



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:37 AM UTC

PDB ID : 1WOI / pdb_00001woi
Title : Crystal Structure of Agmatinase Reveals Structural Conservation and Inhibition Mechanism of the Ureohydrolase Superfamily
Authors : Ahn, H.J.; Kim, K.H.; Lee, J.; Ha, J.-Y.; Lee, H.H.; Kim, D.; Yoon, H.-J.; Kwon, A.-R.; Suh, S.W.
Deposited on : 2004-08-18
Resolution : 1.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

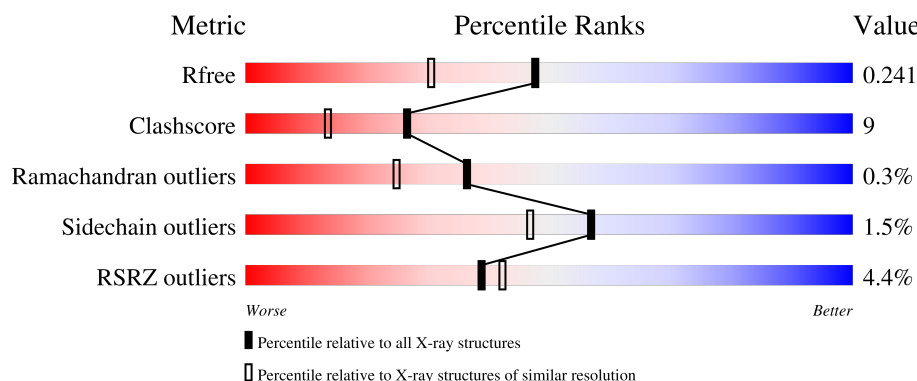
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	305	3% 79% 19% ..
1	B	305	6% 77% 21% ..
1	C	305	4% 80% 19% ..
1	D	305	7% 80% 18% ..
1	E	305	4% 80% 18% ..

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Mol	Chain	Length	Quality of chain
1	F	305	2% 80% 17% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14401 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 agmatinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2287	1446	409	425	7			
1	B	303	Total	C	N	O	S	0	0	0
			2287	1446	409	425	7			
1	C	303	Total	C	N	O	S	0	0	0
			2286	1446	409	424	7			
1	D	303	Total	C	N	O	S	0	0	0
			2287	1446	409	425	7			
1	E	303	Total	C	N	O	S	0	0	0
			2287	1446	409	425	7			
1	F	303	Total	C	N	O	S	0	0	0
			2287	1446	409	425	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	LEU	-	cloning artifact	UNP Q9RZ04
B	305	LEU	-	cloning artifact	UNP Q9RZ04
C	305	LEU	-	cloning artifact	UNP Q9RZ04
D	305	LEU	-	cloning artifact	UNP Q9RZ04
E	305	LEU	-	cloning artifact	UNP Q9RZ04
F	305	LEU	-	cloning artifact	UNP Q9RZ04

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total 2	Mn 2	0	0
2	E	2	Total 2	Mn 2	0	0
2	F	2	Total 2	Mn 2	0	0

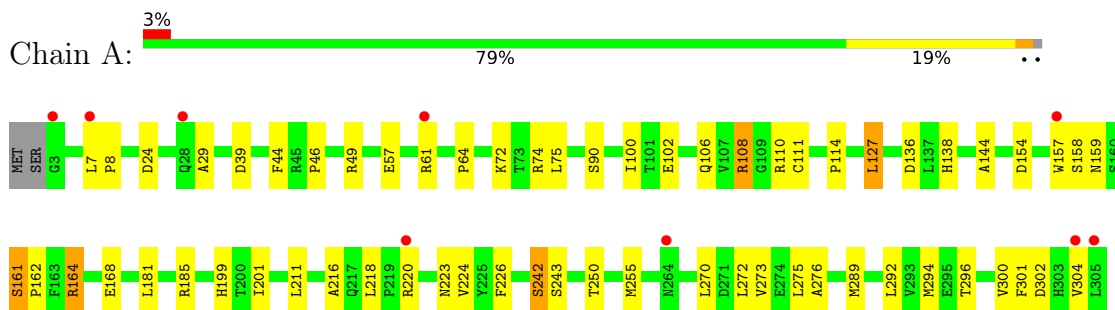
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	134	Total 134	O 134	0	0
3	B	97	Total 97	O 97	0	0
3	C	124	Total 124	O 124	0	0
3	D	92	Total 92	O 92	0	0
3	E	106	Total 106	O 106	0	0
3	F	115	Total 115	O 115	0	0

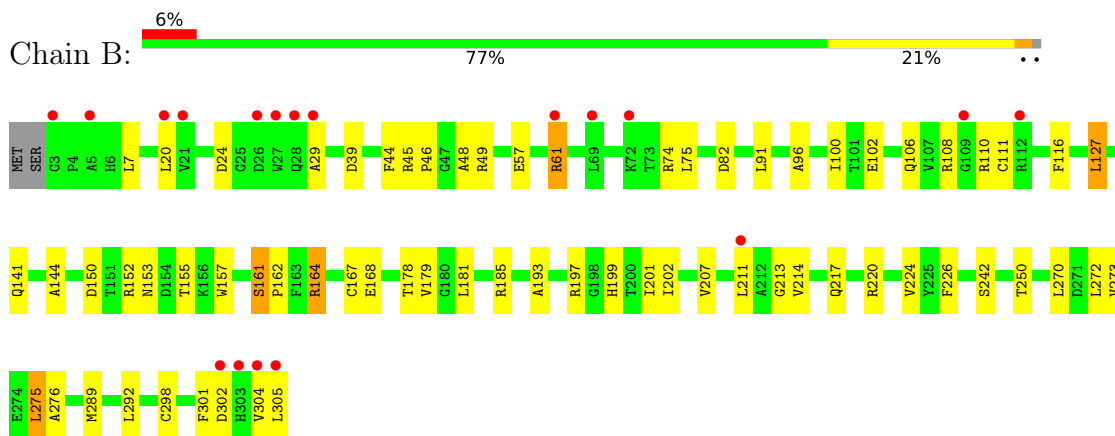
3 Residue-property plots [i](#)

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.

