



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:07 AM UTC

PDB ID : 6RLM / pdb_00006rlm
Title : Crystal structure of AT1412dm Fab fragment
Authors : Neviani, V.; Pearce, N.M.; Pos, W.; Schotte, R.; Spits, H.; Gros, P.
Deposited on : 2019-05-02
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

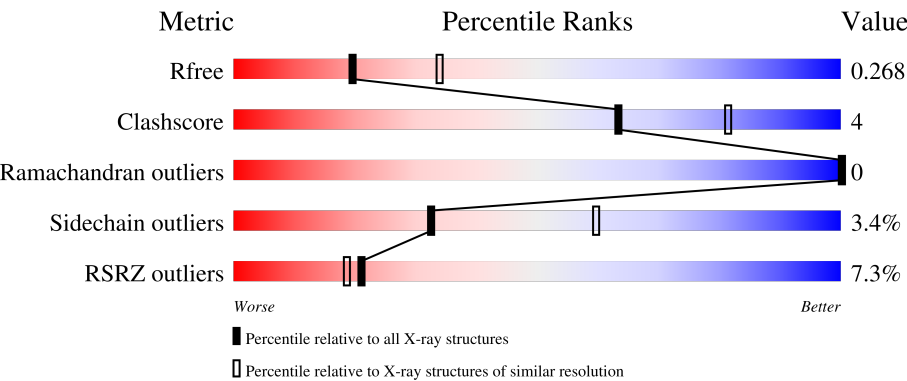
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	227	4% 85%10%5%
1	C	227	5% 86%8%6%
1	E	227	6% 87%9%. .
1	G	227	3% 86%7%6%
1	I	227	12% 89%7%. .

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Mol	Chain	Length	Quality of chain
1	K	227	
1	M	227	
1	O	227	
2	B	220	
2	D	220	
2	F	220	
2	H	220	
2	J	220	
2	L	220	
2	N	220	
2	P	220	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26544 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 AT1412dm Fab (Heavy Chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1630	1041	271	313	5			
1	C	214	Total	C	N	O	S	0	0	0
			1622	1037	269	311	5			
1	E	221	Total	C	N	O	S	0	0	0
			1664	1060	277	322	5			
1	G	213	Total	C	N	O	S	0	0	0
			1613	1031	267	310	5			
1	I	220	Total	C	N	O	S	0	0	0
			1658	1057	276	320	5			
1	K	211	Total	C	N	O	S	0	0	0
			1601	1025	265	306	5			
1	M	215	Total	C	N	O	S	0	0	0
			1626	1039	270	312	5			
1	O	206	Total	C	N	O	S	0	0	0
			1566	1004	259	298	5			

- Molecule 2 is a protein called AT1412dm Fab (Light Chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	0
			1697	1060	284	348	5			
2	D	218	Total	C	N	O	S	0	0	0
			1689	1056	283	345	5			
2	F	219	Total	C	N	O	S	0	0	0
			1697	1060	284	348	5			
2	H	218	Total	C	N	O	S	0	0	0
			1689	1056	283	345	5			
2	J	219	Total	C	N	O	S	0	0	0
			1697	1060	284	348	5			
2	L	219	Total	C	N	O	S	0	0	0
			1697	1060	284	348	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	219	Total	C	N	O	S	0	0	0
			1697	1060	284	348	5			
2	P	219	Total	C	N	O	S	0	0	0
			1697	1060	284	348	5			

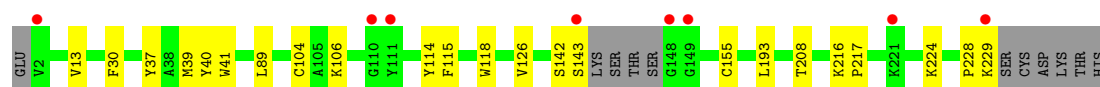
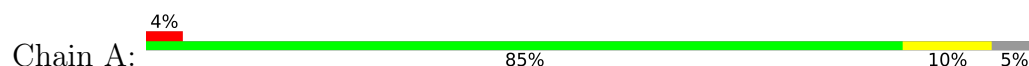
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Cl	0	0
			1	1		
3	G	1	Total	Cl	0	0
			1	1		
3	J	1	Total	Cl	0	0
			1	1		
3	K	1	Total	Cl	0	0
			1	1		

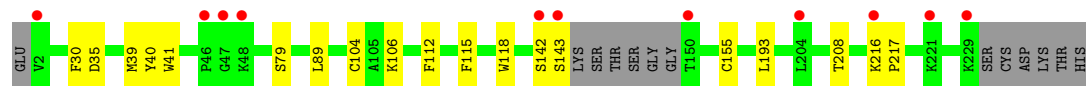
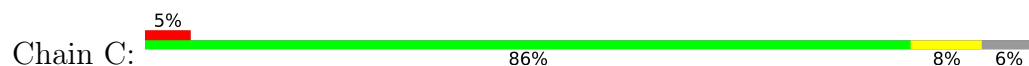
3 Residue-property plots [i](#)

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.

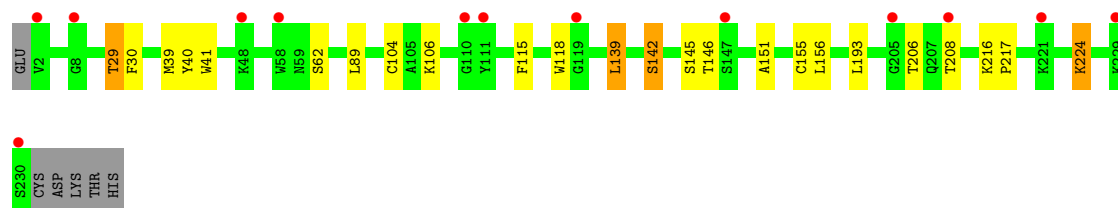
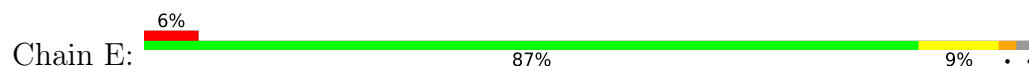
- Molecule 1: AT1412dm Fab (Heavy Chain)



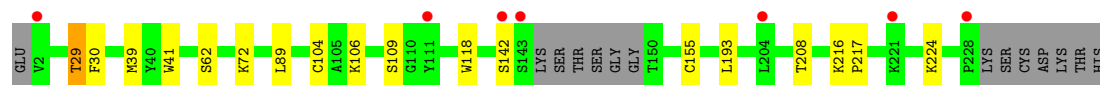
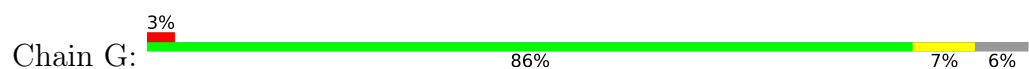
- Molecule 1: AT1412dm Fab (Heavy Chain)



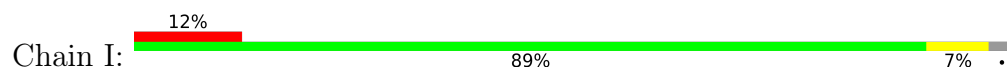
- Molecule 1: AT1412dm Fab (Heavy Chain)

