



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:11 AM UTC

PDB ID : 1RRL / pdb_00001rrl
Title : Soybean Lipoxygenase (LOX-3) at 93K at 2.0 Å resolution
Authors : Borbulevych, O.Y.; Jankun, J.; Skrzypczak-Jankun, E.
Deposited on : 2003-12-08
Resolution : 2.09 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

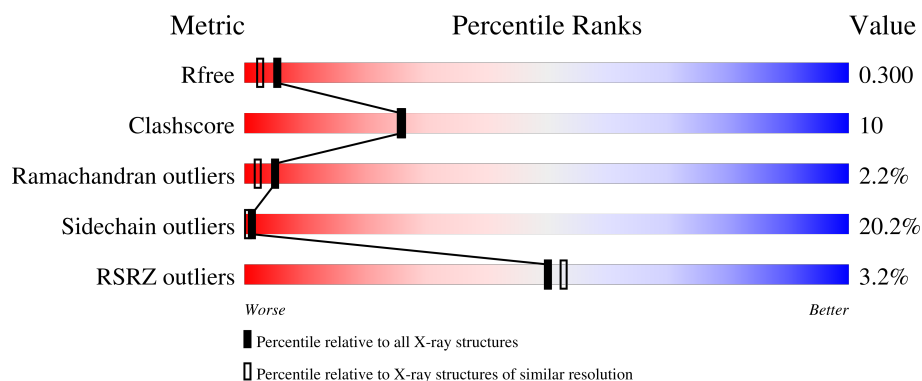
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	857	3% 62% 28% 9% ..
1	B	857	3% 64% 25% 9% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14643 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 Seed lipoxygenase-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	850	Total	C	N	O	S	0	0	0
			6789	4335	1167	1269	18			
1	B	850	Total	C	N	O	S	0	0	0
			6789	4335	1167	1269	18			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ASP	HIS	SEE REMARK 99	UNP P09186
A	57	SER	PRO	SEE REMARK 999	UNP P09186
A	112	PRO	LEU	SEE REMARK 999	UNP P09186
A	201	ILE	VAL	SEE REMARK 999	UNP P09186
A	382	ASP	GLU	SEE REMARK 999	UNP P09186
A	428	ASP	GLY	SEE REMARK 999	UNP P09186
A	630	THR	ALA	SEE REMARK 999	UNP P09186
B	25	ASP	HIS	SEE REMARK 999	UNP P09186
B	57	SER	PRO	SEE REMARK 999	UNP P09186
B	112	PRO	LEU	SEE REMARK 999	UNP P09186
B	201	ILE	VAL	SEE REMARK 999	UNP P09186
B	382	ASP	GLU	SEE REMARK 999	UNP P09186
B	428	ASP	GLY	SEE REMARK 999	UNP P09186
B	630	THR	ALA	SEE REMARK 999	UNP P09186

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

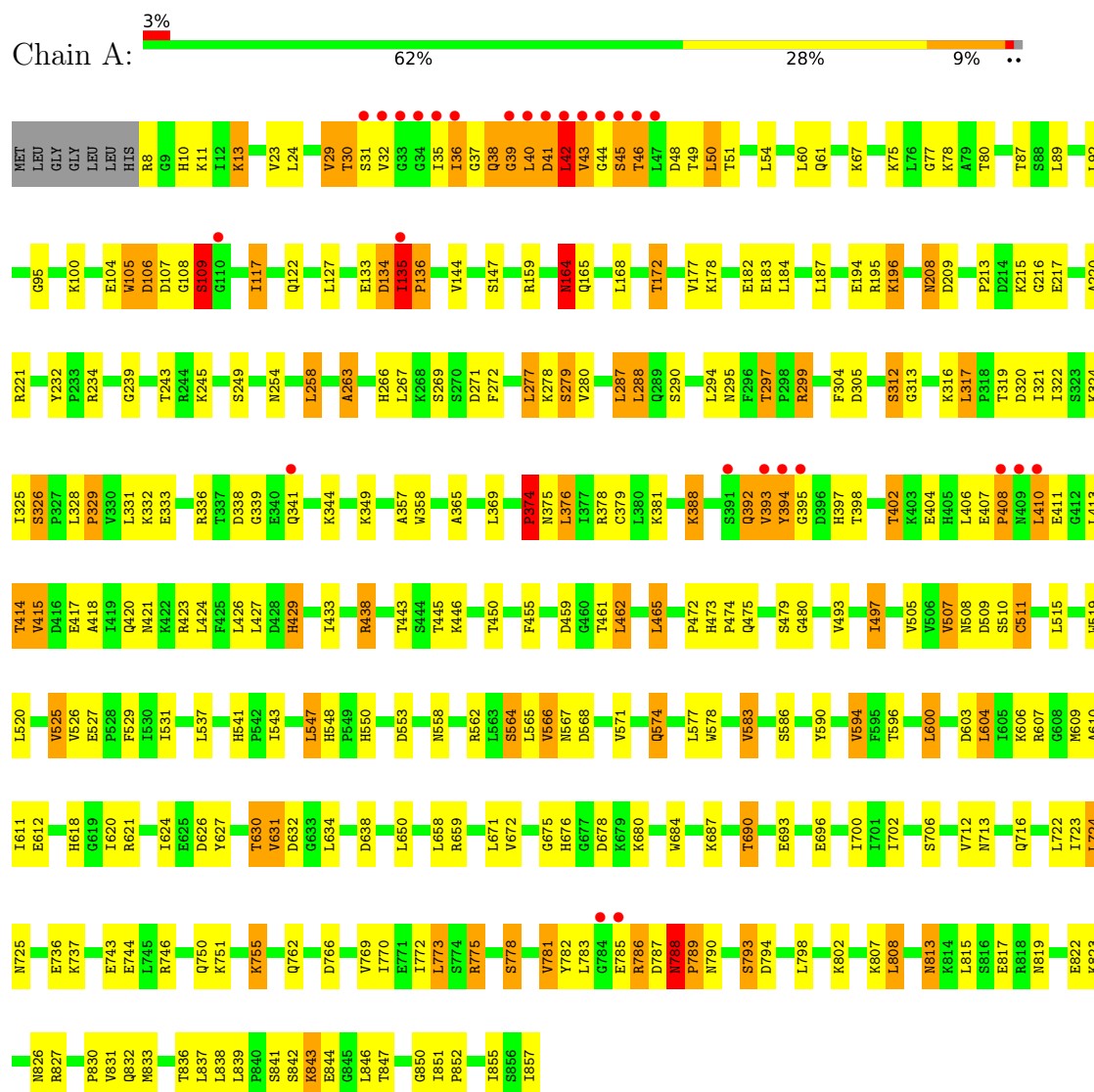
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	500	Total 500	O 500	0	0
3	B	563	Total 563	O 563	0	0

