O	3:U:34:ASN:ND2	2.43	0.52
1:A:87:ARG:HH11	1:A:89:GLU:HB2	1.75	0.51
3:J:98:GLU:HG3	2:M:34:ASN:HB3	1.92	0.51
2:B:157:ASP:OD2	2:B:195:HIS:HB3	2.11	0.51
3:U:134:ILE:CD1	3:U:134:ILE:C	2.77	0.51
3:U:46:LYS:O	3:U:59:CYS:HA	2.10	0.51
1:C:152:PRO:O	1:C:153:VAL:HG13	2.11	0.51
1:C:173:LEU:HB2	1:C:179:TYR:HE1	1.75	0.51
2:D:39:LEU:HD13	2:D:77:PHE:CD1	2.46	0.51
2:B:39:LEU:HG	2:B:40:THR:N	2.24	0.51
1:C:22:CYS:HB3	1:C:79:LEU:HB3	1.93	0.51
2:L:139:VAL:HG22	2:L:184:THR:HG23	1.92	0.51
2:L:98:TYR:CE1	3:V:93:GLN:HG3	2.46	0.51
3:V:47:LEU:HA	3:V:59:CYS:HB2	1.93	0.51
1:E:36:TRP:CG	1:E:81:LEU:HD22	2.46	0.50
3:J:66:GLU:HA	3:J:79:GLN:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:122:PRO:HB3	1:H:148:TYR:HB3	1.94	0.50
3:G:110:HIS:HB3	3:G:122:HIS:CD2	2.47	0.50
2:L:99:THR:HG23	3:V:93:GLN:HA	1.92	0.50
3:V:121:LEU:H	3:V:121:LEU:HD12	1.77	0.50
3:V:47:LEU:HA	3:V:59:CYS:CB	2.42	0.50
1:C:129:PRO:HD3	1:C:141:LEU:HB3	1.93	0.50
1:C:34:MET:HB3	1:C:79:LEU:HD22	1.94	0.50
3:G:28:GLU:HG3	3:J:100:ASP:HB2	1.94	0.50
2:L:207:LEU:HD13	2:L:211:VAL:HG23	1.94	0.50
3:U:135:ALA:HB2	3:U:141:THR:HG23	1.93	0.49
2:F:187:LEU:HD12	2:F:191:ASP:HB3	1.93	0.49
1:H:2:VAL:HG12	1:H:105:VAL:HG11	1.93	0.49
1:E:127:LEU:HB3	2:F:124:PHE:CD2	2.48	0.49
2:F:130:GLN:HG2	2:F:135:THR:O	2.12	0.49
2:B:98:TYR:CD2	2:B:99:THR:HG23	2.48	0.49
3:V:45:GLN:HA	3:V:61:PRO:HA	1.94	0.49
2:D:67:ARG:HB2	2:D:82:SER:O	2.13	0.49
1:E:122:PRO:HD2	1:E:208:THR:HG21	1.95	0.48
2:F:13:VAL:HG23	2:F:84:LEU:HD22	1.95	0.48
2:F:12:ALA:HA	2:F:111:GLU:O	2.12	0.48
2:D:72:GLY:HA3	2:D:77:PHE:HA	1.96	0.48
1:E:13:LYS:HB2	3:G:107:GLU:HG3	1.96	0.48
3:I:32:LEU:HD11	3:I:35:SER:HA	1.95	0.48
1:C:53:SER:OG	3:G:64:GLU:HB3	2.13	0.48
1:H:34:MET:HB3	1:H:79:LEU:HD22	1.96	0.48
2:B:72:GLY:HA3	2:B:77:PHE:HA	1.96	0.48
2:D:169:VAL:HG22	2:D:181:LEU:HD12	1.95	0.48
2:D:2:ILE:HG12	2:D:27:GLN:HB2	1.95	0.48
1:E:68:PHE:CD1	1:E:68:PHE:N	2.82	0.48
2:D:84:LEU:HD11	2:D:110:LEU:HD21	1.96	0.48
2:F:13:VAL:HA	2:F:113:LYS:HE2	1.96	0.47
3:G:70:THR:HG22	3:G:71:TRP:H	1.79	0.47
2:D:99:THR:HG23	3:G:93:GLN:HA	1.96	0.47
2:B:67:ARG:HB2	2:B:82:SER:O	2.14	0.47
3:J:79:GLN:CB	1:K:55:ARG:HH22	2.28	0.47
2:F:114:ARG:HD3	2:F:115:THR:O	2.15	0.47
