



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:45 AM UTC

PDB ID : 1AOS / pdb_00001aos
Title : HUMAN ARGININOSUCCINATE LYASE
Authors : Turner, M.A.; Simpson, A.; Mcinnes, R.R.; Howell, P.L.
Deposited on : 1997-07-10
Resolution : 4.20 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

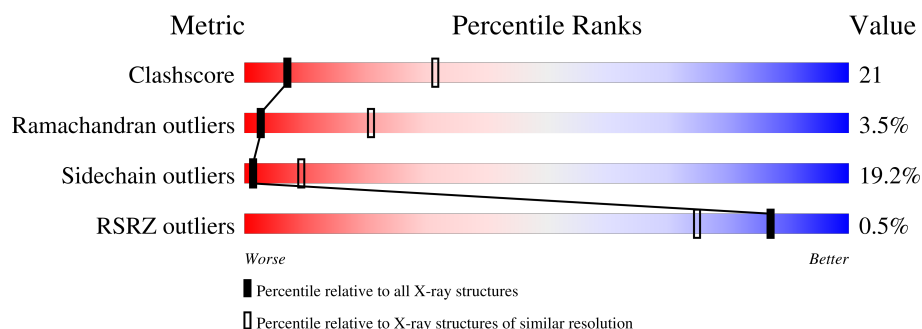
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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))
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	464	
1	B	464	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6788 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 ARGININOSUCCINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	0
			3394	2134	602	639	19			
1	B	434	Total	C	N	O	S	0	0	0
			3394	2134	602	639	19			

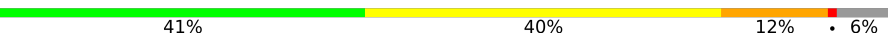
There are 2 discrepancies between the modelled and reference sequences:

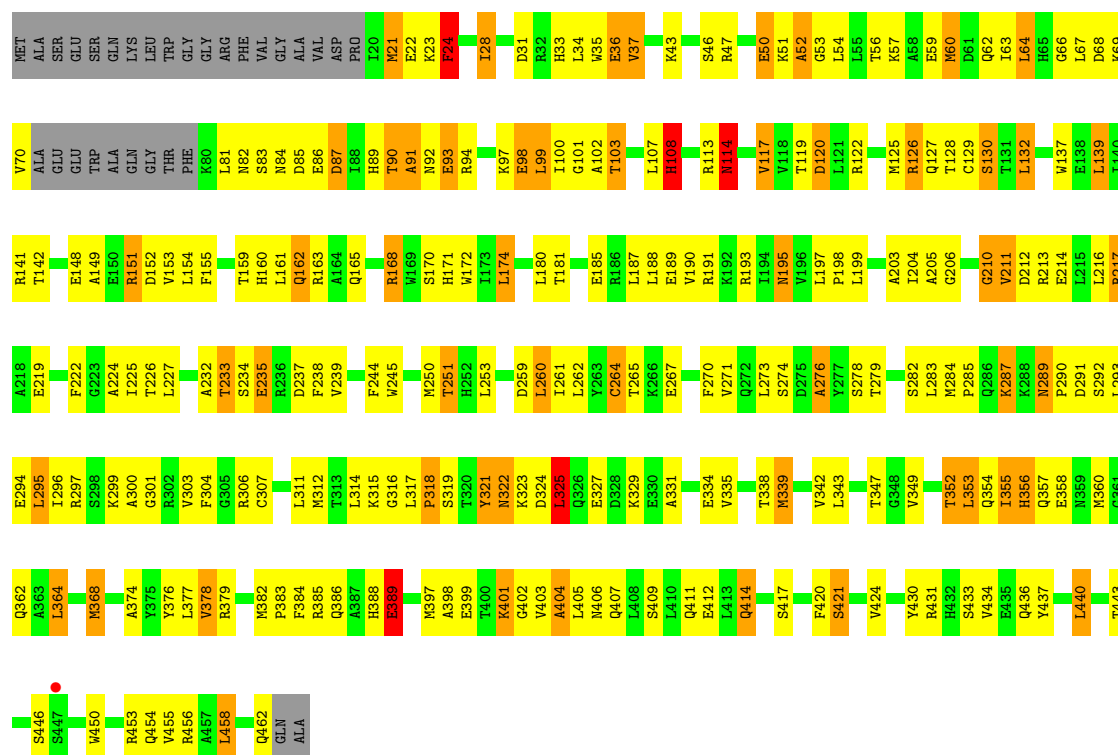
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLN	GLY	conflict	UNP P04424
B	6	GLN	GLY	conflict	UNP P04424

3 Residue-property plots

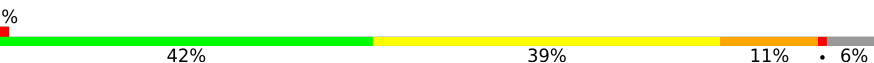
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