3 Residue-property plots

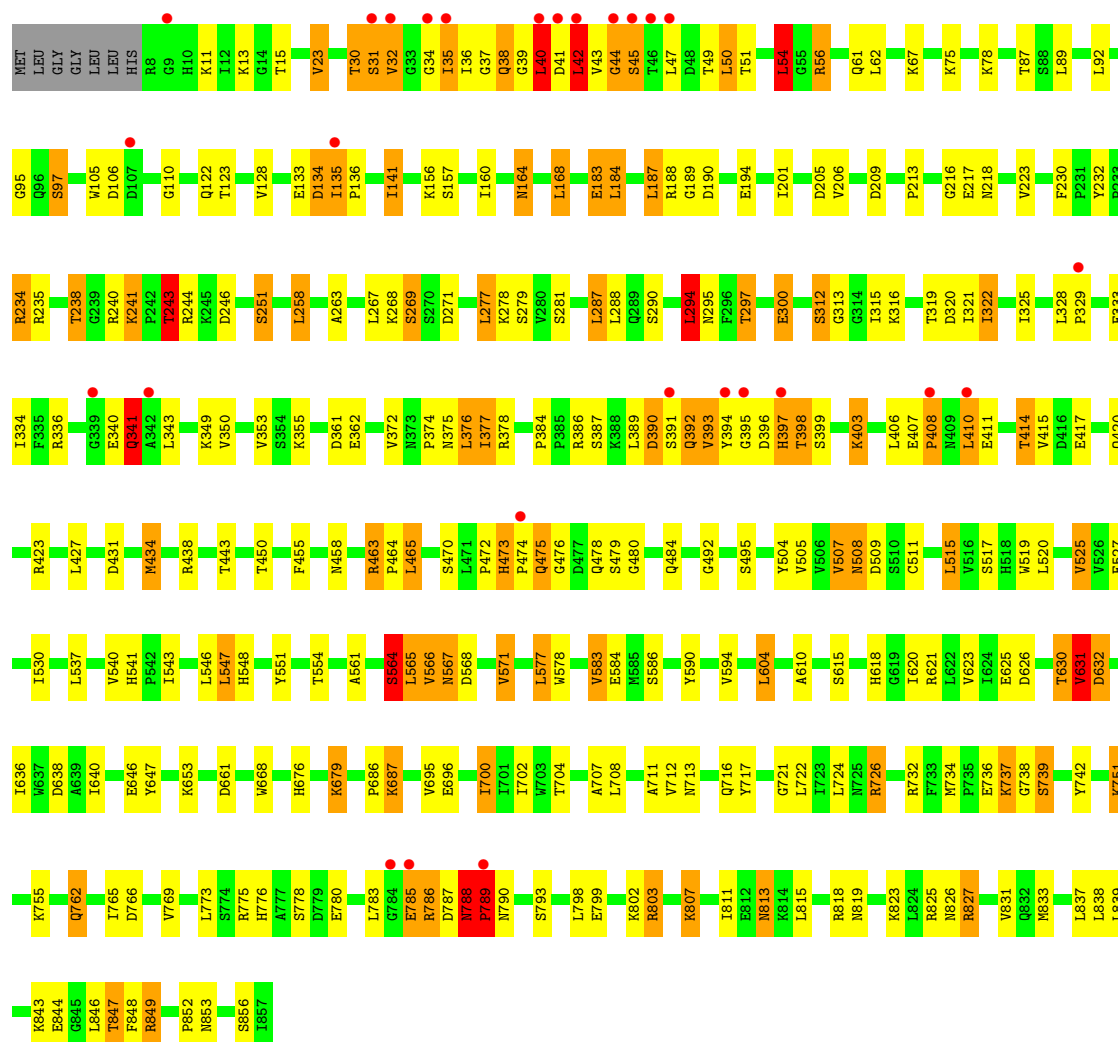
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Seed lipoxygenase-3



• Molecule 1: Seed lipoxygenase-3





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.40Å 133.50Å 60.70Å 90.00° 97.30° 90.00°	Depositor
Resolution (Å)	10.00 – 2.09 10.00 – 2.09	Depositor EDS
% Data completeness (in resolution range)	65.4 (10.00-2.09) 64.8 (10.00-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.207 , 0.305 0.209 , 0.300	Depositor DCC
R_{free} test set	3245 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.3	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	0.95	EDS
Total number of atoms	14643	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2683e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: FE2

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	1.04	5/6961 (0.1%)	1.48	74/9453 (0.8%)
1	B	1.08	11/6961 (0.2%)	1.47	62/9453 (0.7%)
All	All	1.06	16/13922 (0.1%)	1.47	136/18906 (0.7%)

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	5
1	B	0	3
All	All	0	8

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	734	MET	SD-CE	-8.51	1.58	1.79
1	A	263	ALA	CA-CB	-6.62	1.44	1.53
1	B	853	ASN	CA-C	-6.51	1.43	1.52
1	B	434	MET	CG-SD	-6.39	1.64	1.80
1	A	135	ILE	CA-CB	6.34	1.62	1.54
1	B	566	VAL	CA-CB	6.11	1.61	1.54
1	A	531	ILE	C-O	-5.82	1.17	1.24
1	B	548	HIS	N-CA	5.69	1.52	1.46
1	B	32	VAL	CA-CB	5.57	1.63	1.54
1	B	443	THR	CA-CB	5.55	1.61	1.53
1	B	35	ILE	CA-CB	5.47	1.61	1.54
1	B	833	MET	SD-CE	5.40	1.93	1.79
1	A	32	VAL	CA-CB	5.09	1.63	1.54
1	B	527	GLU	CA-C	5.05	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	GLU	CA-C	5.01	1.58	1.52
1	B	377	ILE	CA-CB	-5.00	1.49	1.54

