Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 09:55 pm GMT

PDB ID	:	2WRT
Title	:	The 2.4 Angstrom structure of the Fasciola hepatica mu class GST, GST26
Authors	:	Line, K.; Isupov, M.N.; LaCourse, E.J.; Brophy, P.M.; Littlechild, J.A.
Deposited on	:	2009-09-02
Resolution	:	2.40 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:

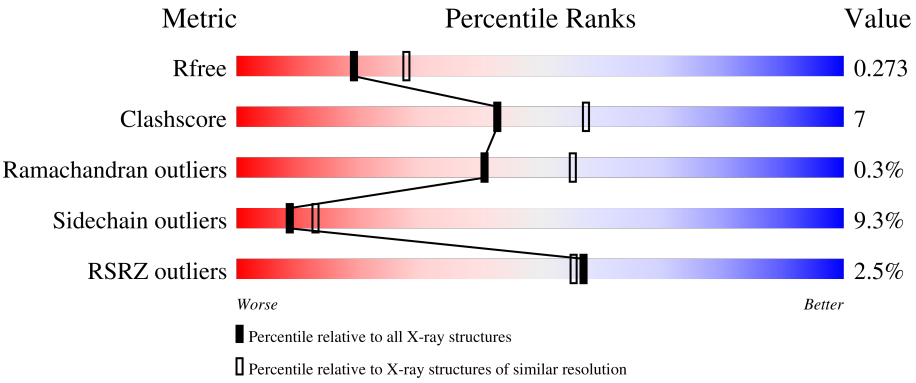
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	218	3% 82% 16% ·
1	B	218	83% 15% ·
1	C	218	6% 78% 19% ·
1	D	218	81% 17% ·
1	E	218	79% 17% ·

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Mol	Chain	Length	Quality of chain
1	F	218	79% 18%
1	G	218	4% 78% 19%
1	H	218	% 81% 17%
1	I	218	3% 78% 20%
1	J	218	% 84% 14%
1	K	218	2% 72% 24%
1	L	218	8% 70% 27%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	F	1219	-	-	X	-
2	CL	G	1219	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22586 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 GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	2	0
			1789	1155	298	323	13			
1	B	217	Total	C	N	O	S	0	1	0
			1778	1148	293	324	13			
1	C	217	Total	C	N	O	S	0	0	0
			1772	1144	293	322	13			
1	D	217	Total	C	N	O	S	0	1	0
			1778	1148	294	323	13			
1	E	217	Total	C	N	O	S	0	0	0
			1772	1144	293	322	13			
1	F	217	Total	C	N	O	S	0	1	0
			1778	1149	294	322	13			
1	G	217	Total	C	N	O	S	0	0	0
			1772	1144	293	322	13			
1	H	217	Total	C	N	O	S	0	2	0
			1786	1153	296	324	13			
1	I	217	Total	C	N	O	S	0	0	0
			1772	1144	293	322	13			
1	J	217	Total	C	N	O	S	0	0	0
			1772	1144	293	322	13			
1	K	217	Total	C	N	O	S	0	0	0
			1772	1144	293	322	13			
1	L	217	Total	C	N	O	S	0	0	0
			1772	1144	293	322	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	LEU	PHE	conflict	UNP P30112
A	84	SER	THR	conflict	UNP P30112
A	147	SER	PRO	conflict	UNP P30112
B	42	LEU	PHE	conflict	UNP P30112

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Chain	Residue	Modelled	Actual	Comment	Reference
B	84	SER	THR	conflict	UNP P30112
B	147	SER	PRO	conflict	UNP P30112
C	42	LEU	PHE	conflict	UNP P30112
C	84	SER	THR	conflict	UNP P30112
C	147	SER	PRO	conflict	UNP P30112
D	42	LEU	PHE	conflict	UNP P30112
D	84	SER	THR	conflict	UNP P30112
D	147	SER	PRO	conflict	UNP P30112
E	42	LEU	PHE	conflict	UNP P30112
E	84	SER	THR	conflict	UNP P30112
E	147	SER	PRO	conflict	UNP P30112
F	42	LEU	PHE	conflict	UNP P30112
F	84	SER	THR	conflict	UNP P30112
F	147	SER	PRO	conflict	UNP P30112
G	42	LEU	PHE	conflict	UNP P30112
G	84	SER	THR	conflict	UNP P30112
G	147	SER	PRO	conflict	UNP P30112
H	42	LEU	PHE	conflict	UNP P30112
H	84	SER	THR	conflict	UNP P30112
H	147	SER	PRO	conflict	UNP P30112
I	42	LEU	PHE	conflict	UNP P30112
I	84	SER	THR	conflict	UNP P30112
I	147	SER	PRO	conflict	UNP P30112
J	42	LEU	PHE	conflict	UNP P30112
J	84	SER	THR	conflict	UNP P30112
J	147	SER	PRO	conflict	UNP P30112
K	42	LEU	PHE	conflict	UNP P30112
K	84	SER	THR	conflict	UNP P30112
K	147	SER	PRO	conflict	UNP P30112
L	42	LEU	PHE	conflict	UNP P30112
L	84	SER	THR	conflict	UNP P30112
L	147	SER	PRO	conflict	UNP P30112

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	D	2	Total Cl 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0
2	H	2	Total Cl 2 2	0	0
2	I	1	Total Cl 1 1	0	0
2	J	2	Total Cl 2 2	0	0

- Molecule 3 is water.

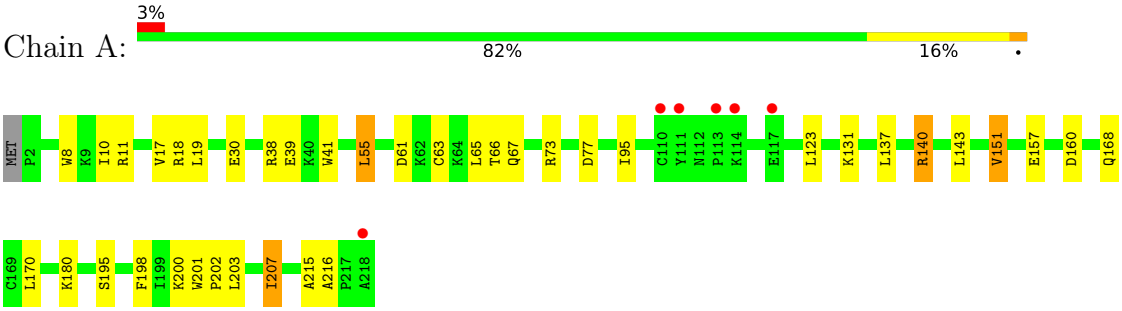
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	99	Total O 99 99	0	0
3	B	136	Total O 136 136	0	0
3	C	81	Total O 81 81	0	0
3	D	153	Total O 153 153	0	0
3	E	122	Total O 122 122	0	0
3	F	105	Total O 105 105	0	0
3	G	85	Total O 85 85	0	0
3	H	149	Total O 149 149	0	0
3	I	88	Total O 88 88	0	0
3	J	93	Total O 93 93	0	0
3	K	106	Total O 106 106	0	0
3	L	44	Total O 44 44	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

