



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:39 PM EDT

PDB ID : 3NO9 / pdb_00003no9
Title : Crystal Structure of apo fumarate hydratase from Mycobacterium tuberculosis
Authors : Li, H.; Swanson, S.; Yu, M.; Hung, L.-W.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2010-06-25
Resolution : 2.48 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

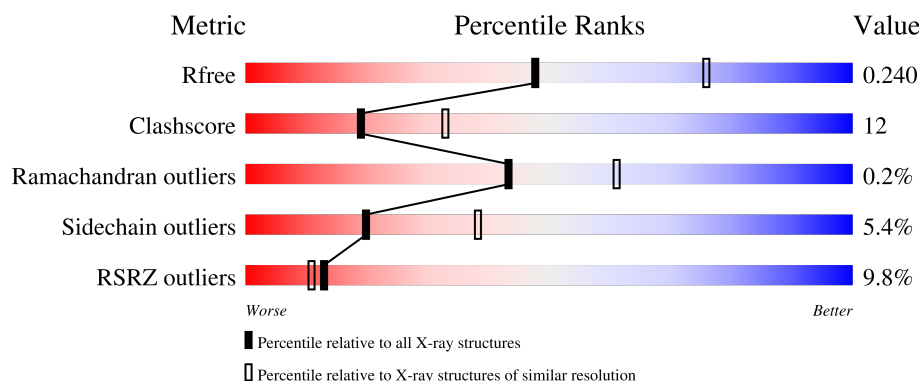
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	475	11% 77% 16% 5%
1	B	475	7% 77% 15% 5%
1	C	475	13% 75% 16% 5%
1	D	475	7% 77% 15% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13623 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 Fumarate hydratase class II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	38	1	0
			3363	2095	609	648	11			
1	B	452	Total	C	N	O	S	16	1	0
			3357	2092	608	646	11			
1	C	453	Total	C	N	O	S	13	1	0
			3368	2098	611	648	11			
1	D	452	Total	C	N	O	S	13	1	0
			3357	2092	608	646	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP O53446
B	0	SER	-	expression tag	UNP O53446
C	0	SER	-	expression tag	UNP O53446
D	0	SER	-	expression tag	UNP O53446

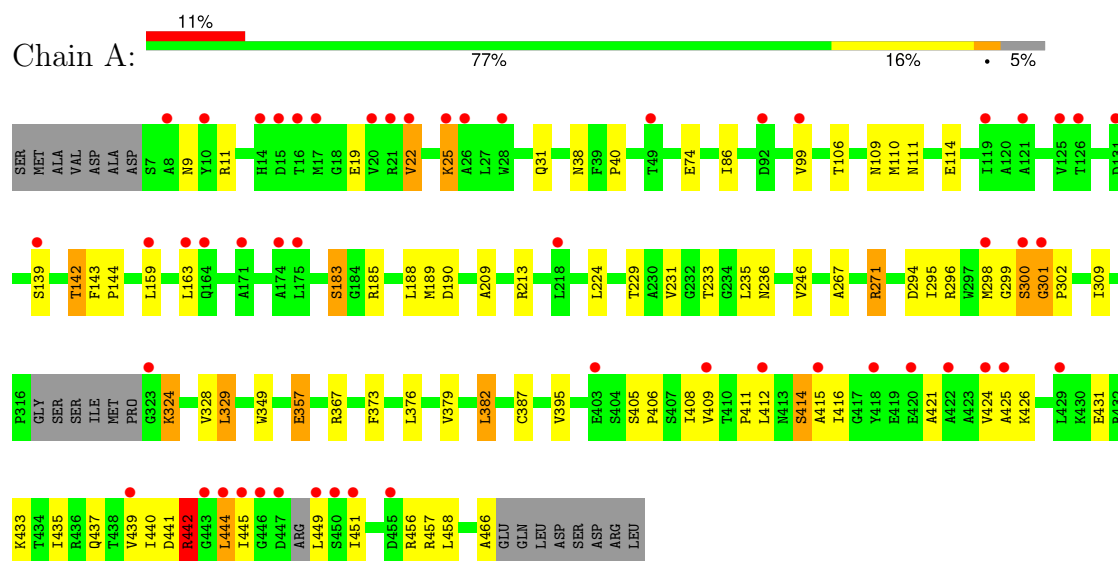
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	37	Total	O	0	0
			37	37		
2	B	55	Total	O	0	0
			55	55		
2	C	38	Total	O	0	0
			38	38		
2	D	48	Total	O	0	0
			48	48		

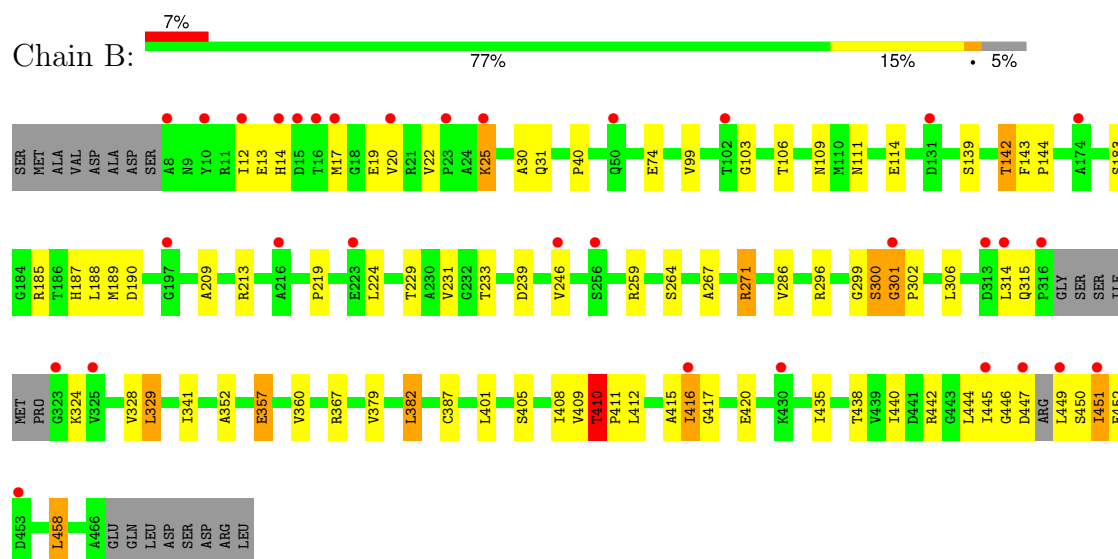
3 Residue-property plots [i](#)

