



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:51 AM UTC

PDB ID : 8YAU / pdb_00008yau
Title : Crystal structure of glucose 1-dehydrogenase mutant2 from Limosilactobacillus fermentum
Authors : Cong, L.; Wei, H.L.; Liu, W.D.; You, S.
Deposited on : 2024-02-10
Resolution : 2.22 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

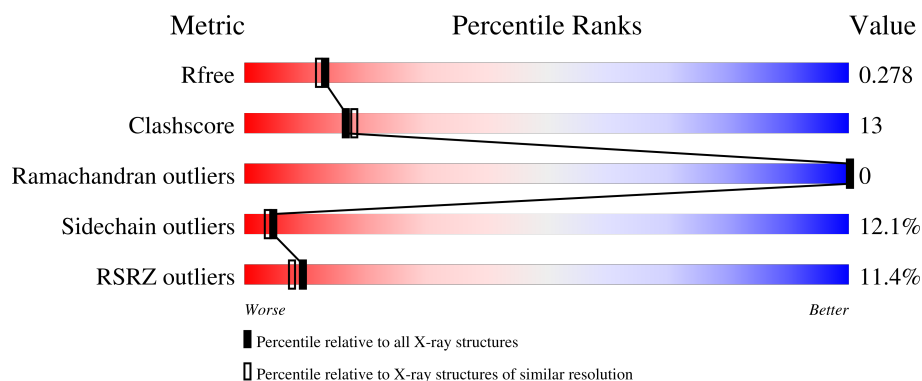
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	247	5% 71% 27% .
1	B	247	5% 77% 21% .
1	C	247	8% 74% 19% .
1	D	247	9% 66% 28% 5%
1	E	247	13% 57% 33% 6%

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Mol	Chain	Length	Quality of chain
1	F	247	26% 57% 28% 8% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10646 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 SDR family oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1801	1133	308	352	8			
1	B	244	Total	C	N	O	S	0	0	0
			1819	1149	309	353	8			
1	C	239	Total	C	N	O	S	0	0	0
			1718	1084	294	332	8			
1	D	234	Total	C	N	O	S	0	0	0
			1719	1081	290	341	7			
1	E	236	Total	C	N	O	S	0	0	0
			1742	1099	296	339	8			
1	F	230	Total	C	N	O	S	0	0	0
			1623	1025	271	319	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	VAL	GLY	engineered mutation	UNP A0A843R2C6
A	146	ASP	GLY	engineered mutation	UNP A0A843R2C6
A	186	ALA	VAL	engineered mutation	UNP A0A843R2C6
B	92	VAL	GLY	engineered mutation	UNP A0A843R2C6
B	146	ASP	GLY	engineered mutation	UNP A0A843R2C6
B	186	ALA	VAL	engineered mutation	UNP A0A843R2C6
C	92	VAL	GLY	engineered mutation	UNP A0A843R2C6
C	146	ASP	GLY	engineered mutation	UNP A0A843R2C6
C	186	ALA	VAL	engineered mutation	UNP A0A843R2C6
D	92	VAL	GLY	engineered mutation	UNP A0A843R2C6
D	146	ASP	GLY	engineered mutation	UNP A0A843R2C6
D	186	ALA	VAL	engineered mutation	UNP A0A843R2C6
E	92	VAL	GLY	engineered mutation	UNP A0A843R2C6
E	146	ASP	GLY	engineered mutation	UNP A0A843R2C6
E	186	ALA	VAL	engineered mutation	UNP A0A843R2C6
F	92	VAL	GLY	engineered mutation	UNP A0A843R2C6
F	146	ASP	GLY	engineered mutation	UNP A0A843R2C6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	186	ALA	VAL	engineered mutation	UNP A0A843R2C6