2:L:39:LEU:HG	2:L:40:THR:N	2.30	0.47
1:A:2:VAL:HG12	1:A:105:VAL:HG11	1.96	0.47
1:E:2:VAL:HG12	1:E:27:PHE:HD2	1.80	0.47
1:E:6:GLU:HG3	1:E:96:CYS:HB3	1.97	0.47
3:U:106:GLU:HB3	3:U:109:TRP:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PRO:HB3	1:A:148:TYR:HB3	1.98	0.46
1:C:151:GLU:HA	1:C:152:PRO:HA	1.54	0.46
3:G:45:GLN:HB3	3:G:59:CYS:HB3	1.96	0.46
1:K:34:MET:HB3	1:K:79:LEU:HD22	1.97	0.46
2:F:89:VAL:HB	2:F:112:ILE:HD11	1.97	0.46
2:F:34:ASN:O	2:F:36:LYS:HG3	2.16	0.46
1:K:14:PRO:HD3	1:K:115:SER:O	2.15	0.46
1:C:173:LEU:HB2	1:C:179:TYR:CE1	2.51	0.46
1:C:87:ARG:NE	1:E:63:THR:HG22	2.30	0.46
1:C:57:ASN:HB3	3:G:82:TYR:CD1	2.50	0.46
2:D:44:GLN:NE2	2:D:48:GLN:O	2.48	0.46
3:G:67:PHE:CE1	3:G:78:HIS:HB2	2.50	0.46
1:H:196:THR:HG23	1:H:213:LYS:HE3	1.98	0.46
2:M:22:ASN:HA	2:M:78:THR:HG22	1.97	0.45
2:B:116:VAL:HG23	5:B:312:HOH:O	2.15	0.45
2:B:203:THR:HG23	2:B:210:PRO:HG3	1.97	0.45
2:F:142:LEU:HB2	2:F:181:LEU:HB2	1.99	0.45
1:K:99:SER:HB3	1:K:103:PHE:CD1	2.51	0.45
2:L:65:PRO:HG2	2:L:68:PHE:CD2	2.51	0.45
1:E:199:CYS:O	1:E:211:ASP:HA	2.16	0.45
1:H:36:TRP:NE1	1:H:81:LEU:HB2	2.31	0.45
3:I:45:GLN:HG2	3:I:61:PRO:HA	1.97	0.45
1:C:127:LEU:HB3	2:D:124:PHE:CD1	2.52	0.45
3:G:73:ARG:NH2	3:J:74:GLU:OE1	2.42	0.45
2:D:46:PRO:HB3	2:D:171:GLU:HG3	1.98	0.45
1:K:99:SER:HB3	1:K:103:PHE:HD1	1.81	0.45
1:C:6:GLU:HG2	1:C:96:CYS:HB3	1.98	0.45
2:M:41:TRP:CZ3	2:M:94:CYS:HB3	2.52	0.45
2:B:24:LYS:HA	2:B:75:THR:O	2.17	0.45
2:D:86:ALA:HA	2:D:112:ILE:HD13	1.97	0.45
3:V:66:GLU:HB3	3:V:77:CYS:CB	2.46	0.45
3:I:26:CYS:HB2	3:U:78:HIS:ND1	2.32	0.44
1:E:13:LYS:HA	1:E:115:SER:O	2.17	0.44
1:E:127:LEU:HB3	2:F:124:PHE:CE2	2.53	0.44
1:K:37:VAL:O	1:K:95:TYR:HB2	2.17	0.44
1:C:152:PRO:HB2	1:C:153:VAL:H	1.60	0.44
1:K:70:ILE:HD11	1:K:79:LEU:HD11	2.00	0.44
1:H:57:ASN:HB3	3:V:82:TYR:CD1	2.53	0.44
4:H:302:SO4:O3	2:L:184:THR:OG1	2.24	0.44
2:F:31:ASN:HB3	2:F:34:ASN:OD1	2.18	0.44
1:H:60:TYR:HB2	1:H:65:LYS:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:106:GLU:C	3:I:109:TRP:H	2.21	0.44
2:L:68:PHE:CD1	2:L:81:ILE:HG12	2.53	0.44
3:J:69:ASP:N	3:J:69:ASP:OD1	2.48	0.44
2:L:67:ARG:HB2	2:L:82:SER:O	2.18	0.44
2:B:39:LEU:HD22	2:B:77:PHE:CG	2.53	0.44