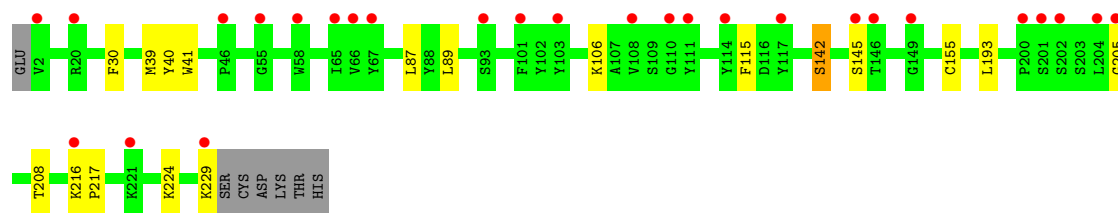


- Molecule 1: AT1412dm Fab (Heavy Chain)

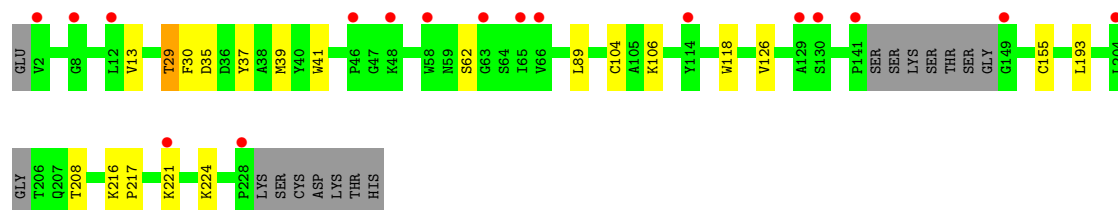
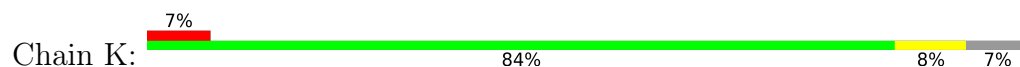


- Molecule 1: AT1412dm Fab (Heavy Chain)

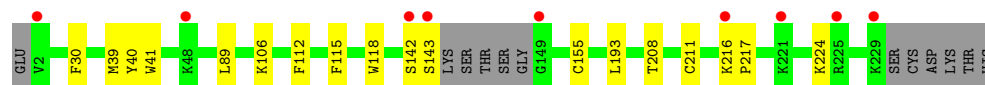
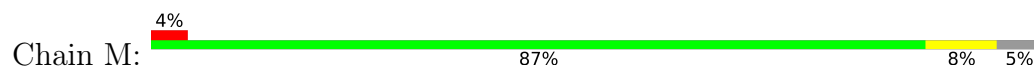




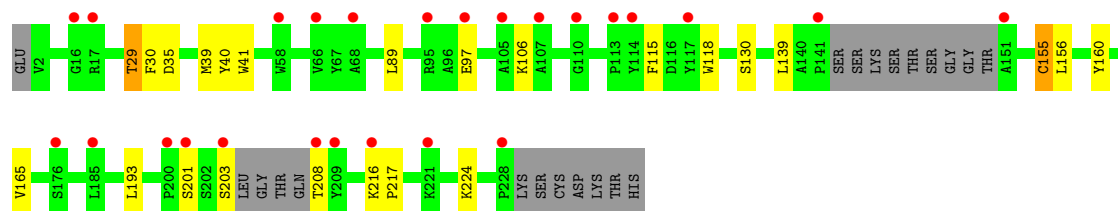
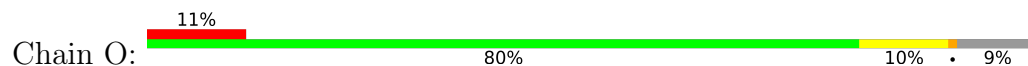
• Molecule 1: AT1412dm Fab (Heavy Chain)



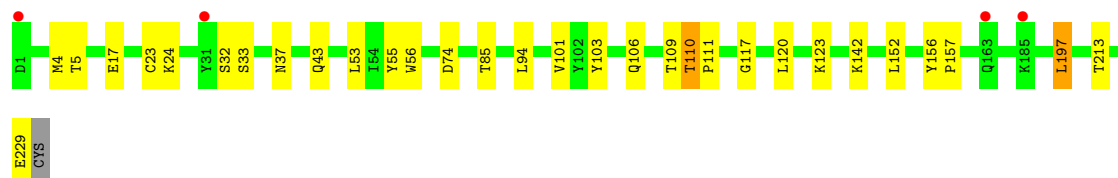
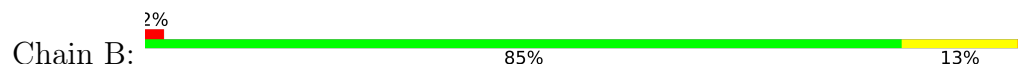
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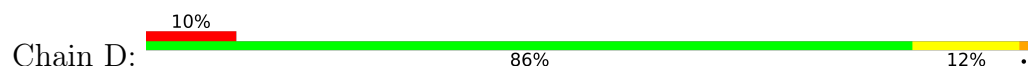
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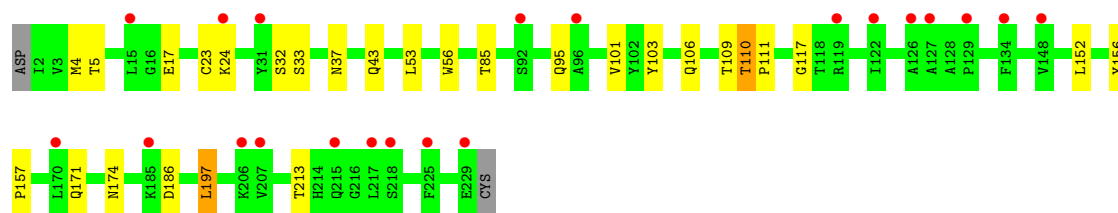


• Molecule 2: AT1412dm Fab (Light Chain)

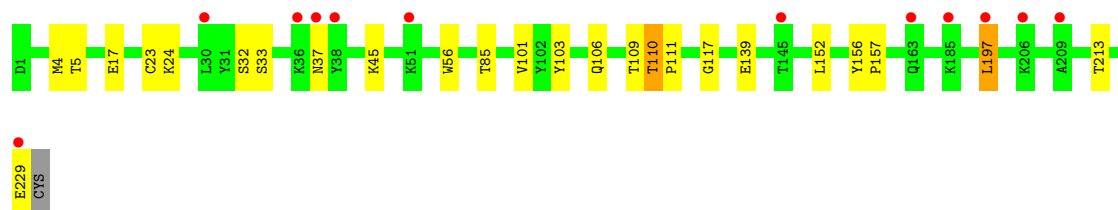
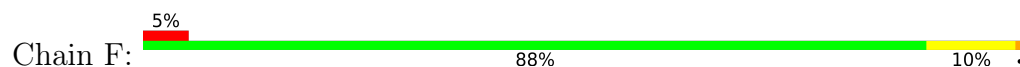


• Molecule 2: AT1412dm Fab (Light Chain)

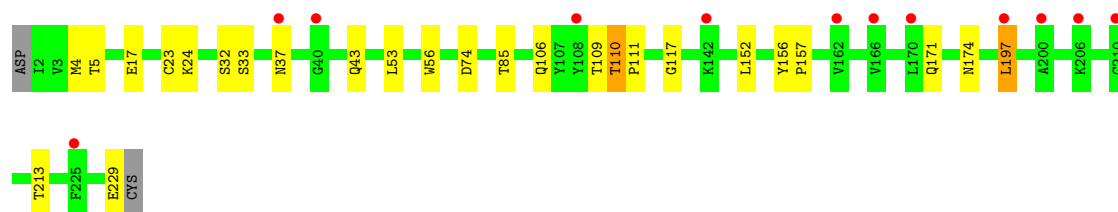
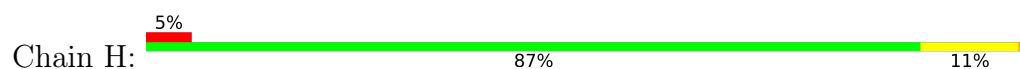