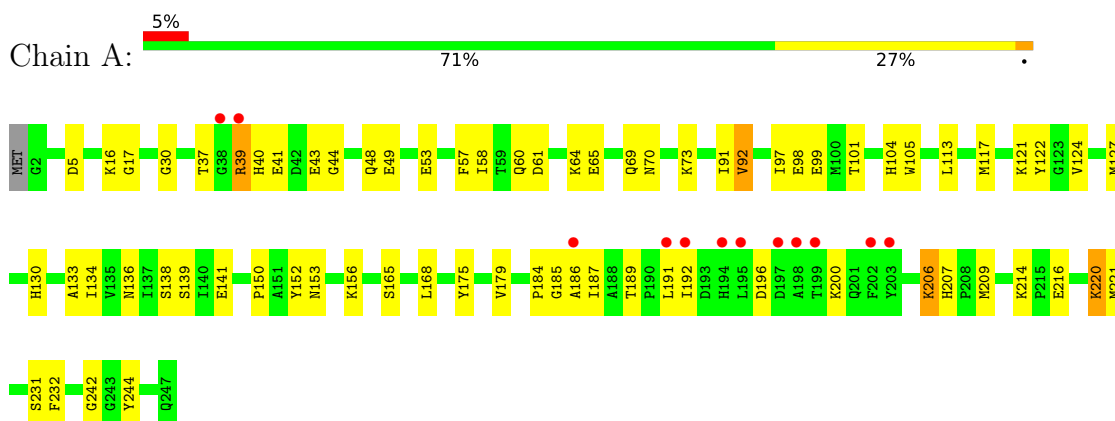
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	52	Total 52	O 52	0	0
2	B	52	Total 52	O 52	0	0
2	C	25	Total 25	O 25	0	0
2	D	44	Total 44	O 44	0	0
2	E	31	Total 31	O 31	0	0
2	F	20	Total 20	O 20	0	0

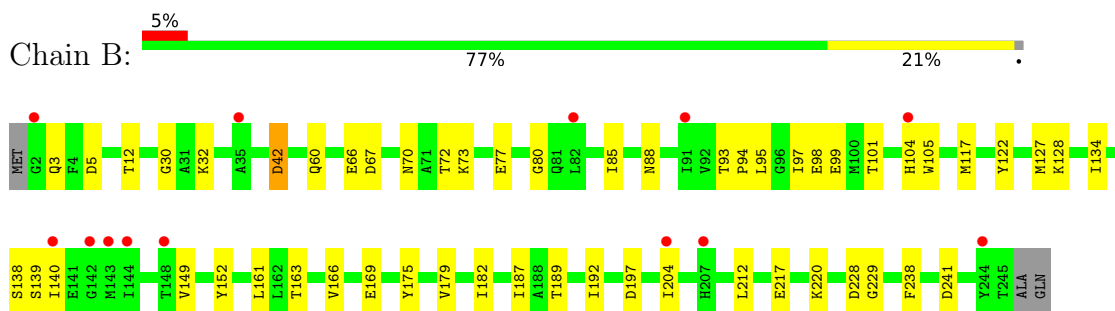
3 Residue-property plots [i](#)