2:L:39:LEU:HD22	2:L:77:PHE:CG	2.53	0.44
3:U:93:GLN:HB3	3:U:102:ILE:HD12	1.99	0.44
2:B:95:GLN:HG3	2:B:104:PHE:CE2	2.53	0.43
1:E:169:PHE:HD2	1:E:182:SER:O	2.01	0.43
2:F:114:ARG:HG2	2:F:115:THR:H	1.83	0.43
2:D:9:ASP:O	2:D:108:THR:HA	2.19	0.43
2:F:72:GLY:HA3	2:F:77:PHE:HA	2.00	0.43
3:G:41:CYS:O	3:G:71:TRP:HA	2.19	0.43
2:M:96:ASN:OD1	2:M:98:TYR:N	2.51	0.43
2:D:99:THR:HG21	3:G:92:GLN:C	2.39	0.43
2:M:12:ALA:HA	2:M:111:GLU:HB2	2.00	0.43
1:H:29:PHE:O	1:H:72:ARG:NH2	2.51	0.43
2:D:149:GLU:H	2:D:149:GLU:CD	2.21	0.43
3:G:83:CYS:HB2	3:G:91:VAL:HG22	2.00	0.43
1:H:108:GLN:HA	2:L:49:PRO:HG3	2.00	0.43
1:E:48:VAL:HG13	1:E:64:VAL:HG11	2.01	0.43
2:F:34:ASN:HB3	3:U:98:GLU:HG3	1.99	0.43
2:D:10:SER:HB3	2:D:109:LYS:HB3	2.00	0.43
3:G:67:PHE:CE2	3:G:100:ASP:HB2	2.54	0.43
1:H:62:ASP:HA	1:H:65:LYS:HD3	1.99	0.43
2:M:41:TRP:CG	2:M:79:LEU:HD13	2.54	0.43
3:U:140:ASP:OD1	3:U:141:THR:N	2.47	0.43
3:U:31:TYR:CG	3:U:73:ARG:HD3	2.54	0.43
1:C:67:ARG:C	1:C:68:PHE:HD1	2.22	0.43
3:U:60:LEU:HD23	3:U:60:LEU:HA	1.78	0.43
1:E:27:PHE:HE1	1:E:29:PHE:HA	1.84	0.43
2:D:89:VAL:HG23	2:D:111:GLU:HA	2.01	0.42
1:E:155:VAL:HG22	1:E:201:VAL:HG22	2.00	0.42
2:F:145:PHE:HD2	2:F:204:HIS:HE2	1.67	0.42
2:B:125:PRO:HB3	2:B:215:PHE:CE2	2.54	0.42
3:U:34:ASN:CG	3:U:35:SER:N	2.73	0.42
3:V:82:TYR:CE2	3:V:84:ASP:HA	2.54	0.42
3:G:140:ASP:OD1	3:G:141:THR:N	2.53	0.42
3:G:142:ILE:HA	3:G:142:ILE:HD13	1.87	0.42
3:I:47:LEU:HD22	3:I:73:ARG:HB2	2.02	0.42
1:A:11:LEU:HD13	1:A:150:PRO:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:GLU:OE1	1:C:96:CYS:N	2.52	0.42
2:F:196:LYS:HE2	2:F:196:LYS:HB3	1.93	0.42
1:E:173:LEU:HD13	1:E:179:TYR:CE1	2.55	0.42
2:B:41:TRP:CE2	2:B:79:LEU:HB2	2.55	0.42
1:K:21:SER:HA	1:K:79:LEU:O	2.20	0.42
2:L:130:GLN:HE22	2:L:137:SER:HB2	1.85	0.42
2:F:40:THR:HG22	2:F:41:TRP:N	2.35	0.41
2:L:65:PRO:HG2	2:L:68:PHE:CE2	2.55	0.41
1:C:12:VAL:O	1:C:114:VAL:HA	2.20	0.41
3:V:113:SER:C	3:V:115:ALA:H	2.23	0.41
1:A:87:ARG:NH1	1:A:89:GLU:HB2	2.35	0.41
2:B:131:LEU:HD23	2:B:131:LEU:HA	1.79	0.41
2:D:114:ARG:HG2	2:D:115:THR:H	1.81	0.41
3:G:48:VAL:HB	3:G:58:GLU:HG3	2.02	0.41
2:L:149:GLU:CD	2:L:149:GLU:H	2.24	0.41
2:L:39:LEU:HD22	2:L:77:PHE:CB	2.50	0.41