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: Fumarate hydratase class II

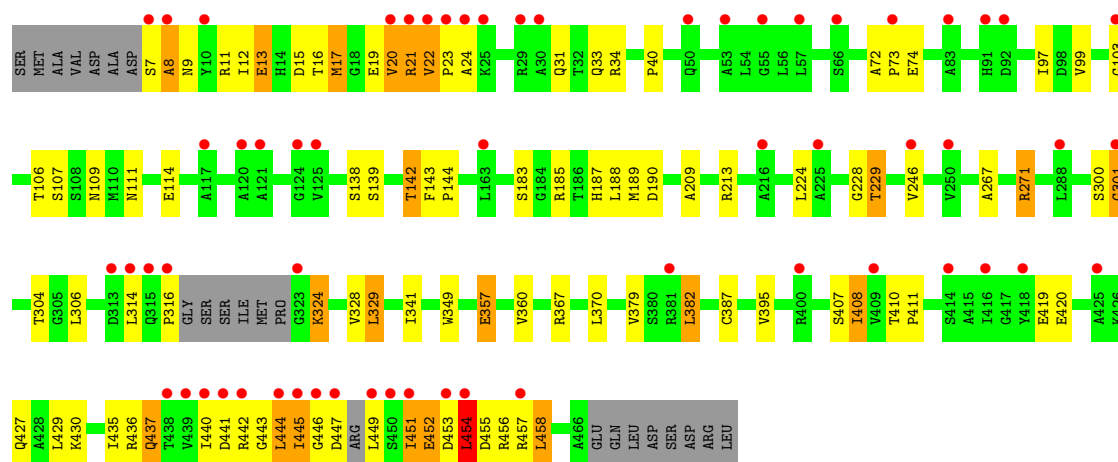


• Molecule 1: Fumarate hydratase class II



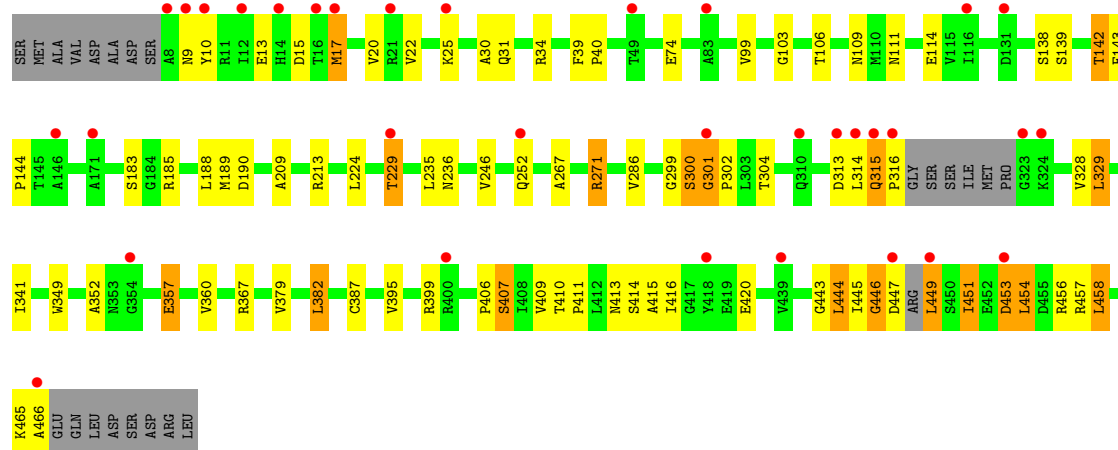
• Molecule 1: Fumarate hydratase class II

Chain C: 



• Molecule 1: Fumarate hydratase class II

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	271.22Å 96.56Å 89.89Å 90.00° 102.99° 90.00°	Depositor
Resolution (Å)	48.52 – 2.48 48.52 – 2.48	Depositor EDS
% Data completeness (in resolution range)	88.4 (48.52-2.48) 88.4 (48.52-2.48)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.206 , 0.241 0.209 , 0.240	Depositor DCC
R_{free} test set	3534 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13623	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% 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

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	0.55	0/3411	0.86	5/4635 (0.1%)
1	B	0.59	0/3405	0.89	9/4627 (0.2%)
1	C	0.57	1/3417 (0.0%)	0.94	12/4643 (0.3%)
1	D	0.58	0/3405	0.87	7/4627 (0.2%)
All	All	0.57	1/13638 (0.0%)	0.89	33/18532 (0.2%)

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	A	0	3
1	B	0	4
1	C	0	3
1	D	0	3
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	441	ASP	C-N	-8.44	1.20	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	451	ILE	N-CA-C	13.14	123.03	110.42
1	C	20	VAL	N-CA-C	10.88	121.71	110.72
1	A	456	ARG	N-CA-C	10.59	122.83	111.28
1	B	12	ILE	CB-CA-C	8.63	123.56	110.96
1	B	12	ILE	N-CA-C	-7.77	96.54	107.80
1	C	22	VAL	CA-C-N	7.68	127.44	119.76
1	C	22	VAL	C-N-CA	7.68	127.44	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	21	ARG	N-CA-C	7.50	122.02	111.52
1	B	13	GLU	N-CA-C	-7.24	98.52	110.17
1	C	408	ILE	N-CA-C	7.09	124.08	109.34
1	A	456	ARG	N-CA-CB	-6.97	99.88	110.12
1	C	441	ASP	O-C-N	-6.47	113.77	122.43
1	D	395	VAL	N-CA-C	6.34	117.02	110.36
1	C	452	GLU	CB-CA-C	6.33	122.34	110.63
1	C	229	THR	CB-CA-C	-6.22	109.42	116.63
1	D	407	SER	CA-C-N	-5.81	115.05	122.26
1	D	407	SER	C-N-CA	-5.81	115.05	122.26
1	A	229	THR	CB-CA-C	-5.57	110.17	116.63
1	D	30	ALA	N-CA-C	5.51	120.40	111.37
1	C	395	VAL	N-CA-C	5.45	116.09	110.36
1	D	229	THR	CB-CA-C	-5.37	108.83	116.34
1	C	441	ASP	CB-CA-C	5.35	121.48	110.31
1	D	446	GLY	N-CA-C	-5.34	106.02	112.48
1	B	229	THR	CB-CA-C	-5.33	108.87	116.34
1	A	395	VAL	N-CA-C	5.30	115.93	110.36
1	B	410	THR	CA-C-N	-5.26	113.26	119.84
1	B	410	THR	C-N-CA	-5.26	113.26	119.84
1	D	17	MET	N-CA-C	-5.21	105.66	113.89
1	B	416	ILE	CA-C-N	-5.15	117.17	122.27
1	B	416	ILE	C-N-CA	-5.15	117.17	122.27
1	B	30	ALA	N-CA-C	5.13	117.27	111.11
1	A	442	ARG	N-CA-C	-5.04	106.73	112.92
1	C	407	SER	CB-CA-C	5.03	119.23	110.68