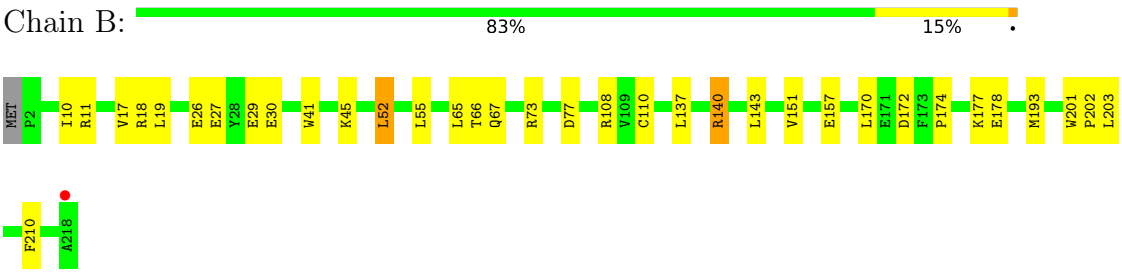
• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51

Chain A:



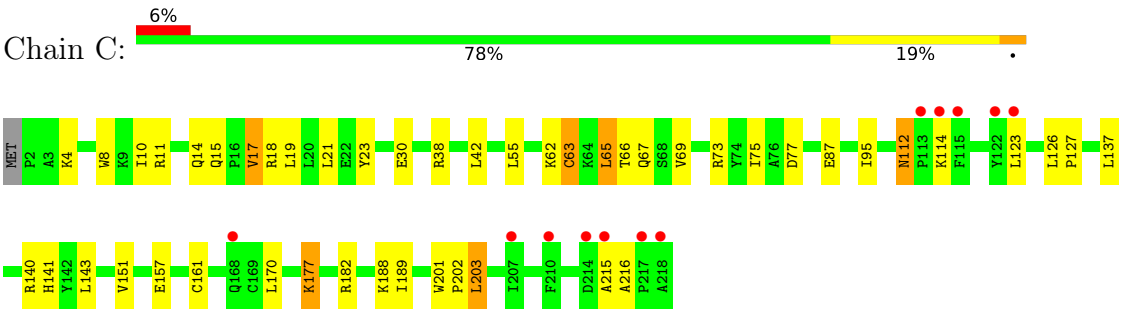
• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51

Chain B:



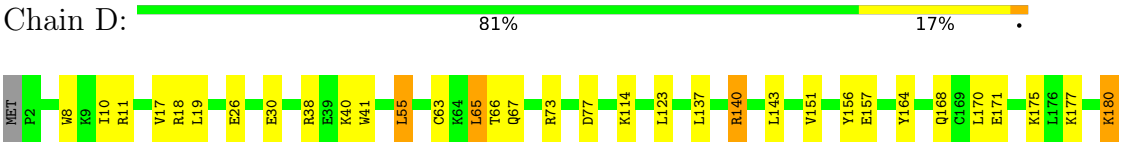
• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51

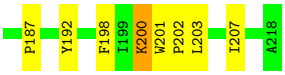
Chain C:



• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51

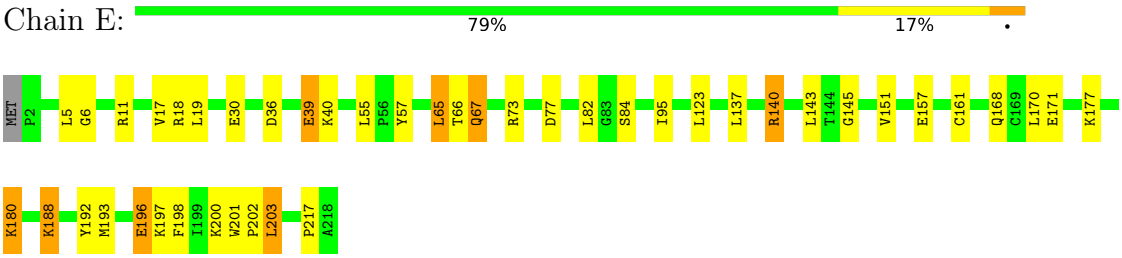
Chain D:





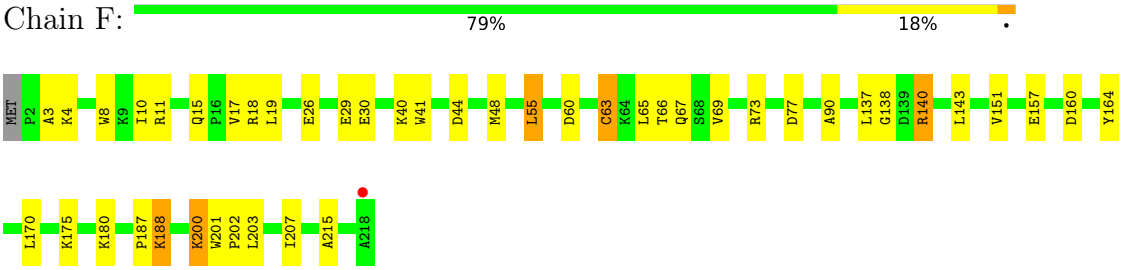
• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51

Chain E:



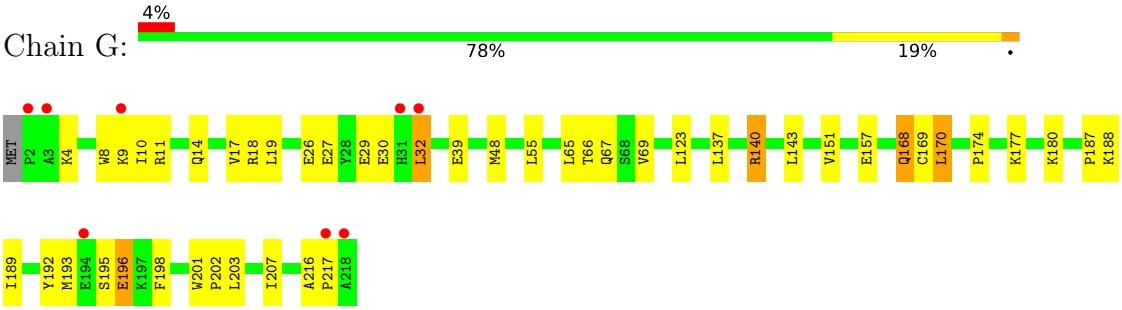
• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51

Chain F:



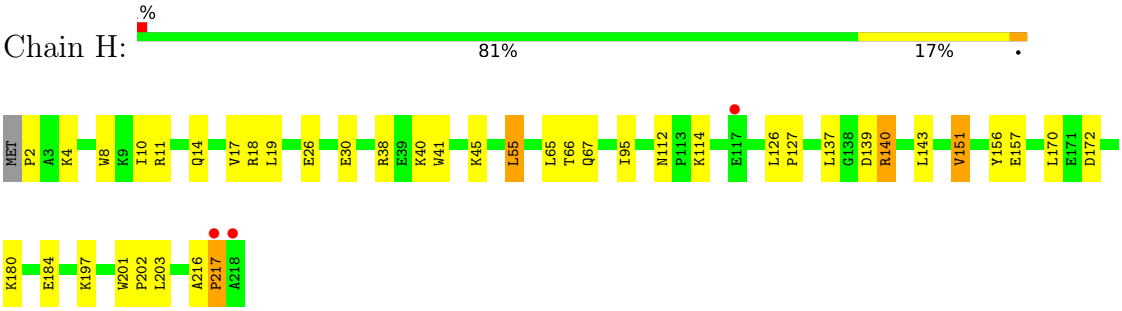
• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51

