WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:02 PM GMT

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

1 Overall quality at a glance (i)

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.
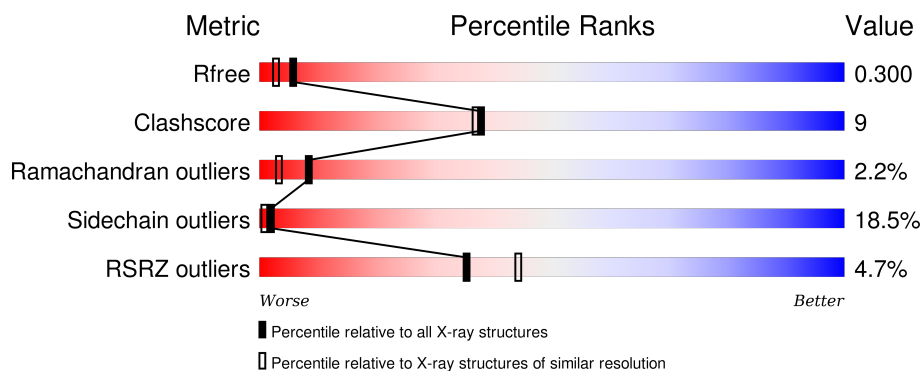
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	
1	B	857	

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 REMARK9 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 (three-letter code: FE2) (formula: Fe).

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

- Molecule 3 is water.