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

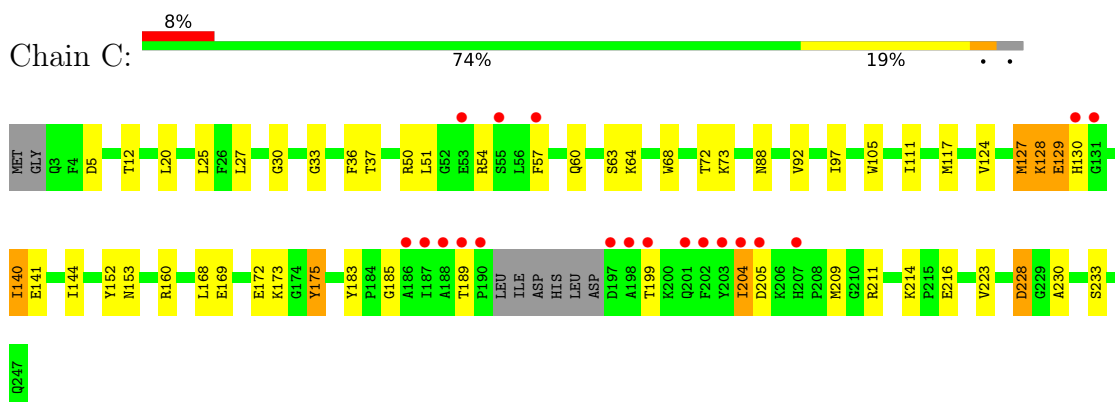
- Molecule 1: SDR family oxidoreductase



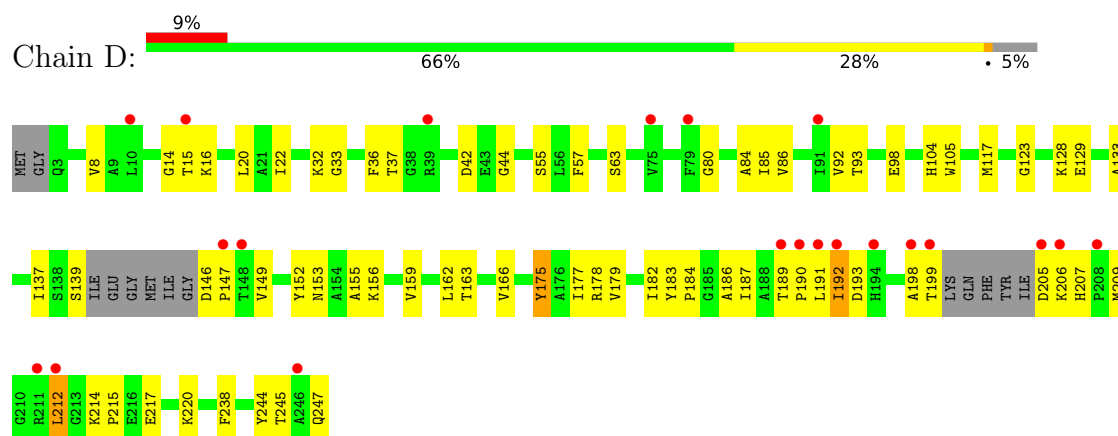
- Molecule 1: SDR family oxidoreductase



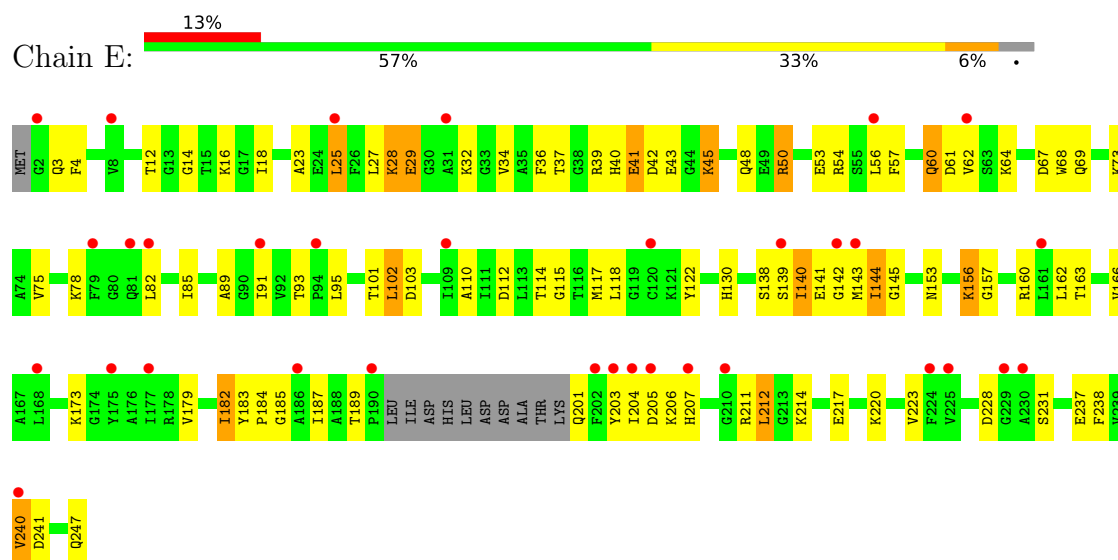
- Molecule 1: SDR family oxidoreductase



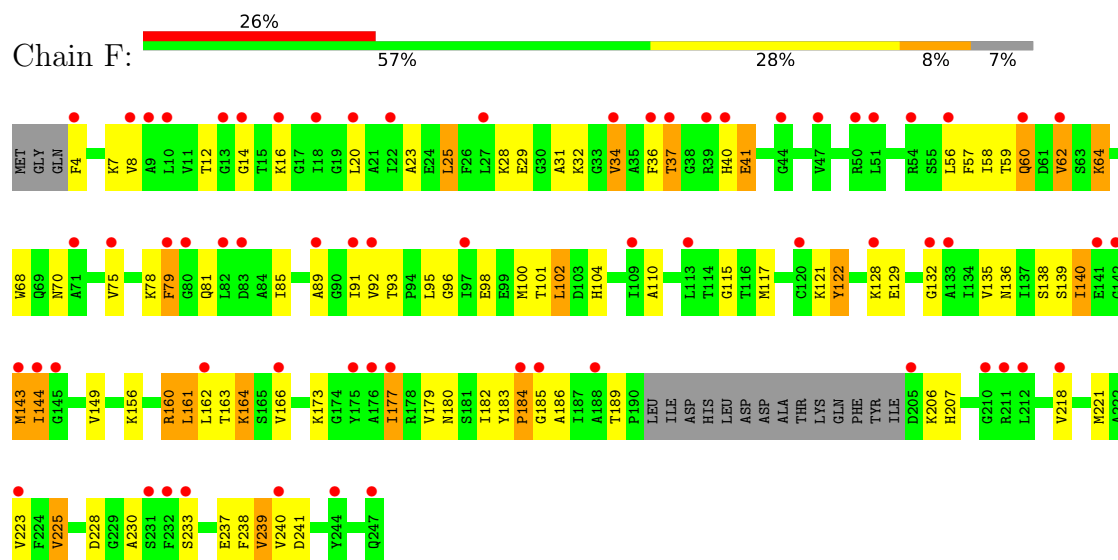
• Molecule 1: SDR family oxidoreductase



• Molecule 1: SDR family oxidoreductase



• Molecule 1: SDR family oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	61.75Å 139.52Å 331.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.56 – 2.22 32.56 – 2.22	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.56-2.22) 99.9 (32.56-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.22Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.238 , 0.272 0.257 , 0.278	Depositor DCC
R_{free} test set	3553 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10646	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.09% 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	0.39	1/1828 (0.1%)	0.72	6/2470 (0.2%)
1	B	0.25	0/1849	0.53	0/2496
1	C	0.48	0/1743	0.73	1/2357 (0.0%)