Chain G:



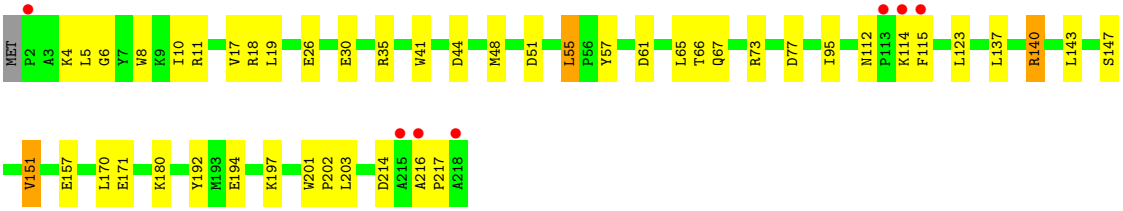
• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51

Chain H:



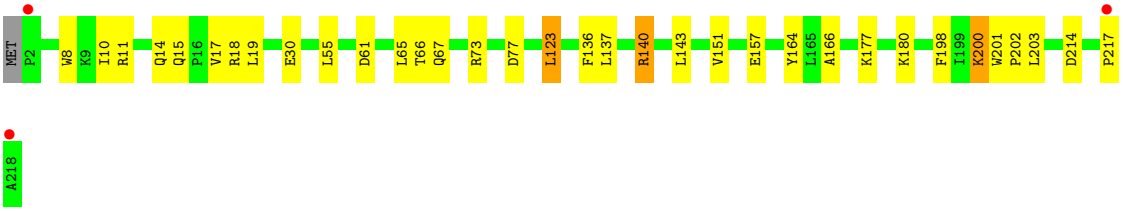
• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51

Chain I:



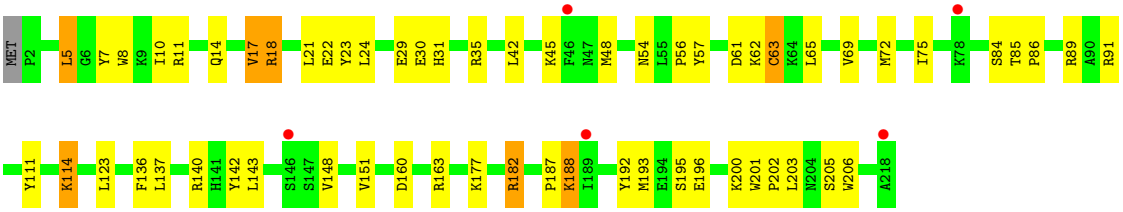
• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51

Chain J:



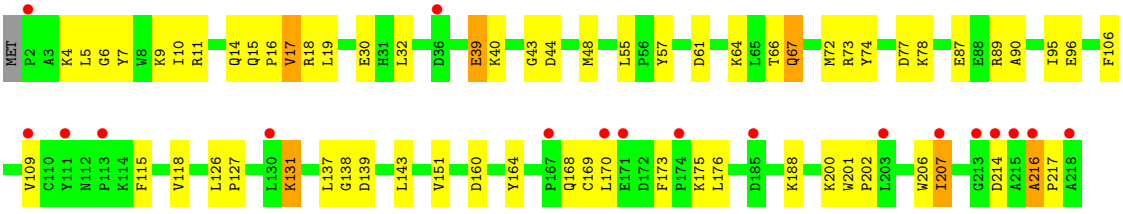
• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51

Chain K:



• Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.31Å 92.50Å 166.42Å 90.00° 94.55° 90.00°	Depositor
Resolution (Å)	166.67 – 2.40 45.82 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (166.67-2.40) 99.8 (45.82-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.205 , 0.281 0.202 , 0.273	Depositor DCC
R_{free} test set	5463 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.9	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22586	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.47	1/1839 (0.1%)	0.61	0/2475
1	B	0.49	0/1828	0.66	2/2462 (0.1%)
1	C	0.49	1/1819 (0.1%)	0.61	0/2450
1	D	0.52	0/1828	0.64	0/2462
1	E	0.48	0/1819	0.62	0/2450
1	F	0.48	1/1828 (0.1%)	0.60	0/2461
1	G	0.47	0/1819	0.62	0/2450
1	H	0.46	0/1839	0.61	0/2476
1	I	0.46	0/1819	0.60	0/2450
1	J	0.44	0/1819	0.59	0/2450
1	K	0.48	0/1819	0.63	0/2450
1	L	0.43	0/1819	0.56	0/2450
All	All	0.47	3/21895 (0.0%)	0.61	2/29486 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	63	CYS	CB-SG	-7.12	1.70	1.82
1	A	63	CYS	CB-SG	-5.18	1.73	1.81
1	F	63	CYS	CB-SG	-5.03	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	52	LEU	CA-CB-CG	6.05	129.21	115.30
1	B	52	LEU	CB-CG-CD1	5.63	120.57	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	62	LYS	Peptide

