



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:41 PM UTC

PDB ID : 2WRT / pdb_00002wrt
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 : 4-5-2 with Phenix2.0
Xtrriage (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

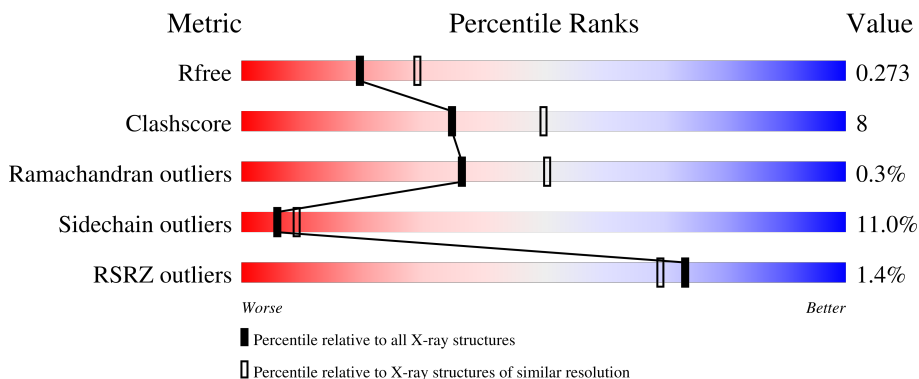
1 Overall quality at a glance

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	218	
1	B	218	
1	C	218	
1	D	218	
1	E	218	

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Mol	Chain	Length	Quality of chain
1	F	218	 77% 18% 5%
1	G	218	 3% 78% 18% .
1	H	218	 78% 18% .
1	I	218	 2% 76% 22% .
1	J	218	 80% 17% .
1	K	218	 5% 72% 24% .
1	L	218	 3% 68% 28% .

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	D	1219	-	-	X	-
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
			Total	C	N	O	S			
1	A	217	1789	1155	298	323	13	0	2	0
1	B	217	1778	1148	293	324	13	0	1	0
1	C	217	1772	1144	293	322	13	0	0	0
1	D	217	1778	1148	294	323	13	0	1	0
1	E	217	1772	1144	293	322	13	0	0	0
1	F	217	1778	1149	294	322	13	0	1	0
1	G	217	1772	1144	293	322	13	0	0	0
1	H	217	1786	1153	296	324	13	0	2	0
1	I	217	1772	1144	293	322	13	0	0	0
1	J	217	1772	1144	293	322	13	0	0	0
1	K	217	1772	1144	293	322	13	0	0	0
1	L	217	1772	1144	293	322	13	0	0	0

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 (CCD ID: 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 1	Cl 1	0	0
2	F	1	Total 1	Cl 1	0	0
2	G	1	Total 1	Cl 1	0	0
2	H	2	Total 2	Cl 2	0	0
2	I	1	Total 1	Cl 1	0	0
2	J	2	Total 2	Cl 2	0	0

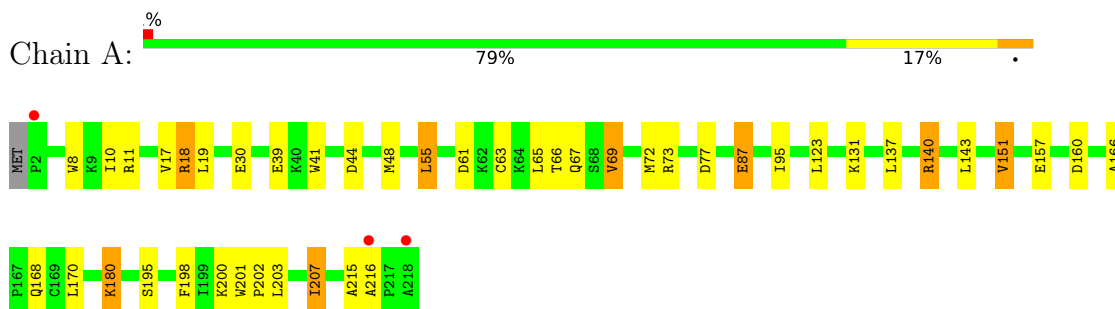
- Molecule 3 is water.