3:U:67:PHE:CE1	3:U:78:HIS:HB2	2.55	0.41
1:E:6:GLU:HA	1:E:21:SER:O	2.20	0.41
1:E:20:LEU:HA	1:E:20:LEU:HD23	1.73	0.41
3:G:129:PHE:N	3:G:129:PHE:CD1	2.87	0.41
3:G:72:ASN:OD1	3:G:74:GLU:HB2	2.21	0.41
3:J:82:TYR:CD1	1:K:57:ASN:HB3	2.55	0.41
3:U:32:LEU:HD12	3:U:36:GLN:O	2.20	0.41
1:C:203:HIS:CE1	1:C:205:PRO:HB2	2.56	0.41
3:G:68:LEU:HD23	3:G:68:LEU:HA	1.75	0.41
2:M:92:TYR:HE2	2:M:110:LEU:HD22	1.86	0.41
1:E:151:GLU:HG2	1:E:152:PRO:HA	2.02	0.41
1:E:127:LEU:HD12	1:E:143:CYS:N	2.36	0.41
1:E:16:GLY:O	1:E:86:LEU:HD12	2.20	0.41
2:L:143:ASN:ND2	2:L:144:ASN:OD1	2.53	0.41
1:E:36:TRP:CE2	1:E:81:LEU:HB2	2.56	0.41
2:L:176:ASP:O	2:L:178:THR:HG23	2.19	0.41
2:B:146:TYR:CG	2:B:147:PRO:HA	2.56	0.41
2:D:39:LEU:HD13	2:D:77:PHE:CG	2.56	0.41
1:E:144:LEU:HD12	2:F:139:VAL:HG21	2.03	0.41
2:M:6:GLN:HA	2:M:23:CYS:HA	2.03	0.41
1:A:203:HIS:CE1	1:A:205:PRO:HG2	2.56	0.40
2:F:125:PRO:HA	2:F:126:PRO:HD2	1.91	0.40
3:U:123:ARG:O	3:U:141:THR:OG1	2.34	0.40
1:C:122:PRO:HD2	1:C:208:THR:HG21	2.02	0.40
2:D:6:GLN:NE2	2:D:108:THR:OG1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:CYS:HB2	1:E:157:TRP:CH2	2.56	0.40
1:K:4:LEU:HB3	1:K:22:CYS:SG	2.62	0.40
1:K:18:LEU:HB3	1:K:83:MET:HE2	2.04	0.40
2:M:86:ALA:O	2:M:89:VAL:HG12	2.21	0.40
1:A:3:GLN:HB2	1:A:25:SER:OG	2.21	0.40
2:B:146:TYR:CD1	2:B:147:PRO:HA	2.57	0.40
2:D:164:ASN:OD1	2:D:164:ASN:N	2.52	0.40
3:V:94:LYS:HG2	3:V:95:GLY:N	2.37	0.40
2:B:14:SER:HA	2:B:113:LYS:HB2	2.04	0.40
2:L:95:GLN:HG3	2:L:104:PHE:CE1	2.56	0.40
1:A:147:ASP:OD1	1:A:174:GLN:NE2	2.49	0.40
1:C:6:GLU:OE2	1:C:109:GLY:N	2.53	0.40
1:C:125:PHE:CE1	2:D:130:GLN:HB3	2.57	0.40
2:F:182:SER:OG	2:F:182:SER:O	2.32	0.40
3:J:93:GLN:HG3	2:M:98:TYR:CZ	2.56	0.40
1:K:36:TRP:CD1	1:K:81:LEU:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	209/223 (94%)	200 (96%)	9 (4%)	0	100	100
1	C	209/223 (94%)	193 (92%)	14 (7%)	2 (1%)	15	47
1	E	206/223 (92%)	191 (93%)	15 (7%)	0	100	100
1	H	210/223 (94%)	201 (96%)	9 (4%)	0	100	100
1	K	114/223 (51%)	107 (94%)	7 (6%)	0	100	100
2	B	217/220 (99%)	208 (96%)	9 (4%)	0	100	100
2	D	218/220 (99%)	203 (93%)	15 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	218/220 (99%)	209 (96%)	9 (4%)	0	100	100