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	1789	0	1777	16	0
1	B	1778	0	1758	15	0
1	C	1772	0	1752	25	0
1	D	1778	0	1760	20	0
1	E	1772	0	1752	24	0
1	F	1778	0	1765	25	0
1	G	1772	0	1752	23	0
1	H	1786	0	1771	25	0
1	I	1772	0	1752	19	0
1	J	1772	0	1752	17	0
1	K	1772	0	1752	44	0
1	L	1772	0	1752	41	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	2	0	0	1	0
2	E	1	0	0	1	0
2	F	1	0	0	2	0
2	G	1	0	0	3	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0
2	J	2	0	0	0	0
3	A	99	0	0	0	0
3	B	136	0	0	5	0
3	C	81	0	0	1	0
3	D	153	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	122	0	0	5	0
3	F	105	0	0	4	0
3	G	85	0	0	2	0
3	H	149	0	0	7	0
3	I	88	0	0	2	0
3	J	93	0	0	1	0
3	K	106	0	0	9	0
3	L	44	0	0	4	0
All	All	22586	0	21095	290	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 (290) 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)
1:H:216:ALA:HB1	1:H:217:PRO:HD2	1.12	1.10
1:K:182:ARG:HD3	3:K:2087:HOH:O	1.60	1.02
1:K:30:GLU:HB3	3:K:2019:HOH:O	1.62	1.00
1:H:216:ALA:CB	1:H:217:PRO:HD2	1.98	0.93
1:K:48:MET:HG2	3:K:2035:HOH:O	1.70	0.89
1:D:168[B]:GLN:HE21	1:D:168[B]:GLN:HA	1.38	0.87
1:H:216:ALA:HB1	1:H:217:PRO:CD	2.03	0.85
1:L:78:LYS:HA	3:L:2023:HOH:O	1.80	0.81
1:D:168[B]:GLN:HA	1:D:168[B]:GLN:NE2	1.97	0.79
1:G:196:GLU:CD	1:G:196:GLU:H	1.89	0.75
1:F:138:GLY:O	1:F:175[B]:LYS:HD3	1.89	0.73
1:C:215:ALA:HB3	1:C:216:ALA:HA	1.70	0.72
1:L:138:GLY:O	1:L:175:LYS:HD2	1.90	0.72
1:C:170:LEU:HB3	1:C:177:LYS:HG3	1.72	0.71
1:L:216:ALA:N	1:L:217:PRO:HD3	2.05	0.71
1:C:112:ASN:HD22	1:C:114:LYS:H	1.37	0.71
1:E:196:GLU:HG2	3:E:2109:HOH:O	1.90	0.71
1:K:114:LYS:NZ	1:K:114:LYS:HB3	2.06	0.70
1:H:26:GLU:HG2	3:H:2019:HOH:O	1.92	0.68
1:A:198:PHE:HE1	1:A:200:LYS:HG3	1.59	0.68
1:I:171:GLU:HB2	3:I:2082:HOH:O	1.94	0.68
1:K:5:LEU:O	1:K:30:GLU:HA	1.95	0.67
1:K:5:LEU:HD11	1:K:21:LEU:HD11	1.75	0.67
1:H:126:LEU:HB3	1:H:127:PRO:HD3	1.79	0.65
1:G:69:VAL:HG23	3:H:2030:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLU:OE1	1:A:39:GLU:HA	1.98	0.64
1:F:164:TYR:OH	1:F:200:LYS:HE3	1.96	0.64
1:L:10:ILE:HG22	1:L:202:PRO:HG2	1.81	0.62
1:K:18:ARG:NH1	1:K:30:GLU:OE2	2.30	0.62
1:I:140:ARG:HH11	1:I:140:ARG:HG2	1.64	0.62
1:D:171:GLU:HG2	3:D:2118:HOH:O	1.99	0.61
1:J:123:LEU:HD11	1:J:166:ALA:HB2	1.81	0.61
1:G:216:ALA:HB1	1:G:217:PRO:HD2	1.81	0.61
1:K:63:CYS:CB	3:K:2044:HOH:O	2.49	0.60
1:C:8:TRP:HB2	1:C:10:ILE:HG12	1.82	0.60
1:K:24:LEU:HD12	1:K:75:ILE:HG22	1.82	0.60
1:L:7:TYR:CD2	1:L:14:GLN:HB2	2.36	0.59
1:L:131:LYS:HA	1:L:173:PHE:HE1	1.67	0.59
1:H:139:ASP:OD2	3:H:2097:HOH:O	2.16	0.59
1:D:140:ARG:HG2	1:D:140:ARG:HH11	1.67	0.59
1:G:140:ARG:HH11	1:G:140:ARG:HG2	1.68	0.59
1:H:26:GLU:CG	3:H:2019:HOH:O	2.50	0.59
1:A:10:ILE:HG22	1:A:202:PRO:HG2	1.85	0.58
1:K:18:ARG:HG2	1:K:192:TYR:OH	2.03	0.57
1:K:63:CYS:HB2	3:K:2044:HOH:O	2.04	0.57
1:E:39:GLU:CD	1:E:39:GLU:H	2.07	0.57
1:F:188:LYS:HG3	2:F:1219:CL:CL	2.41	0.57
1:C:141:HIS:HA	1:C:182:ARG:HH11	1.70	0.57
1:D:18:ARG:HD2	1:D:30:GLU:OE1	2.05	0.57
1:J:140:ARG:HG2	1:J:140:ARG:HH11	1.70	0.57
1:K:111:TYR:OH	1:K:205:SER:HB3	2.05	0.57
1:B:193:MET:CE	3:B:2038:HOH:O	2.53	0.56
1:K:23:TYR:HA	1:K:188:LYS:HG3	1.86	0.56
1:B:140:ARG:HH11	1:B:140:ARG:HG2	1.70	0.56
1:C:66:THR:O	1:C:67:GLN:HB2	2.05	0.56
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.69	0.56
1:B:29[B]:GLU:HA	1:B:29[B]:GLU:OE1	2.05	0.56
1:I:216:ALA:HB1	1:I:217:PRO:HD2	1.88	0.56
1:F:69:VAL:HG23	3:F:2053:HOH:O	2.06	0.56
1:K:21:LEU:HG	1:K:75:ILE:HD13	1.87	0.56
1:G:27:GLU:O	3:G:2006:HOH:O	2.18	0.56
1:G:192:TYR:CE2	1:G:198:PHE:HD2	2.23	0.56
1:L:131:LYS:HA	1:L:173:PHE:CE1	2.40	0.56
1:L:201:TRP:CG	1:L:202:PRO:HA	2.41	0.56
1:A:8:TRP:HB2	1:A:10:ILE:HG12	1.87	0.55
1:K:201:TRP:CG	1:K:202:PRO:HA	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2031:HOH:O	1:K:177:LYS:HD3	2.06	0.55
1:J:18:ARG:HD2	1:J:30:GLU:OE1	2.06	0.55
1:H:140:ARG:HG2	1:H:140:ARG:HH11	1.70	0.55
1:F:201:TRP:CG	1:F:202:PRO:HA	2.42	0.55
1:E:66:THR:O	1:E:67:GLN:HB2	2.07	0.54
1:G:8:TRP:HB2	1:G:10:ILE:HG12	1.88	0.54
1:L:126:LEU:HB3	1:L:127:PRO:HD3	1.89	0.54
1:C:11:ARG:HD3	1:C:157:GLU:OE1	2.07	0.54
1:K:14:GLN:O	1:K:14:GLN:HG3	2.06	0.54
1:L:9:LYS:HG3	1:L:32:LEU:HD13	1.90	0.54
1:A:18:ARG:HD2	1:A:30:GLU:OE1	2.08	0.54
1:B:66:THR:O	1:B:67:GLN:HB2	2.08	0.54
1:G:11:ARG:NH2	3:G:2002:HOH:O	2.38	0.54
1:G:189:ILE:O	1:G:193:MET:HG3	2.08	0.54
1:D:201:TRP:CG	1:D:202:PRO:HA	2.43	0.53
1:E:5:LEU:HB3	1:E:30:GLU:HG3	1.90	0.53
1:J:201:TRP:CG	1:J:202:PRO:HA	2.43	0.53
1:K:14:GLN:OE1	1:K:56:PRO:CB	2.56	0.53
1:F:18:ARG:HD2	1:F:30:GLU:OE1	2.08	0.53
1:I:201:TRP:CG	1:I:202:PRO:HA	2.44	0.53
1:B:193:MET:HE2	3:B:2038:HOH:O	2.09	0.53
1:B:201:TRP:CG	1:B:202:PRO:HA	2.44	0.53