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	299	GLY	Peptide
1	A	300	SER	Peptide
1	A	301	GLY	Peptide
1	B	299	GLY	Peptide
1	B	300	SER	Peptide
1	B	301	GLY	Peptide
1	B	415	ALA	Peptide
1	C	300	SER	Peptide
1	C	301	GLY	Peptide
1	C	8	ALA	Peptide
1	D	299	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	D	300	SER	Peptide
1	D	301	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3363	0	3399	103	0
1	B	3357	0	3394	67	0
1	C	3368	0	3404	108	0
1	D	3357	0	3394	92	0
2	A	37	0	0	3	0
2	B	55	0	0	4	0
2	C	38	0	0	2	0
2	D	48	0	0	5	0
All	All	13623	0	13591	317	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 12.

All (317) 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:C:22:VAL:HG12	1:C:33:GLN:OE1	1.24	1.26
1:C:437:GLN:NE2	1:C:440:ILE:HD12	1.59	1.16
1:A:295:ILE:HA	1:A:298:MET:HE2	1.31	1.06
1:C:324:LYS:HZ2	1:C:324:LYS:HB3	1.19	1.05
1:A:415:ALA:HB1	1:A:449:LEU:HD13	1.39	1.04
1:C:22:VAL:CG1	1:C:33:GLN:OE1	2.08	1.02
1:C:324:LYS:HB3	1:C:324:LYS:NZ	1.74	0.99
1:D:449:LEU:N	1:D:449:LEU:HD23	1.72	0.99
1:D:449:LEU:N	1:D:449:LEU:CD2	2.29	0.95
1:C:13:GLU:HB3	1:C:20:VAL:CG2	1.97	0.94
1:C:437:GLN:HE22	1:C:440:ILE:HD12	1.27	0.94
1:C:22:VAL:HG12	1:C:33:GLN:CD	1.93	0.94
1:C:22:VAL:HB	1:C:23:PRO:HD2	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ILE:HA	1:A:298:MET:CE	2.01	0.91
1:C:17:MET:SD	1:D:315:GLN:O	2.28	0.91
1:D:314:LEU:C	1:D:316:PRO:CD	2.45	0.89
1:D:449:LEU:HD23	1:D:449:LEU:O	1.72	0.88
1:B:189:MET:CE	1:C:301:GLY:HA2	2.04	0.87
1:A:99:VAL:HG11	1:A:367:ARG:HD2	1.58	0.85
1:A:294:ASP:O	1:A:298:MET:HG3	1.77	0.85
1:D:314:LEU:C	1:D:316:PRO:HD2	2.00	0.84
1:C:21:ARG:O	1:C:21:ARG:HG2	1.78	0.84
1:B:99:VAL:HG11	1:B:367:ARG:HD2	1.59	0.82
1:D:99:VAL:HG11	1:D:367:ARG:HD2	1.61	0.82
1:C:446:GLY:N	1:C:449:LEU:O	2.10	0.82
1:D:315:GLN:N	1:D:316:PRO:CD	2.43	0.81
1:D:449:LEU:CD2	1:D:449:LEU:O	2.30	0.80
1:D:445:ILE:HG21	1:D:451:ILE:HG13	1.64	0.80
1:A:439:VAL:O	1:A:444:LEU:HD13	1.82	0.80
1:C:437:GLN:HE21	1:C:437:GLN:HA	1.48	0.79
1:B:14:HIS:HA	1:B:19:GLU:HG2	1.65	0.78
1:A:295:ILE:CA	1:A:298:MET:HE2	2.12	0.78
1:A:415:ALA:CB	1:A:449:LEU:HD13	2.13	0.78
1:D:314:LEU:O	1:D:316:PRO:HD2	1.83	0.77
1:C:445:ILE:H	1:C:445:ILE:HD12	1.49	0.77
1:B:302:PRO:HD2	1:C:190:ASP:OD2	1.85	0.77
1:C:99:VAL:HG11	1:C:367:ARG:HD2	1.67	0.76
1:A:324:LYS:NZ	1:A:324:LYS:HB3	2.02	0.75
1:D:314:LEU:C	1:D:316:PRO:HD3	2.11	0.75
1:B:445:ILE:HD13	1:B:451:ILE:HG12	1.69	0.75
1:D:209:ALA:O	1:D:213:ARG:HG2	1.85	0.75
1:C:34:ARG:NE	2:C:497:HOH:O	2.20	0.74
1:D:445:ILE:HD11	1:D:454:LEU:HD12	1.70	0.73
1:A:190:ASP:OD2	1:D:302:PRO:HD2	1.87	0.73
1:A:324:LYS:HB3	1:A:324:LYS:HZ3	1.54	0.72
1:D:106:THR:HA	1:D:139:SER:OG	1.90	0.72
1:B:106:THR:HA	1:B:139:SER:OG	1.90	0.72
1:A:324:LYS:NZ	1:A:324:LYS:CB	2.53	0.71
1:A:439:VAL:HG13	1:A:444:LEU:HD22	1.72	0.71
1:A:106:THR:HA	1:A:139:SER:OG	1.89	0.71
1:A:159:LEU:HD22	1:A:373:PHE:CD1	2.27	0.70
1:C:106:THR:HA	1:C:139:SER:OG	1.91	0.69
1:A:300:SER:HB2	1:D:188:LEU:HB3	1.74	0.69
1:C:209:ALA:O	1:C:213:ARG:HG2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:ARG:HB3	1:C:444:LEU:HD23	1.73	0.69
1:A:442:ARG:HB2	1:A:444:LEU:HD11	1.75	0.67
1:A:301:GLY:CA	1:D:189:MET:CE	2.72	0.67
1:A:444:LEU:N	1:A:444:LEU:HD12	2.09	0.67
1:C:9:ASN:OD1	1:C:9:ASN:C	2.34	0.66
1:A:209:ALA:O	1:A:213:ARG:HG2	1.95	0.66
1:C:454:LEU:O	1:C:456:ARG:N	2.29	0.66
1:B:189:MET:CE	1:C:301:GLY:CA	2.74	0.66
1:B:189:MET:HA	1:C:301:GLY:HA3	1.76	0.65
1:C:442:ARG:HB3	1:C:444:LEU:CD2	2.25	0.65
1:B:189:MET:HE1	1:C:301:GLY:HA2	1.78	0.65
1:A:442:ARG:C	1:A:444:LEU:HD12	2.21	0.65
1:C:7:SER:OG	1:C:8:ALA:N	2.30	0.65
1:C:453:ASP:O	1:C:456:ARG:HB3	1.97	0.64
1:D:313:ASP:O	1:D:316:PRO:HD3	1.97	0.64