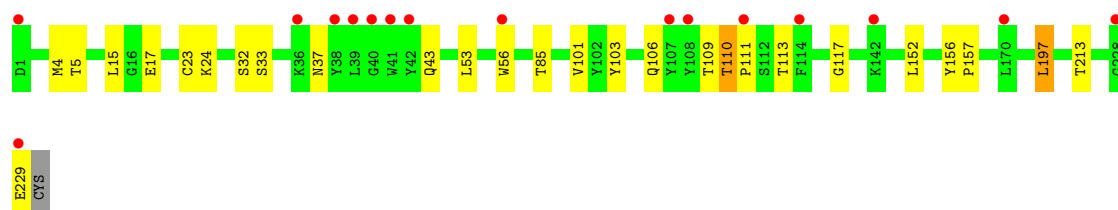
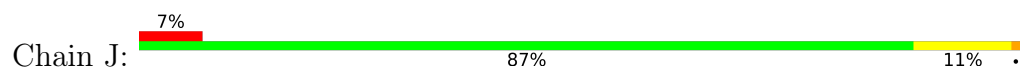
• Molecule 2: AT1412dm Fab (Light Chain)



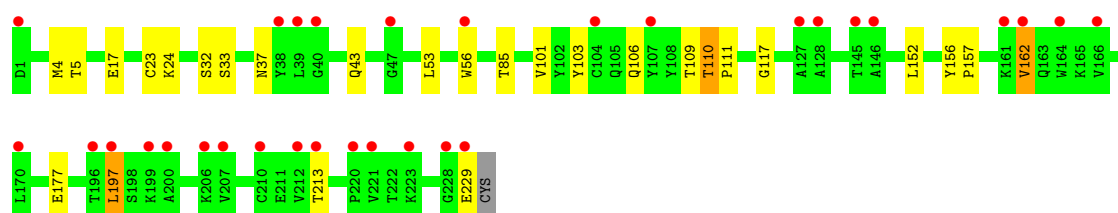
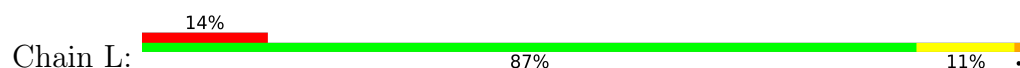
• Molecule 2: AT1412dm Fab (Light Chain)



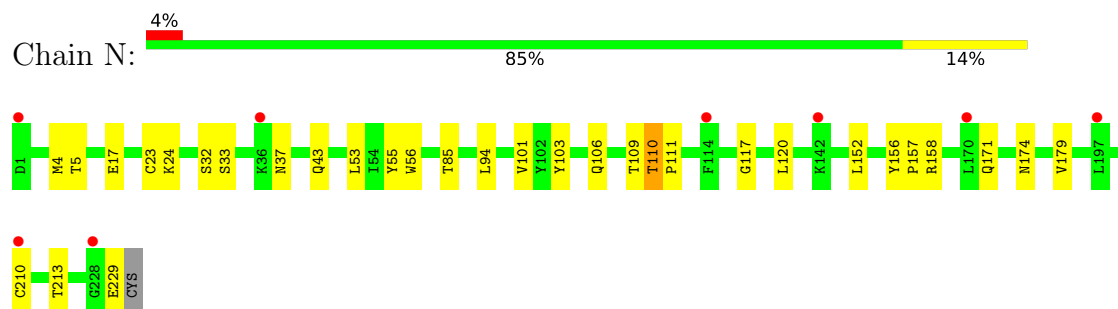
• Molecule 2: AT1412dm Fab (Light Chain)



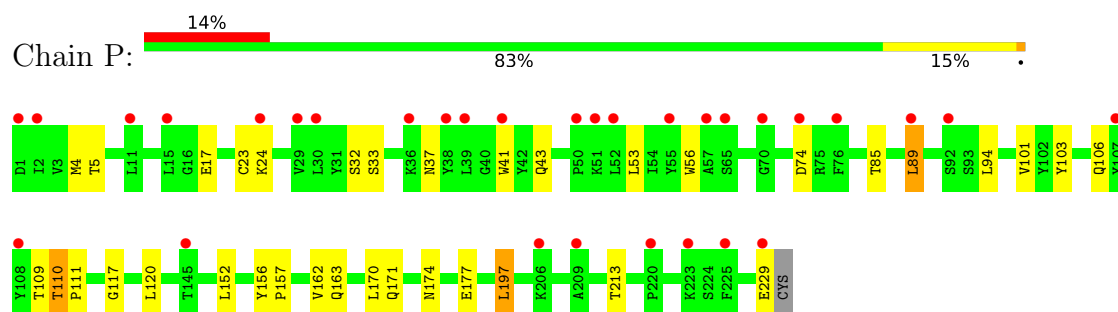
• Molecule 2: AT1412dm Fab (Light Chain)



- Molecule 2: AT1412dm Fab (Light Chain)



- Molecule 2: AT1412dm Fab (Light Chain)