1:H:201:TRP:CG	1:H:202:PRO:HA	2.44	0.53
1:C:95:ILE:HG21	1:C:151:VAL:HG11	1.91	0.52
1:E:201:TRP:CG	1:E:202:PRO:HA	2.45	0.52
1:G:18:ARG:HD2	1:G:30:GLU:OE1	2.09	0.52
1:G:201:TRP:CG	1:G:202:PRO:HA	2.44	0.52
1:E:73:ARG:O	1:E:77:ASP:HB2	2.11	0.52
1:C:18:ARG:HD2	1:C:30:GLU:OE1	2.11	0.51
1:C:141:HIS:HA	1:C:182:ARG:NH1	2.25	0.51
1:F:140:ARG:HG2	1:F:140:ARG:HH11	1.75	0.51
1:I:51:ASP:HB3	1:J:136:PHE:CD1	2.46	0.51
1:I:18:ARG:HD2	1:I:30:GLU:OE1	2.10	0.51
1:K:114:LYS:HB3	1:K:114:LYS:HZ3	1.72	0.51
1:L:9:LYS:HA	1:L:32:LEU:HD22	1.92	0.51
1:L:168:GLN:HB3	3:L:2040:HOH:O	2.10	0.51
1:K:31:HIS:HA	3:K:2021:HOH:O	2.10	0.51
1:G:66:THR:O	1:G:67:GLN:HB2	2.11	0.50
1:D:8:TRP:HB2	1:D:10:ILE:HG12	1.94	0.50
1:I:41:TRP:CH2	1:I:55:LEU:HD13	2.46	0.50
1:K:63:CYS:HB3	3:K:2044:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:ASP:OD1	1:F:180:LYS:NZ	2.44	0.50
1:H:66:THR:O	1:H:67:GLN:HB2	2.11	0.50
1:I:112:ASN:ND2	1:I:114:LYS:O	2.43	0.50
1:J:201:TRP:CH2	1:J:217:PRO:HD3	2.47	0.49
1:K:8:TRP:HB2	1:K:10:ILE:HG12	1.94	0.49
1:L:173:PHE:HB3	1:L:176:LEU:HD12	1.93	0.49
1:C:201:TRP:CG	1:C:202:PRO:HA	2.48	0.49
1:G:188:LYS:HG2	2:G:1219:CL:CL	2.50	0.49
1:L:66:THR:O	1:L:67:GLN:HB2	2.12	0.49
1:F:175[B]:LYS:HB2	3:F:2068:HOH:O	2.13	0.49
1:H:18:ARG:HD2	1:H:30:GLU:OE1	2.13	0.49
1:I:11:ARG:HD2	1:I:157:GLU:OE1	2.13	0.49
1:E:11:ARG:HD2	1:E:157:GLU:OE1	2.13	0.49
1:L:106:PHE:HA	1:L:109:VAL:HG12	1.95	0.48
1:E:11:ARG:NH2	3:E:2006:HOH:O	2.44	0.48
1:F:187:PRO:HD2	2:F:1219:CL:CL	2.51	0.48
1:I:192:TYR:HE1	1:I:197:LYS:HG3	1.78	0.48
1:B:110:CYS:SG	1:B:210:PHE:HB3	2.54	0.48
1:K:85:THR:HB	1:K:86:PRO:HD2	1.95	0.48
1:A:201:TRP:CG	1:A:202:PRO:HA	2.49	0.48
1:B:174:PRO:O	1:B:178:GLU:HB2	2.14	0.48
1:K:187:PRO:HD2	1:K:188:LYS:NZ	2.28	0.48
1:L:169:CYS:O	1:L:170:LEU:HB2	2.13	0.48
1:G:188:LYS:CG	2:G:1219:CL:CL	2.98	0.48
1:H:41:TRP:CZ2	1:H:45:LYS:HG3	2.49	0.48
1:J:177:LYS:HD2	3:J:2078:HOH:O	2.14	0.48
1:K:17:VAL:HB	1:K:72:MET:HG3	1.94	0.48
1:D:10:ILE:HG22	1:D:202:PRO:HG2	1.96	0.48
1:L:170:LEU:HA	1:L:173:PHE:HB2	1.96	0.48
1:B:18:ARG:HD2	1:B:30:GLU:OE1	2.13	0.47
1:G:169:CYS:SG	1:G:170:LEU:HD22	2.53	0.47
1:J:8:TRP:HB2	1:J:10:ILE:HG12	1.95	0.47
1:E:200:LYS:HB2	3:E:2114:HOH:O	2.14	0.47
1:J:198:PHE:CE1	1:J:200:LYS:HG2	2.49	0.47
1:K:14:GLN:HA	1:K:17:VAL:HG13	1.96	0.47
1:B:140:ARG:CD	3:B:2094:HOH:O	2.63	0.47
1:E:180:LYS:HD2	3:E:2098:HOH:O	2.15	0.47
1:B:10:ILE:HG22	1:B:202:PRO:HG2	1.96	0.47
1:G:10:ILE:HG22	1:G:202:PRO:HG2	1.97	0.47
1:G:11:ARG:HD2	1:G:157:GLU:OE1	2.14	0.47
1:I:66:THR:O	1:I:67:GLN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:LYS:HB2	3:E:2019:HOH:O	2.13	0.47
1:F:8:TRP:HB2	1:F:10:ILE:HG12	1.96	0.47
1:F:11:ARG:HD2	1:F:157:GLU:OE1	2.14	0.47
1:J:11:ARG:HD2	1:J:157:GLU:OE1	2.15	0.47
1:A:207:ILE:HG12	1:A:207:ILE:O	2.14	0.47
1:C:23:TYR:HB2	1:C:189:ILE:HD11	1.97	0.46
1:G:187:PRO:HD2	2:G:1219:CL:CL	2.51	0.46
1:D:66:THR:O	1:D:67:GLN:HB2	2.15	0.46
1:L:14:GLN:HG3	1:L:18:ARG:HD3	1.97	0.46
1:D:192:TYR:O	1:D:198:PHE:HB2	2.15	0.46
1:H:126:LEU:HB3	1:H:127:PRO:CD	2.45	0.46
1:A:201:TRP:CZ2	1:A:216:ALA:HB3	2.50	0.46
1:K:14:GLN:OE1	1:K:56:PRO:HB3	2.16	0.46
1:J:66:THR:O	1:J:67:GLN:HB2	2.15	0.46
1:C:215:ALA:N	1:C:216:ALA:HB2	2.31	0.46
1:K:142:TYR:HB3	3:K:2073:HOH:O	2.15	0.46
1:L:216:ALA:N	1:L:217:PRO:CD	2.77	0.46
1:B:140:ARG:HD3	3:B:2094:HOH:O	2.15	0.46
1:F:3:ALA:HA	1:F:60:ASP:HB3	1.98	0.46
1:I:147:SER:HB2	3:I:2066:HOH:O	2.15	0.46
1:E:6:GLY:HA3	1:E:57:TYR:CZ	2.51	0.45
1:L:207:ILE:O	1:L:207:ILE:HG23	2.16	0.45
1:H:40:LYS:HB3	3:H:2038:HOH:O	2.16	0.45
1:L:9:LYS:HB3	1:L:206:TRP:HZ2	1.81	0.45
1:A:95:ILE:HG21	1:A:151:VAL:HG11	1.99	0.45
1:D:187:PRO:HD2	2:D:1219:CL:CL	2.54	0.45
1:E:168:GLN:O	1:E:171:GLU:HB2	2.17	0.45
1:K:7:TYR:HB2	1:K:14:GLN:NE2	2.32	0.45
1:K:84:SER:O	1:K:89:ARG:NH1	2.49	0.45
1:K:142:TYR:CE2	1:K:148:VAL:HG22	2.51	0.45
1:L:17:VAL:HG12	1:L:72:MET:HG3	1.98	0.45
1:F:66:THR:O	1:F:67:GLN:HB2	2.17	0.45
1:F:201:TRP:CD1	1:F:215:ALA:HA	2.52	0.45
1:F:40:LYS:HB2	3:F:2014:HOH:O	2.17	0.45
1:H:41:TRP:CH2	1:H:55:LEU:HD13	2.52	0.45
1:K:10:ILE:HG22	1:K:202:PRO:HG2	1.98	0.45
1:A:11:ARG:HD2	1:A:157:GLU:OE1	2.17	0.45
1:K:29:GLU:O	1:K:29:GLU:HG2	2.16	0.45
1:K:7:TYR:CD2	1:K:14:GLN:HB3	2.52	0.45
1:D:156:TYR:CE2	1:D:180:LYS:HD3	2.51	0.45
1:K:177:LYS:HA	1:K:177:LYS:HD2	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:10:ILE:HA	1:L:202:PRO:HD2	1.99	0.45
1:L:95:ILE:H	1:L:95:ILE:HG13	1.52	0.45
1:C:21:LEU:HD21	1:C:75:ILE:HD13	2.00	0.44
1:H:11:ARG:NH2	3:H:2007:HOH:O	2.42	0.44
1:C:63:CYS:SG	1:C:65:LEU:HD22	2.58	0.44
1:F:10:ILE:HG22	1:F:202:PRO:HG2	1.99	0.44
1:H:11:ARG:HD2	1:H:157:GLU:OE1	2.18	0.44
1:H:95:ILE:HG21	1:H:151:VAL:HG11	2.00	0.44