1	D	0.43	0/1745	0.73	3/2359 (0.1%)
1	E	0.93	0/1770	1.41	3/2389 (0.1%)
1	F	0.98	0/1648	1.43	7/2233 (0.3%)
All	All	0.63	1/10583 (0.0%)	0.98	20/14304 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	LEU	CA-C	5.61	1.57	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	GLN	CA-C-N	-7.98	109.98	122.67
1	A	48	GLN	C-N-CA	-7.98	109.98	122.67
1	C	140	ILE	N-CA-C	-7.59	102.88	110.62
1	A	49	GLU	CA-C-N	-6.17	110.19	120.68
1	A	49	GLU	C-N-CA	-6.17	110.19	120.68
1	F	136	ASN	CA-C-N	-5.96	114.92	122.43
1	F	136	ASN	C-N-CA	-5.96	114.92	122.43
1	A	136	ASN	CA-C-N	-5.76	115.39	122.93
1	A	136	ASN	C-N-CA	-5.76	115.39	122.93
1	D	190	PRO	N-CA-C	-5.76	105.53	113.53
1	F	184	PRO	N-CA-C	5.72	121.06	113.40
1	F	122	TYR	CB-CA-C	5.60	120.37	110.85
1	D	215	PRO	N-CA-C	-5.56	105.81	113.53
1	E	122	TYR	CB-CA-C	5.47	120.14	110.85
1	D	187	ILE	CA-C-O	-5.45	117.37	121.68
1	F	110	ALA	CA-C-N	-5.32	113.75	120.56
1	F	110	ALA	C-N-CA	-5.32	113.75	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	140	ILE	N-CA-C	-5.27	104.46	111.05
1	E	50	ARG	N-CA-C	5.13	116.96	111.36
1	F	140	ILE	N-CA-C	-5.04	104.75	111.05

There are no chirality outliers.

