Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:51 am BST

PDB ID	:	4EVN
Title	:	Crystal Structure of Fab CR6261 (somatic heavy chain with germline-reverted light chain)
Authors	:	Whittle, J.R.R.
Deposited on	:	2012-04-26
Resolution	:	2.85 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:

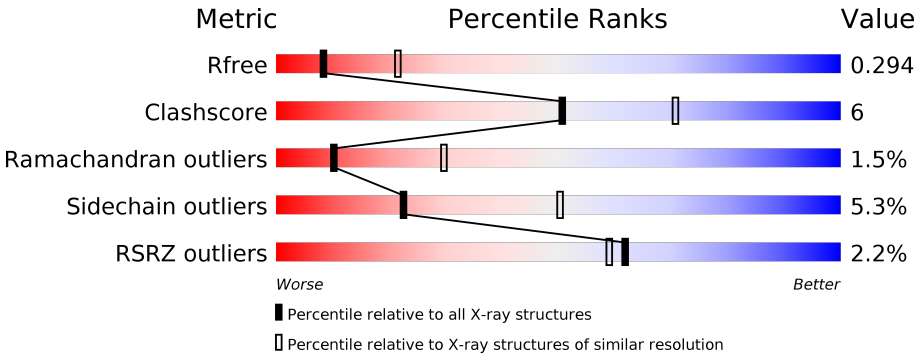
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 <=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	242	73% 17% • 9%
1	C	242	3% 70% 19% • 9%
1	E	242	2% 71% 18% • 9%
1	G	242	3% 73% 17% • 9%
1	I	242	3% 74% 16% • 9%
1	K	242	2% 70% 19% • 9%

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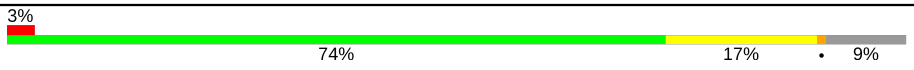
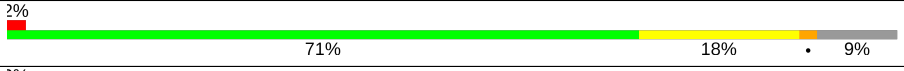
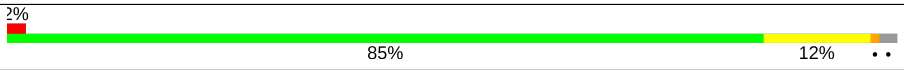
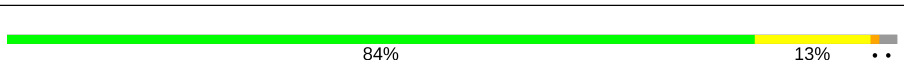
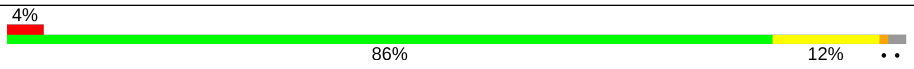
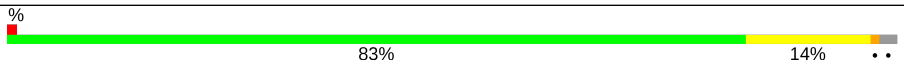
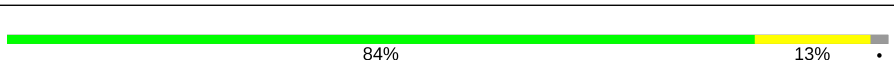
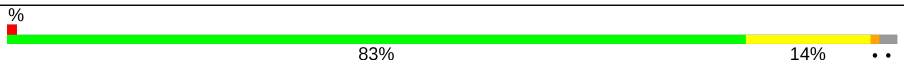
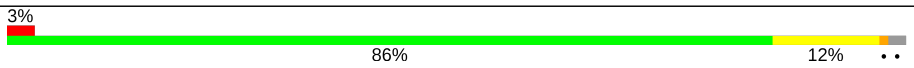
Mol	Chain	Length	Quality of chain
1	M	242	
1	O	242	
2	B	217	
2	D	217	
2	F	217	
2	H	217	
2	J	217	
2	L	217	
2	N	217	
2	P	217	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25293 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	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			
1	C	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			
1	E	221	Total	C	N	O	S	0	0	0
			1625	1029	269	318	9			
1	G	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			
1	I	221	Total	C	N	O	S	0	0	0
			1625	1029	269	318	9			
1	K	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			
1	M	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			
1	O	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			

- Molecule 2 is a protein called Fab Lambda Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1541	972	251	314	4			
2	D	213	Total	C	N	O	S	0	0	0
			1537	969	250	314	4			
2	F	213	Total	C	N	O	S	0	0	0
			1537	969	250	314	4			
2	H	213	Total	C	N	O	S	0	0	0
			1537	969	250	314	4			
2	J	213	Total	C	N	O	S	0	0	0
			1537	969	250	314	4			
2	L	213	Total	C	N	O	S	0	0	0
			1540	970	251	315	4			

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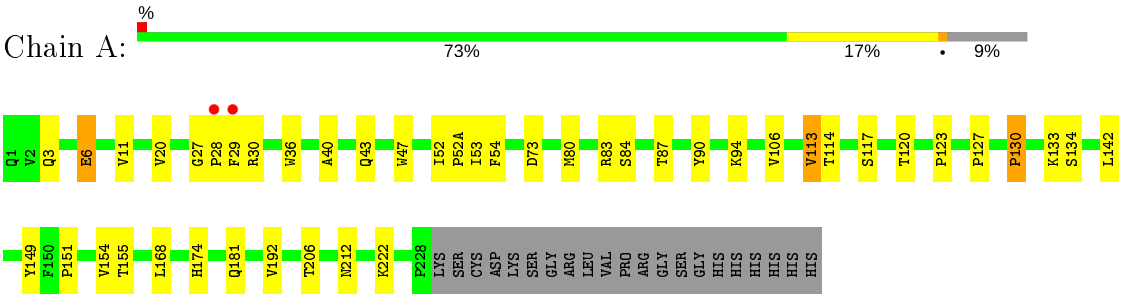
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	213	Total	C	N	O	S	0	0	0
			1537	969	250	314	4			
2	P	213	Total	C	N	O	S	0	0	0
			1539	970	251	314	4			

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.