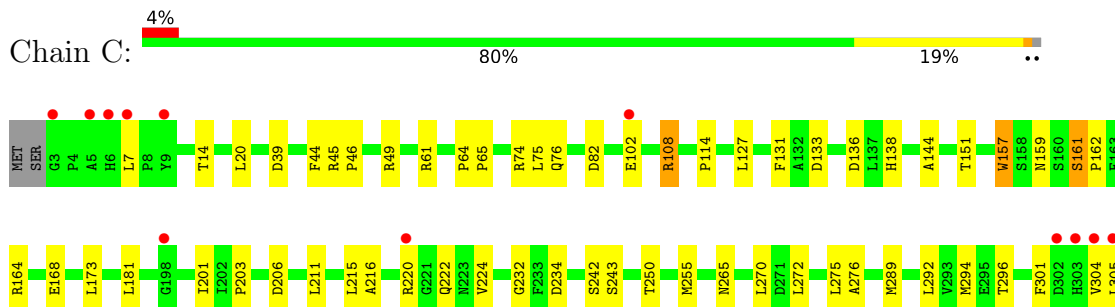
• Molecule 1: agmatinase



• Molecule 1: agmatinase

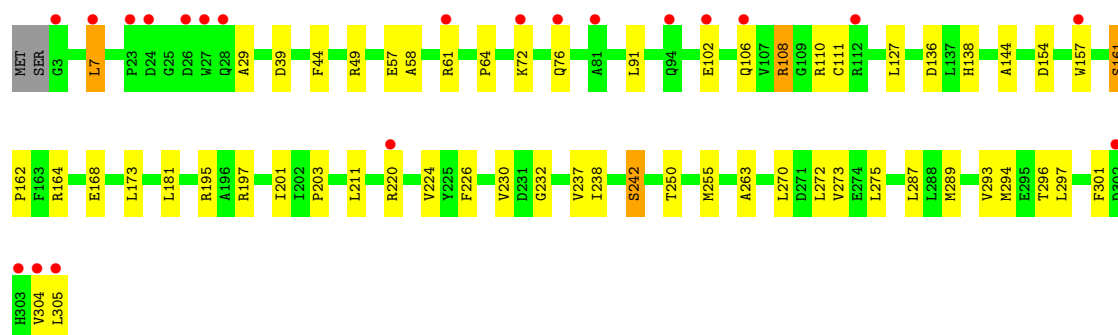


• Molecule 1: agmatinase



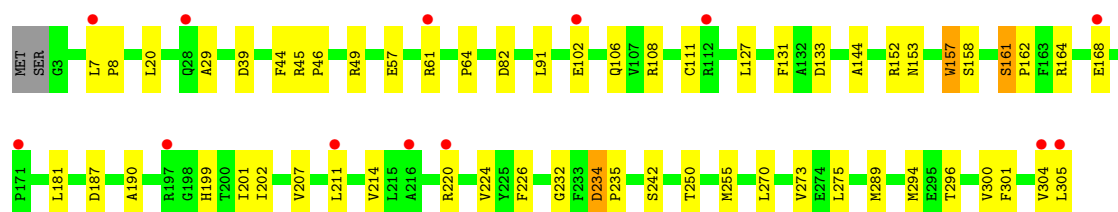
• Molecule 1: agmatinase

Chain D:  7% 80% 18% ..



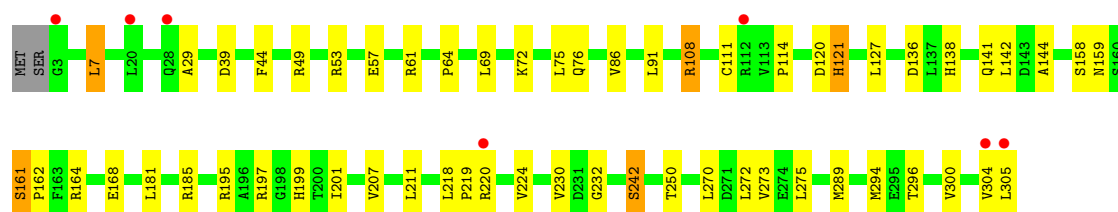
• Molecule 1: agmatinase

Chain E:  4% 80% 18% ..



• Molecule 1: agmatinase

Chain F:  2% 80% 17% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.76Å 130.76Å 168.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 1.85 29.99 – 1.85	Depositor EDS
% Data completeness (in resolution range)	93.5 (29.99-1.85) 93.6 (29.99-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.82 (at 1.85Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.241 0.210 , 0.241	Depositor DCC
R_{free} test set	14355 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14401	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.43	2/2342 (0.1%)	0.93	12/3202 (0.4%)
1	B	0.37	0/2342	0.93	10/3202 (0.3%)
1	C	0.43	1/2341 (0.0%)	0.94	12/3200 (0.4%)
1	D	0.36	0/2342	0.92	9/3202 (0.3%)
1	E	0.39	1/2342 (0.0%)	0.95	11/3202 (0.3%)
1	F	0.44	2/2342 (0.1%)	0.93	10/3202 (0.3%)
All	All	0.40	6/14051 (0.0%)	0.93	64/19210 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	159	ASN	C-N	9.27	1.47	1.33
1	F	159	ASN	C-N	-7.77	1.22	1.33
1	E	158	SER	C-N	-6.94	1.23	1.33
1	A	158	SER	C-N	-6.57	1.23	1.33
1	A	159	ASN	C-N	-6.22	1.24	1.33
1	F	158	SER	C-N	-6.13	1.24	1.33