There are no planarity outliers.

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	1801	0	1777	56	0
1	B	1819	0	1811	45	0
1	C	1718	0	1683	36	0
1	D	1719	0	1680	45	0
1	E	1742	0	1716	55	0
1	F	1623	0	1560	51	0
2	A	52	0	0	3	0
2	B	52	0	0	5	0
2	C	25	0	0	0	0
2	D	44	0	0	5	0
2	E	31	0	0	2	0
2	F	20	0	0	0	0
All	All	10646	0	10227	264	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 13.

All (264) 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:39:ARG:HG3	1:A:39:ARG:HH11	1.03	1.18
1:E:185:GLY:HA3	1:E:241:ASP:HA	1.39	1.02
1:B:93:THR:HG21	1:B:104:HIS:NE2	1.77	0.99
1:A:39:ARG:HD2	1:E:40:HIS:CG	1.99	0.97
1:F:185:GLY:HA3	1:F:241:ASP:HA	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:HH11	1:A:39:ARG:CG	1.81	0.88
1:E:14:GLY:HA3	1:E:36:PHE:HB2	1.60	0.83
1:A:39:ARG:HG3	1:A:39:ARG:NH1	1.85	0.82
1:A:70:ASN:HA	1:A:73:LYS:HD2	1.63	0.78
1:A:39:ARG:HD2	1:E:40:HIS:CD2	2.18	0.77
1:D:139:SER:HA	1:D:184:PRO:HG2	1.66	0.76
1:F:14:GLY:HA3	1:F:36:PHE:HB2	1.67	0.76
1:E:185:GLY:CA	1:E:241:ASP:HA	2.16	0.76
1:F:25:LEU:HB3	1:F:223:VAL:HG21	1.69	0.75
1:F:182:ILE:HD13	1:F:238:PHE:HB2	1.69	0.75
1:E:39:ARG:NH2	1:E:61:ASP:CG	2.45	0.75
1:A:209:MET:HE3	1:A:242:GLY:HA2	1.69	0.74
1:B:70:ASN:ND2	2:B:301:HOH:O	2.22	0.72
1:E:32:LYS:O	1:E:54:ARG:HG2	1.89	0.71
1:C:63:SER:OG	1:C:64:LYS:NZ	2.23	0.71
1:F:182:ILE:HD11	1:F:225:VAL:HG11	1.72	0.71
1:E:25:LEU:HB3	1:E:223:VAL:HG21	1.73	0.71
1:D:32:LYS:NZ	1:D:80:GLY:H	1.89	0.70
1:F:62:VAL:HB	1:F:115:GLY:HA3	1.74	0.70
1:F:140:ILE:HG21	1:F:241:ASP:HB3	1.74	0.69
1:B:93:THR:CG2	1:B:104:HIS:CE1	2.76	0.69
1:C:228:ASP:O	1:D:220:LYS:NZ	2.27	0.68
1:D:16:LYS:NZ	2:D:301:HOH:O	2.20	0.68
1:D:156:LYS:HD2	1:D:183:TYR:HD2	1.59	0.67
1:B:93:THR:HG21	1:B:104:HIS:CE1	2.30	0.66
1:F:180:ASN:HB2	1:F:225:VAL:HG21	1.77	0.66
1:F:183:TYR:CE1	1:F:237:GLU:HB3	2.31	0.65
1:B:32:LYS:NZ	1:B:80:GLY:H	1.95	0.65
1:E:25:LEU:HD21	1:E:220:LYS:HG3	1.79	0.64
1:E:60:GLN:HG2	1:E:67:ASP:HB3	1.80	0.63
1:F:138:SER:O	1:F:184:PRO:HD3	1.98	0.63