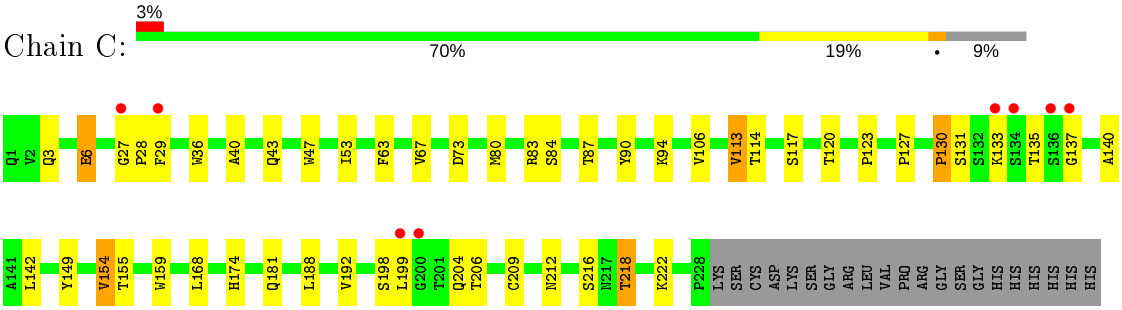
- Molecule 1: Fab Heavy Chain

Chain A:



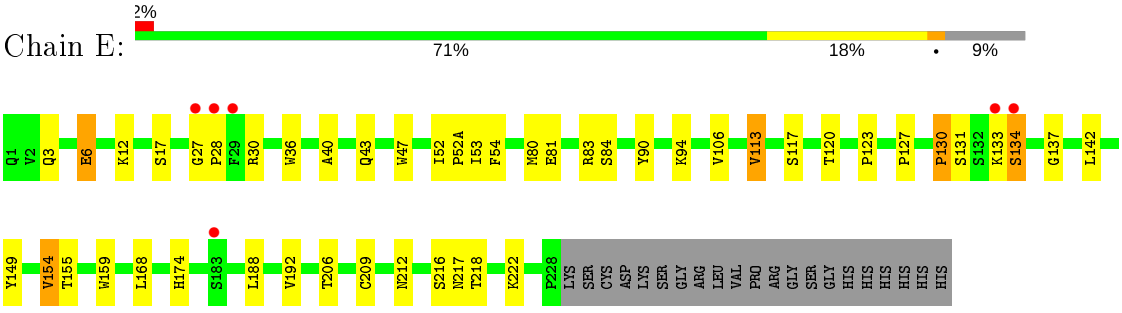
- Molecule 1: Fab Heavy Chain

Chain C:



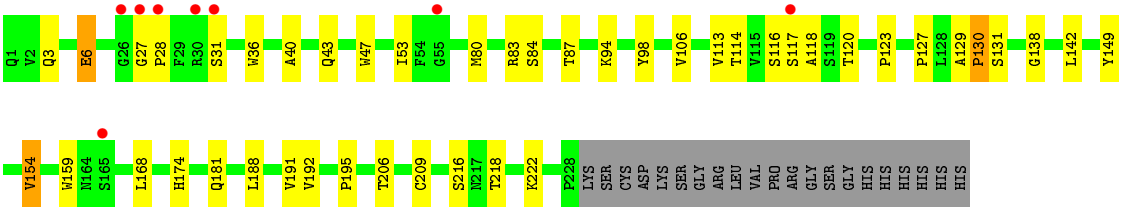
- Molecule 1: Fab Heavy Chain

Chain E:

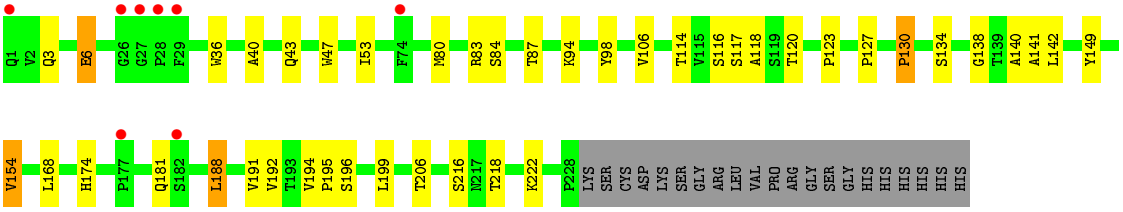


- Molecule 1: Fab Heavy Chain

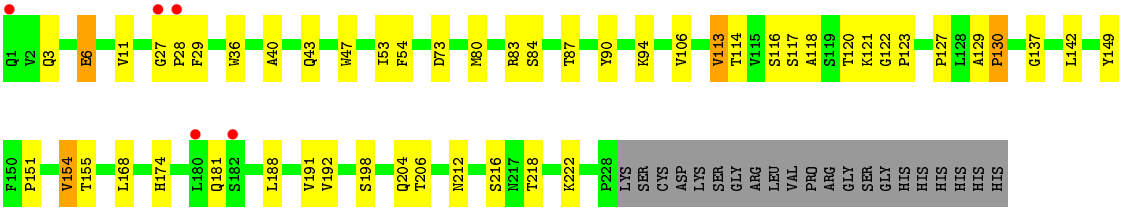
Chain G:



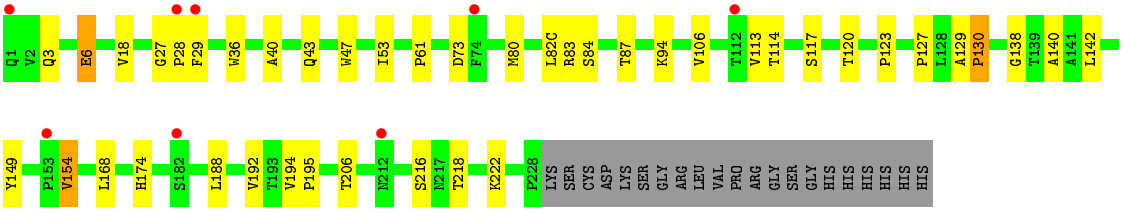
• Molecule 1: Fab Heavy Chain



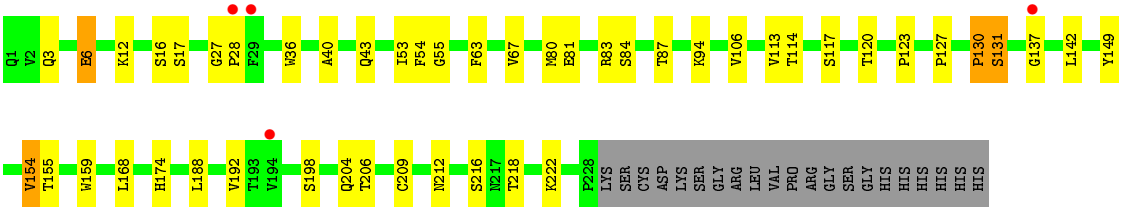
• Molecule 1: Fab Heavy Chain



• Molecule 1: Fab Heavy Chain

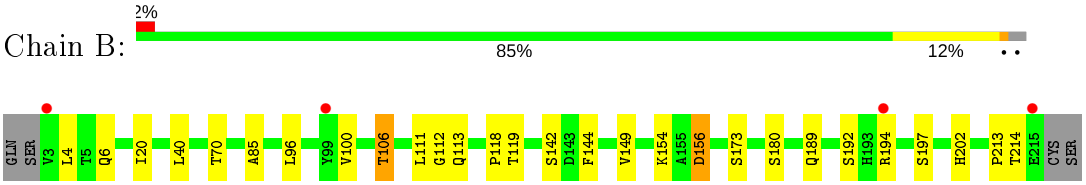


• Molecule 1: Fab Heavy Chain



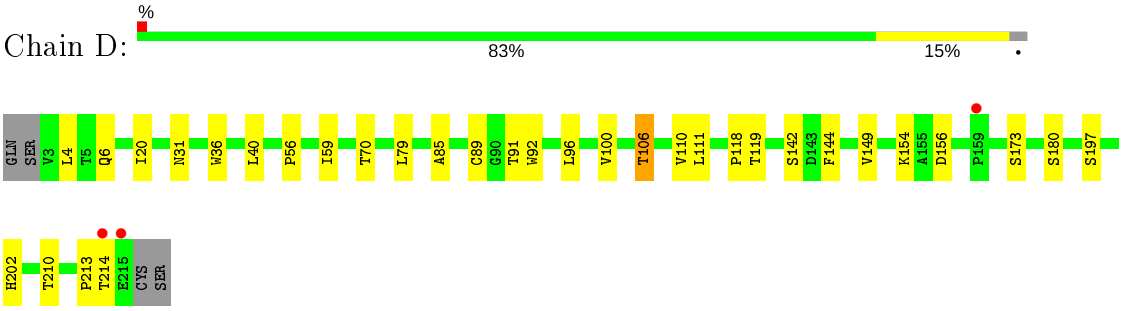
• Molecule 2: Fab Lambda Light Chain

Chain B:



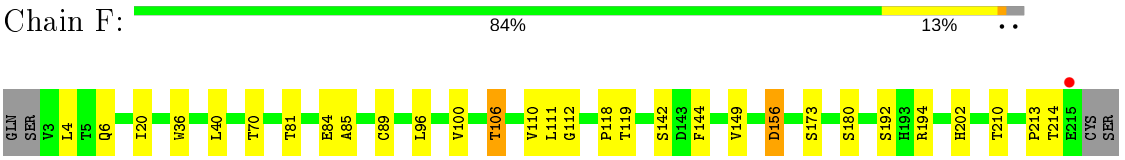
• Molecule 2: Fab Lambda Light Chain

Chain D:



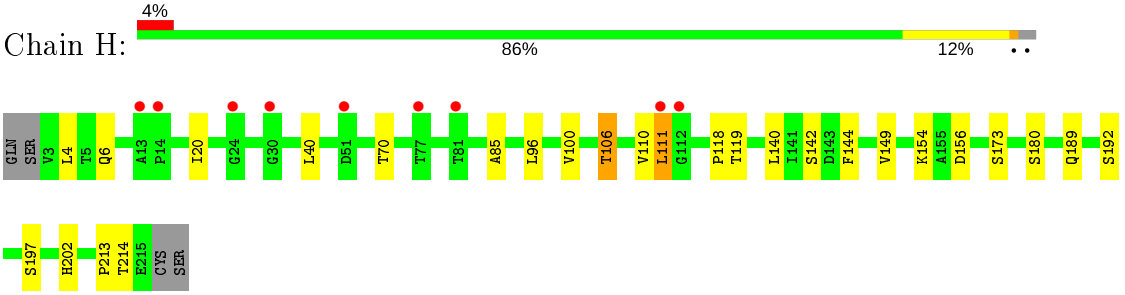
• Molecule 2: Fab Lambda Light Chain

Chain F:



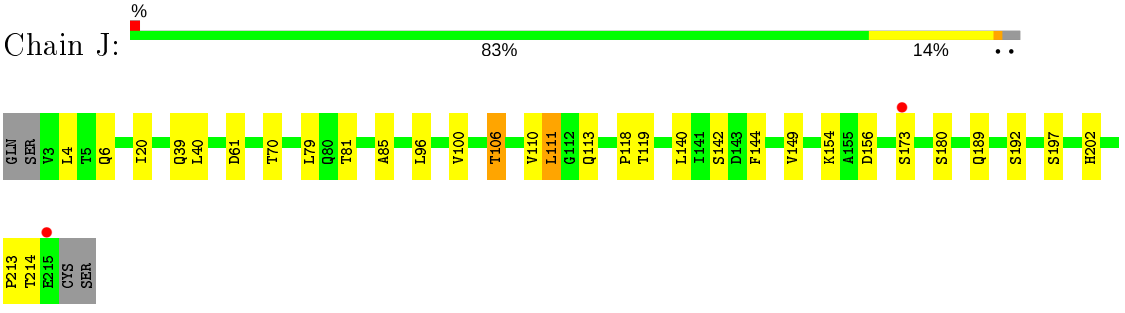
• Molecule 2: Fab Lambda Light Chain

Chain H:



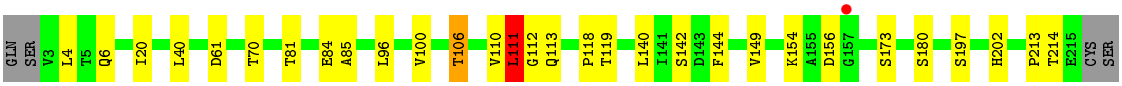
• Molecule 2: Fab Lambda Light Chain

Chain J:



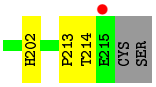
• Molecule 2: Fab Lambda Light Chain

Chain L:



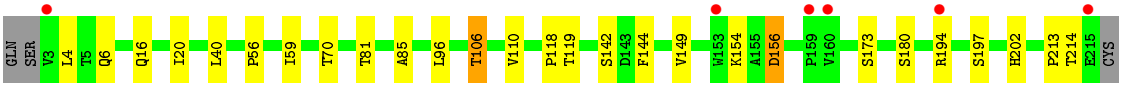
- Molecule 2: Fab Lambda Light Chain

Chain N:



- Molecule 2: Fab Lambda Light Chain

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.11Å 159.27Å 176.44Å 90.00° 89.73° 90.00°	Depositor
Resolution (Å)	55.01 – 2.85 176.44 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.3 (55.01-2.85) 92.7 (176.44-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.230 , 0.293 0.228 , 0.294	Depositor DCC
R_{free} test set	2024 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å^2)	53.9	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 2.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.069 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	25293	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.09% 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

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	0.48	0/1664	0.59	0/2270
1	C	0.53	1/1664 (0.1%)	0.62	0/2270
1	E	0.57	0/1666	0.66	0/2272
1	G	0.50	0/1664	0.61	0/2270
1	I	0.52	0/1666	0.63	0/2272
1	K	0.53	0/1664	0.66	0/2270
1	M	0.49	0/1664	0.57	0/2270
1	O	0.51	0/1664	0.62	0/2270
2	B	0.46	0/1580	0.60	1/2168 (0.0%)
2	D	0.48	0/1576	0.61	0/2164
2	F	0.46	0/1576	0.62	0/2164
2	H	0.42	0/1576	0.56	0/2164
2	J	0.44	0/1576	0.59	0/2164
2	L	0.43	0/1579	0.60	0/2168
2	N	0.43	0/1576	0.59	0/2164
2	P	0.45	0/1578	0.60	0/2166
All	All	0.48	1/25933 (0.0%)	0.61	1/35486 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	GLN	CD-NE2	6.42	1.49	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	113	GLN	N-CA-C	-5.67	95.69	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1623	0	1580	21	0
1	C	1623	0	1580	23	0
1	E	1625	0	1587	33	0
1	G	1623	0	1580	28	0
1	I	1625	0	1587	23	0
1	K	1623	0	1580	27	0
1	M	1623	0	1580	18	1
1	O	1623	0	1580	25	0
2	B	1541	0	1444	11	0
2	D	1537	0	1433	18	0
2	F	1537	0	1433	15	0
2	H	1537	0	1433	11	0
2	J	1537	0	1433	16	0
2	L	1540	0	1437	15	0
2	N	1537	0	1433	18	0
2	P	1539	0	1440	12	1
All	All	25293	0	24140	282	1

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 6.