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	7	LEU	N-CA-C	-8.68	100.15	110.13
1	D	250	THR	N-CA-C	-8.55	99.50	110.53
1	E	250	THR	N-CA-C	-8.21	99.93	110.53
1	A	250	THR	N-CA-C	-8.04	100.16	110.53
1	C	250	THR	N-CA-C	-7.90	100.34	110.53
1	B	250	THR	N-CA-C	-7.90	99.89	110.55
1	F	7	LEU	N-CA-C	-7.87	101.08	110.13
1	F	250	THR	N-CA-C	-7.73	100.55	110.53
1	E	7	LEU	N-CA-C	-7.39	101.63	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	LEU	N-CA-C	-7.29	101.74	110.13
1	C	7	LEU	N-CA-C	-6.94	102.15	110.13
1	E	232	GLY	N-CA-C	-6.76	105.98	114.16
1	B	7	LEU	N-CA-C	-6.56	102.59	110.13
1	F	242	SER	N-CA-C	6.36	117.88	111.07
1	F	224	VAL	N-CA-C	6.29	116.91	108.11
1	C	242	SER	N-CA-C	6.24	117.75	111.07
1	A	144	ALA	N-CA-C	-6.22	105.51	113.23
1	D	144	ALA	N-CA-C	-6.21	105.53	113.23
1	C	224	VAL	N-CA-C	6.18	117.38	108.48
1	B	224	VAL	N-CA-C	6.17	117.36	108.48
1	A	242	SER	N-CA-C	6.10	117.60	111.07
1	D	273	VAL	N-CA-C	6.08	117.59	108.96
1	C	14	THR	N-CA-C	-6.07	100.74	110.14
1	F	144	ALA	N-CA-C	-6.04	105.74	113.23
1	E	242	SER	N-CA-C	5.99	118.30	111.11
1	F	273	VAL	N-CA-C	5.96	117.43	108.96
1	C	157	TRP	N-CA-C	5.96	119.51	112.72
1	F	142	LEU	N-CA-C	-5.90	99.62	109.24
1	E	224	VAL	N-CA-C	5.85	116.90	108.48
1	B	273	VAL	N-CA-C	5.82	117.30	108.80
1	C	144	ALA	N-CA-C	-5.82	106.02	113.23
1	A	273	VAL	N-CA-C	5.73	117.10	108.96
1	E	234	ASP	CA-C-N	5.73	125.58	119.28
1	E	234	ASP	C-N-CA	5.73	125.58	119.28
1	D	232	GLY	N-CA-C	-5.69	105.75	113.37
1	A	276	ALA	CA-C-N	5.65	125.33	119.05
1	A	276	ALA	C-N-CA	5.65	125.33	119.05
1	B	276	ALA	CA-C-N	5.64	125.75	119.32
1	B	276	ALA	C-N-CA	5.64	125.75	119.32
1	B	144	ALA	N-CA-C	-5.55	106.00	112.89
1	F	86	VAL	N-CA-C	-5.54	102.44	109.58
1	F	232	GLY	N-CA-C	-5.53	105.96	113.37
1	B	242	SER	N-CA-C	5.49	117.70	111.11
1	A	90	SER	N-CA-C	-5.46	100.80	109.76
1	D	242	SER	N-CA-C	5.40	117.59	111.11
1	C	232	GLY	N-CA-C	-5.38	106.16	113.37
1	E	91	LEU	CB-CA-C	-5.37	110.41	116.63
1	E	144	ALA	N-CA-C	-5.37	106.24	112.89
1	D	224	VAL	N-CA-C	5.36	116.19	108.48
1	E	273	VAL	N-CA-C	5.34	116.54	108.96
1	D	154	ASP	N-CA-C	5.33	119.06	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	ARG	N-CA-C	-5.32	105.39	111.14
1	F	121	HIS	N-CA-C	5.28	118.82	112.38
1	C	234	ASP	CA-C-N	5.24	125.04	119.28
1	C	234	ASP	C-N-CA	5.24	125.04	119.28
1	D	157	TRP	N-CA-C	5.24	118.98	112.59
1	A	164	ARG	N-CA-C	-5.22	105.50	111.14
1	B	157	TRP	N-CA-C	5.20	119.31	112.92
1	A	154	ASP	N-CA-C	5.19	118.88	112.24
1	A	223	ASN	N-CA-C	-5.12	100.83	108.96
1	C	276	ALA	CA-C-N	5.09	125.12	119.32
1	C	276	ALA	C-N-CA	5.09	125.12	119.32
1	A	224	VAL	N-CA-C	5.09	115.81	108.48
1	E	157	TRP	N-CA-C	5.01	118.43	112.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2287	0	2266	44	0
1	B	2287	0	2266	54	0
1	C	2286	0	2266	45	0
1	D	2287	0	2266	47	0
1	E	2287	0	2266	43	0
1	F	2287	0	2266	48	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	134	0	0	2	0
3	B	97	0	0	3	0
3	C	124	0	0	2	0
3	D	92	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	106	0	0	4	0
3	F	115	0	0	7	0
All	All	14401	0	13596	254	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 9.