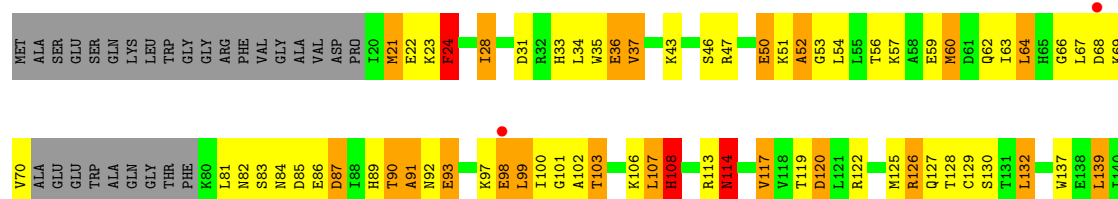
• Molecule 1: ARGININOSUCCINATE LYASE

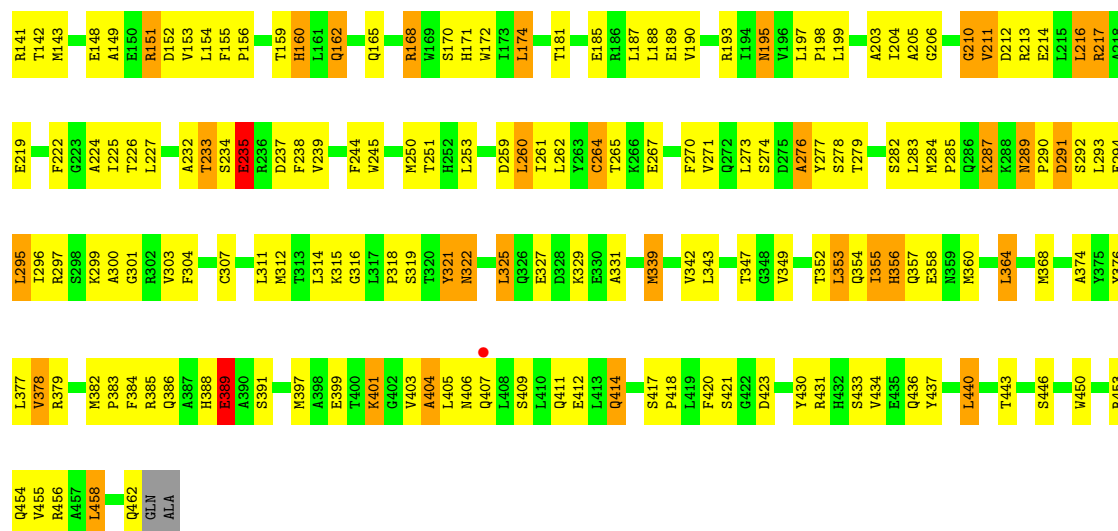
Chain A: 



• Molecule 1: ARGININOSUCCINATE LYASE

Chain B: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.60Å 104.60Å 183.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 4.20 8.00 – 4.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-4.20) 78.7 (8.00-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 4.00Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.188 , 0.298 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.074 for -h,-k,l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6788	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 3.83% 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	0.89	2/3452 (0.1%)	1.34	52/4665 (1.1%)
1	B	0.88	1/3452 (0.0%)	1.35	52/4665 (1.1%)
All	All	0.89	3/6904 (0.0%)	1.35	104/9330 (1.1%)

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	A	0	2
1	B	0	3
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	VAL	CA-CB	6.41	1.61	1.54
1	A	153	VAL	CA-CB	5.38	1.60	1.54
1	A	352	THR	CA-CB	5.25	1.61	1.53