All (282) 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)
2:B:192:SER:HB2	2:P:96:LEU:HD12	1.49	0.94
1:E:81:GLU:OE2	1:O:12:LYS:NZ	2.02	0.93
2:P:81:THR:HA	2:P:110:VAL:HG21	1.52	0.91
1:I:138:GLY:O	1:I:196:SER:N	2.06	0.89
2:D:96:LEU:HD12	2:F:192:SER:HB2	1.51	0.88
1:K:11:VAL:HG21	1:K:151:PRO:HG3	1.54	0.86
1:E:217:ASN:ND2	1:O:55:GLY:O	2.13	0.82
1:O:127:PRO:HD3	1:O:222:LYS:HE2	1.66	0.78
1:M:127:PRO:HD3	1:M:222:LYS:HE2	1.65	0.78
1:E:127:PRO:HD3	1:E:222:LYS:HE2	1.65	0.78
1:A:127:PRO:HD3	1:A:222:LYS:HE2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:ILE:HG21	1:G:98:TYR:CZ	2.20	0.76
1:I:127:PRO:HD3	1:I:222:LYS:HE2	1.68	0.74
1:K:127:PRO:HD3	1:K:222:LYS:HE2	1.69	0.74
2:P:40:LEU:HD23	2:P:85:ALA:HB2	1.70	0.73
1:G:127:PRO:HD3	1:G:222:LYS:HE2	1.69	0.72
2:B:40:LEU:HD23	2:B:85:ALA:HB2	1.71	0.72
2:H:40:LEU:HD23	2:H:85:ALA:HB2	1.71	0.72
1:C:127:PRO:HD3	1:C:222:LYS:HE2	1.72	0.70
2:J:40:LEU:HD23	2:J:85:ALA:HB2	1.73	0.70
2:B:149:VAL:HG12	2:B:202:HIS:HB2	1.74	0.70
2:D:40:LEU:HD23	2:D:85:ALA:HB2	1.73	0.69
2:N:40:LEU:HD23	2:N:85:ALA:HB2	1.72	0.69
2:F:40:LEU:HD23	2:F:85:ALA:HB2	1.76	0.69
2:L:40:LEU:HD23	2:L:85:ALA:HB2	1.74	0.68
1:E:12:LYS:NZ	1:O:81:GLU:OE2	2.26	0.68
2:F:149:VAL:HG12	2:F:202:HIS:HB2	1.77	0.67
1:M:123:PRO:HB3	1:M:149:TYR:HB3	1.76	0.67
2:N:149:VAL:HG12	2:N:202:HIS:HB2	1.78	0.66
1:A:123:PRO:HB3	1:A:149:TYR:HB3	1.78	0.65
1:E:40:ALA:HB3	1:E:43:GLN:HG3	1.79	0.64
1:C:123:PRO:HB3	1:C:149:TYR:HB3	1.79	0.64
1:O:40:ALA:HB3	1:O:43:GLN:HG3	1.80	0.64
1:I:140:ALA:N	1:I:194:VAL:O	2.31	0.64
1:I:123:PRO:HB3	1:I:149:TYR:HB3	1.80	0.63
1:O:123:PRO:HB3	1:O:149:TYR:HB3	1.78	0.63
1:E:54:PHE:CZ	1:G:98:TYR:HB3	2.34	0.63
2:F:84:GLU:HB2	2:F:110:VAL:HG23	1.81	0.63
1:E:123:PRO:HB3	1:E:149:TYR:HB3	1.80	0.62
1:M:40:ALA:HB3	1:M:43:GLN:HG3	1.81	0.61
2:P:149:VAL:HG12	2:P:202:HIS:HB2	1.81	0.61
2:D:149:VAL:HG12	2:D:202:HIS:HB2	1.81	0.61
2:H:149:VAL:HG12	2:H:202:HIS:HB2	1.83	0.61
1:G:40:ALA:HB3	1:G:43:GLN:HG3	1.83	0.61
2:L:84:GLU:HB2	2:L:110:VAL:HG23	1.83	0.60
1:C:40:ALA:HB3	1:C:43:GLN:HG3	1.83	0.60
1:E:54:PHE:CE2	1:G:98:TYR:HB3	2.36	0.60
2:J:149:VAL:HG12	2:J:202:HIS:HB2	1.84	0.60
1:C:140:ALA:HB2	1:C:199:LEU:HD11	1.85	0.58
1:G:123:PRO:HB3	1:G:149:TYR:HB3	1.84	0.58
2:F:118:PRO:HB3	2:F:144:PHE:HB3	1.86	0.58
2:L:149:VAL:HG12	2:L:202:HIS:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ALA:HB3	1:A:43:GLN:HG3	1.85	0.57
2:N:79:LEU:HD11	2:N:110:VAL:HG13	1.86	0.57
1:E:133:LYS:HE2	2:F:210:THR:O	2.04	0.57
2:H:189:GLN:O	2:H:192:SER:HB3	2.05	0.56
1:I:40:ALA:HB3	1:I:43:GLN:HG3	1.87	0.56
1:K:123:PRO:HB3	1:K:149:TYR:HB3	1.87	0.56
1:M:140:ALA:N	1:M:194:VAL:O	2.36	0.56
1:A:36:TRP:CE2	1:A:80:MET:HB2	2.41	0.56
1:E:17:SER:HB2	1:O:17:SER:H	1.71	0.56
1:G:138:GLY:O	1:G:195:PRO:HA	2.06	0.55
1:E:52:ILE:HG21	1:G:98:TYR:OH	2.05	0.55
1:I:36:TRP:CE2	1:I:80:MET:HB2	2.41	0.55
2:J:6:GLN:HB3	2:J:106:THR:HG22	1.89	0.55
1:E:54:PHE:HE2	1:G:31:SER:O	1.90	0.55
1:G:36:TRP:CE2	1:G:80:MET:HB2	2.42	0.54
2:H:6:GLN:HB3	2:H:106:THR:HG22	1.90	0.54
1:O:36:TRP:CE2	1:O:80:MET:HB2	2.43	0.54
1:K:40:ALA:HB3	1:K:43:GLN:HG3	1.90	0.54
1:A:54:PHE:CE2	1:I:98:TYR:HB3	2.43	0.54
2:P:118:PRO:HB3	2:P:144:PHE:HB3	1.90	0.53
1:A:87:THR:HG23	1:A:114:THR:HA	1.91	0.53
2:N:6:GLN:HB3	2:N:106:THR:HG22	1.91	0.53
1:C:131:SER:O	1:C:135:THR:OG1	2.24	0.53
1:I:87:THR:HG23	1:I:114:THR:HA	1.91	0.53
1:I:94:LYS:HG2	1:I:106:VAL:HB	1.90	0.53
2:F:6:GLN:HB3	2:F:106:THR:HG22	1.91	0.52
1:O:87:THR:HG23	1:O:114:THR:HA	1.92	0.52
2:D:154:LYS:HB2	2:D:197:SER:HB2	1.92	0.52
1:C:36:TRP:CE2	1:C:80:MET:HB2	2.45	0.52
2:L:6:GLN:HB3	2:L:106:THR:HG22	1.91	0.52
2:L:154:LYS:HB2	2:L:197:SER:HB2	1.90	0.52
1:K:87:THR:HG23	1:K:114:THR:HA	1.91	0.52
2:D:31:ASN:CG	2:N:95:SER:HA	2.30	0.51
2:D:6:GLN:HB3	2:D:106:THR:HG22	1.90	0.51
2:J:79:LEU:CD1	2:J:110:VAL:HG12	2.40	0.51
2:N:81:THR:HA	2:N:110:VAL:HG21	1.91	0.51
2:L:81:THR:HA	2:L:110:VAL:HG21	1.93	0.51
1:K:168:LEU:HD13	1:K:192:VAL:HG21	1.91	0.51
2:B:118:PRO:HB3	2:B:144:PHE:HB3	1.93	0.51
1:I:134:SER:HB2	1:I:141:ALA:HB3	1.93	0.51
1:M:36:TRP:CE2	1:M:80:MET:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:PRO:HB3	2:D:144:PHE:HB3	1.91	0.51
1:E:54:PHE:CZ	1:G:98:TYR:CB	2.94	0.51
1:M:94:LYS:HG2	1:M:106:VAL:HB	1.92	0.50
2:P:6:GLN:HB3	2:P:106:THR:HG22	1.93	0.50
2:H:20:ILE:HG23	2:H:106:THR:HG21	1.94	0.50
2:H:118:PRO:HB3	2:H:144:PHE:HB3	1.93	0.50
1:K:54:PHE:HE1	1:O:54:PHE:CE1	2.30	0.50
1:K:54:PHE:CE1	1:O:54:PHE:HE1	2.30	0.49
2:B:20:ILE:HG23	2:B:106:THR:HG21	1.94	0.49
2:P:20:ILE:HG23	2:P:106:THR:HG21	1.93	0.49
1:E:36:TRP:CE2	1:E:80:MET:HB2	2.47	0.49
2:F:81:THR:HA	2:F:110:VAL:HG21	1.94	0.49
1:G:94:LYS:HG2	1:G:106:VAL:HB	1.93	0.49
1:I:168:LEU:HD13	1:I:192:VAL:HG21	1.95	0.49
1:A:11:VAL:HG21	1:A:151:PRO:HG3	1.93	0.49
1:I:130:PRO:HG3	1:I:142:LEU:HB3	1.95	0.49
1:M:130:PRO:HG3	1:M:142:LEU:HB3	1.95	0.49
1:M:47:TRP:CG	2:N:100:VAL:HB	2.48	0.48
2:P:154:LYS:HB2	2:P:197:SER:HB2	1.94	0.48
1:G:168:LEU:HD13	1:G:192:VAL:HG21	1.95	0.48
1:M:87:THR:HG23	1:M:114:THR:HA	1.96	0.48
1:E:54:PHE:CE2	1:G:31:SER:O	2.66	0.48
1:C:94:LYS:HG2	1:C:106:VAL:HB	1.96	0.48
1:O:94:LYS:HG2	1:O:106:VAL:HB	1.94	0.48
1:A:94:LYS:HG2	1:A:106:VAL:HB	1.95	0.47
2:B:6:GLN:HB3	2:B:106:THR:HG22	1.95	0.47
1:G:47:TRP:CG	2:H:100:VAL:HB	2.48	0.47
1:E:94:LYS:HG2	1:E:106:VAL:HB	1.95	0.47
2:J:20:ILE:HG23	2:J:106:THR:HG21	1.96	0.47
2:N:6:GLN:NE2	2:N:106:THR:HG23	2.29	0.47
1:I:130:PRO:O	1:I:134:SER:OG	2.31	0.47
1:C:130:PRO:HG3	1:C:142:LEU:HB3	1.96	0.47
2:B:189:GLN:O	2:B:192:SER:HB3	2.15	0.47
2:L:111:LEU:O	2:L:113:GLN:N	2.46	0.47
2:H:154:LYS:HB2	2:H:197:SER:HB2	1.96	0.47
2:D:96:LEU:HA	2:D:96:LEU:HD23	1.74	0.47
1:M:154:VAL:HG12	1:M:188:LEU:HD21	1.95	0.47
2:J:111:LEU:C	2:J:113:GLN:N	2.68	0.47
2:L:118:PRO:HD3	2:L:202:HIS:ND1	2.30	0.47
2:N:56:PRO:HG2	2:N:59:ILE:HG13	1.97	0.47
2:N:79:LEU:CD1	2:N:110:VAL:HG13	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:ILE:HG23	2:D:106:THR:HG21	1.97	0.46
1:G:154:VAL:HG12	1:G:188:LEU:HD21	1.95	0.46
1:C:90:TYR:CD2	1:C:113:VAL:HG13	2.50	0.46
1:G:130:PRO:HG3	1:G:142:LEU:HB3	1.97	0.46
1:E:159:TRP:CH2	1:E:209:CYS:HB3	2.51	0.46
1:K:130:PRO:HG3	1:K:142:LEU:HB3	1.98	0.46