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

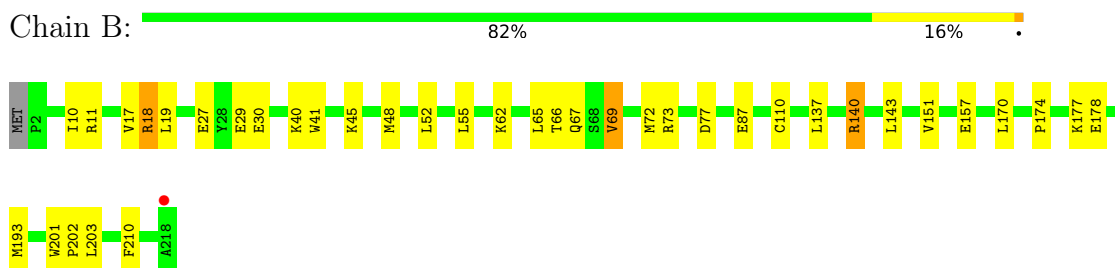
3 Residue-property plots

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.

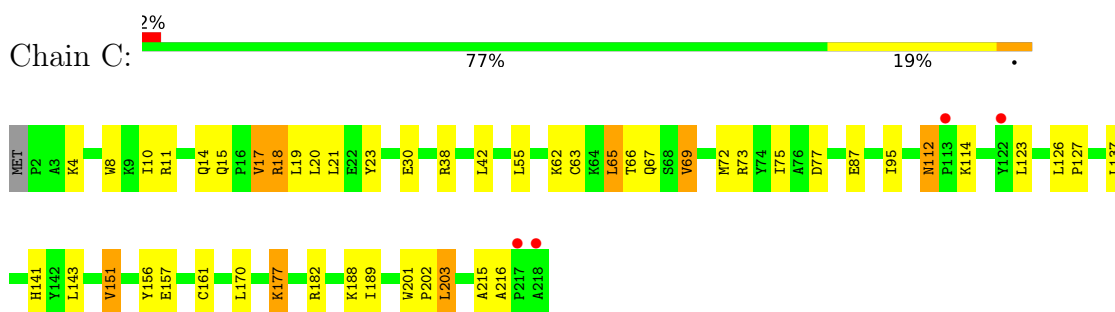
- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51



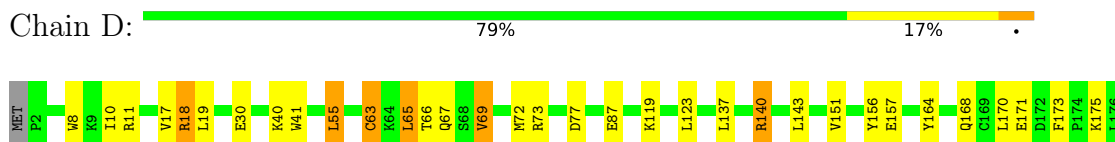
- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51



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



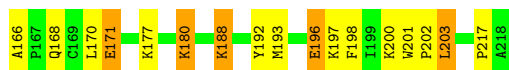
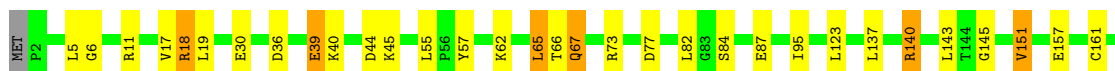
- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51





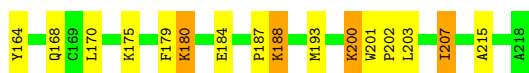
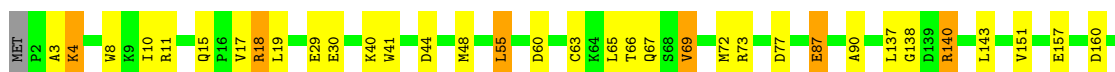
- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51

Chain E: 77% 17% 5%



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

Chain F: 77% 18% 5%



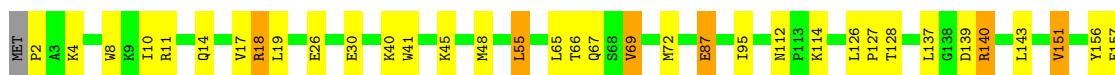
- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51

Chain G: 3% 78% 18% .



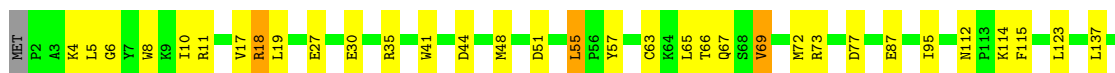
- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51

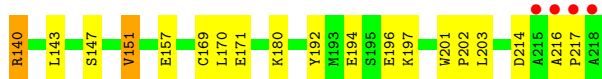
Chain H: 78% 18% .