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	224.91Å 238.59Å 209.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	163.66 – 2.50 163.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (163.66-2.50) 99.4 (163.66-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.52Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.242 , 0.267 0.246 , 0.268	Depositor DCC
R_{free} test set	9465 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26544	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.01	0/1673	1.30	0/2280
1	C	1.02	0/1665	1.29	1/2270 (0.0%)
1	E	1.04	0/1708	1.33	3/2328 (0.1%)
1	G	1.01	0/1656	1.32	3/2259 (0.1%)
1	I	1.03	0/1702	1.31	0/2320
1	K	0.99	0/1643	1.29	4/2240 (0.2%)
1	M	1.01	0/1669	1.30	0/2275
1	O	1.01	0/1608	1.32	4/2192 (0.2%)
2	B	1.02	0/1734	1.34	4/2356 (0.2%)
2	D	1.05	0/1726	1.32	4/2345 (0.2%)
2	F	1.06	0/1734	1.33	4/2356 (0.2%)
2	H	1.04	0/1726	1.32	4/2345 (0.2%)
2	J	1.04	0/1734	1.33	3/2356 (0.1%)
2	L	1.05	0/1734	1.31	3/2356 (0.1%)
2	N	1.05	0/1734	1.32	3/2356 (0.1%)
2	P	1.05	0/1734	1.33	4/2356 (0.2%)
All	All	1.03	0/27180	1.32	44/36990 (0.1%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	117	GLY	CA-C-O	-7.30	117.48	122.22
2	F	117	GLY	CA-C-O	-7.21	117.53	122.22
2	L	117	GLY	CA-C-O	-7.08	117.62	122.22
2	D	117	GLY	CA-C-O	-6.86	117.76	122.22
2	B	117	GLY	CA-C-O	-6.78	117.81	122.22
2	J	117	GLY	CA-C-O	-6.29	118.13	122.22
2	N	117	GLY	CA-C-O	-6.27	118.14	122.22
2	P	74	ASP	CA-CB-CG	6.26	118.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	32	SER	CA-C-N	5.98	128.62	120.54
2	H	32	SER	C-N-CA	5.98	128.62	120.54
2	N	32	SER	CA-C-N	5.94	128.56	120.54
2	N	32	SER	C-N-CA	5.94	128.56	120.54
2	J	32	SER	CA-C-N	5.88	128.48	120.54
2	J	32	SER	C-N-CA	5.88	128.48	120.54
1	G	29	THR	CB-CA-C	5.84	120.91	111.05
2	B	32	SER	CA-C-N	5.77	128.33	120.54
2	B	32	SER	C-N-CA	5.77	128.33	120.54
2	H	117	GLY	CA-C-O	-5.77	118.47	122.22
2	F	32	SER	CA-C-N	5.72	128.26	120.54
2	F	32	SER	C-N-CA	5.72	128.26	120.54
2	P	32	SER	CA-C-N	5.72	128.26	120.54
2	P	32	SER	C-N-CA	5.72	128.26	120.54
1	O	29	THR	CB-CA-C	5.62	120.56	111.05
2	L	32	SER	CA-C-N	5.54	128.02	120.54
2	L	32	SER	C-N-CA	5.54	128.02	120.54
1	C	35	ASP	CA-CB-CG	5.48	118.08	112.60
1	K	35	ASP	CA-CB-CG	5.48	118.08	112.60
2	D	32	SER	CA-C-N	5.44	127.88	120.54
2	D	32	SER	C-N-CA	5.44	127.88	120.54
1	E	29	THR	CB-CA-C	5.35	120.09	111.05
2	F	45	LYS	CB-CA-C	5.32	117.08	109.11
2	H	74	ASP	CA-CB-CG	5.28	117.88	112.60
1	O	201	SER	CA-C-N	5.26	128.06	120.38
1	O	201	SER	C-N-CA	5.26	128.06	120.38
1	O	35	ASP	CA-CB-CG	5.23	117.83	112.60
1	K	29	THR	CB-CA-C	5.20	119.84	111.05
1	K	62	SER	CA-C-N	5.13	125.53	119.94
1	K	62	SER	C-N-CA	5.13	125.53	119.94
1	G	62	SER	CA-C-N	5.12	125.52	119.94
1	G	62	SER	C-N-CA	5.12	125.52	119.94
2	B	74	ASP	CA-CB-CG	5.08	117.68	112.60
2	D	186	ASP	CA-CB-CG	5.04	117.64	112.60
1	E	62	SER	CA-C-N	5.02	125.41	119.94
1	E	62	SER	C-N-CA	5.02	125.41	119.94

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	1630	0	1585	14	0
1	C	1622	0	1579	11	0
1	E	1664	0	1621	13	0
1	G	1613	0	1566	8	0
1	I	1658	0	1616	11	0
1	K	1601	0	1555	9	0
1	M	1626	0	1582	8	0
1	O	1566	0	1519	12	0
2	B	1697	0	1637	16	0
2	D	1689	0	1630	15	0
2	F	1697	0	1637	13	0
2	H	1689	0	1630	14	0
2	J	1697	0	1637	14	0
2	L	1697	0	1637	14	0
2	N	1697	0	1637	18	0
2	P	1697	0	1637	25	0
3	C	1	0	0	0	0
3	G	1	0	0	0	0
3	J	1	0	0	1	0
3	K	1	0	0	0	0
All	All	26544	0	25705	207	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 4.