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	SER	N-CA-C	-13.33	95.95	108.75
1	A	785	GLU	N-CA-C	-11.87	98.79	113.28
1	B	37	GLY	N-CA-C	-11.28	98.83	115.63
1	B	785	GLU	N-CA-C	-10.72	97.55	112.45
1	B	238	THR	N-CA-C	-10.66	92.66	109.72
1	A	294	LEU	CA-C-N	-10.54	108.65	123.20
1	A	294	LEU	C-N-CA	-10.54	108.65	123.20
1	B	31	SER	N-CA-C	-10.21	89.04	110.80
1	B	23	VAL	N-CA-C	-9.71	103.66	113.47
1	A	687	LYS	CA-C-N	-9.57	108.26	122.24
1	A	687	LYS	C-N-CA	-9.57	108.26	122.24
1	A	671	LEU	N-CA-C	-9.53	100.45	111.03
1	B	134	ASP	N-CA-C	9.23	125.49	109.80
1	A	847	THR	CA-C-N	-9.14	109.55	123.17
1	A	847	THR	C-N-CA	-9.14	109.55	123.17
1	B	294	LEU	CA-C-N	-8.26	110.19	122.24
1	B	294	LEU	C-N-CA	-8.26	110.19	122.24
1	B	393	VAL	N-CA-C	8.21	121.36	111.09
1	B	566	VAL	N-CA-C	-7.83	103.63	111.77
1	B	475	GLN	N-CA-C	7.62	122.32	112.41
1	A	109	SER	N-CA-C	-7.56	98.25	110.20
1	A	295	ASN	N-CA-C	7.55	119.18	108.54
1	A	280	VAL	CB-CA-C	-7.53	101.97	112.14
1	A	450	THR	N-CA-C	7.52	121.20	110.14
1	A	566	VAL	N-CA-CB	-7.41	102.42	112.28
1	A	847	THR	N-CA-C	-7.27	99.70	110.46
1	B	695	VAL	N-CA-C	-7.19	103.52	110.42
1	B	294	LEU	N-CA-C	-7.18	101.05	110.53
1	B	566	VAL	CB-CA-C	7.18	122.01	112.46
1	B	554	THR	N-CA-C	6.93	118.49	111.07
1	A	426	LEU	N-CA-C	6.85	119.63	108.26
1	B	726	ARG	NE-CZ-NH2	6.72	125.25	119.20
1	B	40	LEU	N-CA-C	-6.69	103.43	112.26
1	B	847	THR	N-CA-C	-6.66	99.44	110.17
1	A	49	THR	N-CA-C	-6.45	103.85	112.94
1	A	675	GLY	CA-C-N	-6.43	113.58	123.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	675	GLY	C-N-CA	-6.43	113.58	123.17
1	A	511	CYS	N-CA-C	6.43	118.09	111.14
1	A	566	VAL	N-CA-C	-6.42	106.07	112.17
1	B	849	ARG	N-CA-C	6.40	116.90	107.88
1	A	395	GLY	N-CA-C	-6.39	105.68	115.66
1	A	393	VAL	N-CA-C	6.38	122.61	109.34
1	A	279	SER	N-CA-C	6.32	118.17	111.28
1	A	37	GLY	N-CA-C	-6.27	98.31	113.18
1	B	848	PHE	CB-CA-C	6.23	119.54	111.50
1	B	431	ASP	N-CA-C	6.21	121.20	112.75
1	B	737	LYS	N-CA-C	6.15	123.89	110.80
1	B	707	ALA	N-CA-C	6.12	118.03	111.36
1	B	450	THR	N-CA-C	6.06	119.54	110.14
1	A	519	TRP	N-CA-C	6.04	118.39	111.02
1	B	34	GLY	N-CA-C	6.04	127.50	113.18
1	A	786	ARG	N-CA-C	6.02	119.30	109.24
1	B	847	THR	CA-C-N	-6.01	111.16	122.27
1	B	847	THR	C-N-CA	-6.01	111.16	122.27
1	A	105	TRP	N-CA-C	-6.00	100.28	108.38
1	A	794	ASP	N-CA-C	-5.99	100.52	109.15
1	B	128	VAL	N-CA-C	-5.99	105.88	111.45
1	A	328	LEU	CA-C-N	5.97	127.31	119.84
1	A	328	LEU	C-N-CA	5.97	127.31	119.84
1	A	209	ASP	N-CA-CB	-5.95	102.98	110.90
1	B	23	VAL	CB-CA-C	5.95	117.04	110.62
1	A	631	VAL	CB-CA-C	-5.94	104.03	112.22
1	B	700	ILE	N-CA-C	-5.92	105.94	111.45
1	B	687	LYS	N-CA-C	-5.90	101.55	110.28
1	A	527	GLU	N-CA-C	5.87	120.89	113.25
1	A	564	SER	N-CA-C	5.85	122.13	114.75
1	A	164	ASN	N-CA-C	5.83	119.21	111.75
1	B	123	THR	OG1-CB-CG2	-5.79	97.72	109.30
1	B	168	LEU	N-CA-C	-5.79	102.09	110.08
1	B	631	VAL	CB-CA-C	-5.71	102.86	112.16
1	A	374	PRO	CA-C-N	5.69	130.87	121.99
1	A	374	PRO	C-N-CA	5.69	130.87	121.99
1	A	50	LEU	N-CA-C	-5.69	105.06	112.23
1	A	851	ILE	N-CA-C	5.65	112.70	107.56
1	B	632	ASP	N-CA-C	-5.65	104.74	111.69
1	A	574	GLN	CA-CB-CG	5.63	125.35	114.10
1	B	391	SER	N-CA-C	5.60	117.07	111.07
1	B	508	ASN	CB-CA-C	-5.59	101.50	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	799	GLU	N-CA-C	-5.58	105.19	111.28
1	A	855	ILE	N-CA-CB	-5.58	105.30	111.66
1	B	23	VAL	N-CA-CB	-5.58	105.69	112.33
1	B	190	ASP	N-CA-C	5.55	119.68	113.02
1	A	851	ILE	CB-CA-C	-5.54	104.52	110.95
1	A	852	PRO	CA-C-O	-5.54	114.98	122.08
1	B	30	THR	N-CA-C	5.54	117.13	109.15
1	A	725	ASN	N-CA-C	5.54	117.12	111.14
1	A	39	GLY	N-CA-C	-5.50	100.15	113.18
1	B	97	SER	N-CA-C	-5.48	101.19	109.85
1	B	341	GLN	CA-C-N	-5.47	114.29	122.39
1	B	341	GLN	C-N-CA	-5.47	114.29	122.39
1	A	497	ILE	N-CA-C	-5.46	105.20	110.72
1	B	300	GLU	N-CA-C	5.46	117.98	109.52
1	B	564	SER	CA-C-N	-5.46	113.07	122.79
1	B	564	SER	C-N-CA	-5.46	113.07	122.79
1	A	574	GLN	CB-CA-C	-5.43	100.24	110.67
1	B	209	ASP	N-CA-CB	-5.43	102.77	110.81
1	A	548	HIS	N-CA-C	5.43	120.87	113.16
1	A	134	ASP	N-CA-C	5.40	122.30	110.80
1	B	295	ASN	N-CA-C	5.39	117.44	110.65
1	A	288	LEU	CA-C-N	5.39	127.81	120.54
1	A	288	LEU	C-N-CA	5.39	127.81	120.54
1	A	144	VAL	CB-CA-C	-5.38	103.11	110.96
1	A	713	ASN	N-CA-C	5.36	119.81	112.68
1	B	726	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	A	328	LEU	O-C-N	5.34	126.14	121.18
1	A	672	VAL	N-CA-C	5.33	115.54	110.53
1	A	329	PRO	N-CA-C	5.31	123.40	112.47
1	A	600	LEU	N-CA-C	5.30	120.14	113.25
1	A	30	THR	CA-C-N	5.26	128.76	123.13
1	A	30	THR	C-N-CA	5.26	128.76	123.13
1	B	328	LEU	O-C-N	5.26	125.93	121.20
1	B	243	THR	N-CA-CB	-5.24	102.33	110.04
1	A	294	LEU	O-C-N	-5.24	115.34	122.36
1	B	577	LEU	N-CA-C	5.24	117.39	111.11
1	A	168	LEU	N-CA-C	-5.21	102.57	110.39
1	A	243	THR	N-CA-C	-5.19	103.68	110.53
1	A	716	GLN	N-CA-C	5.18	116.61	110.97
1	B	294	LEU	O-C-N	-5.17	116.90	122.79
1	A	510	SER	CB-CA-C	-5.16	102.18	110.74
1	A	326	SER	N-CA-C	5.14	121.17	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	LEU	N-CA-C	-5.14	106.86	113.23
1	B	134	ASP	CB-CA-C	-5.12	105.12	113.37
1	B	504	TYR	N-CA-C	5.11	117.58	111.71
1	A	832	GLN	N-CA-C	5.11	118.37	111.17
1	A	42	LEU	CA-C-N	5.10	129.38	120.86
1	A	42	LEU	C-N-CA	5.10	129.38	120.86
1	A	830	PRO	CA-C-N	5.10	129.41	121.35
1	A	830	PRO	C-N-CA	5.10	129.41	121.35
1	A	687	LYS	O-C-N	-5.09	116.99	122.79
1	A	30	THR	N-CA-C	5.09	117.84	108.58
1	B	813	ASN	N-CA-C	5.07	117.70	111.82
1	B	223	VAL	CB-CA-C	-5.05	105.17	111.08
1	B	789	PRO	N-CA-C	5.04	122.84	112.47
1	B	54	LEU	CB-CA-C	-5.03	102.92	111.02
1	B	297	THR	OG1-CB-CG2	-5.03	99.23	109.30
1	A	429	HIS	N-CA-C	-5.00	104.65	111.56