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	LYS	N-CA-C	-12.47	98.01	113.97
1	B	69	LYS	N-CA-C	-12.21	98.35	113.97
1	B	28	ILE	N-CA-C	10.57	121.40	110.62
1	A	28	ILE	N-CA-C	10.50	121.33	110.62
1	B	24	PHE	N-CA-C	-9.73	101.17	113.43
1	A	24	PHE	N-CA-C	-9.70	101.21	113.43
1	A	276	ALA	N-CA-C	-8.61	102.59	113.43
1	A	384	PHE	N-CA-C	8.40	120.13	110.97
1	B	384	PHE	N-CA-C	8.39	120.12	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	ALA	N-CA-C	-8.33	102.94	113.43
1	B	289	ASN	CA-C-N	8.25	128.20	120.03
1	B	289	ASN	C-N-CA	8.25	128.20	120.03
1	B	130	SER	N-CA-C	-8.24	102.25	111.07
1	B	347	THR	N-CA-C	-8.17	102.46	111.36
1	A	401	LYS	N-CA-C	-7.92	103.07	112.89
1	B	401	LYS	N-CA-C	-7.77	103.25	112.89
1	B	155	PHE	CA-C-N	-7.77	112.19	120.66
1	B	155	PHE	C-N-CA	-7.77	112.19	120.66
1	A	130	SER	N-CA-C	-7.76	102.76	111.07
1	A	289	ASN	CA-C-N	7.73	128.19	119.92
1	A	289	ASN	C-N-CA	7.73	128.19	119.92
1	B	122	ARG	N-CA-C	-7.62	102.92	111.07
1	B	244	PHE	N-CA-C	-7.56	102.98	111.07
1	A	244	PHE	N-CA-C	-7.44	103.11	111.07
1	A	347	THR	N-CA-C	-7.43	102.55	111.69
1	B	60	MET	N-CA-C	-7.11	103.61	111.36
1	A	122	ARG	N-CA-C	-6.95	103.63	111.07
1	A	185	GLU	N-CA-C	-6.90	103.20	111.69
1	A	60	MET	N-CA-C	-6.87	103.87	111.36
1	A	152	ASP	N-CA-C	6.87	121.51	113.20
1	B	185	GLU	N-CA-C	-6.86	103.25	111.69
1	A	23	LYS	N-CA-C	-6.85	105.34	113.21
1	A	155	PHE	CA-C-N	-6.84	113.20	120.66
1	A	155	PHE	C-N-CA	-6.84	113.20	120.66
1	B	23	LYS	N-CA-C	-6.82	105.37	113.21
1	B	289	ASN	N-CA-C	6.82	124.88	109.81
1	B	152	ASP	N-CA-C	6.71	121.32	113.20
1	A	289	ASN	N-CA-C	6.69	124.58	109.81
1	B	251	THR	N-CA-C	-6.67	104.01	111.28
1	B	389	GLU	N-CA-C	-6.60	104.26	112.90
1	A	389	GLU	N-CA-C	-6.55	104.32	112.90
1	A	251	THR	N-CA-C	-6.46	104.24	111.28
1	A	83	SER	N-CA-C	6.46	119.13	111.71
1	B	155	PHE	CB-CA-C	6.45	118.63	110.76
1	A	52	ALA	N-CA-C	-6.41	105.28	113.23
1	A	205	ALA	N-CA-C	-6.39	101.33	110.59
1	B	205	ALA	N-CA-C	-6.38	101.34	110.59
1	A	160	HIS	N-CA-C	-6.25	101.99	110.68
1	B	83	SER	N-CA-C	6.22	118.86	111.71
1	B	294	GLU	N-CA-C	-6.20	105.61	113.43
1	A	172	TRP	N-CA-C	-6.14	103.19	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	GLU	N-CA-C	-6.11	105.74	113.43
1	B	355	ILE	N-CA-C	6.08	117.35	108.53
1	A	148	GLU	N-CA-C	-6.05	104.60	111.07
1	A	46	SER	N-CA-C	-6.04	104.62	111.14
1	A	355	ILE	N-CA-C	5.99	117.22	108.53
1	B	52	ALA	N-CA-C	-5.97	105.82	113.23
1	A	405	LEU	N-CA-C	5.93	118.50	111.33
1	A	155	PHE	CB-CA-C	5.90	117.96	110.76
1	B	33	HIS	N-CA-C	5.88	119.28	111.75
1	A	108	HIS	N-CA-C	5.88	120.24	112.25
1	B	160	HIS	N-CA-C	-5.86	102.53	110.68
1	A	357	GLN	N-CA-C	5.86	118.14	111.11
1	B	172	TRP	N-CA-C	-5.84	103.63	112.04
1	B	117	VAL	N-CA-C	5.84	116.62	110.72
1	A	279	THR	N-CA-C	5.83	119.41	110.20
1	A	114	ASN	N-CA-C	5.80	119.17	111.75
1	B	46	SER	N-CA-C	-5.78	104.90	111.14
1	B	108	HIS	N-CA-C	5.71	120.02	112.25
1	A	117	VAL	N-CA-C	5.68	116.42	110.62
1	A	168	ARG	N-CA-C	5.67	118.50	110.50
1	A	331	ALA	N-CA-C	5.64	117.23	111.14
1	B	357	GLN	N-CA-C	5.62	117.85	111.11
1	B	405	LEU	N-CA-C	5.59	118.91	111.75
1	A	233	THR	N-CA-C	5.57	118.19	111.40
1	B	339	MET	N-CA-C	5.56	117.02	111.07
1	B	114	ASN	N-CA-C	5.56	118.87	111.75
1	B	331	ALA	N-CA-C	5.54	117.12	111.14
1	B	233	THR	N-CA-C	5.54	118.15	111.40
1	B	168	ARG	N-CA-C	5.53	118.29	110.50
1	A	33	HIS	N-CA-C	5.51	119.50	112.34
1	B	279	THR	N-CA-C	5.44	118.80	110.20
1	B	212	ASP	N-CA-C	5.36	118.00	109.96
1	A	307	CYS	N-CA-C	-5.34	105.54	111.36
1	A	339	MET	N-CA-C	5.33	116.77	111.07
1	B	322	ASN	N-CA-C	-5.32	102.18	110.42
1	A	210	GLY	N-CA-C	5.31	122.40	115.40
1	B	235	GLU	N-CA-C	5.29	118.44	109.76
1	A	127	GLN	N-CA-C	-5.27	105.12	112.45
1	B	127	GLN	N-CA-C	-5.27	105.12	112.45
1	B	210	GLY	N-CA-C	5.26	122.34	115.40
1	B	391	SER	N-CA-C	-5.26	105.55	111.28
1	B	37	VAL	CB-CA-C	-5.23	106.46	111.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	PRO	N-CA-C	5.23	120.50	111.77
1	B	307	CYS	N-CA-C	-5.20	105.53	111.14
1	A	212	ASP	N-CA-C	5.18	117.73	109.96
1	A	37	VAL	CB-CA-C	-5.17	106.51	111.06
1	B	148	GLU	N-CA-C	-5.16	104.92	111.11
1	B	149	ALA	N-CA-C	5.04	116.47	111.07
1	A	338	THR	N-CA-C	-5.03	105.26	111.40
1	A	94	ARG	N-CA-C	-5.03	106.41	112.54
1	A	322	ASN	N-CA-C	-5.03	102.62	110.42
1	A	149	ALA	N-CA-C	5.01	116.74	111.28
1	A	362	GLN	N-CA-C	-5.01	106.95	113.16

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	376	TYR	Sidechain
1	A	437	TYR	Sidechain
1	B	277	TYR	Sidechain
1	B	376	TYR	Sidechain
1	B	437	TYR	Sidechain

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	3394	0	3391	148	0
1	B	3394	0	3391	139	0
All	All	6788	0	6782	284	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 21.