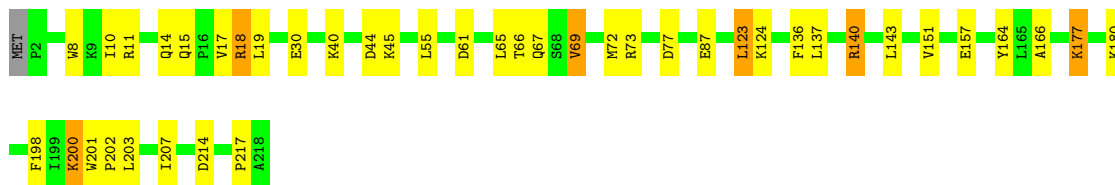
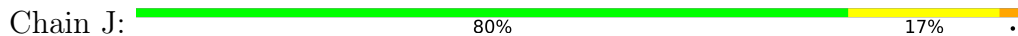
- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51

Chain I: 2% 76% 22% .

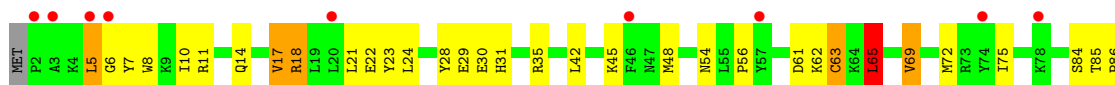
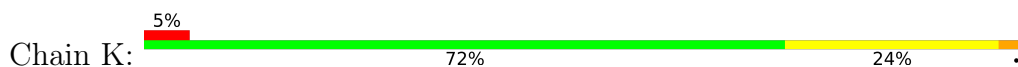




- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME 51



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



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



4 Data and refinement statistics

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 – 2.40 165.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (166.67-2.40) 99.8 (165.90-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.39Å)	Xtrriage
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	Xtrriage
Anisotropy	0.622	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

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	0.53	0/1839	0.85	3/2475 (0.1%)
1	B	0.58	0/1828	0.86	0/2462
1	C	0.57	0/1819	0.86	0/2450
1	D	0.59	0/1828	0.86	3/2462 (0.1%)
1	E	0.58	0/1819	0.86	2/2450 (0.1%)
1	F	0.54	0/1828	0.85	0/2461
1	G	0.56	0/1819	0.85	0/2450
1	H	0.57	0/1839	0.86	2/2476 (0.1%)
1	I	0.54	0/1819	0.84	2/2450 (0.1%)
1	J	0.53	0/1819	0.81	0/2450
1	K	0.57	0/1819	0.93	3/2450 (0.1%)
1	L	0.52	0/1819	0.86	0/2450
All	All	0.56	0/21895	0.86	15/29486 (0.1%)

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

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	186	LEU	CA-C-N	6.16	125.64	119.24
1	H	186	LEU	C-N-CA	6.16	125.64	119.24
1	K	6	GLY	N-CA-C	5.79	119.56	110.71
1	A	63	CYS	N-CA-C	5.69	117.06	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	65	LEU	N-CA-C	5.52	117.43	108.26
1	A	166	ALA	CA-C-N	5.48	125.09	119.56
1	A	166	ALA	C-N-CA	5.48	125.09	119.56
1	E	166	ALA	CA-C-N	5.42	125.08	119.56
1	E	166	ALA	C-N-CA	5.42	125.08	119.56
1	I	63	CYS	N-CA-C	5.35	116.54	108.46
1	D	63	CYS	N-CA-C	5.34	117.88	108.75
1	K	63	CYS	N-CA-C	5.24	117.35	109.23
1	I	169	CYS	N-CA-C	5.02	117.49	111.71
1	D	173	PHE	CA-C-N	5.02	125.04	119.32
1	D	173	PHE	C-N-CA	5.02	125.04	119.32

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	19	0
1	B	1778	0	1758	16	0
1	C	1772	0	1752	27	0
1	D	1778	0	1760	22	0
1	E	1772	0	1752	25	0
1	F	1778	0	1765	30	0
1	G	1772	0	1752	25	0
1	H	1786	0	1771	28	0
1	I	1772	0	1752	21	0
1	J	1772	0	1752	19	0
1	K	1772	0	1752	48	0
1	L	1772	0	1752	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	2	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	8	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	318	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 8.