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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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
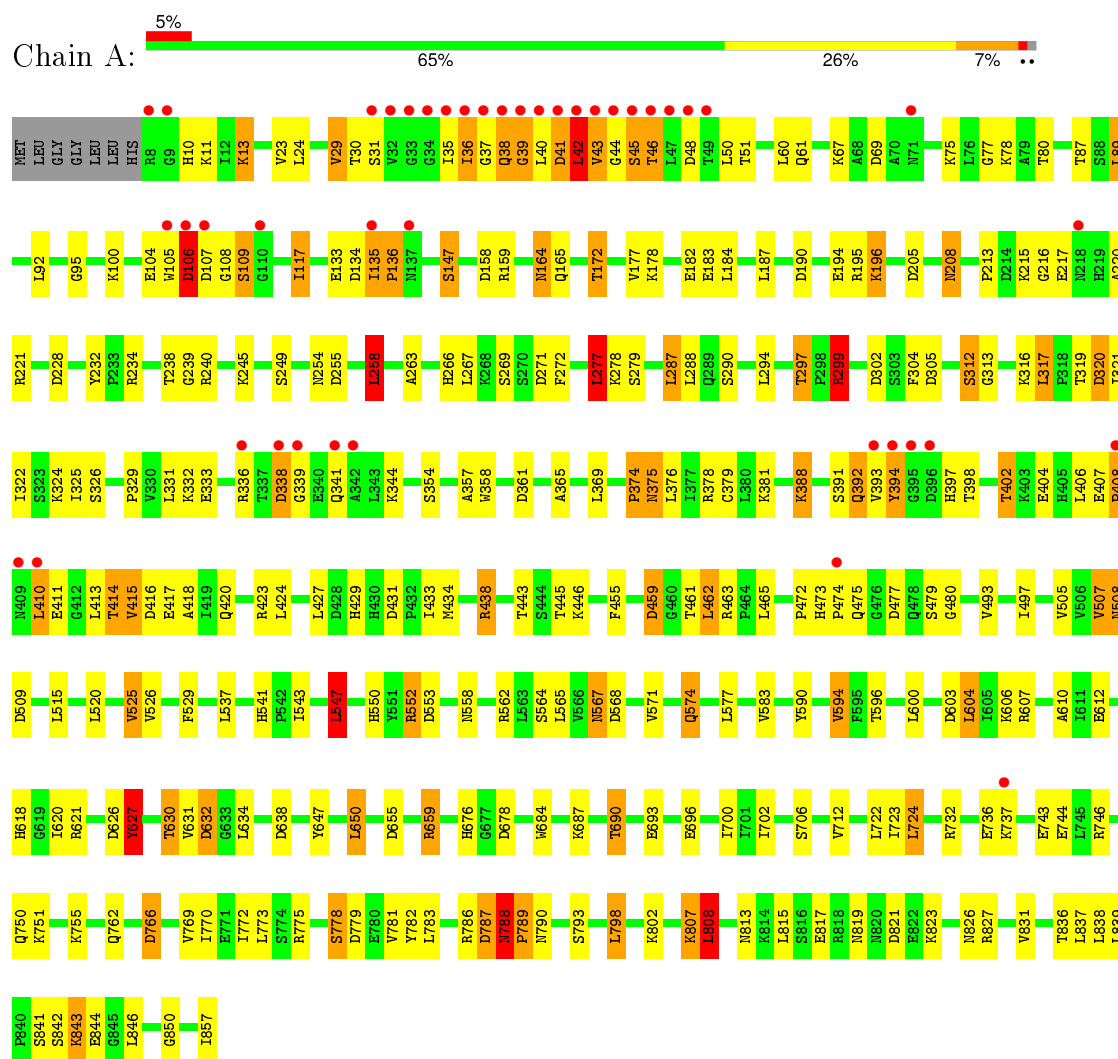
- Molecule 1: Seed lipoxygenase-3
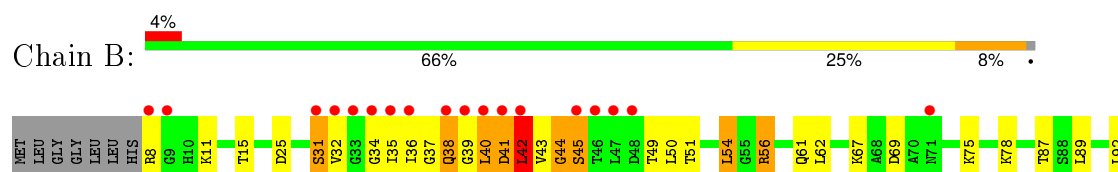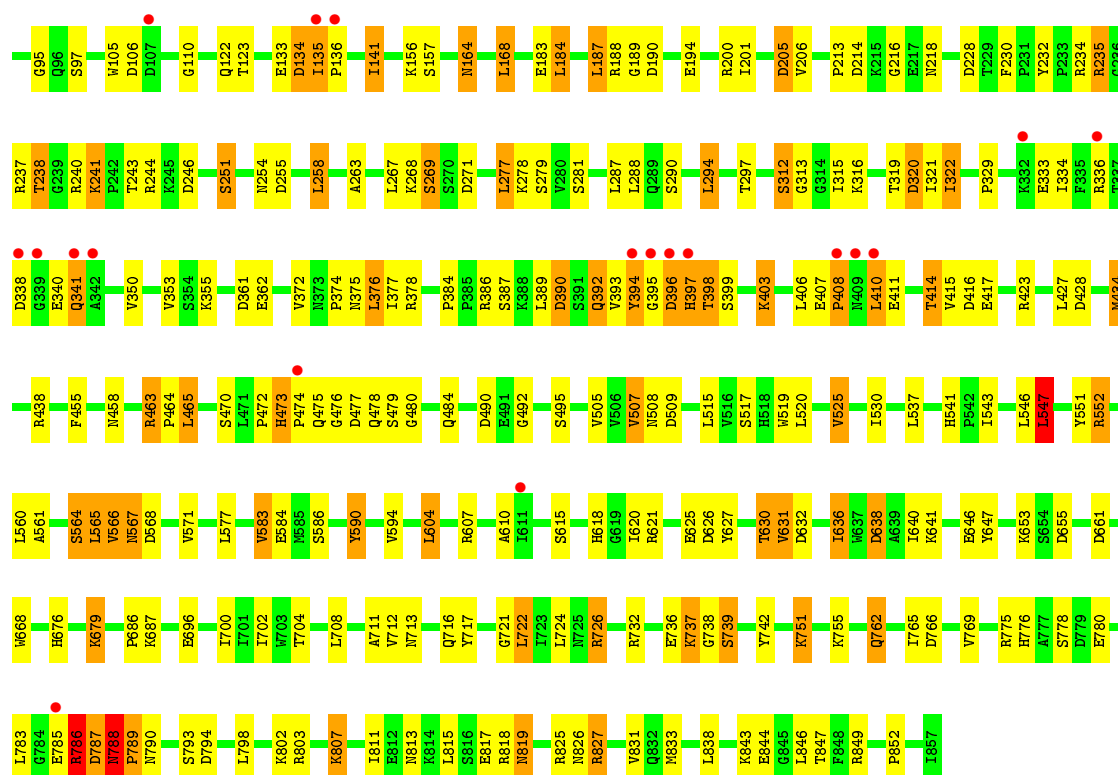
4 Data and refinement statistics (i)