All (254) 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:B:272:LEU:HD21	1:B:289:MET:HE2	1.34	1.09
1:F:230:VAL:HG12	1:F:289:MET:HE2	1.18	1.09
1:C:272:LEU:HD21	1:C:289:MET:HE2	1.32	1.09
1:F:272:LEU:HD21	1:F:289:MET:HE3	1.38	1.04
1:A:272:LEU:HD21	1:A:289:MET:HE2	1.48	0.95
1:F:300:VAL:O	1:F:304:VAL:HG23	1.67	0.94
1:C:181:LEU:HD12	1:C:201:ILE:HG23	1.53	0.89
1:B:181:LEU:HD12	1:B:201:ILE:HG23	1.57	0.87
1:A:272:LEU:HD21	1:A:289:MET:CE	2.05	0.86
1:F:272:LEU:HD21	1:F:289:MET:CE	2.07	0.84
1:E:181:LEU:HD12	1:E:201:ILE:HG23	1.62	0.81
1:C:272:LEU:HD21	1:C:289:MET:CE	2.11	0.80
1:A:181:LEU:HD12	1:A:201:ILE:HG23	1.64	0.80
1:D:238:ILE:HG13	1:D:289:MET:HE1	1.65	0.78
1:D:230:VAL:HB	1:D:289:MET:HE3	1.64	0.78
1:B:289:MET:HE1	1:B:292:LEU:HD22	1.65	0.78
1:D:272:LEU:HD21	1:D:289:MET:HG3	1.73	0.70
1:D:301:PHE:HA	1:D:304:VAL:HG23	1.74	0.70
1:B:46:PRO:HG3	1:E:49:ARG:NH1	2.07	0.69
1:D:61:ARG:HE	1:D:61:ARG:HA	1.57	0.68
1:A:39:ASP:OD2	1:A:49:ARG:HD2	1.94	0.67
1:B:289:MET:HE1	1:B:292:LEU:CD2	2.24	0.67
1:A:300:VAL:O	1:A:304:VAL:HG23	1.94	0.67
1:B:289:MET:HE3	1:B:289:MET:HA	1.76	0.66
1:C:301:PHE:HA	1:C:304:VAL:HG23	1.76	0.66
1:F:207:VAL:HG13	1:F:211:LEU:HD23	1.77	0.66
1:B:272:LEU:HD21	1:B:289:MET:CE	2.21	0.66
1:C:216:ALA:HA	1:C:220:ARG:HH22	1.60	0.65
1:C:39:ASP:OD2	1:C:49:ARG:HD2	1.96	0.65
1:C:203:PRO:HD2	1:C:206:ASP:OD2	1.97	0.65
1:D:181:LEU:HD12	1:D:201:ILE:HG23	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:LEU:HD12	1:F:201:ILE:HG23	1.80	0.63
1:A:44:PHE:CE1	1:C:61:ARG:HD2	2.34	0.62
1:F:164:ARG:O	1:F:168:GLU:HG2	1.99	0.62
1:B:39:ASP:OD2	1:B:49:ARG:HD2	2.00	0.61
1:D:102:GLU:O	1:D:106:GLN:HG3	2.01	0.60
1:B:49:ARG:NH1	1:E:46:PRO:HG3	2.15	0.60
1:B:96:ALA:O	1:B:100:ILE:HG13	2.02	0.60
1:D:164:ARG:O	1:D:168:GLU:HG2	2.00	0.60
1:C:289:MET:HE1	1:C:292:LEU:CD2	2.32	0.60
1:B:298:CYS:O	1:B:302:ASP:HB2	2.03	0.59
1:D:161:SER:N	1:D:162:PRO:HD2	2.18	0.59
1:D:230:VAL:CB	1:D:289:MET:HE3	2.32	0.59
1:A:216:ALA:HA	1:A:220:ARG:HH22	1.66	0.58
1:E:181:LEU:CD1	1:E:201:ILE:HG23	2.31	0.58
1:F:39:ASP:OD2	1:F:49:ARG:HD2	2.04	0.57
1:D:108:ARG:HD3	3:D:1580:HOH:O	2.05	0.57
1:C:301:PHE:HA	1:C:304:VAL:CG2	2.35	0.57
1:B:46:PRO:HG2	1:E:49:ARG:HD3	1.86	0.57
1:D:238:ILE:HG21	1:D:289:MET:CE	2.35	0.57
1:C:164:ARG:O	1:C:168:GLU:HG2	2.05	0.56
1:C:108:ARG:HD3	3:C:1524:HOH:O	2.05	0.56
1:A:46:PRO:HG3	1:F:49:ARG:NH1	2.21	0.56
1:B:181:LEU:CD1	1:B:201:ILE:HG23	2.32	0.56
1:C:270:LEU:HD23	1:C:270:LEU:C	2.31	0.56
1:E:161:SER:N	1:E:162:PRO:HD2	2.20	0.56
1:D:72:LYS:NZ	1:D:72:LYS:HB3	2.21	0.55
1:B:220:ARG:HG3	1:B:220:ARG:HH11	1.71	0.55
1:E:220:ARG:HG3	1:E:220:ARG:HH11	1.72	0.55
1:A:29:ALA:O	1:A:111:CYS:HA	2.07	0.55
1:B:181:LEU:HD12	1:B:201:ILE:CG2	2.33	0.55
3:E:1548:HOH:O	1:F:185:ARG:HG3	2.07	0.55
1:B:164:ARG:O	1:B:168:GLU:HG2	2.07	0.55
1:C:181:LEU:CD1	1:C:201:ILE:HG23	2.31	0.54
1:C:157:TRP:HB2	1:D:91:LEU:CD1	2.37	0.54
1:E:270:LEU:C	1:E:270:LEU:HD23	2.32	0.54
1:A:8:PRO:HG2	1:A:61:ARG:NE	2.22	0.54