All (318) 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:K:184:GLU:HG2	1:K:193:MET:HE1	1.62	0.82
1:L:78:LYS:HA	3:L:2023:HOH:O	1.80	0.81
1:G:196:GLU:CD	1:G:196:GLU:H	1.89	0.79
1:D:168[B]:GLN:HA	1:D:168[B]:GLN:NE2	1.97	0.79
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:B:193:MET:HE3	3:B:2038:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:69:VAL:HA	1:C:72:MET:HE3	1.77	0.65
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:E:39:GLU:CD	1:E:39:GLU:H	2.07	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:A:39:GLU:OE1	1:A:39:GLU:HA	1.98	0.61
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:69:VAL:HA	1:A:72:MET:HE3	1.90	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: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:I:44:ASP:HB3	1:I:48:MET:HE3	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:44:ASP:HB3	1:F:48:MET:HE3	1.93	0.51
1:K:31:HIS:HA	3:K:2021:HOH:O	2.10	0.51
1:B:193:MET:CE	3:B:2038:HOH:O	2.53	0.51
1:L:69:VAL:HA	1:L:72:MET:HE3	1.91	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
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:G:69:VAL:HA	1:G:72:MET:HE3	1.93	0.49
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:F:69:VAL:HA	1:F:72:MET:HE3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O	1:A:207:ILE:HG12	2.14	0.46
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:J:69:VAL:HA	1:J:72:MET:HE3	1.97	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:I:69:VAL:HA	1:I:72:MET:HE3	1.97	0.46
1:K:22:GLU:OE2	1:K:28:TYR:OH	2.29	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:39:GLU:CD	1:L:39:GLU:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:GLU:HG2	1:F:193:MET:HE1	1.97	0.46
1:I:147:SER:HB2	3:I:2066:HOH:O	2.15	0.46
1:L:18:ARG:HH11	1:L:30:GLU:CD	2.24	0.46
1:B:69:VAL:HA	1:B:72:MET:HE3	1.97	0.45
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
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:C:156:TYR:CD1	1:C:156:TYR:C	2.95	0.44
1:D:69:VAL:HA	1:D:72:MET:HE3	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:44:ASP:O	1:E:45:LYS:C	2.61	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:F:179:PHE:O	1:F:180:LYS:C	2.61	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:H:69:VAL:HA	1:H:72:MET:HE3	2.00	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
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:H:87:GLU:H	1:H:87:GLU:CD	2.26	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:A:87:GLU:H	1:A:87:GLU:CD	2.28	0.42
1:L:160:ASP:O	1:L:164:TYR:CE1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:87:GLU:CD	1:G:87:GLU:H	2.26	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:I:44:ASP:HB3	1:I:48:MET:CE	2.49	0.42
1:K:69:VAL:HA	1:K:72:MET:HE3	2.01	0.42
1:K:136:PHE:O	1:K:140:ARG:NH2	2.53	0.42
1:D:188:LYS:NZ	2:D:1219:CL:CL	2.84	0.41
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:A:44:ASP:HB3	1:A:48:MET:HE3	2.03	0.41
1:H:48:MET:HE3	3:H:2039:HOH:O	2.20	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: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
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:87:GLU:CD	1:F:87:GLU:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:187:PRO:HD2	1:K:188:LYS:HZ1	1.86	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:J:44:ASP:O	1:J:45:LYS:C	2.65	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%)	24	37
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%)	24	37
1	F	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
1	G	215/218 (99%)	210 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	217/218 (100%)	208 (96%)	8 (4%)	1 (0%)	24	37
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%)	14	22
1	L	215/218 (99%)	191 (89%)	20 (9%)	4 (2%)	6	8
All	All	2587/2616 (99%)	2473 (96%)	105 (4%)	9 (0%)	36	50

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%)	170 (90%)	20 (10%)	6	10
1	B	189/189 (100%)	170 (90%)	19 (10%)	7	11
1	C	188/189 (100%)	169 (90%)	19 (10%)	7	11
1	D	189/189 (100%)	170 (90%)	19 (10%)	7	11
1	E	188/189 (100%)	166 (88%)	22 (12%)	5	7
1	F	189/189 (100%)	169 (89%)	20 (11%)	6	10
1	G	188/189 (100%)	163 (87%)	25 (13%)	4	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	190/189 (100%)	172 (90%)	18 (10%)	8	13
1	I	188/189 (100%)	166 (88%)	22 (12%)	5	7
1	J	188/189 (100%)	167 (89%)	21 (11%)	6	9
1	K	188/189 (100%)	170 (90%)	18 (10%)	8	12
1	L	188/189 (100%)	162 (86%)	26 (14%)	3	4
All	All	2263/2268 (100%)	2014 (89%)	249 (11%)	6	9