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) 65.4 (10.00-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.32%)	DCC
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 61.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 64208 reflections	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.83	2/6961 (0.0%)	1.14	41/9453 (0.4%)
1	B	0.88	5/6961 (0.1%)	1.17	39/9453 (0.4%)
All	All	0.85	7/13922 (0.1%)	1.16	80/18906 (0.4%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	594	VAL	CB-CG1	6.95	1.67	1.52
1	B	394	TYR	CE2-CZ	-6.47	1.30	1.38
1	B	434	MET	CG-SD	-6.30	1.64	1.81
1	A	647	TYR	CD1-CE1	-6.27	1.29	1.39
1	B	394	TYR	CD2-CE2	-5.53	1.31	1.39
1	B	590	TYR	CD2-CE2	5.26	1.47	1.39
1	A	228	ASP	CB-CG	5.05	1.62	1.51

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	ASP	CB-CG-OD2	11.02	128.21	118.30
1	B	726	ARG	NE-CZ-NH2	9.89	125.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	25	ASP	CB-CG-OD2	8.72	126.15	118.30
1	A	787	ASP	CB-CG-OD2	8.40	125.86	118.30
1	B	726	ARG	NE-CZ-NH1	-8.29	116.15	120.30
1	A	416	ASP	CB-CG-OD2	8.16	125.65	118.30
1	B	31	SER	N-CA-C	-8.13	89.04	111.00
1	A	650	LEU	CB-CG-CD1	-8.09	97.25	111.00
1	B	787	ASP	CB-CG-OD2	7.97	125.47	118.30
1	A	361	ASP	CB-CG-OD2	7.94	125.44	118.30
1	A	302	ASP	CB-CG-OD2	7.67	125.20	118.30
1	B	655	ASP	CB-CG-OD2	7.62	125.16	118.30
1	B	228	ASP	CB-CG-OD2	7.61	125.15	118.30
1	B	477	ASP	CB-CG-OD2	7.58	125.12	118.30
1	B	237	ARG	NE-CZ-NH1	-7.54	116.53	120.30
1	B	552	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	A	228	ASP	CB-CG-OD2	7.04	124.64	118.30
1	A	477	ASP	CB-CG-OD2	6.93	124.54	118.30
1	A	779	ASP	CB-CG-OD2	6.93	124.53	118.30
1	A	320	ASP	CB-CG-OD2	6.80	124.42	118.30
1	B	428	ASP	CB-CG-OD2	6.80	124.42	118.30
1	B	238	THR	N-CA-C	-6.79	92.66	111.00
1	B	168	LEU	CA-CB-CG	6.70	130.70	115.30
1	B	200	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	431	ASP	CB-CG-OD2	6.65	124.29	118.30
1	A	258	LEU	CA-CB-CG	6.54	130.34	115.30
1	B	255	ASP	CB-CG-OD2	6.54	124.19	118.30
1	B	794	ASP	CB-CG-OD2	6.43	124.08	118.30
1	B	636	ILE	CG1-CB-CG2	-6.33	97.47	111.40
1	A	106	ASP	CB-CG-OD2	6.28	123.96	118.30
1	A	158	ASP	CB-CG-OD1	6.16	123.85	118.30
1	A	255	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	808	LEU	CA-CB-CG	6.12	129.37	115.30
1	A	69	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	69	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	320	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	552	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	722	LEU	CB-CG-CD2	5.99	121.17	111.00
1	A	338	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	190	ASP	CB-CG-OD2	5.95	123.65	118.30
1	B	338	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	37	GLY	N-CA-C	-5.91	98.31	113.10
1	A	459	ASP	CB-CG-OD2	5.91	123.61	118.30
1	B	214	ASP	CB-CG-OD2	5.90	123.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	34	GLY	N-CA-C	5.76	127.50	113.10
1	B	37	GLY	N-CA-C	-5.71	98.83	113.10
1	A	655	ASP	CB-CG-OD2	5.68	123.42	118.30
1	A	766	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	396	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	566	VAL	CB-CA-C	5.58	122.01	111.40
1	A	31	SER	N-CA-C	-5.57	95.95	111.00
1	B	547	LEU	CB-CG-CD1	5.46	120.29	111.00
1	A	574	GLN	CA-CB-CG	5.43	125.35	113.40
1	B	552	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	687	LYS	C-N-CA	-5.38	108.26	121.70
1	A	277	LEU	CA-CB-CG	5.37	127.66	115.30
1	B	134	ASP	N-CA-C	5.37	125.49	111.00
1	B	638	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	123	THR	OG1-CB-CG2	-5.34	97.72	110.00
1	A	547	LEU	CA-CB-CG	5.31	127.51	115.30
1	B	416	ASP	CB-CG-OD2	5.29	123.07	118.30
1	A	240	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	294	LEU	C-N-CA	-5.22	108.65	121.70
1	A	798	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	607	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	39	GLY	N-CA-C	-5.18	100.15	113.10
1	A	659	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	190	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	632	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	833	MET	CA-CB-CG	5.10	121.97	113.30
1	A	659	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	574	GLN	CB-CA-C	-5.08	100.24	110.40
1	B	786	ARG	NE-CZ-NH2	5.07	122.84	120.30
1	B	490	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	89	LEU	CA-CB-CG	5.05	126.93	115.30
1	A	299	ARG	NE-CZ-NH2	5.05	122.82	120.30
1	A	627	TYR	N-CA-C	-5.03	97.41	111.00
1	A	238	THR	C-N-CA	-5.01	111.78	122.30
1	A	821	ASP	CB-CG-OD2	5.00	122.80	118.30
1	B	560	LEU	CA-CB-CG	-5.00	103.80	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	GLU	Peptide