All (284) 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:A:312:MET:HG3	1:B:312:MET:HG3	1.45	0.97
1:B:409:SER:O	1:B:412:GLU:HB2	1.80	0.82
1:A:108:HIS:H	1:A:108:HIS:CD2	1.98	0.81
1:A:409:SER:O	1:A:412:GLU:HB2	1.79	0.80
1:B:271:VAL:HG12	1:B:355:ILE:HG22	1.65	0.79
1:A:271:VAL:HG12	1:A:355:ILE:HG22	1.66	0.78
1:B:108:HIS:CD2	1:B:108:HIS:H	2.00	0.78
1:B:89:HIS:CE1	1:B:117:VAL:HG22	2.19	0.77
1:A:89:HIS:CE1	1:A:117:VAL:HG22	2.20	0.76
1:B:265:THR:HG22	1:B:267:GLU:H	1.52	0.75
1:A:108:HIS:H	1:A:108:HIS:HD2	1.33	0.74
1:B:226:THR:HG21	1:B:232:ALA:HB2	1.70	0.73
1:B:99:LEU:HD12	1:B:100:ILE:HG12	1.70	0.73
1:A:226:THR:HG21	1:A:232:ALA:HB2	1.71	0.73
1:B:250:MET:HE1	1:B:342:VAL:HG11	1.71	0.72
1:B:108:HIS:H	1:B:108:HIS:HD2	1.35	0.71
1:A:99:LEU:HD12	1:A:100:ILE:HG12	1.72	0.71
1:A:265:THR:HG22	1:A:267:GLU:H	1.54	0.70
1:A:250:MET:HE1	1:A:342:VAL:HG11	1.72	0.69
1:A:108:HIS:CD2	1:A:108:HIS:N	2.60	0.69
1:B:382:MET:HE2	1:B:386:GLN:HB3	1.74	0.69
1:B:443:THR:HG22	1:B:443:THR:O	1.93	0.69
1:A:443:THR:O	1:A:443:THR:HG22	1.94	0.68
1:A:382:MET:HE2	1:A:386:GLN:HB3	1.76	0.68
1:B:28:ILE:HG13	1:B:86:GLU:O	1.93	0.68
1:A:282:SER:C	1:A:284:MET:H	2.01	0.68
1:B:108:HIS:CD2	1:B:108:HIS:N	2.62	0.68
1:A:187:LEU:HD22	1:A:245:TRP:CZ2	2.29	0.67
1:B:187:LEU:HD22	1:B:245:TRP:CZ2	2.31	0.66
1:A:383:PRO:HG2	1:A:386:GLN:HB2	1.76	0.65
1:B:282:SER:C	1:B:284:MET:H	2.02	0.65
1:A:28:ILE:HG13	1:A:86:GLU:O	1.96	0.65
1:A:154:LEU:HD11	1:A:431:ARG:HG3	1.79	0.64
1:B:404:ALA:HB3	1:B:407:GLN:OE1	1.97	0.64
1:B:113:ARG:O	1:B:117:VAL:HG23	1.98	0.64
1:B:383:PRO:HG2	1:B:386:GLN:HB2	1.79	0.64
1:A:113:ARG:O	1:A:117:VAL:HG23	1.98	0.63
1:B:154:LEU:HD11	1:B:431:ARG:HG3	1.80	0.63
1:B:97:LYS:O	1:B:101:GLY:HA2	1.99	0.63
1:A:168:ARG:H	1:A:443:THR:HG21	1.64	0.62
1:B:197:LEU:HD12	1:B:225:ILE:HG22	1.81	0.62
1:A:404:ALA:HB3	1:A:407:GLN:OE1	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:GLN:O	1:A:458:LEU:HD13	2.00	0.62
1:A:97:LYS:O	1:A:101:GLY:HA2	2.00	0.62
1:B:454:GLN:O	1:B:458:LEU:HD13	1.99	0.62
1:A:203:ALA:O	1:A:204:ILE:HD12	2.00	0.61
1:B:35:TRP:CG	1:B:36:GLU:N	2.68	0.61
1:A:22:GLU:C	1:A:24:PHE:H	2.08	0.61
1:A:260:LEU:HB3	1:A:293:LEU:HD13	1.83	0.61
1:B:168:ARG:H	1:B:443:THR:HG21	1.65	0.61
1:B:315:LYS:O	1:B:315:LYS:HG2	2.00	0.61
1:B:56:THR:HG23	1:B:59:GLU:OE2	2.01	0.60
1:B:203:ALA:O	1:B:204:ILE:HD12	2.02	0.60
1:A:56:THR:HG23	1:A:59:GLU:OE2	2.00	0.60
1:B:22:GLU:C	1:B:24:PHE:H	2.09	0.60
1:B:379:ARG:HH22	1:B:436:GLN:HG3	1.67	0.60
1:A:250:MET:HG3	1:A:303:VAL:HG21	1.83	0.59
1:A:197:LEU:HD12	1:A:225:ILE:HG22	1.84	0.59
1:A:433:SER:O	1:A:436:GLN:HB3	2.02	0.59
1:A:379:ARG:HH22	1:A:436:GLN:HG3	1.67	0.59
1:B:250:MET:HG3	1:B:303:VAL:HG21	1.84	0.59
1:A:35:TRP:CG	1:A:36:GLU:N	2.70	0.59
1:A:315:LYS:O	1:A:315:LYS:HG2	2.03	0.59
1:B:114:ASN:HD21	1:B:203:ALA:HA	1.68	0.59
1:B:195:ASN:OD1	1:B:222:PHE:HD1	1.86	0.59
1:A:114:ASN:HD21	1:A:203:ALA:HA	1.67	0.59
1:A:195:ASN:OD1	1:A:222:PHE:HD1	1.86	0.58
1:B:35:TRP:CD1	1:B:36:GLU:N	2.71	0.58
1:B:260:LEU:HB3	1:B:293:LEU:HD13	1.85	0.58
1:A:35:TRP:CD1	1:A:36:GLU:N	2.72	0.58
1:B:433:SER:O	1:B:436:GLN:HB3	2.03	0.57