1:J:10:ILE:HG22	1:J:202:PRO:HG2	2.00	0.44
1:E:18:ARG:HD2	1:E:30:GLU:OE1	2.18	0.44
1:E:192:TYR:HE1	1:E:197:LYS:HG3	1.82	0.44
1:C:11:ARG:NH2	3:C:2007:HOH:O	2.50	0.44
1:K:160:ASP:O	1:K:163:ARG:HG3	2.18	0.44
1:E:65:LEU:HD21	1:F:90:ALA:HB1	1.98	0.44
1:I:6:GLY:HA3	1:I:57:TYR:CE2	2.53	0.44
1:H:8:TRP:HB2	1:H:10:ILE:HG12	1.99	0.44
1:H:217:PRO:HD3	3:H:2149:HOH:O	2.18	0.44
1:A:160:ASP:HA	1:A:180:LYS:NZ	2.33	0.43
1:H:10:ILE:HG22	1:H:202:PRO:HG2	2.00	0.43
1:C:73:ARG:O	1:C:77:ASP:HB2	2.18	0.43
1:F:73:ARG:O	1:F:77:ASP:HB2	2.17	0.43
1:J:164:TYR:OH	1:J:200:LYS:HE3	2.19	0.43
1:L:6:GLY:HA3	1:L:57:TYR:CE2	2.53	0.43
1:D:63:CYS:SG	1:D:65:LEU:HD22	2.59	0.43
1:A:160:ASP:OD1	1:A:180:LYS:NZ	2.52	0.43
1:D:164:TYR:OH	1:D:200:LYS:HE3	2.18	0.43
1:H:112:ASN:ND2	1:H:114:LYS:H	2.16	0.43
1:K:62:LYS:HB3	1:L:87:GLU:OE2	2.19	0.43
1:L:15:GLN:HB2	1:L:16:PRO:HD3	2.00	0.43
1:L:168:GLN:CB	3:L:2040:HOH:O	2.65	0.43
1:G:174:PRO:HA	1:G:177:LYS:HB2	1.99	0.43
1:K:5:LEU:HD11	1:K:21:LEU:CD1	2.46	0.43
1:F:11:ARG:HA	1:F:15:GLN:HG2	2.01	0.43
1:K:201:TRP:CD1	1:K:202:PRO:HA	2.53	0.43
1:D:41:TRP:CH2	1:D:55:LEU:HD13	2.53	0.43
1:K:22:GLU:HG3	1:K:192:TYR:CG	2.54	0.43
1:L:18:ARG:NH1	1:L:30:GLU:OE2	2.52	0.43
1:C:11:ARG:HA	1:C:15:GLN:HG2	2.01	0.43
1:C:215:ALA:CB	1:C:216:ALA:HA	2.44	0.43
1:E:193:MET:HG2	1:E:198:PHE:CE2	2.54	0.43
1:H:2:PRO:O	1:H:4:LYS:HE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:8:TRP:HB2	1:I:10:ILE:HG12	2.00	0.43
1:L:115:PHE:HA	1:L:118:VAL:HG22	2.01	0.43
1:B:11:ARG:HD2	1:B:157:GLU:OE1	2.17	0.42
1:D:11:ARG:HD2	1:D:157:GLU:OE1	2.19	0.42
1:G:14:GLN:HG3	1:G:18:ARG:HD3	1.99	0.42
1:I:44:ASP:HB3	1:I:48:MET:CE	2.49	0.42
1:J:73:ARG:O	1:J:77:ASP:HB2	2.20	0.42
1:E:95:ILE:HG21	1:E:151:VAL:CG1	2.49	0.42
1:F:4:LYS:HG2	1:F:29:GLU:HG3	2.01	0.42
1:L:160:ASP:O	1:L:164:TYR:CE1	2.73	0.42
1:A:41:TRP:CH2	1:A:55:LEU:HD13	2.54	0.42
1:I:214:ASP:OD2	1:I:214:ASP:N	2.53	0.42
1:A:66:THR:O	1:A:67:GLN:HB2	2.20	0.42
1:D:140:ARG:HH11	1:D:140:ARG:CG	2.33	0.42
1:E:161:CYS:SG	1:E:203:LEU:HG	2.59	0.42
1:J:14:GLN:HG3	1:J:18:ARG:HD3	2.02	0.42
1:C:112:ASN:HD22	1:C:114:LYS:N	2.12	0.42
1:B:41:TRP:CZ2	1:B:45:LYS:HG3	2.54	0.42
1:C:11:ARG:HD2	1:C:203:LEU:HD12	2.01	0.42
1:K:136:PHE:O	1:K:140:ARG:NH2	2.53	0.42
1:K:91:ARG:HB2	3:K:2052:HOH:O	2.19	0.41
1:L:73:ARG:O	1:L:77:ASP:HB2	2.20	0.41
1:L:74:TYR:CE1	1:L:78:LYS:HD2	2.55	0.41
1:G:140:ARG:HH11	1:G:140:ARG:CG	2.34	0.41
1:K:65:LEU:HD21	1:L:90:ALA:HB1	2.02	0.41
1:H:156:TYR:CE2	1:H:184:GLU:HG3	2.55	0.41
1:L:6:GLY:HA3	1:L:57:TYR:CZ	2.55	0.41
1:L:106:PHE:O	1:L:109:VAL:HG12	2.21	0.41
1:L:216:ALA:H	1:L:217:PRO:HD3	1.82	0.41
1:E:188:LYS:HB2	2:E:1219:CL:CL	2.57	0.41
1:F:44:ASP:O	1:F:48:MET:HG3	2.21	0.41
1:L:39:GLU:CD	1:L:39:GLU:H	2.24	0.41
1:G:9:LYS:HG3	1:G:32:LEU:HG	2.03	0.41
1:H:14:GLN:HG3	1:H:18:ARG:HD3	2.02	0.41
1:D:177:LYS:HD2	1:D:177:LYS:HA	1.86	0.41
1:E:201:TRP:CH2	1:E:217:PRO:HD3	2.55	0.41
1:J:11:ARG:HA	1:J:15:GLN:HG2	2.03	0.41
1:L:18:ARG:HH11	1:L:30:GLU:CD	2.24	0.41
1:B:73:ARG:O	1:B:77:ASP:HB2	2.21	0.41
1:C:126:LEU:N	1:C:127:PRO:CD	2.84	0.41
1:C:161:CYS:SG	1:C:203:LEU:HG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:6:GLY:HA3	1:I:57:TYR:CZ	2.56	0.41
1:I:95:ILE:HG21	1:I:151:VAL:HG11	2.03	0.41
1:K:35:ARG:HA	1:K:206:TRP:CZ3	2.56	0.41
1:C:95:ILE:HG21	1:C:151:VAL:CG1	2.51	0.41
1:D:73:ARG:O	1:D:77:ASP:HB2	2.21	0.41
1:F:207:ILE:HG12	1:F:207:ILE:O	2.21	0.41
1:E:95:ILE:HG21	1:E:151:VAL:HG11	2.04	0.40
1:F:11:ARG:NH2	3:F:2005:HOH:O	2.50	0.40
1:D:175:LYS:HD2	1:D:175:LYS:HA	1.85	0.40
1:J:198:PHE:HE1	1:J:200:LYS:HG2	1.84	0.40
1:L:73:ARG:HD2	1:L:96:GLU:OE2	2.20	0.40
1:E:36:ASP:OD1	1:E:36:ASP:N	2.55	0.40
1:E:140:ARG:HG2	1:E:145:GLY:HA2	2.02	0.40
1:G:168:GLN:HE21	1:G:168:GLN:HA	1.86	0.40
1:I:73:ARG:O	1:I:77:ASP:HB2	2.21	0.40
1:L:188:LYS:HD3	3:L:2007:HOH:O	2.21	0.40
1:C:14:GLN:O	1:C:17:VAL:HG13	2.22	0.40
1:F:41:TRP:CH2	1:F:55:LEU:HD13	2.57	0.40
1:A:73:ARG:O	1:A:77:ASP:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	217/218 (100%)	208 (96%)	8 (4%)	1 (0%)	29 41
1	B	216/218 (99%)	211 (98%)	5 (2%)	0	100 100
1	C	215/218 (99%)	199 (93%)	16 (7%)	0	100 100
1	D	216/218 (99%)	213 (99%)	3 (1%)	0	100 100
1	E	215/218 (99%)	209 (97%)	5 (2%)	1 (0%)	29 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	216/218 (99%)	208 (96%)	8 (4%)	0	100 100
1	G	215/218 (99%)	210 (98%)	5 (2%)	0	100 100
1	H	217/218 (100%)	208 (96%)	8 (4%)	1 (0%)	29 41
1	I	215/218 (99%)	209 (97%)	6 (3%)	0	100 100
1	J	215/218 (99%)	210 (98%)	5 (2%)	0	100 100
1	K	215/218 (99%)	197 (92%)	16 (7%)	2 (1%)	17 25
1	L	215/218 (99%)	191 (89%)	20 (9%)	4 (2%)	8 10
All	All	2587/2616 (99%)	2473 (96%)	105 (4%)	9 (0%)	41 55