1:E:47:TRP:CG	2:F:100:VAL:HB	2.50	0.46
2:F:156:ASP:OD1	2:F:194:ARG:HB3	2.15	0.46
2:L:20:ILE:HG23	2:L:106:THR:HG21	1.97	0.46
1:M:138:GLY:O	1:M:195:PRO:HA	2.16	0.46
2:B:96:LEU:HA	2:B:96:LEU:HD23	1.78	0.46
1:C:6:GLU:HG2	1:C:6:GLU:H	1.58	0.46
2:P:96:LEU:HA	2:P:96:LEU:HD23	1.71	0.46
1:K:47:TRP:CG	2:L:100:VAL:HB	2.51	0.46
1:K:36:TRP:CE2	1:K:80:MET:HB2	2.50	0.46
2:N:20:ILE:HG23	2:N:106:THR:HG21	1.97	0.46
2:P:56:PRO:HG2	2:P:59:ILE:HG13	1.98	0.46
1:C:133:LYS:HE3	2:D:210:THR:O	2.16	0.46
2:D:6:GLN:HE21	2:D:106:THR:HG23	1.81	0.46
1:G:216:SER:OG	1:G:218:THR:HG23	2.16	0.46
2:L:118:PRO:HB3	2:L:144:PHE:HB3	1.96	0.46
1:M:168:LEU:HD13	1:M:192:VAL:HG21	1.97	0.46
2:N:6:GLN:HE21	2:N:106:THR:HG23	1.80	0.46
2:F:20:ILE:HG23	2:F:106:THR:HG21	1.97	0.45
2:J:81:THR:HA	2:J:110:VAL:HG11	1.98	0.45
1:E:130:PRO:O	1:E:134:SER:HB3	2.16	0.45
1:E:154:VAL:HG12	1:E:188:LEU:HD21	1.98	0.45
2:F:111:LEU:HD22	2:F:112:GLY:N	2.31	0.45
1:A:36:TRP:NE1	1:A:80:MET:HB2	2.32	0.45
1:K:94:LYS:HG2	1:K:106:VAL:HB	1.98	0.45
1:E:130:PRO:HG3	1:E:142:LEU:HB3	1.98	0.45
2:F:81:THR:HA	2:F:110:VAL:HG11	1.98	0.45
1:C:155:THR:HB	1:C:212:ASN:HB3	1.99	0.45
1:K:116:SER:C	1:K:118:ALA:N	2.70	0.45
1:K:216:SER:OG	1:K:218:THR:HG23	2.17	0.45
1:O:168:LEU:HD13	1:O:192:VAL:HG21	1.98	0.45
1:K:198:SER:HB2	1:K:204:GLN:HB2	1.98	0.44
1:O:130:PRO:O	1:O:131:SER:OG	2.29	0.44
1:A:130:PRO:HG3	1:A:142:LEU:HB3	1.99	0.44
1:A:30:ARG:NH2	1:A:52(A):PRO:HA	2.31	0.44
2:L:81:THR:HA	2:L:110:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:154:LYS:HB2	2:N:197:SER:HB2	1.98	0.44
1:I:216:SER:OG	1:I:218:THR:HG23	2.18	0.44
1:K:54:PHE:CE1	1:O:54:PHE:CE1	3.05	0.44
1:O:27:GLY:HA3	1:O:28:PRO:HA	1.85	0.44
1:E:130:PRO:O	1:E:131:SER:OG	2.31	0.44
1:G:159:TRP:CH2	1:G:209:CYS:HB3	2.53	0.44
1:E:155:THR:HB	1:E:212:ASN:HB3	2.00	0.44
1:G:116:SER:C	1:G:118:ALA:N	2.70	0.44
2:J:118:PRO:HB3	2:J:144:PHE:HB3	1.99	0.44
2:J:154:LYS:HB2	2:J:197:SER:HB2	1.98	0.44
2:J:189:GLN:O	2:J:192:SER:HB3	2.18	0.44
1:G:27:GLY:HA3	1:G:28:PRO:HA	1.86	0.44
1:I:138:GLY:O	1:I:195:PRO:HA	2.18	0.44
2:N:118:PRO:HB3	2:N:144:PHE:HB3	1.99	0.44
2:D:6:GLN:NE2	2:D:106:THR:HG23	2.33	0.44
1:G:87:THR:HG23	1:G:114:THR:HA	2.00	0.44
1:E:27:GLY:HA3	1:E:28:PRO:HA	1.89	0.43
1:O:130:PRO:HG3	1:O:142:LEU:HB3	2.00	0.43
2:B:154:LYS:HB2	2:B:197:SER:HB2	2.00	0.43
1:C:47:TRP:CG	2:D:100:VAL:HB	2.53	0.43
1:A:52:ILE:HG21	1:I:98:TYR:OH	2.18	0.43
2:D:79:LEU:HD11	2:D:110:VAL:HG12	2.00	0.43
1:E:90:TYR:CD2	1:E:113:VAL:HG13	2.52	0.43
1:G:36:TRP:NE1	1:G:80:MET:HB2	2.32	0.43
1:K:155:THR:HB	1:K:212:ASN:HB3	2.00	0.43
1:K:27:GLY:HA3	1:K:28:PRO:HA	1.84	0.43
1:M:129:ALA:HA	1:M:130:PRO:HD3	1.92	0.43
1:M:216:SER:OG	1:M:218:THR:HG23	2.18	0.43
1:E:216:SER:OG	1:E:218:THR:HG23	2.19	0.43
2:D:56:PRO:HG2	2:D:59:ILE:HG13	2.01	0.43
1:G:6:GLU:H	1:G:6:GLU:HG2	1.66	0.43
1:C:168:LEU:HD13	1:C:192:VAL:HG21	2.01	0.43
1:I:47:TRP:CG	2:J:100:VAL:HB	2.54	0.43
1:I:116:SER:C	1:I:118:ALA:N	2.70	0.43
1:I:6:GLU:H	1:I:6:GLU:HG2	1.63	0.43
2:J:6:GLN:NE2	2:J:106:THR:HG23	2.34	0.43
1:M:27:GLY:HA3	1:M:28:PRO:HA	1.87	0.43
1:A:155:THR:HB	1:A:212:ASN:HB3	2.01	0.42
1:C:216:SER:OG	1:C:218:THR:HG23	2.19	0.42
1:G:130:PRO:HB2	1:G:131:SER:H	1.64	0.42
1:O:198:SER:HB2	1:O:204:GLN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLY:HA3	1:A:28:PRO:HA	1.87	0.42
2:J:61:ASP:OD1	2:J:61:ASP:N	2.48	0.42
1:I:36:TRP:NE1	1:I:80:MET:HB2	2.34	0.42
1:K:90:TYR:CD2	1:K:113:VAL:HG13	2.54	0.42
2:N:96:LEU:HD23	2:N:96:LEU:HA	1.74	0.42
1:O:6:GLU:H	1:O:6:GLU:HG2	1.52	0.42
1:A:181:GLN:HE21	1:A:181:GLN:HB2	1.70	0.42
1:G:181:GLN:HE21	1:G:181:GLN:HB2	1.63	0.42
2:J:39:GLN:O	2:J:85:ALA:HB1	2.19	0.42
2:J:96:LEU:HD23	2:J:96:LEU:HA	1.80	0.42
1:K:181:GLN:HE21	1:K:181:GLN:HB2	1.60	0.42
2:L:61:ASP:OD1	2:L:61:ASP:N	2.46	0.42
1:O:155:THR:HB	1:O:212:ASN:HB3	2.00	0.42
2:B:156:ASP:OD1	2:B:194:ARG:HB3	2.20	0.42
1:C:87:THR:HG23	1:C:114:THR:HA	2.02	0.42
2:F:36:TRP:CZ3	2:F:89:CYS:HB3	2.54	0.42
1:K:154:VAL:HG12	1:K:188:LEU:HD21	2.00	0.42
2:D:36:TRP:CZ3	2:D:89:CYS:HB3	2.55	0.42
1:E:159:TRP:CZ3	1:E:209:CYS:HB3	2.55	0.42
2:D:111:LEU:HA	2:D:111:LEU:HD23	1.86	0.42
1:E:17:SER:HB2	1:O:16:SER:HB2	2.01	0.42
1:E:52:ILE:CG2	1:E:52(A):PRO:HD2	2.49	0.42
1:K:129:ALA:HA	1:K:130:PRO:HD3	1.94	0.42
2:F:96:LEU:HA	2:F:96:LEU:HD23	1.85	0.41
1:E:30:ARG:NH2	1:E:52(A):PRO:HA	2.35	0.41
1:G:129:ALA:HA	1:G:130:PRO:HD3	1.95	0.41
1:A:168:LEU:HD13	1:A:192:VAL:HG21	2.02	0.41
1:I:181:GLN:HE21	1:I:181:GLN:HB2	1.61	0.41
1:K:6:GLU:HG2	1:K:6:GLU:H	1.59	0.41
2:L:96:LEU:HA	2:L:96:LEU:HD23	1.77	0.41
1:O:154:VAL:HG12	1:O:188:LEU:HD21	2.03	0.41
1:G:191:VAL:HG21	2:H:140:LEU:HD13	2.01	0.41
1:K:121:LYS:HG2	1:K:122:GLY:O	2.21	0.41
2:N:156:ASP:OD1	2:N:194:ARG:HB3	2.20	0.41
1:O:216:SER:OG	1:O:218:THR:HG23	2.20	0.41
1:C:63:PHE:O	1:C:67:VAL:HG12	2.21	0.41
2:N:125:PRO:HD3	2:N:137:LEU:HD12	2.02	0.41
1:O:159:TRP:CH2	1:O:209:CYS:HB3	2.56	0.41
1:O:63:PHE:O	1:O:67:VAL:HG12	2.20	0.41
1:E:168:LEU:HD13	1:E:192:VAL:HG21	2.02	0.41
1:K:29:PHE:HD1	1:K:73:ASP:HB3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:GLY:HA3	1:C:28:PRO:HA	1.85	0.41
1:I:154:VAL:HG12	1:I:188:LEU:HD21	2.01	0.41
2:P:118:PRO:HD3	2:P:202:HIS:ND1	2.36	0.41
1:A:29:PHE:HD1	1:A:73:ASP:HB3	1.86	0.41
1:C:154:VAL:HG12	1:C:188:LEU:HD21	2.03	0.41
2:H:118:PRO:HD3	2:H:202:HIS:ND1	2.36	0.41
1:M:6:GLU:HG2	1:M:6:GLU:H	1.62	0.41
1:A:20:VAL:HG12	1:A:36:TRP:CH2	2.57	0.40
1:C:159:TRP:CH2	1:C:209:CYS:HB3	2.56	0.40
1:C:36:TRP:NE1	1:C:80:MET:HB2	2.36	0.40
1:E:6:GLU:HG2	1:E:6:GLU:H	1.55	0.40
1:M:18:VAL:HG12	1:M:82(C):LEU:HD11	2.02	0.40
1:A:90:TYR:CD2	1:A:113:VAL:HG13	2.57	0.40
1:A:47:TRP:CG	2:B:100:VAL:HB	2.57	0.40
1:C:29:PHE:HD1	1:C:73:ASP:HB3	1.86	0.40
2:H:96:LEU:HD23	2:H:96:LEU:HA	1.82	0.40
2:N:61:ASP:OD1	2:N:61:ASP:N	2.48	0.40
1:A:6:GLU:HG2	1:A:6:GLU:H	1.53	0.40
1:C:198:SER:HB2	1:C:204:GLN:HB2	2.03	0.40
1:I:191:VAL:HG21	2:J:140:LEU:HD13	2.02	0.40
1:K:36:TRP:NE1	1:K:80:MET:HB2	2.36	0.40
1:K:191:VAL:HG21	2:L:140:LEU:HD13	2.03	0.40
1:M:29:PHE:HD1	1:M:73:ASP:HB3	1.86	0.40
2:D:91:THR:OG1	2:D:92:TRP:N	2.54	0.40
2:P:156:ASP:OD1	2:P:194:ARG:HB3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:61:PRO:O	2:P:16:GLN:NE2[2_555]	2.08	0.12