1:A:431:ARG:O	1:A:434:VAL:HG22	2.03	0.57
1:B:401:LYS:HE3	1:B:403:VAL:HG23	1.85	0.57
1:B:114:ASN:ND2	1:B:203:ALA:HA	2.20	0.57
1:B:197:LEU:HD23	1:B:222:PHE:CD2	2.40	0.57
1:B:89:HIS:NE2	1:B:117:VAL:HG22	2.19	0.56
1:A:401:LYS:HE3	1:A:403:VAL:HG23	1.87	0.56
1:A:114:ASN:ND2	1:A:203:ALA:HA	2.19	0.56
1:B:431:ARG:O	1:B:434:VAL:HG22	2.05	0.56
1:B:213:ARG:HH22	1:B:226:THR:HG22	1.69	0.56
1:A:197:LEU:HD23	1:A:222:PHE:CD2	2.41	0.56
1:A:213:ARG:HH22	1:A:226:THR:HG22	1.71	0.55
1:A:89:HIS:NE2	1:A:117:VAL:HG22	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLU:HG3	1:A:99:LEU:N	2.21	0.54
1:A:284:MET:N	1:A:285:PRO:HD3	2.21	0.54
1:B:98:GLU:HG3	1:B:99:LEU:N	2.22	0.54
1:B:21:MET:O	1:B:24:PHE:HB2	2.07	0.54
1:B:126:ARG:O	1:B:126:ARG:HG2	2.07	0.54
1:B:284:MET:N	1:B:285:PRO:HD3	2.22	0.53
1:B:282:SER:O	1:B:284:MET:N	2.42	0.53
1:A:282:SER:O	1:A:284:MET:N	2.41	0.53
1:A:126:ARG:O	1:A:126:ARG:HG2	2.08	0.52
1:A:287:LYS:HG2	1:B:162:GLN:HB3	1.90	0.52
1:B:274:SER:C	1:B:276:ALA:H	2.18	0.52
1:B:301:GLY:HA2	1:B:304:PHE:HB3	1.90	0.52
1:A:52:ALA:HB3	1:A:54:LEU:HD23	1.93	0.51
1:A:43:LYS:HD2	1:A:67:LEU:O	2.11	0.51
1:A:301:GLY:HA2	1:A:304:PHE:HB3	1.92	0.51
1:A:21:MET:O	1:A:24:PHE:HB2	2.10	0.51
1:B:52:ALA:HB3	1:B:54:LEU:HD23	1.93	0.51
1:B:273:LEU:HD11	1:B:293:LEU:HD12	1.93	0.51
1:A:187:LEU:HD12	1:A:190:VAL:CG1	2.41	0.51
1:A:319:SER:O	1:A:322:ASN:ND2	2.43	0.50
1:B:108:HIS:HD2	1:B:108:HIS:N	2.06	0.50
1:B:430:TYR:O	1:B:434:VAL:HG13	2.11	0.50
1:A:411:GLN:HA	1:A:414:GLN:HB2	1.92	0.50
1:B:450:TRP:HD1	1:B:453:ARG:HH12	1.60	0.50
1:A:139:LEU:HD12	1:A:343:LEU:HD22	1.94	0.50
1:A:430:TYR:O	1:A:434:VAL:HG13	2.11	0.50
1:A:274:SER:C	1:A:276:ALA:H	2.19	0.49
1:B:364:LEU:HB3	1:B:430:TYR:CE1	2.47	0.49
1:A:171:HIS:HB2	1:A:443:THR:HG23	1.94	0.49
1:A:253:LEU:HD11	1:A:343:LEU:HD23	1.93	0.49
1:B:137:TRP:CZ2	1:B:462:GLN:HB3	2.47	0.49
1:B:43:LYS:HD2	1:B:67:LEU:O	2.12	0.49
1:A:233:THR:HG22	1:A:321:TYR:HB2	1.94	0.49
1:A:382:MET:CG	1:A:383:PRO:HD2	2.42	0.49
1:B:187:LEU:HD12	1:B:190:VAL:CG1	2.43	0.49
1:B:319:SER:O	1:B:322:ASN:ND2	2.46	0.49
1:B:411:GLN:HA	1:B:414:GLN:HB2	1.95	0.49
1:A:213:ARG:HB3	1:A:225:ILE:HG21	1.95	0.49
1:A:282:SER:C	1:A:284:MET:N	2.69	0.49
1:B:21:MET:O	1:B:24:PHE:CB	2.61	0.49
1:B:90:THR:O	1:B:92:ASN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LEU:HB3	1:A:430:TYR:CE1	2.48	0.48
1:B:171:HIS:HB2	1:B:443:THR:HG23	1.95	0.48
1:B:213:ARG:NH2	1:B:226:THR:HG22	2.27	0.48
1:B:253:LEU:HD11	1:B:343:LEU:HD23	1.94	0.48
1:B:377:LEU:HD13	1:B:382:MET:SD	2.53	0.48
1:A:86:GLU:HB3	1:A:87:ASP:OD1	2.14	0.48
1:B:197:LEU:HD23	1:B:222:PHE:HD2	1.78	0.48
1:B:356:HIS:O	1:B:360:MET:HG3	2.14	0.48
1:A:197:LEU:HD23	1:A:222:PHE:HD2	1.78	0.48
1:A:377:LEU:HD13	1:A:382:MET:SD	2.53	0.48
1:B:233:THR:HG22	1:B:321:TYR:HB2	1.95	0.48
1:B:282:SER:C	1:B:284:MET:N	2.70	0.48
1:A:93:GLU:HG2	1:A:108:HIS:CE1	2.48	0.48
1:A:213:ARG:NH2	1:A:226:THR:HG22	2.29	0.48
1:B:299:LYS:O	1:B:303:VAL:HG23	2.14	0.48
1:B:139:LEU:HD12	1:B:343:LEU:HD22	1.95	0.48
1:A:21:MET:O	1:A:24:PHE:CB	2.62	0.48
1:A:137:TRP:CZ2	1:A:462:GLN:HB3	2.49	0.47