1:F:305:LEU:HD12	1:F:305:LEU:H	1.72	0.54
1:C:65:PRO:HG3	1:C:76:GLN:HE22	1.72	0.54
1:D:270:LEU:C	1:D:270:LEU:HD23	2.33	0.54
1:B:161:SER:N	1:B:162:PRO:HD2	2.23	0.54
1:F:72:LYS:NZ	1:F:72:LYS:HB3	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:C	1:A:211:LEU:HD13	2.32	0.54
1:F:305:LEU:HD12	1:F:305:LEU:N	2.23	0.54
1:F:108:ARG:HG2	1:F:114:PRO:HG3	1.90	0.53
1:A:164:ARG:O	1:A:168:GLU:HG2	2.09	0.53
1:D:304:VAL:C	1:D:305:LEU:HD12	2.33	0.53
1:E:39:ASP:OD2	1:E:49:ARG:HD2	2.08	0.53
1:F:29:ALA:O	1:F:111:CYS:HA	2.09	0.53
1:A:270:LEU:HD23	1:A:270:LEU:C	2.34	0.53
1:D:161:SER:N	1:D:162:PRO:CD	2.71	0.53
1:B:301:PHE:HA	1:B:304:VAL:HG23	1.91	0.52
1:E:161:SER:N	1:E:162:PRO:CD	2.72	0.52
1:C:46:PRO:HG2	1:D:49:ARG:HD3	1.92	0.52
1:C:46:PRO:HG3	1:D:49:ARG:CZ	2.39	0.52
1:A:161:SER:N	1:A:162:PRO:CD	2.72	0.52
1:C:161:SER:N	1:C:162:PRO:HD2	2.24	0.52
1:E:289:MET:HE2	1:E:289:MET:HA	1.90	0.52
1:D:301:PHE:HA	1:D:304:VAL:CG2	2.39	0.52
1:F:53:ARG:O	1:F:57:GLU:HG3	2.08	0.52
1:F:220:ARG:HG3	1:F:220:ARG:HH11	1.73	0.52
1:A:46:PRO:HG2	1:F:49:ARG:HD3	1.92	0.52
1:E:29:ALA:O	1:E:111:CYS:HA	2.10	0.52
1:F:270:LEU:HD23	1:F:270:LEU:C	2.34	0.52
1:D:44:PHE:CD1	1:F:61:ARG:HD2	2.45	0.52
1:B:24:ASP:HB3	1:B:106:GLN:NE2	2.25	0.52
1:B:161:SER:N	1:B:162:PRO:CD	2.72	0.52
1:B:91:LEU:CD1	1:E:157:TRP:HB2	2.40	0.52
1:F:181:LEU:HD12	1:F:201:ILE:CG2	2.39	0.51
1:A:157:TRP:HB2	1:F:91:LEU:CD1	2.41	0.51
1:C:289:MET:HE1	1:C:292:LEU:HD22	1.91	0.51
1:D:39:ASP:CG	1:D:49:ARG:HD2	2.35	0.51
1:D:211:LEU:C	1:D:211:LEU:HD13	2.35	0.51
1:C:161:SER:N	1:C:162:PRO:CD	2.73	0.51
1:D:29:ALA:O	1:D:111:CYS:HA	2.11	0.51
1:C:102:GLU:HA	1:C:102:GLU:OE2	2.09	0.51
1:C:181:LEU:HD12	1:C:201:ILE:CG2	2.33	0.51
1:B:211:LEU:HD13	1:B:211:LEU:C	2.36	0.51
1:C:20:LEU:HD12	1:C:82:ASP:O	2.11	0.51
1:D:230:VAL:CG1	1:D:289:MET:HE3	2.41	0.51
1:E:20:LEU:HD12	1:E:82:ASP:O	2.11	0.51
1:B:141:GLN:HG2	1:B:178:THR:HG23	1.92	0.50
1:B:185:ARG:HG3	3:B:1558:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ARG:CZ	1:E:46:PRO:HG3	2.41	0.50
1:C:65:PRO:HG3	1:C:76:GLN:NE2	2.27	0.50
1:E:61:ARG:HD3	3:E:1599:HOH:O	2.11	0.50
1:B:179:VAL:HG22	1:B:202:ILE:HD12	1.94	0.50
1:E:152:ARG:HG2	1:E:153:ASN:OD1	2.12	0.50
1:E:108:ARG:HD3	1:E:131:PHE:CE2	2.47	0.50
1:A:185:ARG:HG3	3:A:1549:HOH:O	2.12	0.50
1:A:243:SER:CB	1:C:61:ARG:HH12	2.24	0.50
1:B:289:MET:HE3	1:B:289:MET:CA	2.42	0.50
1:E:61:ARG:HD2	1:F:44:PHE:CD1	2.47	0.50
1:A:161:SER:N	1:A:162:PRO:HD2	2.27	0.49
1:F:197:ARG:HD2	3:F:1593:HOH:O	2.11	0.49
1:A:39:ASP:CG	1:A:49:ARG:HD2	2.37	0.49
1:F:296:THR:O	1:F:300:VAL:HG23	2.13	0.49
1:B:301:PHE:HA	1:B:304:VAL:CG2	2.43	0.49
1:B:20:LEU:HD12	1:B:82:ASP:O	2.13	0.49
1:C:211:LEU:HD13	1:C:211:LEU:C	2.38	0.48
1:B:199:HIS:HE1	3:B:1551:HOH:O	1.96	0.48
1:A:218:LEU:O	1:A:220:ARG:NH1	2.47	0.48
1:B:49:ARG:HD3	1:E:46:PRO:HG2	1.94	0.48
1:F:136:ASP:O	1:F:138:HIS:HD2	1.95	0.48
1:A:72:LYS:NZ	1:A:72:LYS:HB3	2.29	0.48
1:F:161:SER:N	1:F:162:PRO:CD	2.76	0.48
1:A:102:GLU:O	1:A:106:GLN:HG3	2.14	0.47