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	GLU	Peptide
1	A	208	ASN	Peptide
1	A	30	THR	Peptide
1	A	40	LEU	Peptide
1	A	43	VAL	Peptide
1	B	133	GLU	Peptide
1	B	390	ASP	Peptide
1	B	40	LEU	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	6789	0	6714	132	0
1	B	6789	0	6714	128	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	500	0	0	18	0
3	B	563	0	0	18	0
All	All	14643	0	13428	257	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 10.

All (257) 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:708:LEU:HA	3:B:1171:HOH:O	1.63	0.97
1:B:789:PRO:HA	3:B:1136:HOH:O	1.73	0.86
1:A:194:GLU:HA	1:A:239:GLY:HA3	1.58	0.85
1:B:790:ASN:HA	3:B:1071:HOH:O	1.75	0.85
1:A:507:VAL:HG13	1:A:577:LEU:HD13	1.63	0.78
1:B:387:SER:HB3	1:B:395:GLY:HA2	1.66	0.76
1:A:775:ARG:HD3	3:A:943:HOH:O	1.86	0.76
1:B:618:HIS:ND1	1:B:638:ASP:OD2	2.18	0.76
1:B:788:ASN:HB3	1:B:789:PRO:HD3	1.66	0.76
1:B:780:GLU:HG2	3:B:1187:HOH:O	1.86	0.74
1:B:541:HIS:HD2	1:B:543:ILE:H	1.34	0.74
1:A:541:HIS:HD2	1:A:543:ILE:H	1.35	0.71
1:A:349:LYS:HB3	1:A:833:MET:HE3	1.73	0.70
1:B:394:TYR:HA	1:B:397:HIS:HB3	1.73	0.70
1:A:790:ASN:HA	3:A:1204:HOH:O	1.93	0.69
1:B:258:LEU:HD11	1:B:263:ALA:HB2	1.74	0.69
1:A:525:VAL:HG22	1:A:676:HIS:HE1	1.57	0.69
1:B:852:PRO:HG3	3:B:1187:HOH:O	1.94	0.68
1:A:842:SER:HB2	1:A:850:GLY:HA3	1.75	0.68
1:B:525:VAL:HG22	1:B:676:HIS:HE1	1.59	0.65
1:A:258:LEU:HD21	1:A:263:ALA:HB2	1.79	0.65
1:A:455:PHE:HB2	1:A:465:LEU:HD22	1.78	0.65
1:B:776:HIS:NE2	1:B:849:ARG:O	2.24	0.65
1:A:42:LEU:HB2	1:A:95:GLY:H	1.63	0.64
1:A:365:ALA:HB1	1:A:462:LEU:HB3	1.79	0.64
1:B:213:PRO:HG2	1:B:243:THR:HG21	1.79	0.63
1:B:785:GLU:HB3	1:B:786:ARG:HG2	1.81	0.63
1:A:147:SER:OG	1:A:159:ARG:NH2	2.32	0.63
1:A:312:SER:OG	1:A:313:GLY:N	2.32	0.62
1:B:511:CYS:HG	1:B:578:TRP:CG	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:LEU:HD11	1:B:630:THR:OG1	2.01	0.61
1:A:843:LYS:HE3	1:A:843:LYS:H	1.66	0.60
1:A:297:THR:HG22	3:A:1028:HOH:O	2.00	0.60
1:B:316:LYS:HA	1:B:341:GLN:O	2.01	0.60
1:B:241:LYS:O	1:B:251:SER:HB3	2.01	0.60
1:A:44:GLY:HA3	3:A:964:HOH:O	2.02	0.59
1:B:604:LEU:HB3	1:B:610:ALA:HB3	1.85	0.59
1:A:690:THR:HG22	1:A:693:GLU:H	1.67	0.59
1:B:164:ASN:ND2	1:B:790:ASN:O	2.31	0.59
1:B:406:LEU:O	1:B:408:PRO:HD3	2.04	0.58
1:A:511:CYS:HG	1:A:578:TRP:CG	2.21	0.58
1:A:603:ASP:OD2	1:A:607:ARG:NH1	2.36	0.57
1:B:44:GLY:HA3	3:B:965:HOH:O	2.05	0.57
1:A:414:THR:OG1	1:A:415:VAL:N	2.37	0.57
1:B:243:THR:HG22	1:B:246:ASP:H	1.69	0.57
1:A:381:LYS:NZ	3:A:1281:HOH:O	2.36	0.57
1:A:89:LEU:HB2	1:A:92:LEU:HB2	1.87	0.57
1:A:550:HIS:CE1	1:A:702:ILE:HG23	2.40	0.57
1:A:216:GLY:HA3	3:A:1125:HOH:O	2.04	0.56
1:A:35:ILE:H	1:B:320:ASP:HB3	1.71	0.56
1:B:392:GLN:N	3:B:1068:HOH:O	2.26	0.56
1:B:312:SER:OG	1:B:313:GLY:N	2.36	0.56
1:B:455:PHE:HB2	1:B:465:LEU:HD22	1.88	0.56
1:A:411:GLU:OE2	1:A:423:ARG:NH1	2.26	0.56
1:B:411:GLU:OE1	1:B:423:ARG:NH1	2.38	0.56
1:B:492:GLY:O	1:B:495:SER:OG	2.24	0.56
1:A:473:HIS:N	3:A:1090:HOH:O	2.38	0.55
1:B:847:THR:O	3:B:1159:HOH:O	2.18	0.55
1:A:61:GLN:NE2	1:A:77:GLY:O	2.34	0.55
1:A:29:VAL:HG11	1:A:272:PHE:HE1	1.71	0.55
1:B:42:LEU:HB2	1:B:95:GLY:H	1.71	0.55
1:A:459:ASP:OD2	1:A:461:THR:OG1	2.24	0.54
1:A:626:ASP:HB3	1:A:826:ASN:HD22	1.71	0.54
1:A:751:LYS:O	1:A:755:LYS:HG2	2.07	0.54
1:A:819:ASN:ND2	1:A:827:ARG:HE	2.05	0.54
1:B:473:HIS:HB2	1:B:476:GLY:H	1.72	0.54
1:A:287:LEU:HD11	1:A:324:LYS:HB2	1.90	0.54
1:A:379:CYS:SG	1:A:381:LYS:NZ	2.76	0.54
1:A:827:ARG:NH1	3:A:993:HOH:O	2.38	0.54
1:B:297:THR:HG21	1:B:315:ILE:HD11	1.89	0.54
1:A:358:TRP:CZ2	1:A:724:LEU:HB3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ARG:HD2	1:A:473:HIS:HE1	1.73	0.53
1:B:632:ASP:OD1	1:B:827:ARG:NH2	2.38	0.53
1:B:819:ASN:ND2	1:B:827:ARG:HH11	2.05	0.53
1:A:632:ASP:CG	1:A:827:ARG:HH22	2.17	0.53
1:A:788:ASN:HD22	1:A:789:PRO:HD3	1.74	0.53
1:B:389:LEU:HD12	1:B:394:TYR:HE1	1.73	0.53
1:B:414:THR:HG23	1:B:417:GLU:HB2	1.91	0.53
1:A:36:ILE:HG21	1:A:267:LEU:HB3	1.91	0.53