1:B:238:PHE:CE2	1:B:239:VAL:HG13	2.49	0.47
1:A:238:PHE:CE2	1:A:239:VAL:HG13	2.50	0.47
1:A:450:TRP:O	1:A:454:GLN:HG2	2.14	0.47
1:B:119:THR:HG21	1:B:199:LEU:HD22	1.96	0.47
1:B:455:VAL:HA	1:B:458:LEU:HD22	1.96	0.47
1:A:162:GLN:HB3	1:B:287:LYS:HG2	1.96	0.47
1:A:56:THR:H	1:A:59:GLU:HG2	1.79	0.47
1:B:382:MET:CG	1:B:383:PRO:HD2	2.44	0.47
1:A:90:THR:O	1:A:92:ASN:N	2.48	0.47
1:A:273:LEU:HD11	1:A:293:LEU:HD12	1.96	0.47
1:A:450:TRP:HD1	1:A:453:ARG:HH12	1.61	0.47
1:A:455:VAL:HA	1:A:458:LEU:HD22	1.96	0.47
1:B:397:MET:O	1:B:401:LYS:HB2	2.15	0.47
1:A:22:GLU:C	1:A:24:PHE:N	2.70	0.47
1:A:137:TRP:HE1	1:A:462:GLN:NE2	2.13	0.47
1:B:93:GLU:HG2	1:B:108:HIS:CE1	2.49	0.47
1:B:450:TRP:O	1:B:454:GLN:HG2	2.14	0.47
1:A:129:CYS:HA	1:A:132:LEU:HB2	1.97	0.46
1:B:261:ILE:HD11	1:B:297:ARG:NH1	2.30	0.46
1:A:119:THR:HG21	1:A:199:LEU:HD22	1.98	0.46
1:A:132:LEU:HB3	1:A:187:LEU:HD21	1.96	0.46
1:A:261:ILE:HD11	1:A:297:ARG:NH1	2.31	0.46
1:A:299:LYS:O	1:A:303:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ILE:HA	1:B:31:ASP:OD1	2.15	0.46
1:B:137:TRP:HE1	1:B:462:GLN:NE2	2.13	0.46
1:B:270:PHE:HB3	1:B:360:MET:HE3	1.96	0.46
1:A:168:ARG:H	1:A:443:THR:CG2	2.29	0.46
1:A:170:SER:O	1:A:174:LEU:HB2	2.16	0.46
1:A:289:ASN:HA	1:A:290:PRO:HD3	1.69	0.46
1:B:132:LEU:HB3	1:B:187:LEU:HD21	1.97	0.46
1:A:35:TRP:C	1:A:37:VAL:H	2.22	0.46
1:A:270:PHE:HB3	1:A:360:MET:HE3	1.98	0.46
1:A:210:GLY:O	1:A:211:VAL:C	2.59	0.46
1:A:397:MET:O	1:A:401:LYS:HB2	2.16	0.46
1:B:213:ARG:HB3	1:B:225:ILE:HG21	1.97	0.46
1:B:22:GLU:C	1:B:24:PHE:N	2.71	0.46
1:B:35:TRP:CG	1:B:36:GLU:H	2.32	0.46
1:A:35:TRP:CG	1:A:36:GLU:H	2.33	0.45
1:A:235:GLU:HG2	1:A:237:ASP:H	1.81	0.45
1:B:66:GLY:O	1:B:70:VAL:N	2.48	0.45
1:B:35:TRP:C	1:B:37:VAL:H	2.25	0.45
1:B:235:GLU:HG2	1:B:237:ASP:H	1.82	0.45
1:A:50:GLU:O	1:A:53:GLY:N	2.49	0.45
1:B:56:THR:H	1:B:59:GLU:HG2	1.82	0.45
1:B:90:THR:O	1:B:91:ALA:C	2.59	0.45
1:A:66:GLY:O	1:A:70:VAL:N	2.49	0.45
1:B:86:GLU:HB3	1:B:87:ASP:OD1	2.17	0.45
1:B:374:ALA:O	1:B:378:VAL:HG23	2.17	0.45
1:A:28:ILE:HA	1:A:31:ASP:OD1	2.17	0.45
1:B:170:SER:O	1:B:174:LEU:HB2	2.17	0.45
1:A:260:LEU:O	1:A:264:CYS:HB2	2.17	0.45
1:B:66:GLY:C	1:B:68:ASP:H	2.24	0.45
1:A:292:SER:O	1:A:296:ILE:HG13	2.16	0.44
1:B:117:VAL:HA	1:B:120:ASP:HB2	1.99	0.44
1:B:139:LEU:HD22	1:B:143:MET:SD	2.58	0.44
1:B:292:SER:O	1:B:296:ILE:HG13	2.17	0.44
1:A:250:MET:O	1:A:251:THR:C	2.60	0.44
1:B:260:LEU:O	1:B:264:CYS:HB2	2.17	0.44
1:B:129:CYS:HA	1:B:132:LEU:HB2	1.98	0.44
1:A:352:THR:O	1:A:353:LEU:C	2.61	0.44
1:B:21:MET:HE3	1:B:21:MET:HB3	1.79	0.44
1:A:66:GLY:C	1:A:68:ASP:H	2.26	0.44
1:A:90:THR:O	1:A:91:ALA:C	2.60	0.44
1:B:352:THR:O	1:B:353:LEU:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:HA	1:A:120:ASP:HB2	2.00	0.44
1:B:151:ARG:HA	1:B:170:SER:OG	2.17	0.44
1:B:295:LEU:O	1:B:299:LYS:HG2	2.18	0.44
1:B:385:ARG:O	1:B:389:GLU:HB2	2.18	0.44
1:A:250:MET:HE3	1:A:339:MET:SD	2.58	0.44
1:A:417:SER:HB3	1:A:420:PHE:CD2	2.53	0.44
1:A:217:ARG:HD2	1:A:224:ALA:HA	2.00	0.44
1:B:50:GLU:O	1:B:53:GLY:N	2.51	0.44
1:A:87:ASP:OD1	1:A:87:ASP:N	2.51	0.43
1:A:431:ARG:HA	1:A:434:VAL:HG22	2.00	0.43