1:C:255:MET:HE1	1:C:296:THR:HA	1.96	0.47
1:D:220:ARG:HG3	1:D:220:ARG:HH11	1.78	0.47
1:E:202:ILE:HD13	1:E:214:VAL:HG13	1.95	0.47
1:C:46:PRO:HG3	1:D:49:ARG:NH1	2.29	0.47
1:E:39:ASP:CG	1:E:49:ARG:HD2	2.39	0.47
1:C:289:MET:HE1	1:C:292:LEU:HD23	1.95	0.47
1:A:220:ARG:HH11	1:A:220:ARG:HG3	1.80	0.47
1:E:8:PRO:HG2	1:E:61:ARG:NE	2.30	0.47
1:E:45:ARG:HA	1:E:46:PRO:HD3	1.81	0.47
1:A:199:HIS:HD2	3:A:1586:HOH:O	1.97	0.47
1:E:164:ARG:O	1:E:168:GLU:HG2	2.15	0.47
1:E:226:PHE:O	1:E:270:LEU:HA	2.15	0.47
1:F:195:ARG:HG2	1:F:195:ARG:HH11	1.80	0.47
1:A:108:ARG:HG2	1:A:114:PRO:HG3	1.97	0.46
1:F:141:GLN:HG3	3:F:1618:HOH:O	2.14	0.46
1:F:64:PRO:HD3	1:F:294:MET:HE2	1.97	0.46
1:A:44:PHE:CD1	1:C:61:ARG:HD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:ARG:HD2	3:E:1541:HOH:O	2.15	0.46
1:B:167:CYS:HB3	1:B:197:ARG:NH1	2.31	0.46
1:F:211:LEU:C	1:F:211:LEU:HD13	2.40	0.46
1:A:136:ASP:O	1:A:138:HIS:HD2	1.99	0.46
1:D:39:ASP:OD2	1:D:49:ARG:HD2	2.16	0.46
1:A:255:MET:HE1	1:A:296:THR:HA	1.97	0.46
1:E:301:PHE:HA	1:E:304:VAL:HG23	1.97	0.46
1:C:136:ASP:O	1:C:138:HIS:HD2	1.99	0.45
1:D:102:GLU:OE2	1:D:102:GLU:HA	2.16	0.45
1:E:305:LEU:N	1:E:305:LEU:HD12	2.31	0.45
1:A:110:ARG:HG3	1:A:110:ARG:HH11	1.82	0.45
1:B:110:ARG:HH11	1:B:110:ARG:HG3	1.81	0.45
1:F:199:HIS:HE1	3:F:1589:HOH:O	1.99	0.45
1:C:64:PRO:HD3	1:C:294:MET:HE2	1.98	0.45
1:A:24:ASP:HB3	1:A:106:GLN:NE2	2.31	0.45
1:B:29:ALA:O	1:B:111:CYS:HA	2.17	0.45
1:F:39:ASP:HA	1:F:120:ASP:OD2	2.16	0.45
1:A:301:PHE:HA	1:A:304:VAL:HG23	1.99	0.45
1:C:289:MET:HA	1:C:289:MET:HE3	1.98	0.45
1:E:187:ASP:HB3	1:E:190:ALA:HB3	1.99	0.45
1:F:211:LEU:HD13	1:F:211:LEU:O	2.18	0.45
1:B:270:LEU:C	1:B:270:LEU:HD23	2.42	0.44
1:D:230:VAL:HG12	1:D:289:MET:HG2	1.99	0.44
1:A:289:MET:HE1	1:A:292:LEU:HD22	2.00	0.44
1:C:211:LEU:HD13	1:C:215:LEU:HG	1.99	0.44
1:A:61:ARG:HD2	1:B:44:PHE:CD1	2.52	0.44
1:C:108:ARG:NH2	1:C:131:PHE:HA	2.33	0.44
1:E:207:VAL:HG13	1:E:211:LEU:HD23	2.00	0.44
1:B:74:ARG:O	1:B:75:LEU:HB2	2.17	0.44
1:B:305:LEU:N	1:B:305:LEU:HD12	2.33	0.44
1:A:46:PRO:HG3	1:F:49:ARG:CZ	2.48	0.44
1:C:108:ARG:HG2	1:C:114:PRO:HG3	2.00	0.44
1:E:199:HIS:HE1	3:E:1596:HOH:O	2.01	0.44
1:B:152:ARG:HG2	1:B:153:ASN:OD1	2.18	0.43
1:A:289:MET:HE1	1:A:292:LEU:CD2	2.48	0.43
1:B:150:ASP:HB3	3:B:1557:HOH:O	2.18	0.43
1:C:305:LEU:N	1:C:305:LEU:HD12	2.32	0.43
1:B:116:PHE:CB	1:B:127:LEU:HD21	2.48	0.43
1:D:255:MET:HE1	1:D:296:THR:HA	2.00	0.43
1:F:161:SER:N	1:F:162:PRO:HD2	2.33	0.43
1:F:75:LEU:HD23	1:F:75:LEU:HA	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:HIS:HE1	3:F:1618:HOH:O	2.01	0.43
1:F:305:LEU:H	1:F:305:LEU:CD1	2.31	0.43
1:D:197:ARG:NH2	3:D:1542:HOH:O	2.51	0.43
1:D:195:ARG:HH11	1:D:195:ARG:HG2	1.84	0.42
1:D:226:PHE:O	1:D:270:LEU:HA	2.19	0.42
1:A:181:LEU:HD12	1:A:201:ILE:CG2	2.44	0.42
1:B:61:ARG:NH1	1:C:243:SER:OG	2.52	0.42
1:E:296:THR:O	1:E:300:VAL:HG23	2.18	0.42
1:F:72:LYS:HB3	1:F:72:LYS:HZ3	1.84	0.42
1:D:44:PHE:HB3	1:D:242:SER:OG	2.19	0.42
1:C:151:THR:HG22	3:C:1596:HOH:O	2.18	0.42