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	217	PRO
1	A	215	ALA
1	E	67	GLN
1	K	11	ARG
1	K	45	LYS
1	L	43	GLY
1	L	11	ARG
1	L	67	GLN
1	L	216	ALA

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	190/189 (100%)	173 (91%)	17 (9%)	9 14
1	B	189/189 (100%)	173 (92%)	16 (8%)	10 16
1	C	188/189 (100%)	171 (91%)	17 (9%)	9 14
1	D	189/189 (100%)	171 (90%)	18 (10%)	8 12
1	E	188/189 (100%)	171 (91%)	17 (9%)	9 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	189/189 (100%)	175 (93%)	14 (7%)	13 22
1	G	188/189 (100%)	166 (88%)	22 (12%)	5 7
1	H	190/189 (100%)	176 (93%)	14 (7%)	13 22
1	I	188/189 (100%)	169 (90%)	19 (10%)	7 11
1	J	188/189 (100%)	174 (93%)	14 (7%)	13 22
1	K	188/189 (100%)	167 (89%)	21 (11%)	6 8
1	L	188/189 (100%)	168 (89%)	20 (11%)	6 9
All	All	2263/2268 (100%)	2054 (91%)	209 (9%)	9 13

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	19	LEU
1	A	38	ARG
1	A	55	LEU
1	A	61	ASP
1	A	65	LEU
1	A	123	LEU
1	A	131	LYS
1	A	137	LEU
1	A	140	ARG
1	A	143	LEU
1	A	151	VAL
1	A	168	GLN
1	A	170	LEU
1	A	195	SER
1	A	203	LEU
1	A	207	ILE
1	B	17	VAL
1	B	19	LEU
1	B	26	GLU
1	B	27	GLU
1	B	52	LEU
1	B	55	LEU
1	B	65	LEU
1	B	108	ARG
1	B	137	LEU
1	B	140	ARG
1	B	143	LEU

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Mol	Chain	Res	Type
1	B	151	VAL
1	B	170	LEU
1	B	172	ASP
1	B	177	LYS
1	B	203	LEU
1	C	4	LYS
1	C	17	VAL
1	C	19	LEU
1	C	38	ARG
1	C	42	LEU
1	C	55	LEU
1	C	65	LEU
1	C	69	VAL
1	C	87	GLU
1	C	112	ASN
1	C	123	LEU
1	C	137	LEU
1	C	140	ARG
1	C	143	LEU
1	C	177	LYS
1	C	188	LYS
1	C	203	LEU
1	D	17	VAL
1	D	19	LEU
1	D	26	GLU
1	D	38	ARG
1	D	40	LYS
1	D	55	LEU
1	D	65	LEU
1	D	114	LYS
1	D	123	LEU
1	D	137	LEU
1	D	140	ARG
1	D	143	LEU
1	D	151	VAL
1	D	170	LEU
1	D	180	LYS
1	D	200	LYS
1	D	203	LEU
1	D	207	ILE
1	E	17	VAL
1	E	19	LEU

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Mol	Chain	Res	Type
1	E	39	GLU
1	E	55	LEU
1	E	65	LEU
1	E	82	LEU
1	E	84	SER
1	E	123	LEU
1	E	137	LEU
1	E	140	ARG
1	E	143	LEU
1	E	170	LEU
1	E	177	LYS
1	E	180	LYS
1	E	188	LYS
1	E	196	GLU
1	E	203	LEU
1	F	17	VAL
1	F	19	LEU
1	F	26	GLU
1	F	55	LEU
1	F	63	CYS
1	F	65	LEU
1	F	137	LEU
1	F	140	ARG
1	F	143	LEU
1	F	151	VAL
1	F	170	LEU
1	F	188	LYS
1	F	200	LYS
1	F	203	LEU
1	G	4	LYS
1	G	17	VAL
1	G	19	LEU
1	G	26	GLU
1	G	29	GLU
1	G	32	LEU
1	G	39	GLU
1	G	48	MET
1	G	55	LEU
1	G	65	LEU
1	G	123	LEU
1	G	137	LEU
1	G	140	ARG