All (207) 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:P:41:TRP:CG	2:P:89:LEU:HD23	1.61	1.36
2:P:41:TRP:CD2	2:P:89:LEU:HD23	2.02	0.95
2:P:41:TRP:CG	2:P:89:LEU:CD2	2.50	0.94
2:P:41:TRP:CD1	2:P:89:LEU:HD23	2.09	0.88
2:P:162:VAL:HG22	2:P:177:GLU:OE2	1.80	0.81
1:E:139:LEU:HD11	1:E:156:LEU:HB2	1.68	0.75
2:P:162:VAL:CG2	2:P:177:GLU:OE2	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:GLN:HE22	2:D:109:THR:CG2	2.09	0.66
2:H:106:GLN:HE22	2:H:109:THR:CG2	2.08	0.66
2:B:106:GLN:HE22	2:B:109:THR:CG2	2.08	0.66
1:I:142:SER:H	1:I:145:SER:HB3	1.60	0.66
2:P:106:GLN:HE22	2:P:109:THR:CG2	2.10	0.65
2:N:106:GLN:HE22	2:N:109:THR:CG2	2.09	0.65
2:L:106:GLN:HE22	2:L:109:THR:CG2	2.10	0.65
2:F:106:GLN:HE22	2:F:109:THR:CG2	2.09	0.64
2:J:106:GLN:HE22	2:J:109:THR:CG2	2.09	0.64
1:E:206:THR:HG22	1:G:109:SER:HB3	1.80	0.64
2:P:41:TRP:CD1	2:P:89:LEU:CD2	2.79	0.63
2:P:163:GLN:OE1	2:P:170:LEU:HD12	1.98	0.63
2:L:4:MET:HE3	2:L:23:CYS:SG	2.40	0.62
2:L:110:THR:HA	2:L:111:PRO:C	2.25	0.61
2:F:110:THR:HA	2:F:111:PRO:C	2.26	0.61
2:P:110:THR:HA	2:P:111:PRO:C	2.26	0.61
2:F:4:MET:HE3	2:F:23:CYS:SG	2.41	0.60
1:E:30:PHE:CZ	1:E:39:MET:HE3	2.37	0.60
2:B:110:THR:HA	2:B:111:PRO:C	2.26	0.60
1:E:146:THR:HG22	1:E:151:ALA:HB2	1.83	0.60
2:J:110:THR:HA	2:J:111:PRO:C	2.26	0.60
2:P:41:TRP:CB	2:P:89:LEU:HD23	2.29	0.60
2:H:110:THR:HA	2:H:111:PRO:C	2.27	0.60
2:H:4:MET:HE3	2:H:23:CYS:SG	2.42	0.60
1:I:30:PHE:CZ	1:I:39:MET:HE3	2.36	0.59
2:D:197:LEU:N	2:D:197:LEU:HD23	2.18	0.59
2:N:4:MET:HE3	2:N:23:CYS:SG	2.43	0.59
1:K:30:PHE:CZ	1:K:39:MET:HE3	2.38	0.59
1:O:30:PHE:CZ	1:O:39:MET:HE3	2.37	0.59
1:G:30:PHE:CZ	1:G:39:MET:HE3	2.37	0.59
2:N:110:THR:HA	2:N:111:PRO:C	2.26	0.59
2:D:110:THR:HA	2:D:111:PRO:C	2.27	0.58
1:M:30:PHE:CZ	1:M:39:MET:HE3	2.38	0.58
2:J:4:MET:HE3	2:J:23:CYS:SG	2.43	0.58
1:C:79:SER:HB3	1:I:205:GLY:HA3	1.85	0.58
1:C:30:PHE:CZ	1:C:39:MET:HE3	2.38	0.58
2:B:106:GLN:HE22	2:B:109:THR:HG22	1.69	0.57
2:F:197:LEU:HD23	2:F:197:LEU:N	2.19	0.57
2:B:4:MET:HE3	2:B:23:CYS:SG	2.43	0.57
2:J:197:LEU:N	2:J:197:LEU:HD23	2.19	0.57
2:B:197:LEU:N	2:B:197:LEU:HD23	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:4:MET:HE3	2:P:23:CYS:SG	2.44	0.57
2:D:4:MET:HE3	2:D:23:CYS:SG	2.45	0.57
1:A:30:PHE:CZ	1:A:39:MET:HE3	2.39	0.57
2:P:197:LEU:N	2:P:197:LEU:HD23	2.20	0.57
2:F:106:GLN:HE22	2:F:109:THR:HG22	1.71	0.56
2:L:197:LEU:N	2:L:197:LEU:HD23	2.21	0.56
2:D:106:GLN:HE22	2:D:109:THR:HG22	1.71	0.56
2:H:197:LEU:HD23	2:H:197:LEU:N	2.20	0.56
2:N:106:GLN:HE22	2:N:109:THR:HG22	1.71	0.55
1:E:206:THR:HG22	1:G:109:SER:CB	2.37	0.55
1:O:139:LEU:HD23	1:O:155:CYS:C	2.31	0.55
2:P:41:TRP:CB	2:P:89:LEU:CD2	2.84	0.55
2:H:106:GLN:HE22	2:H:109:THR:HG22	1.71	0.54
2:J:106:GLN:HE22	2:J:109:THR:HG22	1.72	0.54
2:L:106:GLN:HE22	2:L:109:THR:HG22	1.72	0.54
1:O:139:LEU:CD2	1:O:156:LEU:N	2.71	0.53
2:P:106:GLN:HE22	2:P:109:THR:HG22	1.73	0.53
1:O:139:LEU:HD21	1:O:156:LEU:HB2	1.90	0.52
1:E:224:LYS:HE2	2:F:139:GLU:OE1	2.10	0.52
2:N:158:ARG:HH12	2:N:179:VAL:HG21	1.76	0.51
2:H:152:LEU:HD12	2:H:152:LEU:N	2.26	0.51
2:N:152:LEU:N	2:N:152:LEU:HD12	2.26	0.51
2:P:152:LEU:HD12	2:P:152:LEU:N	2.26	0.51
2:J:152:LEU:N	2:J:152:LEU:HD12	2.26	0.50
2:B:152:LEU:N	2:B:152:LEU:HD12	2.27	0.50
1:C:40:TYR:CD2	1:C:115:PHE:CE1	3.00	0.49
1:E:40:TYR:CD2	1:E:115:PHE:CE1	3.01	0.49
2:L:152:LEU:N	2:L:152:LEU:HD12	2.27	0.49
2:F:152:LEU:HD12	2:F:152:LEU:N	2.28	0.49
2:D:152:LEU:HD12	2:D:152:LEU:N	2.28	0.49
1:O:40:TYR:CD2	1:O:115:PHE:CE1	3.00	0.49
1:M:40:TYR:CD2	1:M:115:PHE:CE1	3.01	0.49
1:A:37:TYR:CE2	1:A:106:LYS:HD3	2.47	0.49
1:K:37:TYR:CD2	1:K:106:LYS:HG2	2.48	0.48
2:P:37:ASN:O	2:P:56:TRP:HA	2.14	0.48
1:I:40:TYR:CD2	1:I:115:PHE:CE1	3.02	0.47
2:N:37:ASN:O	2:N:56:TRP:HA	2.14	0.47
1:A:40:TYR:CD2	1:A:115:PHE:CE1	3.02	0.47
2:L:37:ASN:O	2:L:56:TRP:HA	2.15	0.47
1:O:139:LEU:CD2	1:O:155:CYS:C	2.88	0.47
2:B:37:ASN:O	2:B:56:TRP:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:ASN:O	2:D:56:TRP:HA	2.15	0.47
2:D:156:TYR:CD1	2:D:157:PRO:HA	2.50	0.47
1:E:142:SER:O	1:E:146:THR:HG23	2.15	0.47
2:F:37:ASN:O	2:F:56:TRP:HA	2.15	0.47
2:J:37:ASN:O	2:J:56:TRP:HA	2.14	0.47
2:B:156:TYR:CG	2:B:157:PRO:HA	2.50	0.47
1:M:142:SER:O	1:M:143:SER:C	2.58	0.47
1:A:142:SER:O	1:A:143:SER:C	2.58	0.46
2:N:156:TYR:CD1	2:N:157:PRO:HA	2.50	0.46
2:P:24:LYS:HA	2:P:85:THR:O	2.15	0.46
2:B:156:TYR:CD1	2:B:157:PRO:HA	2.50	0.46
2:D:24:LYS:HA	2:D:85:THR:O	2.16	0.46
2:J:24:LYS:HA	2:J:85:THR:O	2.15	0.46
2:N:24:LYS:HA	2:N:85:THR:O	2.16	0.46
2:B:101:VAL:HG12	2:B:103:TYR:CE1	2.51	0.46
2:P:156:TYR:CD1	2:P:157:PRO:HA	2.50	0.46
2:H:156:TYR:CG	2:H:157:PRO:HA	2.50	0.46
2:L:156:TYR:CG	2:L:157:PRO:HA	2.50	0.46
1:A:228:PRO:O	1:A:229:LYS:HB2	2.16	0.46
2:H:37:ASN:O	2:H:56:TRP:HA	2.15	0.46
2:F:156:TYR:CD1	2:F:157:PRO:HA	2.51	0.46
2:F:156:TYR:CG	2:F:157:PRO:HA	2.51	0.46
2:J:156:TYR:CD1	2:J:157:PRO:HA	2.51	0.46
2:P:156:TYR:CG	2:P:157:PRO:HA	2.50	0.46
2:D:171:GLN:HE21	2:D:174:ASN:HD21	1.64	0.46
2:H:156:TYR:CD1	2:H:157:PRO:HA	2.50	0.46
2:H:24:LYS:HA	2:H:85:THR:O	2.16	0.45
1:E:106:LYS:HB2	1:E:118:TRP:CD1	2.52	0.45
2:N:158:ARG:NH1	2:N:179:VAL:HG21	2.31	0.45
2:L:156:TYR:CD1	2:L:157:PRO:HA	2.50	0.45
2:N:156:TYR:CG	2:N:157:PRO:HA	2.51	0.45
2:N:171:GLN:HE21	2:N:174:ASN:HD21	1.64	0.45
1:A:216:LYS:N	1:A:217:PRO:CD	2.79	0.45