1:B:184:LEU:HB3	1:B:188:ARG:NH2	2.24	0.53
1:A:543:ILE:HG22	1:A:547:LEU:HD22	1.91	0.52
1:B:216:GLY:HA3	3:B:934:HOH:O	2.09	0.52
1:B:646:GLU:OE1	1:B:803:ARG:NH2	2.23	0.52
1:B:751:LYS:O	1:B:755:LYS:HG2	2.10	0.52
1:B:626:ASP:HB3	1:B:826:ASN:HD22	1.75	0.52
1:A:105:TRP:HB3	1:A:135:ILE:HD11	1.91	0.52
1:A:604:LEU:HD21	1:A:630:THR:OG1	2.11	0.51
1:A:443:THR:O	1:A:446:LYS:NZ	2.44	0.51
1:A:320:ASP:H	1:B:35:ILE:HG13	1.75	0.51
1:A:594:VAL:HB	1:A:684:TRP:CE2	2.46	0.51
1:A:583:VAL:O	1:A:586:SER:OG	2.25	0.51
1:B:567:ASN:HD22	1:B:567:ASN:H	1.58	0.51
1:B:783:LEU:O	1:B:785:GLU:N	2.41	0.51
1:B:739:SER:HB3	1:B:742:TYR:H	1.76	0.50
1:A:604:LEU:HB3	1:A:610:ALA:HB3	1.92	0.50
1:B:561:ALA:HA	1:B:565:LEU:HB2	1.92	0.50
1:A:525:VAL:HG22	1:A:676:HIS:CE1	2.43	0.50
1:A:406:LEU:O	1:A:408:PRO:HD3	2.11	0.50
1:A:445:THR:O	1:A:446:LYS:NZ	2.44	0.50
1:B:583:VAL:O	1:B:586:SER:OG	2.29	0.50
1:A:696:GLU:O	1:A:700:ILE:HG13	2.12	0.50
1:A:438:ARG:HG2	3:A:938:HOH:O	2.12	0.49
1:A:574:GLN:HG2	3:A:1120:HOH:O	2.11	0.49
1:A:304:PHE:H	1:A:750:GLN:HE21	1.60	0.49
1:A:369:LEU:HD11	1:A:462:LEU:HD22	1.93	0.49
1:B:384:PRO:HD2	1:B:398:THR:HG21	1.93	0.49
1:A:287:LEU:HD12	1:A:325:ILE:HG23	1.94	0.49
1:A:414:THR:HG23	1:A:417:GLU:HB2	1.94	0.49
1:A:571:VAL:HG11	1:A:769:VAL:HG21	1.93	0.49
1:B:509:ASP:OD2	1:B:726:ARG:NH2	2.36	0.49
1:A:299:ARG:HH21	1:A:299:ARG:HB3	1.76	0.49
1:B:789:PRO:HB2	1:B:790:ASN:H	1.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ARG:NH1	3:A:1005:HOH:O	2.32	0.49
1:A:788:ASN:HB2	1:A:789:PRO:HD3	1.95	0.49
1:B:751:LYS:HE2	1:B:755:LYS:HE3	1.95	0.49
1:A:60:LEU:HG	1:A:117:ILE:HG13	1.94	0.48
1:B:183:GLU:OE1	1:B:187:LEU:HD22	2.13	0.48
1:B:546:LEU:HB2	1:B:647:TYR:CE1	2.48	0.48
1:B:736:GLU:O	1:B:738:GLY:N	2.47	0.48
1:B:234:ARG:NH1	3:B:899:HOH:O	2.36	0.48
1:A:770:ILE:HA	1:A:773:LEU:HB2	1.96	0.48
1:B:32:VAL:HA	1:B:269:SER:OG	2.14	0.48
1:B:819:ASN:HD22	1:B:827:ARG:HD3	1.78	0.48
1:B:636:ILE:HD12	1:B:811:ILE:HG21	1.94	0.47
1:A:659:ARG:NH2	3:A:1020:HOH:O	2.46	0.47
1:B:230:PHE:CE1	1:B:584:GLU:HB2	2.49	0.47
1:B:397:HIS:CD2	1:B:398:THR:H	2.32	0.47
1:A:392:GLN:HB2	1:A:394:TYR:CE2	2.50	0.47
1:A:164:ASN:HB3	1:A:793:SER:OG	2.15	0.47
1:A:277:LEU:HD13	1:A:772:ILE:HG21	1.96	0.47
1:B:394:TYR:HD2	1:B:480:GLY:HA2	1.80	0.47
1:A:10:HIS:HD2	1:A:135:ILE:HG12	1.79	0.46
1:A:38:GLN:HB3	1:A:39:GLY:H	1.58	0.46
1:A:394:TYR:HB2	3:A:947:HOH:O	2.15	0.46
1:B:38:GLN:HB3	1:B:39:GLY:H	1.57	0.46
1:A:632:ASP:OD2	1:A:827:ARG:NH2	2.48	0.46
1:A:786:ARG:HD3	3:A:995:HOH:O	2.14	0.46
1:A:392:GLN:HB2	1:A:394:TYR:HE2	1.81	0.46
1:B:389:LEU:HD12	1:B:394:TYR:CE1	2.50	0.46
1:A:13:LYS:HE3	1:A:13:LYS:HB2	1.37	0.46
1:B:713:ASN:OD1	1:B:716:GLN:NE2	2.49	0.46
1:B:235:ARG:HD2	1:B:235:ARG:C	2.40	0.45
1:A:394:TYR:CD2	1:A:480:GLY:HA2	2.52	0.45
1:B:408:PRO:HB2	3:B:1290:HOH:O	2.14	0.45
1:B:474:PRO:HD2	3:B:1015:HOH:O	2.15	0.45
1:B:515:LEU:HD13	1:B:515:LEU:HA	1.78	0.45
1:B:590:TYR:O	1:B:679:LYS:HE3	2.17	0.45
1:B:717:TYR:O	1:B:721:GLY:N	2.45	0.45
1:B:398:THR:HB	1:B:399:SER:H	1.54	0.45
1:B:407:GLU:HA	1:B:408:PRO:HD3	1.76	0.45
1:B:484:GLN:NE2	3:B:860:HOH:O	2.32	0.45
1:B:564:SER:C	1:B:567:ASN:ND2	2.75	0.45
1:A:213:PRO:HB3	1:A:220:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:THR:HG23	1:A:404:GLU:H	1.80	0.45
1:A:526:VAL:O	1:A:529:PHE:HB2	2.16	0.45
1:B:807:LYS:HA	1:B:807:LYS:HD3	1.61	0.45
1:B:577:LEU:HD12	1:B:577:LEU:HA	1.81	0.45
1:A:376:LEU:HD12	1:A:376:LEU:HA	1.44	0.44
1:B:294:LEU:H	1:B:294:LEU:HG	1.52	0.44
1:B:164:ASN:HB3	1:B:793:SER:OG	2.16	0.44
1:B:711:ALA:HB3	3:B:1171:HOH:O	2.18	0.44
1:A:567:ASN:H	1:A:567:ASN:HD22	1.64	0.44
1:A:836:THR:HA	1:A:839:LEU:HD13	1.99	0.44
1:B:105:TRP:HB3	1:B:135:ILE:HD11	1.98	0.44
1:A:317:LEU:HD12	1:A:317:LEU:HA	1.83	0.44
1:A:165:GLN:NE2	3:A:1111:HOH:O	2.44	0.44
1:B:394:TYR:HD2	1:B:480:GLY:C	2.25	0.44
1:A:234:ARG:HH22	1:A:678:ASP:CG	2.26	0.44
1:A:520:LEU:HD21	1:A:590:TYR:HB2	2.00	0.44
1:A:388:LYS:HD2	1:A:388:LYS:HA	1.64	0.44
1:A:493:VAL:HG21	1:A:746:ARG:HG2	1.99	0.44