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	219/242 (90%)	211 (96%)	6 (3%)	2 (1%)	17	43
1	C	219/242 (90%)	210 (96%)	6 (3%)	3 (1%)	11	31
1	E	219/242 (90%)	207 (94%)	9 (4%)	3 (1%)	11	31
1	G	219/242 (90%)	207 (94%)	10 (5%)	2 (1%)	17	43
1	I	219/242 (90%)	209 (95%)	7 (3%)	3 (1%)	11	31
1	K	219/242 (90%)	209 (95%)	7 (3%)	3 (1%)	11	31
1	M	219/242 (90%)	209 (95%)	8 (4%)	2 (1%)	17	43
1	O	219/242 (90%)	208 (95%)	7 (3%)	4 (2%)	8	25
2	B	211/217 (97%)	200 (95%)	7 (3%)	4 (2%)	8	24
2	D	211/217 (97%)	202 (96%)	6 (3%)	3 (1%)	11	31
2	F	211/217 (97%)	201 (95%)	7 (3%)	3 (1%)	11	31
2	H	211/217 (97%)	199 (94%)	8 (4%)	4 (2%)	8	24
2	J	211/217 (97%)	200 (95%)	7 (3%)	4 (2%)	8	24
2	L	211/217 (97%)	199 (94%)	7 (3%)	5 (2%)	6	19
2	N	211/217 (97%)	199 (94%)	8 (4%)	4 (2%)	8	24
2	P	211/217 (97%)	202 (96%)	6 (3%)	3 (1%)	11	31
All	All	3440/3672 (94%)	3272 (95%)	116 (3%)	52 (2%)	10	30