1:B:106:LYS:O	1:B:107:LEU:C	2.60	0.43
1:A:299:LYS:O	1:A:300:ALA:C	2.60	0.43
1:B:210:GLY:O	1:B:211:VAL:C	2.61	0.43
1:B:250:MET:HE1	1:B:342:VAL:CG1	2.46	0.43
1:B:417:SER:HA	1:B:418:PRO:HD3	1.91	0.43
1:A:214:GLU:O	1:A:217:ARG:HG3	2.17	0.43
1:A:317:LEU:HA	1:A:318:PRO:HD2	1.83	0.43
1:A:82:ASN:HB3	1:A:85:ASP:OD2	2.19	0.43
1:B:349:VAL:O	1:B:353:LEU:HB2	2.19	0.43
1:A:151:ARG:HA	1:A:170:SER:OG	2.18	0.43
1:A:174:LEU:HD12	1:A:174:LEU:HA	1.75	0.43
1:A:353:LEU:HA	1:A:353:LEU:HD12	1.77	0.43
1:A:374:ALA:O	1:A:378:VAL:HG23	2.19	0.43
1:B:60:MET:O	1:B:64:LEU:HB2	2.19	0.43
1:B:188:LEU:HD23	1:B:188:LEU:HA	1.78	0.43
1:A:306:ARG:HH22	1:A:334:GLU:CD	2.27	0.43
1:B:214:GLU:O	1:B:217:ARG:HG3	2.19	0.43
1:B:417:SER:HB3	1:B:420:PHE:CD2	2.53	0.43
1:A:125:MET:SD	1:A:239:VAL:HG12	2.58	0.42
1:A:385:ARG:O	1:A:389:GLU:HB2	2.19	0.42
1:B:168:ARG:HH22	1:B:431:ARG:CZ	2.31	0.42
1:B:289:ASN:HA	1:B:290:PRO:HD3	1.69	0.42
1:A:63:ILE:HG23	1:A:103:THR:HB	2.01	0.42
1:B:87:ASP:OD1	1:B:87:ASP:N	2.51	0.42
1:B:299:LYS:O	1:B:300:ALA:C	2.62	0.42
1:A:60:MET:O	1:A:64:LEU:HB2	2.19	0.42
1:B:216:LEU:HD12	1:B:216:LEU:HA	1.85	0.42
1:A:28:ILE:HG13	1:A:28:ILE:H	1.71	0.42
1:B:217:ARG:HD2	1:B:224:ALA:HA	2.01	0.42
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.79	0.42
1:A:306:ARG:HD3	1:A:306:ARG:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.70	0.42
1:A:168:ARG:HH22	1:A:431:ARG:CZ	2.32	0.41
1:A:356:HIS:O	1:A:360:MET:HG3	2.20	0.41
1:B:168:ARG:H	1:B:443:THR:CG2	2.29	0.41
1:A:52:ALA:CB	1:A:54:LEU:HD23	2.50	0.41
1:A:213:ARG:HH22	1:A:226:THR:CG2	2.33	0.41
1:B:125:MET:SD	1:B:239:VAL:HG12	2.61	0.41
1:B:250:MET:HE3	1:B:339:MET:SD	2.61	0.41
1:B:431:ARG:HA	1:B:434:VAL:HG22	2.02	0.41
1:A:137:TRP:HE1	1:A:462:GLN:HE21	1.67	0.41
1:A:322:ASN:O	1:A:325:LEU:HD13	2.21	0.41
1:B:261:ILE:HD11	1:B:297:ARG:HH12	1.85	0.41
1:A:265:THR:HG22	1:A:267:GLU:HB2	2.03	0.41
1:A:295:LEU:O	1:A:299:LYS:HG2	2.20	0.41
1:A:82:ASN:ND2	1:A:84:ASN:OD1	2.53	0.41
1:A:398:ALA:O	1:A:402:GLY:N	2.54	0.41
1:A:421:SER:O	1:A:424:VAL:HG13	2.20	0.41
1:B:82:ASN:HB3	1:B:85:ASP:OD2	2.21	0.41
1:B:160:HIS:CD2	1:B:160:HIS:N	2.88	0.41
1:B:287:LYS:HE2	1:B:287:LYS:HB3	1.87	0.41
1:A:56:THR:O	1:A:60:MET:N	2.49	0.41
1:A:303:VAL:HG13	1:A:335:VAL:HG13	2.02	0.41
1:B:187:LEU:HD12	1:B:190:VAL:HG11	2.03	0.41
1:B:82:ASN:ND2	1:B:84:ASN:OD1	2.54	0.40
1:B:137:TRP:HZ2	1:B:462:GLN:HB3	1.86	0.40
1:A:130:SER:HA	1:A:191:ARG:CZ	2.51	0.40
1:A:163:ARG:HD3	1:A:368:MET:HE3	2.03	0.40
1:A:287:LYS:HE2	1:A:287:LYS:HB3	1.86	0.40
1:A:349:VAL:O	1:A:353:LEU:HB2	2.21	0.40
1:B:52:ALA:CB	1:B:54:LEU:HD23	2.51	0.40
1:B:54:LEU:N	1:B:54:LEU:HD22	2.36	0.40
1:A:21:MET:HE3	1:A:21:MET:HB3	1.82	0.40
1:A:323:LYS:O	1:A:324:ASP:C	2.65	0.40
1:A:443:THR:O	1:A:443:THR:CG2	2.64	0.40
1:B:63:ILE:HG23	1:B:103:THR:HB	2.02	0.40
1:A:139:LEU:HD13	1:A:180:LEU:HD13	2.03	0.40
1:B:265:THR:HG22	1:B:267:GLU:N	2.29	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	430/464 (93%)	383 (89%)	32 (7%)	15 (4%)	3	21
1	B	430/464 (93%)	384 (89%)	31 (7%)	15 (4%)	3	21
All	All	860/928 (93%)	767 (89%)	63 (7%)	30 (4%)	3	21