1:D:454:LEU:HD22	1:D:458:LEU:HD22	1.79	0.64
1:C:329:LEU:HD23	1:C:387:CYS:HB2	1.80	0.63
1:B:209:ALA:O	1:B:213:ARG:HG2	1.98	0.63
1:A:382:LEU:HD21	1:B:40:PRO:HD2	1.80	0.63
1:A:301:GLY:HA2	1:D:189:MET:CE	2.29	0.63
1:B:267:ALA:O	1:B:271:ARG:NH2	2.32	0.62
1:A:445:ILE:HG23	1:A:449:LEU:O	2.00	0.62
1:C:437:GLN:HE21	1:C:437:GLN:CA	2.13	0.62
1:C:440:ILE:HA	1:C:445:ILE:HD11	1.82	0.62
1:D:267:ALA:O	1:D:271:ARG:NH2	2.31	0.62
1:D:9:ASN:OD1	1:D:10:TYR:CE2	2.53	0.61
1:C:437:GLN:NE2	1:C:437:GLN:HA	2.16	0.61
1:B:185:ARG:O	1:D:357:GLU:HG2	2.01	0.61
1:C:454:LEU:C	1:C:456:ARG:H	2.08	0.61
1:A:298:MET:HE3	1:A:309:ILE:CD1	2.31	0.60
1:B:189:MET:HE3	1:C:301:GLY:HA2	1.83	0.60
1:A:267:ALA:O	1:A:271:ARG:NH2	2.34	0.60
1:C:437:GLN:HE22	1:C:440:ILE:CD1	2.08	0.60
1:A:301:GLY:HA3	1:D:189:MET:HE3	1.82	0.60
1:C:13:GLU:HB3	1:C:20:VAL:HG23	1.83	0.60
1:A:442:ARG:HG3	1:A:444:LEU:HD11	1.83	0.59
1:B:187:HIS:O	1:B:188:LEU:HB2	2.02	0.59
1:A:301:GLY:N	1:D:189:MET:SD	2.75	0.59
1:B:189:MET:SD	1:C:301:GLY:CA	2.91	0.59
1:A:440:ILE:HG12	1:A:445:ILE:HD12	1.84	0.59
1:B:219:PRO:HA	2:B:527:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ARG:CB	1:A:444:LEU:HD11	2.31	0.59
1:D:444:LEU:O	1:D:449:LEU:HD21	2.03	0.59
1:B:357:GLU:HG2	1:D:185:ARG:O	2.03	0.59
1:C:454:LEU:C	1:C:456:ARG:N	2.59	0.59
1:D:446:GLY:O	1:D:447:ASP:HB2	2.03	0.58
1:C:453:ASP:HA	1:C:456:ARG:HE	1.67	0.58
1:A:426:LYS:O	1:A:426:LYS:HD3	2.04	0.58
1:D:329:LEU:HD23	1:D:387:CYS:HB2	1.86	0.58
1:D:454:LEU:CD2	1:D:458:LEU:HD22	2.34	0.58
1:A:302:PRO:HD2	1:D:190:ASP:OD2	2.04	0.57
1:A:444:LEU:H	1:A:444:LEU:CD1	2.17	0.57
1:C:324:LYS:NZ	1:C:324:LYS:CB	2.49	0.57
1:C:382:LEU:HD21	1:D:40:PRO:HD2	1.86	0.57
1:B:213:ARG:NH1	2:B:478:HOH:O	2.37	0.57
1:C:17:MET:HG3	1:C:34:ARG:NH1	2.19	0.57
1:D:20:VAL:CG1	1:D:34:ARG:HE	2.16	0.57
1:B:329:LEU:HD23	1:B:387:CYS:HB2	1.86	0.57
1:A:444:LEU:HD12	1:A:444:LEU:H	1.69	0.56
1:C:111:ASN:C	1:C:111:ASN:HD22	2.12	0.56
1:A:142:THR:HG22	1:A:143:PHE:N	2.19	0.56
1:C:328:VAL:HG11	1:D:39:PHE:HZ	1.71	0.56
1:C:349:TRP:CZ3	1:D:341:ILE:HD13	2.40	0.56
1:D:449:LEU:O	1:D:449:LEU:CG	2.48	0.56
1:B:408:ILE:O	1:B:411:PRO:HD2	2.05	0.56
1:A:324:LYS:CB	1:A:324:LYS:HZ2	2.16	0.56
1:B:31:GLN:HB2	1:B:114:GLU:OE2	2.06	0.56
1:C:21:ARG:O	1:C:21:ARG:CG	2.51	0.56
1:D:9:ASN:OD1	1:D:10:TYR:CD2	2.59	0.56
1:D:111:ASN:C	1:D:111:ASN:HD22	2.13	0.56
1:C:267:ALA:O	1:C:271:ARG:NH2	2.39	0.55
1:D:224:LEU:HD12	1:D:246:VAL:HG22	1.87	0.55
1:C:22:VAL:CG1	1:C:33:GLN:CD	2.72	0.55
1:C:411:PRO:HB2	1:C:457:ARG:HB3	1.87	0.55
1:D:31:GLN:HB2	1:D:114:GLU:OE2	2.07	0.54
1:A:295:ILE:HG12	1:A:298:MET:CE	2.37	0.54
1:C:12:ILE:HA	1:C:21:ARG:HA	1.89	0.54
1:B:445:ILE:HG21	1:B:451:ILE:HG12	1.88	0.54
1:A:442:ARG:CG	1:A:444:LEU:HD11	2.38	0.54
1:B:17:MET:HE2	1:B:17:MET:HA	1.90	0.54
1:D:406:PRO:O	1:D:409:VAL:HG22	2.08	0.54
1:A:11:ARG:HH21	1:A:22:VAL:HG21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:HB2	1:A:114:GLU:OE2	2.07	0.54
1:A:329:LEU:HD23	1:A:387:CYS:HB2	1.88	0.54
1:B:324:LYS:O	1:B:324:LYS:HG2	2.06	0.54
1:A:349:TRP:CZ3	1:B:341:ILE:HD13	2.43	0.54
1:D:315:GLN:NE2	2:D:513:HOH:O	2.40	0.54
1:B:189:MET:SD	1:C:301:GLY:N	2.81	0.54
1:D:449:LEU:N	1:D:449:LEU:HD22	2.22	0.54
1:A:301:GLY:CA	1:D:189:MET:HE3	2.37	0.53
1:B:25:LYS:HD2	1:B:25:LYS:O	2.08	0.53
1:A:189:MET:CE	1:D:301:GLY:HA2	2.38	0.53
1:B:264:SER:HB2	2:B:492:HOH:O	2.08	0.53
1:A:411:PRO:HB2	1:A:457:ARG:HB3	1.91	0.53
1:A:159:LEU:HD22	1:A:373:PHE:HD1	1.69	0.53
1:A:440:ILE:HG13	1:A:445:ILE:HD11	1.91	0.53
1:C:15:ASP:OD2	1:C:16:THR:N	2.39	0.53
1:A:301:GLY:HA2	1:D:189:MET:HE1	1.90	0.52
1:A:349:TRP:CH2	1:B:341:ILE:HD13	2.44	0.52
1:B:111:ASN:C	1:B:111:ASN:HD22	2.14	0.52
1:C:19:GLU:O	1:C:19:GLU:HG3	2.09	0.52