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	18	ARG
1	A	19	LEU
1	A	55	LEU
1	A	61	ASP
1	A	65	LEU
1	A	69	VAL
1	A	87	GLU
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	180	LYS
1	A	195	SER
1	A	203	LEU
1	A	207	ILE
1	B	17	VAL
1	B	18	ARG
1	B	19	LEU
1	B	27	GLU
1	B	40	LYS
1	B	48	MET
1	B	52	LEU
1	B	55	LEU
1	B	62	LYS
1	B	65	LEU

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Mol	Chain	Res	Type
1	B	69	VAL
1	B	87	GLU
1	B	137	LEU
1	B	140	ARG
1	B	143	LEU
1	B	151	VAL
1	B	170	LEU
1	B	177	LYS
1	B	203	LEU
1	C	4	LYS
1	C	17	VAL
1	C	18	ARG
1	C	19	LEU
1	C	20	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	143	LEU
1	C	151	VAL
1	C	177	LYS
1	C	188	LYS
1	C	203	LEU
1	D	17	VAL
1	D	18	ARG
1	D	19	LEU
1	D	40	LYS
1	D	55	LEU
1	D	65	LEU
1	D	69	VAL
1	D	87	GLU
1	D	119	LYS
1	D	123	LEU
1	D	137	LEU
1	D	140	ARG
1	D	143	LEU
1	D	151	VAL

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Mol	Chain	Res	Type
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	18	ARG
1	E	19	LEU
1	E	39	GLU
1	E	55	LEU
1	E	62	LYS
1	E	65	LEU
1	E	82	LEU
1	E	84	SER
1	E	87	GLU
1	E	123	LEU
1	E	137	LEU
1	E	140	ARG
1	E	143	LEU
1	E	151	VAL
1	E	170	LEU
1	E	171	GLU
1	E	177	LYS
1	E	180	LYS
1	E	188	LYS
1	E	196	GLU
1	E	203	LEU
1	F	4	LYS
1	F	17	VAL
1	F	18	ARG
1	F	19	LEU
1	F	55	LEU
1	F	63	CYS
1	F	65	LEU
1	F	69	VAL
1	F	87	GLU
1	F	137	LEU
1	F	140	ARG
1	F	143	LEU
1	F	151	VAL
1	F	168	GLN
1	F	170	LEU

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Mol	Chain	Res	Type
1	F	180	LYS
1	F	188	LYS
1	F	200	LYS
1	F	203	LEU
1	F	207	ILE
1	G	4	LYS
1	G	17	VAL
1	G	18	ARG
1	G	19	LEU
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	69	VAL
1	G	87	GLU
1	G	123	LEU
1	G	137	LEU
1	G	140	ARG
1	G	143	LEU
1	G	151	VAL
1	G	168	GLN
1	G	170	LEU
1	G	180	LYS
1	G	188	LYS
1	G	195	SER
1	G	196	GLU
1	G	203	LEU
1	G	207	ILE
1	H	17	VAL
1	H	18	ARG
1	H	19	LEU
1	H	55	LEU
1	H	65	LEU
1	H	69	VAL
1	H	87	GLU
1	H	128	THR
1	H	137	LEU
1	H	140	ARG
1	H	143	LEU
1	H	151	VAL

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Mol	Chain	Res	Type
1	H	170	LEU
1	H	172	ASP
1	H	180	LYS
1	H	197	LYS
1	H	203	LEU
1	H	207	ILE
1	I	4	LYS
1	I	5	LEU
1	I	17	VAL
1	I	18	ARG
1	I	19	LEU
1	I	27	GLU
1	I	35	ARG
1	I	55	LEU
1	I	65	LEU
1	I	69	VAL
1	I	87	GLU
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	196	GLU
1	I	203	LEU
1	J	17	VAL
1	J	18	ARG
1	J	19	LEU
1	J	40	LYS
1	J	55	LEU
1	J	61	ASP
1	J	65	LEU
1	J	69	VAL
1	J	87	GLU
1	J	123	LEU
1	J	124	LYS
1	J	137	LEU
1	J	140	ARG
1	J	143	LEU

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Mol	Chain	Res	Type
1	J	151	VAL
1	J	177	LYS
1	J	180	LYS
1	J	200	LYS
1	J	203	LEU
1	J	207	ILE
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	61	ASP
1	K	65	LEU
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	188	LYS
1	K	193	MET
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	18	ARG
1	L	19	LEU
1	L	39	GLU
1	L	40	LYS
1	L	44	ASP
1	L	48	MET
1	L	55	LEU
1	L	61	ASP
1	L	64	LYS
1	L	69	VAL
1	L	89	ARG
1	L	92	ILE
1	L	95	ILE
1	L	135	ASN