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Mol	Chain	Res	Type
1	G	143	LEU
1	G	151	VAL
1	G	168	GLN
1	G	170	LEU
1	G	180	LYS
1	G	195	SER
1	G	196	GLU
1	G	203	LEU
1	G	207	ILE
1	H	17	VAL
1	H	19	LEU
1	H	38	ARG
1	H	55	LEU
1	H	65	LEU
1	H	137	LEU
1	H	140	ARG
1	H	143	LEU
1	H	151	VAL
1	H	170	LEU
1	H	172	ASP
1	H	180	LYS
1	H	197	LYS
1	H	203	LEU
1	I	4	LYS
1	I	5	LEU
1	I	17	VAL
1	I	19	LEU
1	I	26	GLU
1	I	35	ARG
1	I	55	LEU
1	I	61	ASP
1	I	65	LEU
1	I	115	PHE
1	I	123	LEU
1	I	137	LEU
1	I	140	ARG
1	I	143	LEU
1	I	151	VAL
1	I	170	LEU
1	I	180	LYS
1	I	194	GLU
1	I	203	LEU

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Mol	Chain	Res	Type
1	J	17	VAL
1	J	19	LEU
1	J	55	LEU
1	J	61	ASP
1	J	65	LEU
1	J	123	LEU
1	J	137	LEU
1	J	140	ARG
1	J	143	LEU
1	J	151	VAL
1	J	180	LYS
1	J	200	LYS
1	J	203	LEU
1	J	214	ASP
1	K	5	LEU
1	K	17	VAL
1	K	18	ARG
1	K	42	LEU
1	K	54	ASN
1	K	57	TYR
1	K	61	ASP
1	K	63	CYS
1	K	69	VAL
1	K	114	LYS
1	K	123	LEU
1	K	137	LEU
1	K	143	LEU
1	K	151	VAL
1	K	182	ARG
1	K	188	LYS
1	K	193	MET
1	K	195	SER
1	K	196	GLU
1	K	200	LYS
1	K	203	LEU
1	L	4	LYS
1	L	5	LEU
1	L	17	VAL
1	L	19	LEU
1	L	39	GLU
1	L	40	LYS
1	L	44	ASP

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Mol	Chain	Res	Type
1	L	48	MET
1	L	55	LEU
1	L	61	ASP
1	L	64	LYS
1	L	89	ARG
1	L	131	LYS
1	L	137	LEU
1	L	139	ASP
1	L	143	LEU
1	L	151	VAL
1	L	200	LYS
1	L	207	ILE
1	L	214	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	112	ASN
1	C	141	HIS
1	D	141	HIS
1	E	47	ASN
1	E	141	HIS
1	H	112	ASN
1	J	47	ASN
1	K	54	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 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

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	217/218 (99%)	-0.24	6 (2%) 53 51	22, 38, 76, 95	0
1	B	217/218 (99%)	-0.18	1 (0%) 91 89	17, 32, 60, 79	0
1	C	217/218 (99%)	-0.01	12 (5%) 25 24	19, 43, 107, 117	0
1	D	217/218 (99%)	-0.46	0 100 100	16, 29, 45, 64	0
1	E	217/218 (99%)	-0.61	0 100 100	18, 30, 52, 70	0
1	F	217/218 (99%)	-0.31	1 (0%) 91 89	22, 38, 60, 80	0
1	G	217/218 (99%)	0.01	8 (3%) 41 41	22, 38, 73, 92	0
1	H	217/218 (99%)	-0.28	3 (1%) 75 73	16, 32, 63, 85	0
1	I	217/218 (99%)	-0.24	7 (3%) 47 46	21, 34, 71, 105	0
1	J	217/218 (99%)	-0.41	3 (1%) 75 73	22, 35, 58, 70	0
1	K	217/218 (99%)	-0.13	5 (2%) 60 58	17, 45, 70, 86	0
1	L	217/218 (99%)	0.60	18 (8%) 11 10	27, 68, 99, 116	0
All	All	2604/2616 (99%)	-0.19	64 (2%) 57 55	16, 36, 77, 117	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	218	ALA	7.1
1	I	218	ALA	7.0
1	L	215	ALA	5.3
1	C	215	ALA	5.2
1	C	207	ILE	5.1
1	C	214	ASP	4.8
1	C	210	PHE	4.2
1	K	46	PHE	3.9
1	B	218	ALA	3.8
1	A	218	ALA	3.8
1	L	216	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	I	114	LYS	3.7
1	L	185	ASP	3.5
1	L	218	ALA	3.5
1	I	113	PRO	3.5
1	J	218	ALA	3.4
1	F	218	ALA	3.2
1	G	218	ALA	3.1
1	C	113	PRO	3.0
1	L	130	LEU	3.0
1	A	114	LYS	2.9
1	G	2	PRO	2.9
1	L	214	ASP	2.9
1	I	2	PRO	2.9
1	A	113	PRO	2.8
1	J	2	PRO	2.8
1	L	167	PRO	2.8
1	C	218	ALA	2.8
1	L	2	PRO	2.8
1	L	109	VAL	2.7
1	C	168	GLN	2.7
1	C	115	PHE	2.6
1	G	31	HIS	2.6
1	K	189	ILE	2.6
1	A	117	GLU	2.6
1	I	215	ALA	2.5
1	G	32	LEU	2.5
1	L	207	ILE	2.5
1	K	218	ALA	2.5
1	G	3	ALA	2.5
1	I	216	ALA	2.5
1	H	117	GLU	2.5
1	K	146	SER	2.4
1	C	114	LYS	2.4
1	L	174	PRO	2.4
1	L	111	TYR	2.4
1	A	110	CYS	2.4
1	H	217	PRO	2.4
1	L	203	LEU	2.4
1	G	217	PRO	2.4
1	L	36	ASP	2.4
1	L	170	LEU	2.3
1	C	217	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	217	PRO	2.3
1	L	213	GLY	2.3
1	C	123	LEU	2.3
1	L	171	GLU	2.1
1	A	111	TYR	2.1
1	C	122	TYR	2.1
1	G	9	LYS	2.1
1	K	78	LYS	2.0
1	L	113	PRO	2.0
1	I	115	PHE	2.0
1	G	194	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	G	1219	1/1	0.69	0.15	79,79,79,79	0
2	CL	H	1220	1/1	0.93	0.16	43,43,43,43	0
2	CL	I	1219	1/1	0.94	0.17	78,78,78,78	0
2	CL	D	1220	1/1	0.95	0.17	54,54,54,54	0
2	CL	J	1220	1/1	0.95	0.21	52,52,52,52	0
2	CL	H	1219	1/1	0.97	0.10	40,40,40,40	0
2	CL	F	1219	1/1	0.97	0.08	59,59,59,59	0
2	CL	A	1219	1/1	0.98	0.12	64,64,64,64	0
2	CL	J	1219	1/1	0.98	0.13	48,48,48,48	0
2	CL	E	1219	1/1	0.98	0.06	47,47,47,47	0
2	CL	D	1219	1/1	0.99	0.06	38,38,38,38	0
2	CL	B	1219	1/1	0.99	0.11	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.