1:M:41:TRP:NE1	1:M:89:LEU:HB2	2.32	0.45
1:C:142:SER:O	1:C:143:SER:C	2.59	0.45
2:F:101:VAL:HG12	2:F:103:TYR:CE1	2.52	0.45
2:H:106:GLN:HE22	2:H:109:THR:HG23	1.81	0.45
2:B:24:LYS:HA	2:B:85:THR:O	2.15	0.45
2:D:106:GLN:HE22	2:D:109:THR:HG23	1.82	0.45
1:O:139:LEU:HD21	1:O:156:LEU:N	2.32	0.45
2:J:106:GLN:HE22	2:J:109:THR:HG23	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:156:TYR:CG	2:D:157:PRO:HA	2.52	0.45
2:J:156:TYR:CG	2:J:157:PRO:HA	2.52	0.45
1:O:160:TYR:CE2	1:O:165:VAL:HG13	2.52	0.45
1:E:41:TRP:NE1	1:E:89:LEU:HB2	2.33	0.44
1:I:142:SER:N	1:I:145:SER:HB3	2.30	0.44
1:A:41:TRP:NE1	1:A:89:LEU:HB2	2.32	0.44
1:I:41:TRP:NE1	1:I:89:LEU:HB2	2.32	0.44
1:C:41:TRP:NE1	1:C:89:LEU:HB2	2.32	0.44
1:C:79:SER:CB	1:I:205:GLY:HA3	2.48	0.44
2:L:24:LYS:HA	2:L:85:THR:O	2.16	0.44
2:P:171:GLN:HE21	2:P:174:ASN:HD21	1.65	0.44
1:A:37:TYR:CD2	1:A:106:LYS:HG2	2.53	0.44
2:B:106:GLN:NE2	2:B:109:THR:HG22	2.31	0.44
2:F:24:LYS:HA	2:F:85:THR:O	2.16	0.44
1:K:106:LYS:HB2	1:K:118:TRP:CD1	2.53	0.44
1:O:41:TRP:NE1	1:O:89:LEU:HB2	2.32	0.44
2:J:43:GLN:HB2	2:J:53:LEU:HD11	2.00	0.44
1:G:41:TRP:NE1	1:G:89:LEU:HB2	2.33	0.44
1:M:216:LYS:N	1:M:217:PRO:CD	2.81	0.44
2:B:142:LYS:HE3	1:C:112:PHE:CE2	2.53	0.44
2:J:101:VAL:HG12	2:J:103:TYR:CE1	2.53	0.44
2:N:101:VAL:HG12	2:N:103:TYR:CE1	2.53	0.44
1:O:216:LYS:N	1:O:217:PRO:CD	2.81	0.44
1:K:41:TRP:NE1	1:K:89:LEU:HB2	2.33	0.43
2:D:43:GLN:HB2	2:D:53:LEU:HD11	2.00	0.43
2:P:101:VAL:HG12	2:P:103:TYR:CE1	2.53	0.43
1:C:104:CYS:HB2	1:C:118:TRP:O	2.17	0.43
1:G:216:LYS:N	1:G:217:PRO:CD	2.81	0.43
1:E:193:LEU:HD12	1:E:193:LEU:C	2.44	0.43
2:P:106:GLN:HE22	2:P:109:THR:HG23	1.81	0.43
2:H:171:GLN:HE21	2:H:174:ASN:HD21	1.65	0.43
1:I:216:LYS:N	1:I:217:PRO:CD	2.81	0.43
1:O:193:LEU:HD12	1:O:193:LEU:C	2.44	0.43
1:A:106:LYS:HB2	1:A:118:TRP:CD1	2.54	0.43
2:L:101:VAL:HG12	2:L:103:TYR:CE1	2.54	0.43
1:G:106:LYS:HB2	1:G:118:TRP:CD1	2.54	0.43
1:K:193:LEU:C	1:K:193:LEU:HD12	2.44	0.43
2:L:162:VAL:HG12	2:L:177:GLU:OE2	2.18	0.43
1:M:193:LEU:C	1:M:193:LEU:HD12	2.44	0.43
2:N:43:GLN:HB2	2:N:53:LEU:HD11	2.01	0.43
2:N:106:GLN:HE22	2:N:109:THR:HG23	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:LYS:N	1:E:217:PRO:CD	2.82	0.43
1:K:216:LYS:N	1:K:217:PRO:CD	2.81	0.43
1:A:193:LEU:C	1:A:193:LEU:HD12	2.43	0.42
1:C:216:LYS:N	1:C:217:PRO:CD	2.82	0.42
1:I:193:LEU:C	1:I:193:LEU:HD12	2.44	0.42
1:K:104:CYS:HB2	1:K:118:TRP:O	2.19	0.42
2:N:106:GLN:NE2	2:N:109:THR:HG22	2.33	0.42
1:C:106:LYS:HB2	1:C:118:TRP:CD1	2.54	0.42
2:H:43:GLN:HB2	2:H:53:LEU:HD11	2.01	0.42
2:B:94:LEU:HD11	2:B:120:LEU:HD21	2.01	0.42
1:C:193:LEU:C	1:C:193:LEU:HD12	2.45	0.42
2:D:106:GLN:NE2	2:D:109:THR:HG22	2.33	0.42
2:P:43:GLN:HB2	2:P:53:LEU:HD11	2.01	0.42
1:E:104:CYS:HB2	1:E:118:TRP:O	2.19	0.42
2:D:101:VAL:HG12	2:D:103:TYR:CE1	2.55	0.42
1:K:37:TYR:CD2	1:K:106:LYS:CD	3.03	0.42
2:H:106:GLN:NE2	2:H:109:THR:HG22	2.33	0.41
1:G:193:LEU:HD12	1:G:193:LEU:C	2.45	0.41
2:J:113:THR:HA	3:J:301:CL:CL	2.57	0.41
2:L:106:GLN:HE22	2:L:109:THR:HG23	1.83	0.41
1:O:106:LYS:HB2	1:O:118:TRP:CD1	2.55	0.41
1:A:114:TYR:CE2	2:B:55:TYR:HB2	2.56	0.41
1:G:104:CYS:HB2	1:G:118:TRP:O	2.19	0.41
2:L:43:GLN:HB2	2:L:53:LEU:HD11	2.03	0.41
2:B:43:GLN:HB2	2:B:53:LEU:HD11	2.02	0.41
1:K:13:VAL:O	1:K:126:VAL:HA	2.21	0.41
1:A:37:TYR:CD2	1:A:106:LYS:HD3	2.56	0.41
2:F:106:GLN:NE2	2:F:109:THR:HG22	2.33	0.41
1:M:106:LYS:HB2	1:M:118:TRP:CD1	2.55	0.41
1:A:104:CYS:HB2	1:A:118:TRP:O	2.20	0.41
1:A:13:VAL:O	1:A:126:VAL:HA	2.21	0.41
1:I:30:PHE:CE1	1:I:39:MET:HE3	2.56	0.41
2:N:94:LEU:HD11	2:N:120:LEU:HD21	2.04	0.40
2:P:94:LEU:HD11	2:P:120:LEU:HD21	2.04	0.40
1:I:39:MET:HB3	1:I:87:LEU:HD22	2.04	0.40
1:M:112:PHE:HE2	2:N:55:TYR:CE2	2.39	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	212/227 (93%)	210 (99%)	2 (1%)	0	100	100
1	C	210/227 (92%)	207 (99%)	3 (1%)	0	100	100
1	E	219/227 (96%)	215 (98%)	4 (2%)	0	100	100
1	G	209/227 (92%)	207 (99%)	2 (1%)	0	100	100
1	I	218/227 (96%)	215 (99%)	3 (1%)	0	100	100
1	K	205/227 (90%)	201 (98%)	4 (2%)	0	100	100
1	M	211/227 (93%)	209 (99%)	2 (1%)	0	100	100
1	O	200/227 (88%)	197 (98%)	3 (2%)	0	100	100
2	B	217/220 (99%)	208 (96%)	9 (4%)	0	100	100
2	D	216/220 (98%)	206 (95%)	10 (5%)	0	100	100
2	F	217/220 (99%)	208 (96%)	9 (4%)	0	100	100
2	H	216/220 (98%)	208 (96%)	8 (4%)	0	100	100
2	J	217/220 (99%)	208 (96%)	9 (4%)	0	100	100
2	L	217/220 (99%)	209 (96%)	8 (4%)	0	100	100
2	N	217/220 (99%)	207 (95%)	10 (5%)	0	100	100
2	P	217/220 (99%)	207 (95%)	10 (5%)	0	100	100
All	All	3418/3576 (96%)	3322 (97%)	96 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	179/190 (94%)	176 (98%)	3 (2%)	53	78
1	C	179/190 (94%)	177 (99%)	2 (1%)	65	84
1	E	184/190 (97%)	177 (96%)	7 (4%)	29	56
1	G	178/190 (94%)	172 (97%)	6 (3%)	32	60
1	I	183/190 (96%)	177 (97%)	6 (3%)	33	61
1	K	176/190 (93%)	171 (97%)	5 (3%)	38	66
1	M	179/190 (94%)	175 (98%)	4 (2%)	45	73
1	O	172/190 (90%)	165 (96%)	7 (4%)	27	53
2	B	194/195 (100%)	186 (96%)	8 (4%)	27	53
2	D	193/195 (99%)	186 (96%)	7 (4%)	31	58
2	F	194/195 (100%)	187 (96%)	7 (4%)	31	58
2	H	193/195 (99%)	186 (96%)	7 (4%)	31	58
2	J	194/195 (100%)	186 (96%)	8 (4%)	27	53
2	L	194/195 (100%)	186 (96%)	8 (4%)	27	53
2	N	194/195 (100%)	187 (96%)	7 (4%)	31	58
2	P	194/195 (100%)	186 (96%)	8 (4%)	27	53
All	All	2980/3080 (97%)	2880 (97%)	100 (3%)	32	60