2	L	218/220 (99%)	209 (96%)	9 (4%)	0	100	100
2	M	111/220 (50%)	101 (91%)	10 (9%)	0	100	100
3	G	119/173 (69%)	110 (92%)	9 (8%)	0	100	100
3	I	93/173 (54%)	87 (94%)	6 (6%)	0	100	100
3	J	77/173 (44%)	72 (94%)	5 (6%)	0	100	100
3	U	117/173 (68%)	104 (89%)	11 (9%)	2 (2%)	9	34
3	V	74/173 (43%)	65 (88%)	9 (12%)	0	100	100
All	All	2410/3080 (78%)	2260 (94%)	146 (6%)	4 (0%)	47	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	152	PRO
1	C	153	VAL
3	U	125	CYS
3	U	35	SER

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	177/187 (95%)	170 (96%)	7 (4%)	31	62
1	C	173/187 (92%)	168 (97%)	5 (3%)	42	70
1	E	173/187 (92%)	170 (98%)	3 (2%)	60	82
1	H	177/187 (95%)	175 (99%)	2 (1%)	73	88
1	K	86/187 (46%)	84 (98%)	2 (2%)	50	75
2	B	192/195 (98%)	184 (96%)	8 (4%)	30	60
2	D	192/195 (98%)	186 (97%)	6 (3%)	40	69
2	F	190/195 (97%)	185 (97%)	5 (3%)	46	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	194/195 (100%)	188 (97%)	6 (3%)	40	69
2	M	98/195 (50%)	96 (98%)	2 (2%)	55	79
3	G	97/157 (62%)	92 (95%)	5 (5%)	23	53
3	I	86/157 (55%)	84 (98%)	2 (2%)	50	75
3	J	66/157 (42%)	64 (97%)	2 (3%)	41	70
3	U	103/157 (66%)	99 (96%)	4 (4%)	32	63
3	V	66/157 (42%)	65 (98%)	1 (2%)	65	84
All	All	2070/2695 (77%)	2010 (97%)	60 (3%)	42	70

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ARG
1	A	120	LYS
1	A	183	SER
1	A	199	CYS
1	A	200	ASN
1	A	212	LYS
1	A	219	CYS
2	B	9	ASP
2	B	10	SER
2	B	18	ARG
2	B	66	ASP
2	B	97	ASP
2	B	114	ARG
2	B	153	GLN
2	B	219	GLU
1	C	1	GLU
1	C	6	GLU
1	C	99	SER
1	C	100	TRP
1	C	203	HIS
2	D	7	SER
2	D	14	SER
2	D	71	SER
2	D	97	ASP
2	D	130	GLN
2	D	133	SER
1	E	78	SER
1	E	143	CYS

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Mol	Chain	Res	Type
1	E	151	GLU
2	F	39	LEU
2	F	97	ASP
2	F	114	ARG
2	F	162	SER
2	F	189	LYS
3	G	47	LEU
3	G	69	ASP
3	G	72	ASN
3	G	79	GLN
3	G	116	CYS
1	H	65	LYS
1	H	83	MET
3	I	73	ARG
3	I	117	GLU
3	J	31	TYR
3	J	50	ASP
1	K	98	ARG
1	K	100	TRP
2	L	7	SER
2	L	10	SER
2	L	18	ARG
2	L	25	SER
2	L	137	SER
2	L	168	SER
2	M	35	GLN
2	M	97	ASP
3	U	26	CYS
3	U	34	ASN
3	U	118	SER
3	U	126	SER
3	V	65	SER

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

Mol	Chain	Res	Type
2	B	143	ASN
2	B	144	ASN
3	I	42	GLN