1:C:222:GLN:O	1:C:265:ASN:HB3	2.19	0.42
1:B:45:ARG:HA	1:B:46:PRO:HD3	1.81	0.42
1:D:136:ASP:O	1:D:138:HIS:HD2	2.02	0.42
1:E:108:ARG:NH2	1:E:133:ASP:OD2	2.51	0.42
1:A:8:PRO:HG2	1:A:61:ARG:CZ	2.50	0.42
1:A:44:PHE:HB3	1:A:242:SER:OG	2.20	0.42
1:A:100:ILE:CG2	1:A:127:LEU:HD13	2.50	0.42
1:C:45:ARG:HA	1:C:46:PRO:HD3	1.81	0.42
1:C:108:ARG:NH2	1:C:133:ASP:OD2	2.53	0.42
1:B:152:ARG:O	1:B:155:THR:HG22	2.21	0.41
1:E:211:LEU:HD13	1:E:211:LEU:C	2.45	0.41
1:B:226:PHE:O	1:B:270:LEU:HA	2.20	0.41
1:A:57:GLU:OE1	1:E:57:GLU:OE1	2.37	0.41
1:B:116:PHE:HB3	1:B:127:LEU:HD21	2.01	0.41
1:F:181:LEU:CD1	1:F:201:ILE:HG23	2.48	0.41
1:D:64:PRO:HD3	1:D:294:MET:HE2	2.02	0.41
1:D:7:LEU:N	1:D:7:LEU:HD22	2.36	0.41
1:F:199:HIS:HD2	3:F:1574:HOH:O	2.03	0.41
1:F:218:LEU:HB3	1:F:219:PRO:HD2	2.03	0.41
1:F:220:ARG:HG3	1:F:220:ARG:NH1	2.35	0.41
1:B:48:ALA:HA	1:B:275:LEU:O	2.20	0.41
1:B:61:ARG:HD2	1:C:44:PHE:CD1	2.56	0.41
1:E:255:MET:HE1	1:E:296:THR:HA	2.02	0.41
1:B:213:GLY:O	1:B:217:GLN:HG3	2.21	0.41
1:D:61:ARG:HD2	1:E:44:PHE:CD1	2.55	0.41
1:D:76:GLN:NE2	1:D:76:GLN:HA	2.36	0.41
1:D:293:VAL:O	1:D:297:LEU:HG	2.21	0.41
1:E:102:GLU:O	1:E:106:GLN:HG3	2.20	0.41
1:E:181:LEU:HD12	1:E:201:ILE:CG2	2.43	0.41
1:F:44:PHE:HB3	1:F:242:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:GLN:HB2	3:F:1544:HOH:O	2.20	0.41
1:A:64:PRO:HD3	1:A:294:MET:HE2	2.03	0.41
1:A:226:PHE:O	1:A:270:LEU:HA	2.21	0.41
1:B:46:PRO:CG	1:E:49:ARG:HD3	2.50	0.40
1:B:57:GLU:OE1	1:D:57:GLU:OE1	2.39	0.40
1:B:102:GLU:O	1:B:106:GLN:HG3	2.20	0.40
1:D:203:PRO:HG3	1:F:69:LEU:CD2	2.51	0.40
1:D:237:VAL:O	1:D:238:ILE:HD13	2.21	0.40
1:E:64:PRO:HD3	1:E:294:MET:HE2	2.02	0.40
1:A:74:ARG:O	1:A:75:LEU:HB2	2.21	0.40
1:B:193:ALA:O	1:B:197:ARG:HG3	2.21	0.40
1:C:74:ARG:O	1:C:75:LEU:HB2	2.20	0.40
1:D:263:ALA:HB2	3:D:1599:HOH:O	2.21	0.40
1:E:234:ASP:HA	1:E:235:PRO:HD3	1.88	0.40
1:F:7:LEU:HD23	3:F:1594:HOH:O	2.22	0.40
1:D:58:ALA:HB1	1:D:287:LEU:HA	2.04	0.40
1:D:110:ARG:HG3	1:D:110:ARG:HH11	1.85	0.40
1:B:207:VAL:HA	1:B:214:VAL:HG21	2.03	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	301/305 (99%)	291 (97%)	9 (3%)	1 (0%)	36	25
1	B	301/305 (99%)	290 (96%)	10 (3%)	1 (0%)	36	25
1	C	301/305 (99%)	290 (96%)	10 (3%)	1 (0%)	36	25
1	D	301/305 (99%)	292 (97%)	8 (3%)	1 (0%)	36	25
1	E	301/305 (99%)	292 (97%)	8 (3%)	1 (0%)	36	25
1	F	301/305 (99%)	291 (97%)	9 (3%)	1 (0%)	36	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1806/1830 (99%)	1746 (97%)	54 (3%)	6 (0%)	36 25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	161	SER
1	A	161	SER
1	C	161	SER
1	D	161	SER
1	F	161	SER
1	E	161	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	240/242 (99%)	236 (98%)	4 (2%)	53 42
1	B	240/242 (99%)	236 (98%)	4 (2%)	53 42
1	C	240/242 (99%)	236 (98%)	4 (2%)	53 42
1	D	240/242 (99%)	236 (98%)	4 (2%)	53 42
1	E	240/242 (99%)	238 (99%)	2 (1%)	73 67
1	F	240/242 (99%)	237 (99%)	3 (1%)	61 51
All	All	1440/1452 (99%)	1419 (98%)	21 (2%)	57 47