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	404	ALA
1	A	440	LEU
1	B	404	ALA
1	B	440	LEU
1	A	102	ALA
1	A	206	GLY
1	A	283	LEU
1	A	321	TYR
1	B	102	ALA
1	B	206	GLY
1	B	283	LEU
1	B	321	TYR
1	A	91	ALA
1	A	195	ASN
1	A	291	ASP
1	A	318	PRO
1	A	325	LEU
1	B	91	ALA
1	B	195	ASN
1	B	291	ASP
1	B	318	PRO
1	B	325	LEU
1	B	353	LEU
1	A	353	LEU
1	B	198	PRO

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Mol	Chain	Res	Type
1	A	151	ARG
1	A	198	PRO
1	B	151	ARG
1	A	316	GLY
1	B	316	GLY

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	364/389 (94%)	295 (81%)	69 (19%)	1	10
1	B	364/389 (94%)	293 (80%)	71 (20%)	1	9
All	All	728/778 (94%)	588 (81%)	140 (19%)	1	9

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	MET
1	A	24	PHE
1	A	34	LEU
1	A	36	GLU
1	A	47	ARG
1	A	50	GLU
1	A	51	LYS
1	A	57	LYS
1	A	62	GLN
1	A	64	LEU
1	A	81	LEU
1	A	87	ASP
1	A	90	THR
1	A	93	GLU
1	A	98	GLU
1	A	99	LEU
1	A	103	THR
1	A	107	LEU

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Mol	Chain	Res	Type
1	A	108	HIS
1	A	114	ASN
1	A	120	ASP
1	A	126	ARG
1	A	128	THR
1	A	132	LEU
1	A	139	LEU
1	A	141	ARG
1	A	142	THR
1	A	159	THR
1	A	162	GLN
1	A	165	GLN
1	A	174	LEU
1	A	181	THR
1	A	189	GLU
1	A	193	ARG
1	A	211	VAL
1	A	216	LEU
1	A	217	ARG
1	A	219	GLU
1	A	227	LEU
1	A	234	SER
1	A	235	GLU
1	A	259	ASP
1	A	260	LEU
1	A	262	LEU
1	A	264	CYS
1	A	278	SER
1	A	287	LYS
1	A	295	LEU
1	A	311	LEU
1	A	314	LEU
1	A	325	LEU
1	A	327	GLU
1	A	329	LYS
1	A	354	GLN
1	A	356	HIS
1	A	358	GLU
1	A	364	LEU
1	A	368	MET
1	A	378	VAL
1	A	388	HIS

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Mol	Chain	Res	Type
1	A	389	GLU
1	A	399	GLU
1	A	406	ASN
1	A	414	GLN
1	A	421	SER
1	A	440	LEU
1	A	446	SER
1	A	456	ARG
1	A	458	LEU
1	B	21	MET
1	B	24	PHE
1	B	34	LEU
1	B	36	GLU
1	B	47	ARG
1	B	50	GLU
1	B	51	LYS
1	B	57	LYS
1	B	62	GLN
1	B	64	LEU
1	B	81	LEU
1	B	87	ASP
1	B	90	THR
1	B	93	GLU
1	B	98	GLU
1	B	99	LEU
1	B	103	THR
1	B	107	LEU
1	B	108	HIS
1	B	114	ASN
1	B	120	ASP
1	B	126	ARG
1	B	128	THR
1	B	132	LEU
1	B	139	LEU
1	B	141	ARG
1	B	142	THR
1	B	159	THR
1	B	162	GLN
1	B	165	GLN
1	B	174	LEU
1	B	181	THR
1	B	189	GLU

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Mol	Chain	Res	Type
1	B	193	ARG
1	B	211	VAL
1	B	216	LEU
1	B	217	ARG
1	B	219	GLU
1	B	227	LEU
1	B	234	SER
1	B	235	GLU
1	B	259	ASP
1	B	260	LEU
1	B	262	LEU
1	B	264	CYS
1	B	278	SER
1	B	287	LYS
1	B	291	ASP
1	B	295	LEU
1	B	311	LEU
1	B	314	LEU
1	B	325	LEU
1	B	327	GLU
1	B	329	LYS
1	B	354	GLN
1	B	356	HIS
1	B	358	GLU
1	B	364	LEU
1	B	368	MET
1	B	378	VAL
1	B	388	HIS
1	B	389	GLU
1	B	399	GLU
1	B	406	ASN
1	B	414	GLN
1	B	421	SER
1	B	423	ASP
1	B	440	LEU
1	B	446	SER
1	B	456	ARG
1	B	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	108	HIS
1	A	114	ASN
1	A	162	GLN
1	A	207	ASN
1	A	326	GLN
1	A	344	GLN
1	A	362	GLN
1	A	462	GLN
1	B	40	GLN
1	B	65	HIS
1	B	108	HIS
1	B	114	ASN
1	B	162	GLN
1	B	326	GLN
1	B	344	GLN
1	B	356	HIS
1	B	362	GLN
1	B	462	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](#)

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 ⓘ

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	434/464 (93%)	-0.15	1 (0%) 91 83	20, 20, 20, 20	0
1	B	434/464 (93%)	-0.16	3 (0%) 84 70	20, 20, 20, 20	0
All	All	868/928 (93%)	-0.16	4 (0%) 87 75	20, 20, 20, 20	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	98	GLU	2.3
1	A	447	SER	2.1
1	B	68	ASP	2.1
1	B	407	GLN	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.