1:A:520:LEU:O	1:A:525:VAL:HB	2.17	0.44
1:A:46:THR:HA	3:A:1156:HOH:O	2.18	0.43
1:B:50:LEU:HD13	1:B:50:LEU:HA	1.79	0.43
1:A:414:THR:HG23	1:A:417:GLU:H	1.84	0.43
1:A:842:SER:HB2	1:A:850:GLY:CA	2.46	0.43
1:B:403:LYS:HB2	3:B:1261:HOH:O	2.18	0.43
1:A:10:HIS:HB3	1:A:135:ILE:HD13	2.00	0.43
1:A:221:ARG:HD3	1:A:221:ARG:HA	1.82	0.43
1:B:322:ILE:HD13	1:B:322:ILE:HA	1.84	0.43
1:B:410:LEU:HD21	1:B:458:ASN:H	1.83	0.43
1:B:463:ARG:NH1	3:B:1076:HOH:O	2.51	0.43
1:A:196:LYS:HA	1:A:196:LYS:HD2	1.91	0.43
1:A:407:GLU:HA	1:A:408:PRO:HD3	1.75	0.43
1:A:782:TYR:O	1:A:786:ARG:HB2	2.18	0.43
1:B:361:ASP:HB3	1:B:464:PRO:HD2	2.00	0.43
1:A:462:LEU:HD12	1:A:462:LEU:HA	1.79	0.43
1:A:394:TYR:HD2	1:A:480:GLY:HA2	1.83	0.43
1:B:631:VAL:HB	1:B:818:ARG:NH1	2.33	0.43
1:A:271:ASP:OD2	1:A:778:SER:HB2	2.18	0.43
1:B:187:LEU:HD12	1:B:187:LEU:HA	1.88	0.43
1:B:704:THR:HA	1:B:708:LEU:HB3	2.01	0.43
1:B:89:LEU:HB2	1:B:92:LEU:HB2	1.99	0.43
1:A:781:VAL:HG12	1:A:786:ARG:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:VAL:HG21	1:B:769:VAL:HG21	2.00	0.43
1:A:620:ILE:HD11	1:A:634:LEU:HD21	2.01	0.42
1:B:736:GLU:O	1:B:739:SER:HB2	2.19	0.42
1:B:668:TRP:NE1	1:B:686:PRO:O	2.52	0.42
1:A:266:HIS:NE2	3:A:1000:HOH:O	2.37	0.42
1:A:424:LEU:HD23	1:A:424:LEU:HA	1.60	0.42
1:B:455:PHE:HB2	1:B:465:LEU:CD2	2.48	0.42
1:A:789:PRO:HB2	1:A:790:ASN:H	1.31	0.42
1:B:543:ILE:HG22	1:B:547:LEU:HD22	2.02	0.42
1:B:640:ILE:HD13	1:B:702:ILE:HG22	2.01	0.42
1:A:234:ARG:NH2	1:A:678:ASP:OD2	2.52	0.42
1:A:429:HIS:NE2	1:A:509:ASP:OD1	2.42	0.42
1:A:607:ARG:NH2	1:A:627:TYR:OH	2.43	0.42
1:B:194:GLU:HG3	1:B:240:ARG:HA	2.02	0.42
1:B:376:LEU:HD12	1:B:376:LEU:HA	1.81	0.42
1:B:361:ASP:HB3	1:B:464:PRO:CD	2.50	0.42
1:B:205:ASP:OD1	1:B:206:VAL:N	2.51	0.42
1:B:414:THR:OG1	1:B:415:VAL:N	2.52	0.42
1:B:632:ASP:CG	1:B:827:ARG:HH22	2.26	0.42
1:A:36:ILE:HD12	1:A:36:ILE:HA	1.88	0.42
1:A:618:HIS:ND1	1:A:638:ASP:OD2	2.52	0.42
1:B:38:GLN:HE21	1:B:38:GLN:HB2	1.62	0.42
1:B:394:TYR:HD2	1:B:480:GLY:CA	2.33	0.42
1:A:505:VAL:O	1:A:508:ASN:HB2	2.19	0.41
1:A:438:ARG:CD	1:A:473:HIS:HE1	2.31	0.41
1:B:825:ARG:HD3	3:B:945:HOH:O	2.20	0.41
1:A:558:ASN:O	1:A:562:ARG:HG3	2.20	0.41
1:A:609:MET:HE1	1:A:624:ILE:HD12	2.01	0.41
1:B:505:VAL:O	1:B:508:ASN:HB2	2.19	0.41
1:A:723:ILE:HD12	1:A:723:ILE:HA	1.84	0.41
1:B:141:ILE:HG23	1:B:141:ILE:HD13	1.80	0.41
1:B:278:LYS:HB2	1:B:278:LYS:HE3	1.87	0.41
1:A:29:VAL:HG11	1:A:272:PHE:CE1	2.53	0.41
1:A:702:ILE:O	1:A:706:SER:OG	2.27	0.41
1:B:696:GLU:O	1:B:700:ILE:HG13	2.21	0.41
1:A:106:ASP:HB2	1:A:107:ASP:H	1.40	0.41
1:A:135:ILE:HB	1:A:136:PRO:HD3	2.02	0.41
1:A:414:THR:O	1:A:418:ALA:N	2.54	0.41
1:B:56:ARG:HH11	1:B:56:ARG:HD3	1.70	0.41
1:B:530:ILE:HG12	1:B:551:TYR:CG	2.56	0.41
1:B:541:HIS:HE1	1:B:661:ASP:OD2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:765:ILE:HD13	1:B:765:ILE:HG21	1.70	0.41
1:B:783:LEU:C	1:B:785:GLU:H	2.28	0.41
1:A:172:THR:HB	1:A:177:VAL:HG22	2.03	0.41
1:B:411:GLU:CD	1:B:423:ARG:HH12	2.29	0.41
1:B:520:LEU:O	1:B:525:VAL:HB	2.21	0.41
1:A:320:ASP:HB2	1:B:35:ILE:HG13	2.03	0.40
1:B:105:TRP:NE1	1:B:110:GLY:O	2.47	0.40
1:A:375:ASN:O	1:A:375:ASN:ND2	2.52	0.40
1:B:54:LEU:HD12	1:B:54:LEU:HA	1.85	0.40
1:B:189:GLY:HA3	1:B:201:ILE:HD13	2.03	0.40
1:A:105:TRP:CD2	1:A:109:SER:HB2	2.56	0.40
1:B:271:ASP:OD2	1:B:778:SER:HB3	2.22	0.40
1:A:208:ASN:HB2	1:A:249:SER:HA	2.04	0.40
1:A:604:LEU:HB3	1:A:610:ALA:CB	2.52	0.40
1:A:813:ASN:ND2	3:A:1152:HOH:O	2.54	0.40
1:B:56:ARG:NH2	3:B:982:HOH:O	2.55	0.40
1:B:277:LEU:HD12	1:B:277:LEU:HA	1.91	0.40
1:A:600:LEU:HG	1:A:604:LEU:HD22	2.03	0.40
1:A:600:LEU:HD23	1:A:634:LEU:HD23	2.03	0.40
1:A:783:LEU:HG	1:A:808:LEU:HD21	2.03	0.40
1:B:507:VAL:HG13	1:B:577:LEU:HD13	2.03	0.40
1:B:762:GLN:HE21	1:B:762:GLN:H	1.68	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	848/857 (99%)	767 (90%)	61 (7%)	20 (2%)	4	2
1	B	848/857 (99%)	772 (91%)	59 (7%)	17 (2%)	6	2
All	All	1696/1714 (99%)	1539 (91%)	120 (7%)	37 (2%)	5	2