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Mol	Chain	Res	Type	Group
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6789	0	6714	128	0
1	B	6789	0	6714	124	0
2	A	1	0	0	0	0
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	249	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (249) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:312:SER:OG	1:B:313:GLY:N	2.36	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:CYS:SG	1:A:381:LYS:NZ	2.76	0.56
1:B:847:THR:O	3:B:1159:HOH:O	2.18	0.55
1:A:473:HIS:N	3:A:1090:HOH:O	2.38	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:751:LYS:O	1:A:755:LYS:HG2	2.07	0.54
1:B:473:HIS:HB2	1:B:476:GLY:H	1.72	0.54
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:819:ASN:ND2	1:A:827:ARG:HE	2.05	0.54
1:A:287:LEU:HD11	1:A:324:LYS:HB2	1.90	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
1:B:492:GLY:O	1:B:495:SER:OG	2.24	0.54
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:B:389:LEU:HD12	1:B:394:TYR:HE1	1.73	0.53
1:A:788:ASN:HD22	1:A:789:PRO:HD3	1.74	0.53
1:B:414:THR:HG23	1:B:417:GLU:HB2	1.91	0.53
1:B:184:LEU:HB3	1:B:188:ARG:NH2	2.24	0.53
1:A:36:ILE:HG21	1:A:267:LEU:HB3	1.91	0.53
1:A:543:ILE:HG22	1:A:547:LEU:HD22	1.91	0.52
1:B:646:GLU:OE1	1:B:803:ARG:NH2	2.23	0.52
1:B:216:GLY:HA3	3:B:934:HOH:O	2.09	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:594:VAL:HB	1:A:684:TRP:CE2	2.46	0.51
1:A:320:ASP:H	1:B:35:ILE:HG13	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:369:LEU:HD11	1:A:462:LEU:HD22	1.93	0.49
1:A:304:PHE:H	1:A:750:GLN:HE21	1.60	0.49
1:B:384:PRO:HD2	1:B:398:THR:HG21	1.93	0.49
1:A:414:THR:HG23	1:A:417:GLU:HB2	1.94	0.49
1:A:287:LEU:HD12	1:A:325:ILE:HG23	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:B:789:PRO:HB2	1:B:790:ASN:H	1.33	0.49
1:A:299:ARG:HH21	1:A:299:ARG:HB3	1.76	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:195:ARG:NH1	3:A:1005:HOH:O	2.32	0.49
1:A:60:LEU:HG	1:A:117:ILE:HG13	1.94	0.48
1:A:445:THR:O	1:A:446:LYS:NZ	2.44	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:A:632:ASP:CG	1:A:827:ARG:HH22	2.17	0.48
1:B:234:ARG:NH1	3:B:899:HOH:O	2.36	0.48
1:B:819:ASN:HD22	1:B:827:ARG:HD3	1.78	0.48
1:B:32:VAL:HA	1:B:269:SER:OG	2.14	0.48
1:A:770:ILE:HA	1:A:773:LEU:HB2	1.96	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:397:HIS:CD2	1:B:398:THR:H	2.32	0.47
1:B:230:PHE:CE1	1:B:584:GLU:HB2	2.49	0.47
1:A:392:GLN:HB2	1:A:394:TYR:CE2	2.50	0.47
1:B:583:VAL:O	1:B:586:SER:OG	2.29	0.47
1:A:164:ASN:HB3	1:A:793:SER:OG	2.15	0.47
1:B:394:TYR:HD2	1:B:480:GLY:HA2	1.80	0.47
1:A:277:LEU:HD13	1:A:772:ILE:HG21	1.96	0.47
1:A:10:HIS:HD2	1:A:135:ILE:HG12	1.79	0.46
1:A:394:TYR:HB2	3:A:947:HOH:O	2.15	0.46
1:A:38:GLN:HB3	1:A:39:GLY:H	1.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HA	1:B:515:LEU:HD13	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:807:LYS:HD3	1:B:807:LYS:HA	1.61	0.45
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:A:213:PRO:HB3	1:A:220:ALA:HB2	1.99	0.45
1:B:577:LEU:HA	1:B:577:LEU:HD12	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:711:ALA:HB3	3:B:1171:HOH:O	2.18	0.44
1:B:164:ASN:HB3	1:B:793:SER:OG	2.16	0.44
1:A:807:LYS:HG2	1:A:807:LYS:HZ3	1.70	0.44
1:A:836:THR:HA	1:A:839:LEU:HD13	1.99	0.44
1:A:567:ASN:H	1:A:567:ASN:HD22	1.64	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:A:520:LEU:HD21	1:A:590:TYR:HB2	2.00	0.44