1:B:224:LEU:HD12	1:B:246:VAL:HG22	1.92	0.52
1:C:31:GLN:HB2	1:C:114:GLU:OE2	2.10	0.52
1:C:408:ILE:O	1:C:411:PRO:HD2	2.09	0.52
1:D:415:ALA:HB2	1:D:457:ARG:CZ	2.40	0.52
1:B:143:PHE:N	1:B:144:PRO:HD2	2.24	0.52
1:D:252:GLN:NE2	2:D:515:HOH:O	2.23	0.52
1:C:11:ARG:N	1:C:22:VAL:O	2.42	0.51
1:C:143:PHE:N	1:C:144:PRO:HD2	2.25	0.51
1:D:315:GLN:O	1:D:316:PRO:C	2.51	0.51
1:C:22:VAL:HB	1:C:23:PRO:CD	2.31	0.51
1:A:231:VAL:HG23	1:A:233:THR:HG23	1.91	0.51
1:A:298:MET:HE3	1:A:309:ILE:HD11	1.91	0.51
1:A:406:PRO:O	1:A:409:VAL:HG22	2.11	0.51
1:B:189:MET:HE3	1:C:301:GLY:CA	2.41	0.51
1:A:444:LEU:N	1:A:444:LEU:CD1	2.72	0.51
1:C:349:TRP:CH2	1:D:341:ILE:HD13	2.46	0.51
1:B:416:ILE:HB	1:B:420:GLU:HB2	1.93	0.51
1:A:301:GLY:CA	1:D:189:MET:SD	2.99	0.51
1:A:224:LEU:HD12	1:A:246:VAL:HG22	1.91	0.51
1:B:259:ARG:NH2	2:B:527:HOH:O	2.42	0.51
1:C:13:GLU:HB3	1:C:20:VAL:HG22	1.88	0.50
1:C:109:ASN:OD1	1:C:142:THR:HG21	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ARG:HB2	1:B:444:LEU:CD2	2.41	0.50
1:D:413:ASN:O	1:D:416:ILE:O	2.29	0.50
1:A:301:GLY:HA3	1:D:189:MET:CE	2.39	0.50
1:A:405:SER:O	1:A:408:ILE:HG12	2.11	0.50
1:D:445:ILE:HD13	1:D:451:ILE:HG13	1.93	0.50
1:A:189:MET:CE	1:D:301:GLY:CA	2.90	0.50
1:A:295:ILE:HG12	1:A:298:MET:HE1	1.94	0.49
1:A:367:ARG:HG2	1:A:367:ARG:HH11	1.77	0.49
1:C:34:ARG:CZ	2:C:497:HOH:O	2.58	0.49
1:C:446:GLY:O	1:C:447:ASP:HB2	2.12	0.49
1:B:187:HIS:O	1:B:188:LEU:CB	2.60	0.49
1:D:142:THR:HG22	1:D:143:PHE:N	2.26	0.49
1:A:440:ILE:HG12	1:A:445:ILE:CD1	2.42	0.49
1:B:438:THR:O	1:B:442:ARG:HG3	2.13	0.49
1:D:143:PHE:N	1:D:144:PRO:HD2	2.27	0.49
1:A:111:ASN:HD22	1:A:111:ASN:C	2.21	0.49
1:B:109:ASN:OD1	1:B:142:THR:HG21	2.13	0.49
1:A:445:ILE:HD13	1:A:451:ILE:HG12	1.95	0.48
1:A:40:PRO:HD2	1:B:382:LEU:HD21	1.93	0.48
1:B:301:GLY:HA2	1:C:189:MET:CE	2.42	0.48
1:D:315:GLN:N	1:D:316:PRO:HD3	2.20	0.48
1:D:449:LEU:O	1:D:449:LEU:HG	2.12	0.48
1:C:138:SER:HB3	1:C:229:THR:HA	1.94	0.48
1:A:445:ILE:HG21	1:A:451:ILE:HG13	1.95	0.48
1:C:410:THR:N	1:C:411:PRO:CD	2.77	0.48
1:A:185:ARG:O	1:C:357:GLU:HG2	2.14	0.47
1:B:352:ALA:HA	1:D:286:VAL:HG13	1.96	0.47
1:C:443:GLY:C	1:C:445:ILE:HD12	2.39	0.47
1:D:20:VAL:HG13	1:D:34:ARG:HE	1.79	0.47
1:D:329:LEU:HD12	1:D:329:LEU:HA	1.80	0.47
1:A:143:PHE:N	1:A:144:PRO:HD2	2.30	0.47
1:C:224:LEU:HD12	1:C:246:VAL:HG22	1.95	0.47
1:C:420:GLU:OE2	1:C:444:LEU:HD21	2.14	0.47
1:C:367:ARG:HG2	1:C:367:ARG:HH11	1.80	0.46
1:A:409:VAL:O	1:A:412:LEU:HB2	2.14	0.46
1:A:466:ALA:N	2:A:495:HOH:O	2.47	0.46
1:B:324:LYS:O	1:B:324:LYS:CG	2.63	0.46
1:C:20:VAL:HB	1:C:33:GLN:HG2	1.98	0.46
1:C:314:LEU:C	1:C:316:PRO:HD3	2.41	0.46
1:A:295:ILE:CG1	1:A:298:MET:CE	2.94	0.46
1:C:103:GLY:HA3	1:C:360:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:MET:HE3	1:A:309:ILE:HD13	1.98	0.46
1:D:109:ASN:OD1	1:D:142:THR:HG21	2.16	0.46
1:D:410:THR:OG1	1:D:411:PRO:HD3	2.16	0.46
1:D:465:LYS:O	1:D:466:ALA:C	2.57	0.46
1:A:433:LYS:HE2	1:A:441:ASP:OD2	2.16	0.46
1:B:296:ARG:HG3	1:C:188:LEU:HD12	1.96	0.46
1:D:235:LEU:O	1:D:236:ASN:HB2	2.15	0.46
1:B:409:VAL:O	1:B:412:LEU:HB2	2.16	0.46
1:C:451:ILE:H	1:C:451:ILE:HG13	1.51	0.46
1:D:15:ASP:C	1:D:17:MET:H	2.23	0.46
1:B:440:ILE:HG12	1:B:445:ILE:HD12	1.97	0.45
1:C:187:HIS:O	1:C:188:LEU:HB2	2.15	0.45
1:C:454:LEU:O	1:C:457:ARG:N	2.49	0.45
1:D:445:ILE:CG2	1:D:451:ILE:HG13	2.42	0.45
1:A:235:LEU:O	1:A:236:ASN:HB2	2.15	0.45
1:A:440:ILE:CG1	1:A:445:ILE:HD11	2.47	0.45
1:B:142:THR:HG22	1:B:143:PHE:N	2.31	0.45
1:D:15:ASP:OD1	1:D:34:ARG:NH1	2.49	0.45
1:A:38:ASN:HD21	1:B:315:GLN:HG3	1.82	0.45
1:A:433:LYS:HE3	1:A:437:GLN:HG3	1.98	0.45
1:B:367:ARG:HG2	1:B:367:ARG:HH11	1.81	0.45
1:D:453:ASP:O	1:D:457:ARG:HG3	2.17	0.45
1:A:412:LEU:O	1:A:416:ILE:HG12	2.17	0.45