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	CYS
1	A	208	THR
1	A	224	LYS
2	B	5	THR
2	B	17	GLU
2	B	33	SER
2	B	110	THR
2	B	123	LYS
2	B	197	LEU
2	B	213	THR
2	B	229	GLU
1	C	155	CYS
1	C	208	THR
2	D	5	THR
2	D	17	GLU
2	D	33	SER

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Mol	Chain	Res	Type
2	D	95	GLN
2	D	110	THR
2	D	197	LEU
2	D	213	THR
1	E	29	THR
1	E	139	LEU
1	E	142	SER
1	E	145	SER
1	E	155	CYS
1	E	208	THR
1	E	224	LYS
2	F	5	THR
2	F	17	GLU
2	F	33	SER
2	F	110	THR
2	F	197	LEU
2	F	213	THR
2	F	229	GLU
1	G	29	THR
1	G	72	LYS
1	G	142	SER
1	G	155	CYS
1	G	208	THR
1	G	224	LYS
2	H	5	THR
2	H	17	GLU
2	H	33	SER
2	H	110	THR
2	H	197	LEU
2	H	213	THR
2	H	229	GLU
1	I	106	LYS
1	I	142	SER
1	I	155	CYS
1	I	208	THR
1	I	224	LYS
1	I	229	LYS
2	J	5	THR
2	J	15	LEU
2	J	17	GLU
2	J	33	SER
2	J	110	THR

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Mol	Chain	Res	Type
2	J	197	LEU
2	J	213	THR
2	J	229	GLU
1	K	29	THR
1	K	155	CYS
1	K	208	THR
1	K	221	LYS
1	K	224	LYS
2	L	5	THR
2	L	17	GLU
2	L	33	SER
2	L	110	THR
2	L	162	VAL
2	L	197	LEU
2	L	213	THR
2	L	229	GLU
1	M	155	CYS
1	M	208	THR
1	M	211	CYS
1	M	224	LYS
2	N	5	THR
2	N	17	GLU
2	N	33	SER
2	N	110	THR
2	N	210	CYS
2	N	213	THR
2	N	229	GLU
1	O	29	THR
1	O	97	GLU
1	O	130	SER
1	O	155	CYS
1	O	203	SER
1	O	208	THR
1	O	224	LYS
2	P	5	THR
2	P	17	GLU
2	P	33	SER
2	P	89	LEU
2	P	110	THR
2	P	197	LEU
2	P	213	THR
2	P	229	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	85	ASN
1	A	207	GLN
2	B	43	GLN
2	B	44	GLN
2	B	226	ASN
1	C	44	GLN
1	C	186	GLN
1	C	207	GLN
2	D	44	GLN
2	D	171	GLN
1	E	85	ASN
2	F	22	ASN
2	F	163	GLN
2	F	215	GLN
2	F	226	ASN
1	G	3	GLN
1	G	44	GLN
1	G	85	ASN
1	G	186	GLN
1	G	207	GLN
2	H	27	GLN
2	H	44	GLN
2	H	171	GLN
2	H	215	GLN
2	H	226	ASN
1	I	3	GLN
1	I	44	GLN
1	I	207	GLN
2	J	22	ASN
2	J	44	GLN
2	J	215	GLN
2	J	226	ASN
1	K	85	ASN
1	K	207	GLN
2	L	226	ASN
1	M	207	GLN
2	N	163	GLN
2	N	171	GLN
2	N	215	GLN
2	N	226	ASN

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Mol	Chain	Res	Type
1	O	44	GLN
2	P	44	GLN
2	P	95	GLN
2	P	171	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	216/227 (95%)	0.28	8 (3%) 45 40	42, 68, 96, 114	0
1	C	214/227 (94%)	0.36	11 (5%) 33 29	40, 62, 119, 136	0
1	E	221/227 (97%)	0.58	13 (5%) 28 24	48, 75, 105, 132	0
1	G	213/227 (93%)	0.29	7 (3%) 49 45	46, 66, 110, 128	0
1	I	220/227 (96%)	0.98	27 (12%) 8 7	51, 82, 116, 132	0
1	K	211/227 (92%)	0.93	17 (8%) 18 15	61, 86, 118, 137	0
1	M	215/227 (94%)	0.59	9 (4%) 40 36	51, 73, 108, 123	0
1	O	206/227 (90%)	0.99	25 (12%) 8 7	57, 82, 123, 157	0
2	B	219/220 (99%)	0.28	4 (1%) 67 64	42, 66, 94, 124	0
2	D	218/220 (99%)	0.90	21 (9%) 13 11	49, 84, 116, 128	0
2	F	219/220 (99%)	0.76	12 (5%) 30 27	48, 75, 104, 121	0
2	H	218/220 (99%)	0.54	12 (5%) 30 27	45, 72, 113, 132	0
2	J	219/220 (99%)	0.78	16 (7%) 21 19	56, 78, 106, 137	0
2	L	219/220 (99%)	1.00	31 (14%) 6 5	60, 89, 132, 147	0
2	N	219/220 (99%)	0.76	8 (3%) 45 40	53, 77, 104, 130	0
2	P	219/220 (99%)	1.14	31 (14%) 6 5	70, 105, 138, 148	0
All	All	3466/3576 (96%)	0.70	252 (7%) 21 19	40, 78, 118, 157	0