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	130	PRO
2	J	111	LEU
2	L	111	LEU
2	N	111	LEU
2	B	214	THR
1	C	137	GLY
2	D	214	THR
1	E	137	GLY
2	F	214	THR
1	G	53	ILE
2	H	111	LEU
2	H	214	THR
1	I	130	PRO
2	J	214	THR

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Mol	Chain	Res	Type
1	K	130	PRO
2	L	214	THR
2	N	214	THR
1	O	131	SER
2	P	214	THR
1	A	53	ILE
2	B	112	GLY
2	B	156	ASP
2	B	213	PRO
1	C	130	PRO
2	D	213	PRO
1	E	53	ILE
2	F	156	ASP
2	F	213	PRO
2	H	213	PRO
1	I	53	ILE
2	J	156	ASP
2	J	213	PRO
1	K	53	ILE
2	L	112	GLY
2	L	156	ASP
2	L	213	PRO
1	M	53	ILE
2	N	156	ASP
2	N	213	PRO
1	O	53	ILE
1	O	130	PRO
2	P	213	PRO
1	C	53	ILE
2	D	156	ASP
2	H	156	ASP
1	M	130	PRO
2	P	156	ASP
1	A	130	PRO
1	I	199	LEU
1	O	137	GLY
1	E	130	PRO
1	K	137	GLY

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	178/202 (88%)	166 (93%)	12 (7%)	16	39
1	C	178/202 (88%)	167 (94%)	11 (6%)	18	43
1	E	179/202 (89%)	168 (94%)	11 (6%)	18	43
1	G	178/202 (88%)	168 (94%)	10 (6%)	21	47
1	I	179/202 (89%)	169 (94%)	10 (6%)	21	47
1	K	178/202 (88%)	168 (94%)	10 (6%)	21	47
1	M	178/202 (88%)	168 (94%)	10 (6%)	21	47
1	O	178/202 (88%)	168 (94%)	10 (6%)	21	47
2	B	164/182 (90%)	156 (95%)	8 (5%)	25	54
2	D	163/182 (90%)	156 (96%)	7 (4%)	29	59
2	F	163/182 (90%)	156 (96%)	7 (4%)	29	59
2	H	163/182 (90%)	154 (94%)	9 (6%)	21	49
2	J	163/182 (90%)	156 (96%)	7 (4%)	29	59
2	L	164/182 (90%)	156 (95%)	8 (5%)	25	54
2	N	163/182 (90%)	155 (95%)	8 (5%)	25	54
2	P	164/182 (90%)	157 (96%)	7 (4%)	29	59
All	All	2733/3072 (89%)	2588 (95%)	145 (5%)	22	50

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	6	GLU
1	A	83	ARG
1	A	84	SER
1	A	113	VAL
1	A	117	SER
1	A	120	THR
1	A	133	LYS