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	SER
1	A	136	PRO
1	A	408	PRO
1	A	410	LEU
1	A	789	PRO
1	B	45	SER
1	B	390	ASP
1	B	408	PRO
1	B	737	LYS
1	B	788	ASN
1	B	789	PRO
1	A	41	ASP
1	A	135	ILE
1	A	788	ASN
1	B	41	ASP
1	B	397	HIS
1	B	472	PRO
1	A	341	GLN
1	A	357	ALA
1	A	393	VAL
1	B	42	LEU
1	B	136	PRO
1	B	410	LEU
1	B	519	TRP
1	A	42	LEU
1	A	108	GLY
1	A	397	HIS
1	B	135	ILE
1	B	329	PRO
1	B	374	PRO
1	A	48	ASP
1	A	472	PRO
1	A	329	PRO
1	A	339	GLY
1	A	374	PRO
1	A	474	PRO
1	B	44	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	744/749 (99%)	596 (80%)	148 (20%)	1	0
1	B	744/749 (99%)	592 (80%)	152 (20%)	1	0
All	All	1488/1498 (99%)	1188 (80%)	300 (20%)	1	0

All (300) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	11	LYS
1	A	13	LYS
1	A	23	VAL
1	A	24	LEU
1	A	29	VAL
1	A	36	ILE
1	A	38	GLN
1	A	40	LEU
1	A	41	ASP
1	A	42	LEU
1	A	43	VAL
1	A	45	SER
1	A	46	THR
1	A	50	LEU
1	A	51	THR
1	A	54	LEU
1	A	67	LYS
1	A	75	LYS
1	A	78	LYS
1	A	80	THR
1	A	87	THR
1	A	100	LYS
1	A	104	GLU
1	A	106	ASP
1	A	109	SER
1	A	117	ILE

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Mol	Chain	Res	Type
1	A	122	GLN
1	A	127	LEU
1	A	134	ASP
1	A	135	ILE
1	A	164	ASN
1	A	172	THR
1	A	178	LYS
1	A	182	GLU
1	A	183	GLU
1	A	184	LEU
1	A	187	LEU
1	A	196	LYS
1	A	215	LYS
1	A	217	GLU
1	A	232	TYR
1	A	245	LYS
1	A	254	ASN
1	A	258	LEU
1	A	269	SER
1	A	277	LEU
1	A	278	LYS
1	A	279	SER
1	A	287	LEU
1	A	288	LEU
1	A	290	SER
1	A	297	THR
1	A	299	ARG
1	A	305	ASP
1	A	312	SER
1	A	316	LYS
1	A	317	LEU
1	A	319	THR
1	A	321	ILE
1	A	322	ILE
1	A	326	SER
1	A	331	LEU
1	A	332	LYS
1	A	333	GLU
1	A	336	ARG
1	A	338	ASP
1	A	344	LYS
1	A	374	PRO

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Mol	Chain	Res	Type
1	A	376	LEU
1	A	378	ARG
1	A	388	LYS
1	A	392	GLN
1	A	394	TYR
1	A	398	THR
1	A	402	THR
1	A	410	LEU
1	A	413	LEU
1	A	414	THR
1	A	415	VAL
1	A	420	GLN
1	A	421	ASN
1	A	427	LEU
1	A	433	ILE
1	A	438	ARG
1	A	462	LEU
1	A	465	LEU
1	A	475	GLN
1	A	479	SER
1	A	497	ILE
1	A	507	VAL
1	A	515	LEU
1	A	525	VAL
1	A	537	LEU
1	A	547	LEU
1	A	553	ASP
1	A	564	SER
1	A	565	LEU
1	A	566	VAL
1	A	568	ASP
1	A	583	VAL
1	A	594	VAL
1	A	596	THR
1	A	604	LEU
1	A	606	LYS
1	A	611	ILE
1	A	612	GLU
1	A	621	ARG
1	A	630	THR
1	A	631	VAL
1	A	650	LEU

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Mol	Chain	Res	Type
1	A	658	LEU
1	A	680	LYS
1	A	690	THR
1	A	712	VAL
1	A	722	LEU
1	A	724	LEU
1	A	736	GLU
1	A	737	LYS
1	A	743	GLU
1	A	744	GLU
1	A	755	LYS
1	A	762	GLN
1	A	766	ASP
1	A	773	LEU
1	A	775	ARG
1	A	778	SER
1	A	781	VAL
1	A	787	ASP
1	A	788	ASN
1	A	793	SER
1	A	798	LEU
1	A	802	LYS
1	A	807	LYS
1	A	808	LEU
1	A	813	ASN
1	A	815	LEU
1	A	817	GLU
1	A	822	GLU
1	A	823	LYS
1	A	831	VAL
1	A	837	LEU
1	A	838	LEU
1	A	841	SER
1	A	843	LYS
1	A	844	GLU
1	A	846	LEU
1	A	857	ILE
1	B	11	LYS
1	B	13	LYS
1	B	15	THR
1	B	23	VAL
1	B	30	THR