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Mol	Chain	Res	Type
1	L	137	LEU
1	L	139	ASP
1	L	143	LEU
1	L	151	VAL
1	L	175	LYS
1	L	180	LYS
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 (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	B	79	HIS
1	C	67	GLN
1	C	112	ASN
1	C	141	HIS
1	D	47	ASN
1	D	141	HIS
1	E	141	HIS
1	E	168	GLN
1	F	47	ASN
1	G	168	GLN
1	H	112	ASN
1	J	67	GLN
1	K	54	ASN
1	L	15	GLN
1	L	67	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 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 [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 i

6.1 Protein, DNA and RNA chains i

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	217/218 (99%)	-0.11	3 (1%) 73 69	18, 38, 76, 95	2 (0%)
1	B	217/218 (99%)	-0.20	1 (0%) 87 85	17, 32, 60, 79	1 (0%)
1	C	217/218 (99%)	0.03	4 (1%) 67 63	19, 43, 107, 117	0
1	D	217/218 (99%)	-0.35	0 100 100	14, 29, 45, 64	1 (0%)
1	E	217/218 (99%)	-0.47	0 100 100	18, 30, 52, 70	0
1	F	217/218 (99%)	-0.12	0 100 100	22, 38, 60, 80	1 (0%)
1	G	217/218 (99%)	0.17	6 (2%) 55 51	22, 38, 73, 92	0
1	H	217/218 (99%)	-0.21	1 (0%) 87 85	16, 32, 63, 85	2 (0%)
1	I	217/218 (99%)	-0.09	4 (1%) 67 63	21, 34, 71, 105	0
1	J	217/218 (99%)	-0.22	0 100 100	22, 35, 58, 70	0
1	K	217/218 (99%)	0.28	11 (5%) 33 30	17, 45, 70, 86	0
1	L	217/218 (99%)	0.82	7 (3%) 50 46	27, 68, 99, 116	0
All	All	2604/2616 (99%)	-0.04	37 (1%) 73 69	14, 36, 77, 117	7 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	217	PRO	3.9
1	I	215	ALA	3.6
1	I	218	ALA	3.5
1	I	216	ALA	3.4
1	K	3	ALA	3.3
1	L	207	ILE	3.3
1	L	2	PRO	3.1
1	K	6	GLY	3.0
1	B	218	ALA	3.0
1	K	189	ILE	2.9
1	A	2	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	78	LYS	2.7
1	K	5	LEU	2.6
1	L	216	ALA	2.6
1	A	218	ALA	2.5
1	L	109	VAL	2.5
1	G	216	ALA	2.5
1	G	43	GLY	2.4
1	K	2	PRO	2.3
1	A	216	ALA	2.3
1	L	218	ALA	2.3
1	L	215	ALA	2.3
1	K	192	TYR	2.3
1	L	115	PHE	2.2
1	K	57	TYR	2.2
1	G	2	PRO	2.2
1	H	218	ALA	2.2
1	K	20	LEU	2.1
1	C	217	PRO	2.1
1	C	113	PRO	2.1
1	K	46	PHE	2.1
1	C	218	ALA	2.1
1	C	122	TYR	2.1
1	K	74	TYR	2.1
1	G	3	ALA	2.0
1	I	217	PRO	2.0
1	G	218	ALA	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 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(\AA^2)	Q<0.9
2	CL	G	1219	1/1	0.88	0.11	79,79,79,79	0
2	CL	I	1219	1/1	0.89	0.12	78,78,78,78	0
2	CL	H	1220	1/1	0.91	0.08	43,43,43,43	0
2	CL	F	1219	1/1	0.93	0.08	59,59,59,59	0
2	CL	D	1220	1/1	0.93	0.10	54,54,54,54	0
2	CL	A	1219	1/1	0.95	0.08	64,64,64,64	0
2	CL	J	1219	1/1	0.95	0.08	48,48,48,48	0
2	CL	J	1220	1/1	0.97	0.11	52,52,52,52	0
2	CL	B	1219	1/1	0.98	0.03	37,37,37,37	0
2	CL	E	1219	1/1	0.98	0.06	47,47,47,47	0
2	CL	D	1219	1/1	0.99	0.03	38,38,38,38	0
2	CL	H	1219	1/1	0.99	0.04	40,40,40,40	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.