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ARG
1	A	127	LEU
1	A	275	LEU
1	A	302	ASP
1	B	61	ARG
1	B	108	ARG

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Mol	Chain	Res	Type
1	B	127	LEU
1	B	275	LEU
1	C	108	ARG
1	C	127	LEU
1	C	173	LEU
1	C	275	LEU
1	D	108	ARG
1	D	127	LEU
1	D	173	LEU
1	D	275	LEU
1	E	127	LEU
1	E	275	LEU
1	F	108	ARG
1	F	127	LEU
1	F	275	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	199	HIS
1	B	76	GLN
1	B	106	GLN
1	B	138	HIS
1	B	199	HIS
1	C	76	GLN
1	C	138	HIS
1	D	76	GLN
1	D	138	HIS
1	D	199	HIS
1	E	76	GLN
1	E	175	HIS
1	E	199	HIS
1	E	222	GLN
1	F	76	GLN
1	F	138	HIS
1	F	175	HIS
1	F	199	HIS
1	F	217	GLN
1	F	223	ASN
1	F	303	HIS

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 ⓘ

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	303/305 (99%)	-0.03	9 (2%)	52	56	9, 15, 29, 42	0
1	B	303/305 (99%)	0.44	18 (5%)	28	31	10, 22, 36, 67	0
1	C	303/305 (99%)	0.10	12 (3%)	42	46	9, 17, 29, 78	0
1	D	303/305 (99%)	0.43	21 (6%)	23	25	11, 21, 37, 75	0
1	E	303/305 (99%)	0.29	13 (4%)	40	43	12, 20, 32, 48	0
1	F	303/305 (99%)	0.06	7 (2%)	61	64	9, 17, 29, 42	0
All	All	1818/1830 (99%)	0.21	80 (4%)	39	42	9, 18, 33, 78	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	304	VAL	7.9
1	D	304	VAL	7.6
1	F	305	LEU	7.3
1	C	305	LEU	6.8
1	E	305	LEU	6.0
1	D	305	LEU	6.0
1	B	305	LEU	5.2
1	C	303	HIS	4.8
1	A	304	VAL	4.5
1	B	304	VAL	4.5
1	A	305	LEU	4.2
1	C	102	GLU	3.9
1	F	220	ARG	3.8
1	D	302	ASP	3.8
1	D	102	GLU	3.6
1	F	3	GLY	3.5
1	B	26	ASP	3.5
1	F	304	VAL	3.5
1	E	304	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	28	GLN	3.2
1	A	220	ARG	3.2
1	D	303	HIS	3.1
1	A	61	ARG	3.0
1	D	72	LYS	3.0
1	C	5	ALA	3.0
1	B	72	LYS	3.0
1	D	3	GLY	2.9
1	A	3	GLY	2.9
1	C	6	HIS	2.9
1	D	220	ARG	2.9
1	C	198	GLY	2.9
1	F	112	ARG	2.8
1	C	9	TYR	2.7
1	B	112	ARG	2.7
1	C	220	ARG	2.6
1	D	61	ARG	2.6
1	B	3	GLY	2.6
1	A	157	TRP	2.6
1	D	28	GLN	2.6
1	D	76	GLN	2.6
1	A	28	GLN	2.5
1	E	61	ARG	2.5
1	E	220	ARG	2.5
1	C	3	GLY	2.5
1	C	302	ASP	2.5
1	D	81	ALA	2.4
1	D	27	TRP	2.4
1	D	157	TRP	2.4
1	B	29	ALA	2.4
1	E	216	ALA	2.4
1	F	28	GLN	2.4
1	B	303	HIS	2.4
1	E	211	LEU	2.3
1	D	24	ASP	2.3
1	E	197	ARG	2.3
1	B	20	LEU	2.3
1	B	21	VAL	2.3
1	D	26	ASP	2.3
1	A	264	ASN	2.3
1	C	7	LEU	2.3
1	D	7	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	112	ARG	2.2
1	B	69	LEU	2.2
1	E	7	LEU	2.2
1	B	302	ASP	2.2
1	B	27	TRP	2.2
1	B	211	LEU	2.2
1	D	106	GLN	2.2
1	E	28	GLN	2.2
1	F	20	LEU	2.1
1	B	5	ALA	2.1
1	E	102	GLU	2.1
1	A	7	LEU	2.1
1	E	112	ARG	2.1
1	B	109	GLY	2.0
1	D	94	GLN	2.0
1	D	23	PRO	2.0
1	E	171	PRO	2.0
1	B	61	ARG	2.0
1	E	168	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 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
2	MN	E	1509	1/1	0.87	0.34	73,73,73,73	0
2	MN	E	1510	1/1	0.93	0.12	37,37,37,37	0
2	MN	B	1503	1/1	0.95	0.25	42,42,42,42	0
2	MN	D	1507	1/1	0.95	0.28	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	F	1512	1/1	0.97	0.11	27,27,27,27	0
2	MN	A	1501	1/1	0.98	0.21	28,28,28,28	0
2	MN	B	1504	1/1	0.98	0.11	35,35,35,35	0
2	MN	C	1505	1/1	0.98	0.24	36,36,36,36	0
2	MN	F	1511	1/1	0.98	0.25	36,36,36,36	0
2	MN	C	1506	1/1	0.98	0.15	32,32,32,32	0
2	MN	A	1502	1/1	0.99	0.13	21,21,21,21	0
2	MN	D	1508	1/1	0.99	0.16	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.