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Mol	Chain	Res	Type
1	B	31	SER
1	B	36	ILE
1	B	38	GLN
1	B	40	LEU
1	B	42	LEU
1	B	43	VAL
1	B	45	SER
1	B	47	LEU
1	B	49	THR
1	B	50	LEU
1	B	51	THR
1	B	54	LEU
1	B	56	ARG
1	B	61	GLN
1	B	62	LEU
1	B	67	LYS
1	B	75	LYS
1	B	78	LYS
1	B	87	THR
1	B	97	SER
1	B	106	ASP
1	B	122	GLN
1	B	134	ASP
1	B	141	ILE
1	B	156	LYS
1	B	157	SER
1	B	160	ILE
1	B	164	ASN
1	B	168	LEU
1	B	183	GLU
1	B	184	LEU
1	B	187	LEU
1	B	217	GLU
1	B	218	ASN
1	B	232	TYR
1	B	234	ARG
1	B	238	THR
1	B	241	LYS
1	B	243	THR
1	B	244	ARG
1	B	251	SER
1	B	258	LEU

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Mol	Chain	Res	Type
1	B	267	LEU
1	B	268	LYS
1	B	269	SER
1	B	277	LEU
1	B	279	SER
1	B	281	SER
1	B	287	LEU
1	B	288	LEU
1	B	290	SER
1	B	294	LEU
1	B	300	GLU
1	B	312	SER
1	B	319	THR
1	B	321	ILE
1	B	322	ILE
1	B	325	ILE
1	B	333	GLU
1	B	334	ILE
1	B	336	ARG
1	B	340	GLU
1	B	341	GLN
1	B	343	LEU
1	B	349	LYS
1	B	350	VAL
1	B	353	VAL
1	B	355	LYS
1	B	362	GLU
1	B	372	VAL
1	B	375	ASN
1	B	376	LEU
1	B	377	ILE
1	B	378	ARG
1	B	386	ARG
1	B	392	GLN
1	B	393	VAL
1	B	396	ASP
1	B	398	THR
1	B	403	LYS
1	B	414	THR
1	B	420	GLN
1	B	427	LEU
1	B	434	MET

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Mol	Chain	Res	Type
1	B	438	ARG
1	B	463	ARG
1	B	465	LEU
1	B	470	SER
1	B	473	HIS
1	B	475	GLN
1	B	478	GLN
1	B	479	SER
1	B	507	VAL
1	B	515	LEU
1	B	517	SER
1	B	525	VAL
1	B	537	LEU
1	B	540	VAL
1	B	547	LEU
1	B	564	SER
1	B	565	LEU
1	B	566	VAL
1	B	567	ASN
1	B	568	ASP
1	B	571	VAL
1	B	583	VAL
1	B	594	VAL
1	B	604	LEU
1	B	615	SER
1	B	620	ILE
1	B	621	ARG
1	B	623	VAL
1	B	625	GLU
1	B	630	THR
1	B	631	VAL
1	B	653	LYS
1	B	679	LYS
1	B	687	LYS
1	B	712	VAL
1	B	722	LEU
1	B	724	LEU
1	B	732	ARG
1	B	739	SER
1	B	751	LYS
1	B	762	GLN
1	B	766	ASP

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Mol	Chain	Res	Type
1	B	773	LEU
1	B	775	ARG
1	B	786	ARG
1	B	787	ASP
1	B	788	ASN
1	B	798	LEU
1	B	802	LYS
1	B	803	ARG
1	B	807	LYS
1	B	813	ASN
1	B	815	LEU
1	B	823	LYS
1	B	827	ARG
1	B	831	VAL
1	B	837	LEU
1	B	838	LEU
1	B	839	LEU
1	B	843	LYS
1	B	844	GLU
1	B	846	LEU
1	B	856	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	142	HIS
1	A	164	ASN
1	A	165	GLN
1	A	282	GLN
1	A	289	GLN
1	A	295	ASN
1	A	400	GLN
1	A	421	ASN
1	A	458	ASN
1	A	473	HIS
1	A	521	ASN
1	A	541	HIS
1	A	556	ASN
1	A	567	ASN
1	A	750	GLN
1	A	788	ASN

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Mol	Chain	Res	Type
1	A	790	ASN
1	A	806	ASN
1	A	813	ASN
1	A	819	ASN
1	B	10	HIS
1	B	38	GLN
1	B	137	ASN
1	B	164	ASN
1	B	254	ASN
1	B	283	ASN
1	B	289	GLN
1	B	308	HIS
1	B	375	ASN
1	B	397	HIS
1	B	421	ASN
1	B	458	ASN
1	B	473	HIS
1	B	478	GLN
1	B	521	ASN
1	B	541	HIS
1	B	548	HIS
1	B	556	ASN
1	B	567	ASN
1	B	645	HIS
1	B	750	GLN
1	B	762	GLN
1	B	788	ASN
1	B	806	ASN
1	B	819	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	850/857 (99%)	-0.13	27 (3%)	50	53	2, 17, 34, 49	0
1	B	850/857 (99%)	-0.21	27 (3%)	50	53	2, 16, 35, 46	0
All	All	1700/1714 (99%)	-0.17	54 (3%)	50	53	2, 16, 35, 49	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	VAL	5.3
1	A	410	LEU	5.1
1	B	41	ASP	4.4
1	B	32	VAL	4.4
1	B	394	TYR	4.2
1	A	36	ILE	3.9
1	A	33	GLY	3.8
1	B	474	PRO	3.8
1	A	35	ILE	3.7
1	A	34	GLY	3.4
1	B	34	GLY	3.4
1	B	35	ILE	3.4
1	B	45	SER	3.3
1	A	42	LEU	3.3
1	B	391	SER	3.2
1	B	339	GLY	3.2
1	B	397	HIS	3.1
1	A	394	TYR	3.1
1	A	44	GLY	3.1
1	B	410	LEU	3.1
1	A	46	THR	3.0
1	A	135	ILE	3.0
1	B	31	SER	2.9
1	B	44	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	393	VAL	2.8
1	B	9	GLY	2.8
1	A	341	GLN	2.7
1	B	784	GLY	2.7
1	A	47	LEU	2.7
1	A	31	SER	2.7
1	B	46	THR	2.6
1	B	47	LEU	2.6
1	A	408	PRO	2.5
1	B	342	ALA	2.5
1	A	41	ASP	2.5
1	A	40	LEU	2.5
1	A	110	GLY	2.5
1	B	785	GLU	2.4
1	A	43	VAL	2.4
1	A	45	SER	2.4
1	B	42	LEU	2.4
1	A	409	ASN	2.4
1	B	395	GLY	2.4
1	A	784	GLY	2.3
1	B	789	PRO	2.3
1	A	391	SER	2.3
1	A	785	GLU	2.2
1	B	408	PRO	2.2
1	A	39	GLY	2.2
1	B	135	ILE	2.1
1	B	40	LEU	2.1
1	B	107	ASP	2.1
1	A	395	GLY	2.1
1	B	329	PRO	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(Å ²)	Q<0.9
2	FE2	A	858	1/1	0.99	0.08	28,28,28,28	0
2	FE2	B	858	1/1	0.99	0.04	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.