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Mol	Chain	Res	Type
1	A	134	SER
1	A	154	VAL
1	A	174	HIS
1	A	206	THR
2	B	4	LEU
2	B	70	THR
2	B	106	THR
2	B	111	LEU
2	B	119	THR
2	B	142	SER
2	B	173	SER
2	B	180	SER
1	C	3	GLN
1	C	6	GLU
1	C	83	ARG
1	C	84	SER
1	C	113	VAL
1	C	117	SER
1	C	120	THR
1	C	154	VAL
1	C	174	HIS
1	C	206	THR
1	C	218	THR
2	D	4	LEU
2	D	70	THR
2	D	106	THR
2	D	119	THR
2	D	142	SER
2	D	173	SER
2	D	180	SER
1	E	3	GLN
1	E	6	GLU
1	E	83	ARG
1	E	84	SER
1	E	113	VAL
1	E	117	SER
1	E	120	THR
1	E	134	SER
1	E	154	VAL
1	E	174	HIS
1	E	206	THR
2	F	4	LEU

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Mol	Chain	Res	Type
2	F	70	THR
2	F	106	THR
2	F	119	THR
2	F	142	SER
2	F	173	SER
2	F	180	SER
1	G	3	GLN
1	G	6	GLU
1	G	83	ARG
1	G	84	SER
1	G	113	VAL
1	G	117	SER
1	G	120	THR
1	G	154	VAL
1	G	174	HIS
1	G	206	THR
2	H	4	LEU
2	H	70	THR
2	H	106	THR
2	H	110	VAL
2	H	111	LEU
2	H	119	THR
2	H	142	SER
2	H	173	SER
2	H	180	SER
1	I	3	GLN
1	I	6	GLU
1	I	83	ARG
1	I	84	SER
1	I	117	SER
1	I	120	THR
1	I	154	VAL
1	I	174	HIS
1	I	188	LEU
1	I	206	THR
2	J	4	LEU
2	J	70	THR
2	J	106	THR
2	J	119	THR
2	J	142	SER
2	J	173	SER
2	J	180	SER

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Mol	Chain	Res	Type
1	K	3	GLN
1	K	6	GLU
1	K	83	ARG
1	K	84	SER
1	K	113	VAL
1	K	117	SER
1	K	120	THR
1	K	154	VAL
1	K	174	HIS
1	K	206	THR
2	L	4	LEU
2	L	70	THR
2	L	106	THR
2	L	111	LEU
2	L	119	THR
2	L	142	SER
2	L	173	SER
2	L	180	SER
1	M	3	GLN
1	M	6	GLU
1	M	83	ARG
1	M	84	SER
1	M	113	VAL
1	M	117	SER
1	M	120	THR
1	M	154	VAL
1	M	174	HIS
1	M	206	THR
2	N	4	LEU
2	N	70	THR
2	N	106	THR
2	N	110	VAL
2	N	119	THR
2	N	142	SER
2	N	173	SER
2	N	180	SER
1	O	3	GLN
1	O	6	GLU
1	O	83	ARG
1	O	84	SER
1	O	113	VAL
1	O	117	SER

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Mol	Chain	Res	Type
1	O	120	THR
1	O	154	VAL
1	O	174	HIS
1	O	206	THR
2	P	4	LEU
2	P	70	THR
2	P	106	THR
2	P	119	THR
2	P	142	SER
2	P	173	SER
2	P	180	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	217	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 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	221/242 (91%)	-0.35	2 (0%)	84	84	35, 65, 111, 200	0
1	C	221/242 (91%)	-0.32	8 (3%)	42	37	32, 60, 132, 231	0
1	E	221/242 (91%)	-0.19	6 (2%)	54	50	24, 57, 123, 199	0
1	G	221/242 (91%)	-0.06	8 (3%)	42	37	52, 75, 130, 200	0
1	I	221/242 (91%)	-0.20	8 (3%)	42	37	38, 72, 122, 200	0
1	K	221/242 (91%)	-0.19	5 (2%)	60	57	31, 64, 111, 198	0
1	M	221/242 (91%)	0.08	8 (3%)	42	37	48, 76, 133, 200	0
1	O	221/242 (91%)	-0.25	4 (1%)	68	66	28, 68, 146, 199	0
2	B	213/217 (98%)	-0.25	4 (1%)	66	64	38, 75, 107, 163	0
2	D	213/217 (98%)	-0.34	3 (1%)	75	74	30, 64, 104, 165	0
2	F	213/217 (98%)	-0.39	1 (0%)	91	90	31, 65, 105, 162	0
2	H	213/217 (98%)	0.24	9 (4%)	36	31	55, 92, 141, 207	0
2	J	213/217 (98%)	-0.33	2 (0%)	84	84	42, 76, 114, 161	0
2	L	213/217 (98%)	-0.28	1 (0%)	91	90	34, 71, 118, 163	0
2	N	213/217 (98%)	-0.32	2 (0%)	84	84	40, 77, 113, 183	0
2	P	213/217 (98%)	-0.25	6 (2%)	53	48	32, 73, 114, 164	0
All	All	3472/3672 (94%)	-0.21	77 (2%)	62	59	24, 72, 123, 231	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	28	PRO	11.5
1	M	29	PHE	8.1
2	J	173	SER	7.2
1	I	26	GLY	6.8
2	D	215	GLU	6.5

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Mol	Chain	Res	Type	RSRZ
1	I	27	GLY	6.3
1	C	136	SER	5.9
1	C	134	SER	5.9
1	M	1	GLN	5.8
1	I	28	PRO	5.1
1	O	29	PHE	4.9
1	E	29	PHE	4.9
2	B	215	GLU	4.8
1	I	1	GLN	4.3
1	K	182	SER	4.0
1	M	182	SER	4.0
1	E	28	PRO	3.9
1	K	180	LEU	3.6
2	F	215	GLU	3.6
1	K	27	GLY	3.5
2	P	215	GLU	3.5
2	N	215	GLU	3.5
1	K	28	PRO	3.4
1	G	28	PRO	3.3
1	O	28	PRO	3.2
1	G	27	GLY	3.2
1	I	29	PHE	3.2
2	P	153	TRP	3.2
1	E	134	SER	3.1
1	A	28	PRO	3.0
1	G	26	GLY	3.0
2	H	81	THR	3.0
1	C	133	LYS	3.0
1	C	29	PHE	3.0
1	A	29	PHE	2.9
2	H	112	GLY	2.9
2	D	214	THR	2.8
2	J	215	GLU	2.8
1	E	133	LYS	2.8
2	B	194	ARG	2.7
1	G	55	GLY	2.7
1	M	112	THR	2.7
2	L	157	GLY	2.7
2	H	13	ALA	2.7
2	H	111	LEU	2.6
1	I	182	SER	2.6
1	K	1	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	27	GLY	2.6
2	P	159	PRO	2.5
1	I	177	PRO	2.4
2	D	159	PRO	2.4
1	G	31	SER	2.4
1	M	74	PHE	2.3
1	G	165	SER	2.3
1	C	199	LEU	2.3
2	N	157	GLY	2.3
1	M	153	PRO	2.3
1	C	200	GLY	2.3
2	H	30	GLY	2.3
1	E	27	GLY	2.2
1	O	194	VAL	2.2
1	O	137	GLY	2.2
2	P	3	VAL	2.2
2	H	51	ASP	2.2
2	P	194	ARG	2.2
2	P	160	VAL	2.2
1	C	137	GLY	2.1
2	B	3	VAL	2.1
2	H	14	PRO	2.1
2	H	24	GLY	2.1
1	G	30	ARG	2.1
1	G	117	SER	2.0
2	B	99	TYR	2.0
1	I	74	PHE	2.0
1	E	183	SER	2.0
2	H	77	THR	2.0
1	M	212	ASN	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.