1:A:520:LEU:O	1:A:525:VAL:HB	2.17	0.44
1:A:493:VAL:HG21	1:A:746:ARG:HG2	1.99	0.44
1:A:388:LYS:HA	1:A:388:LYS:HD2	1.64	0.44
1:A:381:LYS:NZ	3:A:1281:HOH:O	2.36	0.43
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:842:SER:HB2	1:A:850:GLY:CA	2.46	0.43
1:A:414:THR:HG23	1:A:417:GLU:H	1.84	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: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:221:ARG:HA	1:A:221:ARG:HD3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ILE:HD13	1:B:322:ILE:HA	1.84	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:196:LYS:HD2	1:A:196:LYS:HA	1.91	0.43
1:A:462:LEU:HA	1:A:462:LEU:HD12	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:B:704:THR:HA	1:B:708:LEU:HB3	2.01	0.43
1:B:187:LEU:HA	1:B:187:LEU:HD12	1.88	0.43
1:A:271:ASP:OD2	1:A:778:SER:HB2	2.18	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
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:B:455:PHE:HB2	1:B:465:LEU:CD2	2.48	0.42
1:A:424:LEU:HA	1:A:424:LEU:HD23	1.60	0.42
1:A:266:HIS:NE2	3:A:1000:HOH:O	2.37	0.42
1:B:543:ILE:HG22	1:B:547:LEU:HD22	2.02	0.42
1:A:789:PRO:HB2	1:A:790:ASN:H	1.31	0.42
1:B:640:ILE:HD13	1:B:702:ILE:HG22	2.01	0.42
1:A:607:ARG:NH2	1:A:627:TYR:OH	2.43	0.42
1:A:234:ARG:NH2	1:A:678:ASP:OD2	2.52	0.42
1:B:376:LEU:HD12	1:B:376:LEU:HA	1.81	0.42
1:A:429:HIS:NE2	1:A:509:ASP:OD1	2.42	0.42
1:B:194:GLU:HG3	1:B:240:ARG:HA	2.02	0.42
1:B:361:ASP:HB3	1:B:464:PRO:CD	2.50	0.42
1:B:414:THR:OG1	1:B:415:VAL:N	2.52	0.42
1:B:205:ASP:OD1	1:B:206:VAL:N	2.51	0.42
1:A:36:ILE:HA	1:A:36:ILE:HD12	1.88	0.42
1:B:394:TYR:HD2	1:B:480:GLY:CA	2.33	0.42
1:B:38:GLN:HE21	1:B:38:GLN:HB2	1.62	0.42
1:A:618:HIS:ND1	1:A:638:ASP:OD2	2.52	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:B:505:VAL:O	1:B:508:ASN:HB2	2.19	0.41
1:B:141:ILE:HD13	1:B:141:ILE:HG23	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:ILE:HD12	1:A:723:ILE:HA	1.84	0.41
1:B:278:LYS:HE3	1:B:278:LYS:HB2	1.87	0.41
1:A:702:ILE:O	1:A:706:SER:OG	2.27	0.41
1:A:29:VAL:HG11	1:A:272:PHE:CE1	2.53	0.41
1:B:696:GLU:O	1:B:700:ILE:HG13	2.21	0.41
1:B:541:HIS:HE1	1:B:661:ASP:OD2	2.04	0.41
1:A:414:THR:O	1:A:418:ALA:N	2.54	0.41
1:A:135:ILE:HB	1:A:136:PRO:HD3	2.02	0.41
1:A:106:ASP:HB2	1:A:107:ASP:H	1.40	0.41
1:B:56:ARG:HD3	1:B:56:ARG:HH11	1.70	0.41
1:B:765:ILE:HD13	1:B:765:ILE:HG21	1.70	0.41
1:B:235:ARG:C	1:B:235:ARG:HD2	2.40	0.41
1:B:530:ILE:HG12	1:B:551:TYR:CG	2.56	0.41
1:B:520:LEU:O	1:B:525:VAL:HB	2.21	0.41
1:A:172:THR:HB	1:A:177:VAL:HG22	2.03	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:B:189:GLY:HA3	1:B:201:ILE:HD13	2.03	0.40
1:A:375:ASN:ND2	1:A:375:ASN:O	2.52	0.40
1:B:54:LEU:HD12	1:B:54:LEU:HA	1.85	0.40
1:A:105:TRP:CD2	1:A:109:SER:HB2	2.56	0.40
1:B:564:SER:C	1:B:567:ASN:ND2	2.75	0.40
1:B:271:ASP:OD2	1:B:778:SER:HB3	2.22	0.40
1:B:394:TYR:HD2	1:B:480:GLY:C	2.25	0.40
1:A:604:LEU:HB3	1:A:610:ALA:CB	2.52	0.40
1:B:56:ARG:NH2	3:B:982:HOH:O	2.55	0.40
1:A:208:ASN:HB2	1:A:249:SER:HA	2.04	0.40
1:B:277:LEU:HD12	1:B:277:LEU:HA	1.91	0.40
1:A:813:ASN:ND2	3:A:1152:HOH:O	2.54	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:B:507:VAL:HG13	1:B:577:LEU:HD13	2.03	0.40
1:B:762:GLN:H	1:B:762:GLN:HE21	1.68	0.40
1:A:783:LEU:HG	1:A:808:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	848/857 (99%)	767 (90%)	61 (7%)	20 (2%)	7	3
1	B	848/857 (99%)	772 (91%)	59 (7%)	17 (2%)	9	4
All	All	1696/1714 (99%)	1539 (91%)	120 (7%)	37 (2%)	8	3