1:D:414:SER:OG	1:D:457:ARG:NH2	2.50	0.44
1:C:22:VAL:CB	1:C:23:PRO:HD2	2.24	0.44
1:C:328:VAL:HG11	1:D:39:PHE:CZ	2.51	0.44
1:A:189:MET:HE1	1:D:301:GLY:HA2	2.00	0.44
1:A:439:VAL:HG13	1:A:444:LEU:HB2	1.99	0.44
1:C:329:LEU:HD12	1:C:329:LEU:HA	1.79	0.44
1:C:454:LEU:HD23	1:C:454:LEU:HA	1.75	0.44
1:A:38:ASN:ND2	1:B:315:GLN:HE21	2.16	0.44
1:B:286:VAL:HG13	1:D:352:ALA:HA	2.00	0.44
1:C:40:PRO:HD2	1:D:382:LEU:HD21	2.00	0.44
1:A:25:LYS:HD2	1:A:25:LYS:O	2.18	0.44
1:B:231:VAL:HG23	1:B:233:THR:HG23	1.99	0.44
1:B:435:ILE:HG22	1:B:458:LEU:HD21	1.99	0.44
1:D:13:GLU:HB3	1:D:20:VAL:HG23	1.99	0.44
1:D:410:THR:N	1:D:411:PRO:CD	2.81	0.44
1:D:443:GLY:O	2:D:518:HOH:O	2.21	0.44
1:A:424:VAL:CG1	1:A:435:ILE:HG23	2.48	0.43
1:D:213:ARG:NH1	2:D:477:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ILE:HA	2:A:476:HOH:O	2.19	0.43
1:A:424:VAL:HG11	1:A:435:ILE:HG23	1.99	0.43
1:A:109:ASN:OD1	1:A:142:THR:HG21	2.18	0.43
1:A:431:GLU:OE1	1:A:433:LYS:HD2	2.18	0.43
1:B:329:LEU:HD12	1:B:329:LEU:HA	1.80	0.43
1:B:446:GLY:O	1:B:447:ASP:HB2	2.19	0.43
1:D:103:GLY:HA3	1:D:360:VAL:HB	2.01	0.43
1:B:300:SER:HB2	1:C:188:LEU:HB3	2.01	0.43
1:C:17:MET:HG3	1:C:34:ARG:HH12	1.83	0.43
1:C:22:VAL:CB	1:C:23:PRO:CD	2.93	0.43
1:C:341:ILE:HD13	1:D:349:TRP:CZ3	2.54	0.43
1:A:414:SER:OG	1:A:457:ARG:NH2	2.52	0.43
1:D:314:LEU:HD21	1:D:329:LEU:HD22	2.01	0.43
1:A:296:ARG:O	1:A:300:SER:HB3	2.19	0.43
1:A:367:ARG:NH1	2:A:475:HOH:O	2.52	0.43
1:C:445:ILE:H	1:C:445:ILE:CD1	2.11	0.43
1:C:419:GLU:HA	1:C:419:GLU:OE2	2.18	0.42
1:B:103:GLY:HA3	1:B:360:VAL:HB	2.01	0.42
1:C:228:GLY:O	1:C:229:THR:OG1	2.30	0.42
1:D:453:ASP:OD2	1:D:457:ARG:NH1	2.51	0.42
1:C:11:ARG:NH1	1:C:24:ALA:O	2.53	0.42
1:B:417:GLY:N	1:B:420:GLU:OE1	2.43	0.42
1:A:159:LEU:O	1:A:163:LEU:HG	2.19	0.42
1:C:142:THR:HG22	1:C:143:PHE:N	2.33	0.42
1:C:452:GLU:O	1:C:456:ARG:HB2	2.20	0.42
1:C:429:LEU:HA	1:C:429:LEU:HD23	1.81	0.42
1:B:301:GLY:CA	1:C:189:MET:CE	2.98	0.42
1:D:367:ARG:HH11	1:D:367:ARG:HG2	1.84	0.42
1:A:189:MET:HE3	1:D:301:GLY:CA	2.50	0.42
1:A:376:LEU:HD23	1:A:376:LEU:HA	1.92	0.42
1:A:424:VAL:HG12	1:A:435:ILE:HD12	2.01	0.41
1:A:440:ILE:CG1	1:A:445:ILE:CD1	2.98	0.41
1:D:138:SER:HB3	1:D:229:THR:HA	2.02	0.41
1:D:399:ARG:NH1	2:D:503:HOH:O	2.49	0.41
1:C:454:LEU:HD22	1:C:458:LEU:HD22	2.02	0.41
1:A:357:GLU:HG2	1:C:185:ARG:O	2.20	0.41
1:B:190:ASP:OD1	1:C:304:THR:HG23	2.21	0.41
1:B:452:GLU:OE1	1:B:452:GLU:HA	2.18	0.41
1:C:341:ILE:HD13	1:D:349:TRP:CH2	2.56	0.41
1:C:435:ILE:HG22	1:C:458:LEU:HD21	2.02	0.41
1:A:406:PRO:HB3	1:A:425:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ILE:HD13	1:C:107:SER:HB3	2.01	0.41
1:D:313:ASP:C	1:D:316:PRO:HD3	2.45	0.41
1:B:410:THR:C	1:B:412:LEU:N	2.78	0.41
1:B:401:LEU:HD23	1:B:401:LEU:HA	1.92	0.41
1:C:445:ILE:HD12	1:C:445:ILE:N	2.27	0.41
1:A:183:SER:HB3	1:D:304:THR:HG21	2.04	0.41
1:A:106:THR:CG2	1:A:110:MET:HE3	2.52	0.40
1:A:188:LEU:HB3	1:D:300:SER:HB2	2.03	0.40
1:C:430:LYS:HB2	1:C:430:LYS:HE3	1.65	0.40
1:A:9:ASN:OD1	1:A:9:ASN:N	2.54	0.40
1:A:324:LYS:HZ2	1:A:324:LYS:HB2	1.86	0.40
1:A:421:ALA:O	1:A:424:VAL:N	2.55	0.40
1:B:405:SER:O	1:B:408:ILE:HG12	2.22	0.40
1:B:442:ARG:HB2	1:B:444:LEU:HD23	2.02	0.40
1:C:370:LEU:HD23	1:C:370:LEU:HA	1.96	0.40
1:B:296:ARG:HG3	1:C:188:LEU:CD1	2.52	0.40
1:C:72:ALA:HA	1:C:73:PRO:HD2	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	448/475 (94%)	427 (95%)	21 (5%)	0	100	100
1	B	447/475 (94%)	432 (97%)	15 (3%)	0	100	100
1	C	448/475 (94%)	433 (97%)	12 (3%)	3 (1%)	18	32
1	D	447/475 (94%)	434 (97%)	12 (3%)	1 (0%)	43	61
All	All	1790/1900 (94%)	1726 (96%)	60 (3%)	4 (0%)	43	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	455	ASP
1	C	454	LEU
1	C	444	LEU
1	D	315	GLN