3	U	92	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
4	SO4	H	302	-	4,4,4	0.13	0	6,6,6	0.11	0
4	SO4	H	301	-	4,4,4	0.20	0	6,6,6	0.35	0
4	SO4	I	201	-	4,4,4	0.23	0	6,6,6	0.38	0
4	SO4	A	301	-	4,4,4	0.19	0	6,6,6	0.18	0
4	SO4	L	401	-	4,4,4	0.18	0	6,6,6	0.24	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	302	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	213/223 (95%)	-0.51	0 100 100	32, 46, 65, 118	0
1	C	213/223 (95%)	-0.33	3 (1%) 75 59	36, 62, 100, 136	0
1	E	210/223 (94%)	-0.19	1 (0%) 91 83	41, 63, 136, 144	0
1	H	214/223 (95%)	-0.49	2 (0%) 84 72	29, 40, 68, 146	0
1	K	116/223 (52%)	0.25	5 (4%) 35 17	91, 113, 141, 154	0
2	B	219/220 (99%)	-0.57	0 100 100	30, 45, 75, 92	0
2	D	220/220 (100%)	-0.36	0 100 100	38, 59, 96, 136	0
2	F	220/220 (100%)	-0.06	1 (0%) 91 83	39, 88, 121, 144	0
2	L	220/220 (100%)	-0.48	0 100 100	31, 47, 79, 132	0
2	M	113/220 (51%)	0.25	3 (2%) 54 32	92, 122, 168, 170	0
3	G	121/173 (69%)	0.24	5 (4%) 37 19	57, 92, 138, 152	0
3	I	97/173 (56%)	-0.25	1 (1%) 82 70	31, 45, 129, 137	0
3	J	81/173 (46%)	0.30	4 (4%) 29 14	98, 122, 141, 150	0
3	U	119/173 (68%)	-0.35	0 100 100	37, 49, 89, 101	0
3	V	78/173 (45%)	0.07	5 (6%) 19 8	35, 64, 126, 137	0
All	All	2454/3080 (79%)	-0.24	30 (1%) 79 64	29, 58, 130, 170	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	219	CYS	4.8
2	F	220	CYS	3.9
3	G	73	ARG	3.8
2	M	83	SER	3.4
3	G	47	LEU	3.0
1	K	110	THR	2.9
3	J	49	SER	2.9

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Mol	Chain	Res	Type	RSRZ
3	J	103	CYS	2.8
1	K	9	GLY	2.8
3	V	57	THR	2.7
3	V	49	SER	2.6
1	E	139	ALA	2.6
2	M	85	GLN	2.5
1	K	101	GLY	2.5
3	V	56	GLU	2.5
1	K	10	GLY	2.5
3	J	76	HIS	2.4
1	H	218	SER	2.4
3	G	34	ASN	2.4
1	C	1	GLU	2.3
3	G	35	SER	2.3
1	C	219	CYS	2.3
2	M	111	GLU	2.2
3	G	55	THR	2.2
3	I	24	THR	2.2
3	V	48	VAL	2.2
3	J	104	THR	2.1
1	C	218	SER	2.1
1	K	83	MET	2.1
3	V	41	CYS	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	H	302	5/5	0.92	0.29	147,147,148,148	0
4	SO4	H	301	5/5	0.96	0.13	63,65,71,80	0
4	SO4	A	301	5/5	0.97	0.09	69,70,73,83	0
4	SO4	L	401	5/5	0.98	0.07	50,54,57,63	0
4	SO4	I	201	5/5	0.99	0.13	42,43,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.