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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	744/749 (99%)	604 (81%)	140 (19%)	2	1
1	B	744/749 (99%)	608 (82%)	136 (18%)	2	1
All	All	1488/1498 (99%)	1212 (82%)	276 (18%)	2	1

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	41	ASP
1	A	42	LEU
1	A	43	VAL
1	A	45	SER

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Mol	Chain	Res	Type
1	A	46	THR
1	A	50	LEU
1	A	51	THR
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
1	A	134	ASP
1	A	147	SER
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	205	ASP
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

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Mol	Chain	Res	Type
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	354	SER
1	A	374	PRO
1	A	375	ASN
1	A	378	ARG
1	A	388	LYS
1	A	391	SER
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	427	LEU
1	A	433	ILE
1	A	434	MET
1	A	438	ARG
1	A	462	LEU
1	A	463	ARG
1	A	475	GLN
1	A	479	SER
1	A	497	ILE
1	A	507	VAL
1	A	508	ASN
1	A	515	LEU
1	A	525	VAL
1	A	537	LEU
1	A	547	LEU
1	A	552	ARG

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Mol	Chain	Res	Type
1	A	553	ASP
1	A	564	SER
1	A	565	LEU
1	A	567	ASN
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	612	GLU
1	A	621	ARG
1	A	627	TYR
1	A	630	THR
1	A	631	VAL
1	A	650	LEU
1	A	690	THR
1	A	712	VAL
1	A	722	LEU
1	A	724	LEU
1	A	732	ARG
1	A	736	GLU
1	A	737	LYS
1	A	743	GLU
1	A	744	GLU
1	A	762	GLN
1	A	766	ASP
1	A	778	SER
1	A	787	ASP
1	A	788	ASN
1	A	798	LEU
1	A	802	LYS
1	A	807	LYS
1	A	808	LEU
1	A	815	LEU
1	A	817	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

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Mol	Chain	Res	Type
1	A	844	GLU
1	A	846	LEU
1	A	857	ILE
1	B	8	ARG
1	B	11	LYS
1	B	15	THR
1	B	31	SER
1	B	36	ILE
1	B	38	GLN
1	B	40	LEU
1	B	41	ASP
1	B	42	LEU
1	B	43	VAL
1	B	45	SER
1	B	49	THR
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	164	ASN
1	B	168	LEU
1	B	184	LEU
1	B	187	LEU
1	B	218	ASN
1	B	232	TYR
1	B	235	ARG
1	B	238	THR
1	B	241	LYS
1	B	244	ARG
1	B	251	SER

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Mol	Chain	Res	Type
1	B	254	ASN
1	B	258	LEU
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	312	SER
1	B	319	THR
1	B	321	ILE
1	B	322	ILE
1	B	333	GLU
1	B	334	ILE
1	B	336	ARG
1	B	340	GLU
1	B	341	GLN
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	427	LEU
1	B	434	MET
1	B	438	ARG
1	B	463	ARG
1	B	465	LEU

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Mol	Chain	Res	Type
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	517	SER
1	B	525	VAL
1	B	537	LEU
1	B	547	LEU
1	B	552	ARG
1	B	564	SER
1	B	565	LEU
1	B	566	VAL
1	B	567	ASN
1	B	568	ASP
1	B	583	VAL
1	B	604	LEU
1	B	615	SER
1	B	620	ILE
1	B	621	ARG
1	B	625	GLU
1	B	627	TYR
1	B	630	THR
1	B	631	VAL
1	B	641	LYS
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	737	LYS
1	B	739	SER
1	B	751	LYS
1	B	762	GLN
1	B	766	ASP
1	B	775	ARG
1	B	786	ARG
1	B	787	ASP
1	B	788	ASN