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	346/365 (95%)	329 (95%)	17 (5%)	22	42
1	B	345/365 (94%)	325 (94%)	20 (6%)	18	35
1	C	347/365 (95%)	329 (95%)	18 (5%)	21	39
1	D	345/365 (94%)	325 (94%)	20 (6%)	18	35
All	All	1383/1460 (95%)	1308 (95%)	75 (5%)	20	38

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	22	VAL
1	A	25	LYS
1	A	74	GLU
1	A	142	THR
1	A	183	SER
1	A	271	ARG
1	A	324	LYS
1	A	328	VAL
1	A	329	LEU
1	A	357	GLU
1	A	379	VAL
1	A	382	LEU
1	A	414	SER
1	A	442	ARG
1	A	444	LEU
1	A	458	LEU
1	B	20	VAL

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Mol	Chain	Res	Type
1	B	22	VAL
1	B	25	LYS
1	B	74	GLU
1	B	142	THR
1	B	183	SER
1	B	239	ASP
1	B	271	ARG
1	B	306	LEU
1	B	314	LEU
1	B	328	VAL
1	B	329	LEU
1	B	357	GLU
1	B	379	VAL
1	B	382	LEU
1	B	410	THR
1	B	449	LEU
1	B	450	SER
1	B	451	ILE
1	B	458	LEU
1	C	13	GLU
1	C	17	MET
1	C	74	GLU
1	C	142	THR
1	C	183	SER
1	C	271	ARG
1	C	306	LEU
1	C	324	LYS
1	C	329	LEU
1	C	357	GLU
1	C	379	VAL
1	C	382	LEU
1	C	427	GLN
1	C	436	ARG
1	C	437	GLN
1	C	445	ILE
1	C	454	LEU
1	C	458	LEU
1	D	22	VAL
1	D	25	LYS
1	D	74	GLU
1	D	142	THR
1	D	183	SER

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Mol	Chain	Res	Type
1	D	271	ARG
1	D	328	VAL
1	D	329	LEU
1	D	357	GLU
1	D	379	VAL
1	D	382	LEU
1	D	407	SER
1	D	420	GLU
1	D	444	LEU
1	D	449	LEU
1	D	451	ILE
1	D	453	ASP
1	D	454	LEU
1	D	456	ARG
1	D	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	339	GLN
1	A	353	ASN
1	B	9	ASN
1	B	31	GLN
1	B	38	ASN
1	B	353	ASN
1	B	368	ASN
1	C	38	ASN
1	C	339	GLN
1	C	368	ASN
1	C	437	GLN
1	D	38	ASN
1	D	339	GLN
1	D	368	ASN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