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	229	LYS	5.7
1	E	205	GLY	4.9
1	K	58	TRP	4.2
2	N	170	LEU	4.1
1	O	151	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	I	146	THR	3.9
1	G	143	SER	3.8
2	L	197	LEU	3.8
1	O	228	PRO	3.7
1	C	48	LYS	3.7
2	J	228	GLY	3.7
1	E	229	LYS	3.7
1	C	46	PRO	3.7
2	P	29	VAL	3.6
1	I	221	LYS	3.6
1	O	110	GLY	3.6
1	A	229	LYS	3.5
1	E	230	SER	3.5
2	L	166	VAL	3.4
2	H	206	LYS	3.4
2	P	1	ASP	3.4
2	L	162	VAL	3.4
2	L	221	VAL	3.4
2	P	206	LYS	3.4
1	C	221	LYS	3.4
1	I	202	SER	3.4
1	C	229	LYS	3.3
2	L	207	VAL	3.3
1	O	114	TYR	3.3
2	L	206	LYS	3.3
1	O	113	PRO	3.3
2	J	229	GLU	3.3
2	J	1	ASP	3.2
1	O	201	SER	3.2
1	O	107	ALA	3.1
1	C	143	SER	3.1
1	I	204	LEU	3.1
1	G	221	LYS	3.1
2	F	185	LYS	3.1
2	L	161	LYS	3.1
1	A	2	VAL	3.1
1	E	111	TYR	3.1
2	J	107	TYR	3.1
2	D	206	LYS	3.1
2	B	185	LYS	3.0
1	I	200	PRO	3.0
1	G	142	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	143	SER	3.0
1	O	203	SER	3.0
2	D	15	LEU	3.0
2	J	170	LEU	3.0
2	B	1	ASP	3.0
2	L	47	GLY	3.0
1	E	2	VAL	3.0
1	I	67	TYR	3.0
2	H	108	TYR	3.0
2	P	74	ASP	3.0
1	I	55	GLY	3.0
1	I	205	GLY	3.0
2	L	212	VAL	3.0
2	P	57	ALA	3.0
1	K	228	PRO	3.0
1	O	95	ARG	3.0
2	L	1	ASP	2.9
2	D	127	ALA	2.9
1	O	216	LYS	2.9
1	G	228	PRO	2.9
1	A	148	GLY	2.9
1	I	66	VAL	2.9
1	C	150	THR	2.9
2	F	145	THR	2.9
1	K	204	LEU	2.9
2	P	76	PHE	2.9
1	K	65	ILE	2.8
1	O	221	LYS	2.8
2	P	36	LYS	2.8
1	A	110	GLY	2.8
1	A	149	GLY	2.8
2	P	15	LEU	2.8
2	H	170	LEU	2.8
2	F	51	LYS	2.8
2	F	163	GLN	2.8
1	I	101	PHE	2.8
1	O	176	SER	2.7
1	E	119	GLY	2.7
1	I	110	GLY	2.7
1	M	229	LYS	2.7
2	D	96	ALA	2.7
1	I	114	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	N	197	LEU	2.7
2	N	1	ASP	2.7
2	J	40	GLY	2.7
1	I	65	ILE	2.7
1	K	221	LYS	2.6
2	H	210	CYS	2.6
2	J	108	TYR	2.6
1	C	216	LYS	2.6
2	L	170	LEU	2.6
2	L	229	GLU	2.6
1	M	142	SER	2.6
2	B	31	TYR	2.6
2	L	38	TYR	2.6
2	P	38	TYR	2.6
2	L	199	LYS	2.6
2	F	197	LEU	2.6
2	D	129	PRO	2.6
2	L	104	CYS	2.6
2	L	210	CYS	2.6
1	E	147	SER	2.6
2	P	65	SER	2.6
1	O	17	ARG	2.5
1	O	200	PRO	2.5
2	D	170	LEU	2.5
2	D	215	GLN	2.5
2	F	206	LYS	2.5
2	L	200	ALA	2.5
2	N	210	CYS	2.5
1	I	117	TYR	2.5
1	O	209	TYR	2.5
1	O	16	GLY	2.5
2	J	142	LYS	2.5
2	D	92	SER	2.5
2	L	39	LEU	2.5
2	P	30	LEU	2.5
2	P	51	LYS	2.5
1	G	2	VAL	2.5
1	O	66	VAL	2.5
1	I	201	SER	2.5
2	P	107	TYR	2.5
2	J	39	LEU	2.5
2	P	39	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	2	VAL	2.5
1	I	145	SER	2.5
1	K	130	SER	2.5
2	P	50	PRO	2.4
1	K	149	GLY	2.4
2	H	197	LEU	2.4
2	H	225	PHE	2.4
2	D	207	VAL	2.4
2	L	145	THR	2.4
2	D	218	SER	2.4
2	F	229	GLU	2.4
1	E	8	GLY	2.4
2	D	122	ILE	2.4
1	M	2	VAL	2.4
2	H	200	ALA	2.4
2	P	2	ILE	2.4
1	C	204	LEU	2.4
2	J	38	TYR	2.4
1	I	58	TRP	2.4
2	D	134	PHE	2.4
2	P	55	TYR	2.3
1	I	108	VAL	2.3
1	K	2	VAL	2.3
1	K	66	VAL	2.3
1	O	97	GLU	2.3
2	F	209	ALA	2.3
2	P	220	PRO	2.3
1	A	143	SER	2.3
2	D	119	ARG	2.3
1	K	12	LEU	2.3
2	L	220	PRO	2.3
1	K	63	GLY	2.3
2	N	228	GLY	2.3
2	P	41	TRP	2.3
2	P	92	SER	2.3
1	E	221	LYS	2.3
2	H	142	LYS	2.3
2	L	223	LYS	2.3
1	O	117	TYR	2.3
2	L	213	THR	2.3
1	M	149	GLY	2.3
1	I	93	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	58	TRP	2.3
2	P	52	LEU	2.3
2	D	24	LYS	2.3
2	F	36	LYS	2.3
2	N	36	LYS	2.3
2	D	225	PHE	2.3
2	J	114	PHE	2.3
1	K	129	ALA	2.2
2	F	37	ASN	2.2
2	H	40	GLY	2.2
1	I	216	LYS	2.2
2	L	164	TRP	2.2
2	N	114	PHE	2.2
1	O	105	ALA	2.2
1	G	111	TYR	2.2
2	N	142	LYS	2.2
1	E	58	TRP	2.2
2	J	56	TRP	2.2
2	H	37	ASN	2.2
1	A	221	LYS	2.2
1	I	111	TYR	2.2
1	K	48	LYS	2.2
1	M	221	LYS	2.2
2	F	38	TYR	2.2
2	L	107	TYR	2.2
2	H	162	VAL	2.2
2	P	223	LYS	2.2
1	O	208	THR	2.2
2	L	196	THR	2.2
2	P	145	THR	2.2
2	P	70	GLY	2.2
2	P	89	LEU	2.2
1	M	225	ARG	2.2
1	K	46	PRO	2.2
1	O	141	PRO	2.2
2	P	24	LYS	2.2
2	L	40	GLY	2.1
2	P	11	LEU	2.1
1	A	111	TYR	2.1
1	K	114	TYR	2.1
1	C	142	SER	2.1
2	P	225	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	148	VAL	2.1
1	E	208	THR	2.1
1	O	185	LEU	2.1
2	P	108	TYR	2.1
1	E	48	LYS	2.1
1	I	46	PRO	2.1
2	H	166	VAL	2.1
2	D	126	ALA	2.1
1	I	103	TYR	2.1
2	D	31	TYR	2.1
1	M	216	LYS	2.1
2	D	185	LYS	2.1
1	O	68	ALA	2.1
1	G	204	LEU	2.1
2	J	41	TRP	2.1
1	E	110	GLY	2.1
1	I	20	ARG	2.1
2	D	229	GLU	2.1
1	C	2	VAL	2.0
2	L	127	ALA	2.0
2	L	128	ALA	2.0
2	P	209	ALA	2.0
2	D	217	LEU	2.0
1	C	47	GLY	2.0
1	I	149	GLY	2.0
1	K	8	GLY	2.0
2	L	56	TRP	2.0
2	L	228	GLY	2.0
1	M	48	LYS	2.0
1	K	141	PRO	2.0
2	B	163	GLN	2.0
2	F	30	LEU	2.0
2	L	146	ALA	2.0
2	J	36	LYS	2.0
2	P	229	GLU	2.0
2	J	111	PRO	2.0
2	J	42	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	K	301	1/1	0.89	0.18	82,82,82,82	0
3	CL	J	301	1/1	0.91	0.13	89,89,89,89	0
3	CL	C	301	1/1	0.95	0.14	67,67,67,67	0
3	CL	G	301	1/1	0.96	0.08	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.