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Mol	Chain	Res	Type
1	B	798	LEU
1	B	802	LYS
1	B	807	LYS
1	B	813	ASN
1	B	815	LEU
1	B	817	GLU
1	B	819	ASN
1	B	827	ARG
1	B	831	VAL
1	B	838	LEU
1	B	843	LYS
1	B	844	GLU
1	B	846	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	38	GLN
1	A	137	ASN
1	A	164	ASN
1	A	165	GLN
1	A	282	GLN
1	A	458	ASN
1	A	473	HIS
1	A	521	ASN
1	A	541	HIS
1	A	567	ASN
1	A	750	GLN
1	A	806	ASN
1	A	813	ASN
1	A	819	ASN
1	B	10	HIS
1	B	38	GLN
1	B	254	ASN
1	B	283	ASN
1	B	375	ASN
1	B	397	HIS
1	B	421	ASN
1	B	458	ASN
1	B	473	HIS
1	B	478	GLN

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Mol	Chain	Res	Type
1	B	521	ASN
1	B	541	HIS
1	B	548	HIS
1	B	567	ASN
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 carbohydrates 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 (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	850/857 (99%)	-0.02	43 (5%)	32	40	2, 17, 34, 49	0
1	B	850/857 (99%)	-0.13	37 (4%)	38	47	2, 16, 35, 46	0
All	All	1700/1714 (99%)	-0.08	80 (4%)	35	44	2, 16, 35, 49	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	ILE	7.0
1	A	410	LEU	6.9
1	A	35	ILE	6.2
1	A	33	GLY	6.0
1	A	8	ARG	6.0
1	B	32	VAL	5.7
1	A	39	GLY	5.6
1	A	47	LEU	5.5
1	A	32	VAL	5.2
1	B	339	GLY	5.2
1	B	41	ASP	5.1
1	B	394	TYR	4.8
1	A	135	ILE	4.7
1	A	45	SER	4.7
1	B	397	HIS	4.5
1	B	35	ILE	4.5
1	A	409	ASN	4.5
1	B	8	ARG	4.5
1	B	34	GLY	4.4
1	B	410	LEU	4.4
1	A	42	LEU	4.3
1	A	46	THR	4.3
1	B	338	ASP	4.3
1	B	107	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	45	SER	4.3
1	A	40	LEU	4.2
1	B	39	GLY	4.1
1	A	44	GLY	4.0
1	B	395	GLY	4.0
1	B	474	PRO	3.9
1	B	135	ILE	3.8
1	A	34	GLY	3.8
1	B	47	LEU	3.7
1	B	42	LEU	3.6
1	A	408	PRO	3.6
1	B	409	ASN	3.5
1	B	396	ASP	3.5
1	A	339	GLY	3.3
1	A	9	GLY	3.3
1	B	46	THR	3.1
1	A	43	VAL	3.1
1	A	37	GLY	3.1
1	B	36	ILE	3.0
1	A	341	GLN	2.9
1	A	394	TYR	2.9
1	B	332	LYS	2.9
1	A	342	ALA	2.8
1	B	31	SER	2.8
1	A	41	ASP	2.8
1	A	38	GLN	2.8
1	A	395	GLY	2.7
1	B	33	GLY	2.7
1	B	611	ILE	2.7
1	B	38	GLN	2.7
1	B	342	ALA	2.6
1	B	48	ASP	2.4
1	A	474	PRO	2.4
1	A	338	ASP	2.4
1	B	9	GLY	2.4
1	B	341	GLN	2.4
1	B	408	PRO	2.4
1	A	107	ASP	2.3
1	A	396	ASP	2.3
1	A	393	VAL	2.3
1	B	40	LEU	2.3
1	B	71	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	49	THR	2.3
1	B	785	GLU	2.3
1	A	71	ASN	2.2
1	A	110	GLY	2.2
1	A	137	ASN	2.2
1	A	336	ARG	2.2
1	A	48	ASP	2.2
1	A	31	SER	2.2
1	B	136	PRO	2.1
1	B	336	ARG	2.1
1	A	737	LYS	2.1
1	A	218	ASN	2.1
1	A	105	TRP	2.0
1	A	106	ASP	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	FE2	A	858	1/1	1.00	0.08	-1.13	28,28,28,28	0
2	FE2	B	858	1/1	1.00	0.04	-2.67	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.