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	450/475 (94%)	0.82	52 (11%) 9 8	20, 47, 89, 125	18 (4%)
1	B	452/475 (95%)	0.63	32 (7%) 22 19	20, 46, 73, 113	23 (5%)
1	C	453/475 (95%)	0.93	60 (13%) 7 5	20, 49, 94, 122	19 (4%)
1	D	452/475 (95%)	0.68	33 (7%) 21 18	20, 46, 74, 114	25 (5%)
All	All	1807/1900 (95%)	0.77	177 (9%) 13 11	20, 47, 86, 125	85 (4%)

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	449	LEU	8.8
1	C	124	GLY	7.3
1	D	316	PRO	6.2
1	D	8	ALA	6.0
1	C	451	ILE	5.5
1	B	8	ALA	5.4
1	C	447	ASP	5.1
1	D	16	THR	5.1
1	C	20	VAL	5.1
1	C	316	PRO	5.0
1	D	466	ALA	4.9
1	A	447	ASP	4.8
1	A	444	LEU	4.8
1	B	323	GLY	4.6
1	B	25	LYS	4.6
1	C	21	ARG	4.6
1	A	449	LEU	4.6
1	C	55	GLY	4.6
1	C	30	ALA	4.6
1	D	315	GLN	4.6
1	C	314	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	22	VAL	4.4
1	B	314	LEU	4.4
1	B	453	ASP	4.3
1	C	453	ASP	4.2
1	C	425	ALA	4.2
1	C	450	SER	4.1
1	B	449	LEU	4.1
1	D	453	ASP	4.0
1	D	83	ALA	4.0
1	C	439	VAL	4.0
1	C	29	ARG	3.9
1	C	315	GLN	3.9
1	C	121	ALA	3.9
1	A	300	SER	3.9
1	A	25	LYS	3.9
1	B	16	THR	3.9
1	A	415	ALA	3.8
1	C	418	TYR	3.8
1	C	22	VAL	3.7
1	D	17	MET	3.7
1	A	439	VAL	3.6
1	C	454	LEU	3.6
1	A	301	GLY	3.5
1	A	8	ALA	3.5
1	A	422	ALA	3.5
1	A	26	ALA	3.4
1	C	8	ALA	3.4
1	C	416	ILE	3.4
1	A	92	ASP	3.3
1	B	325	VAL	3.3
1	C	225	ALA	3.3
1	B	10	TYR	3.3
1	C	216	ALA	3.3
1	C	25	LYS	3.3
1	C	83	ALA	3.2
1	C	103	GLY	3.2
1	A	455	ASP	3.2
1	D	314	LEU	3.2
1	C	440	ILE	3.1
1	A	418	TYR	3.1
1	B	451	ILE	3.1
1	C	57	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	446	GLY	3.1
1	C	10	TYR	3.0
1	D	449	LEU	3.0
1	C	125	VAL	2.9
1	B	50	GLN	2.9
1	B	301	GLY	2.9
1	D	354	GLY	2.9
1	C	444	LEU	2.9
1	C	50	GLN	2.9
1	A	412	LEU	2.9
1	C	323	GLY	2.9
1	D	229	THR	2.8
1	A	323	GLY	2.8
1	A	445	ILE	2.8
1	D	14	HIS	2.8
1	A	425	ALA	2.8
1	D	146	ALA	2.8
1	A	49	THR	2.8
1	D	313	ASP	2.8
1	D	25	LYS	2.8
1	D	447	ASP	2.8
1	B	313	ASP	2.7
1	D	116	ILE	2.7
1	C	117	ALA	2.7
1	D	171	ALA	2.7
1	C	400	ARG	2.7
1	D	252	GLN	2.7
1	C	313	ASP	2.7
1	D	323	GLY	2.7
1	C	246	VAL	2.7
1	A	17	MET	2.7
1	A	28	TRP	2.7
1	A	171	ALA	2.7
1	A	174	ALA	2.7
1	D	301	GLY	2.6
1	C	66	SER	2.6
1	B	14	HIS	2.6
1	B	223	GLU	2.6
1	C	446	GLY	2.6
1	D	21	ARG	2.6
1	B	447	ASP	2.5
1	A	119	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	20	VAL	2.5
1	D	131	ASP	2.5
1	C	409	VAL	2.5
1	A	16	THR	2.5
1	C	23	PRO	2.5
1	A	159	LEU	2.5
1	B	131	ASP	2.5
1	D	10	TYR	2.5
1	B	20	VAL	2.5
1	B	174	ALA	2.5
1	A	420	GLU	2.4
1	B	197	GLY	2.4
1	C	301	GLY	2.4
1	D	324	LYS	2.4
1	A	163	LEU	2.4
1	D	310	GLN	2.4
1	B	17	MET	2.4
1	A	409	VAL	2.4
1	B	102	THR	2.4
1	C	163	LEU	2.4
1	D	400	ARG	2.4
1	C	73	PRO	2.4
1	A	10	TYR	2.4
1	A	424	VAL	2.4
1	A	126	THR	2.3
1	A	131	ASP	2.3
1	C	91	HIS	2.3
1	A	403	GLU	2.3
1	C	24	ALA	2.3
1	B	216	ALA	2.3
1	A	21	ARG	2.3
1	A	450	SER	2.3
1	C	7	SER	2.3
1	A	218	LEU	2.3
1	B	430	LYS	2.3
1	B	445	ILE	2.2
1	A	125	VAL	2.2
1	C	288	LEU	2.2
1	B	416	ILE	2.2
1	B	15	ASP	2.2
1	A	14	HIS	2.2
1	D	49	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	175	LEU	2.2
1	B	12	ILE	2.2
1	C	445	ILE	2.2
1	B	256	SER	2.2
1	C	92	ASP	2.2
1	B	246	VAL	2.1
1	C	250	VAL	2.1
1	A	429	LEU	2.1
1	A	443	GLY	2.1
1	A	139	SER	2.1
1	C	457	ARG	2.1
1	C	442	ARG	2.1
1	A	121	ALA	2.1
1	C	53	ALA	2.1
1	C	120	ALA	2.1
1	C	381	ARG	2.1
1	A	451	ILE	2.1
1	D	418	TYR	2.1
1	A	15	ASP	2.1
1	C	441	ASP	2.1
1	A	298	MET	2.1
1	A	99	VAL	2.0
1	D	439	VAL	2.0
1	D	9	ASN	2.0
1	D	12	ILE	2.0
1	B	316	PRO	2.0
1	C	414	SER	2.0
1	A	164[A]	GLN	2.0
1	C	438	THR	2.0
1	B	23	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.