1:E:163:THR:HG23	1:E:179:VAL:HG12	1.82	0.62
1:D:32:LYS:HZ1	1:D:80:GLY:H	1.47	0.62
1:F:37:THR:HG21	1:F:60:GLN:HG2	1.81	0.61
1:B:95:LEU:HD23	1:B:104:HIS:CE1	2.35	0.61
1:E:39:ARG:NH2	1:E:61:ASP:OD1	2.33	0.61
1:E:41:GLU:HA	1:E:57:PHE:CE2	2.36	0.60
1:E:4:PHE:H	1:E:29:GLU:HB3	1.67	0.59
1:A:196:ASP:O	1:A:200:LYS:N	2.36	0.59
1:E:40:HIS:HE1	1:E:42:ASP:HB2	1.68	0.59
1:A:65:GLU:OE2	1:A:121:LYS:NZ	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:GLU:HA	1:F:57:PHE:CE1	2.38	0.59
1:E:185:GLY:O	1:E:187:ILE:HG12	2.03	0.59
1:A:5:ASP:HA	1:A:30:GLY:O	2.03	0.58
1:C:92:VAL:HG22	1:C:152:TYR:CE1	2.38	0.58
1:A:231:SER:OG	1:B:220:LYS:NZ	2.35	0.58
1:A:41:GLU:HA	1:A:57:PHE:CE2	2.39	0.58
1:C:37:THR:HB	1:C:60:GLN:HB3	1.85	0.58
1:D:146:ASP:N	2:D:305:HOH:O	2.37	0.58
1:E:62:VAL:HB	1:E:115:GLY:HA3	1.86	0.57
1:A:16:LYS:HG2	1:A:17:GLY:N	2.20	0.57
1:D:156:LYS:HD2	1:D:183:TYR:CD2	2.40	0.57
1:A:39:ARG:NE	1:E:40:HIS:CE1	2.73	0.57
1:B:166:VAL:HG12	1:B:179:VAL:HG21	1.87	0.57
1:B:163:THR:HG23	1:B:179:VAL:HG12	1.86	0.57
1:F:160:ARG:HD3	1:F:237:GLU:CD	2.30	0.57
1:F:139:SER:HA	1:F:184:PRO:CD	2.34	0.56
1:F:183:TYR:HB2	1:F:239:VAL:HG13	1.87	0.56
1:A:139:SER:C	1:A:141:GLU:N	2.62	0.56
1:C:54:ARG:HG3	1:C:54:ARG:HH11	1.69	0.56
1:C:140:ILE:HG12	1:C:185:GLY:HA2	1.87	0.56
1:D:128:LYS:O	1:D:129:GLU:HB2	2.05	0.56
1:E:157:GLY:O	1:E:160:ARG:HG2	2.05	0.56
1:A:138:SER:O	1:A:184:PRO:HD2	2.05	0.56
1:C:168:LEU:HD21	1:D:247:GLN:HB2	1.87	0.56
1:B:189:THR:OG1	1:B:192:ILE:HG13	2.06	0.56
1:E:183:TYR:CE1	1:E:237:GLU:HB3	2.40	0.55
1:B:32:LYS:HZ1	1:B:80:GLY:H	1.54	0.55
1:B:204:ILE:HG12	1:B:212:LEU:HG	1.88	0.55
1:E:40:HIS:CE1	1:E:42:ASP:HB2	2.42	0.55
1:A:130:HIS:HB2	2:A:335:HOH:O	2.06	0.55
1:C:36:PHE:CZ	1:C:57:PHE:HB2	2.42	0.55
1:A:39:ARG:CG	1:A:39:ARG:NH1	2.49	0.55
1:A:99:GLU:OE2	1:A:99:GLU:N	2.40	0.54
1:D:189:THR:HG23	1:D:192:ILE:HD12	1.88	0.54
1:A:165:SER:OG	1:D:153:ASN:OD1	2.25	0.54
1:F:163:THR:HG23	1:F:179:VAL:HG12	1.90	0.54
1:B:73:LYS:HE3	1:B:77:GLU:OE1	2.07	0.54
1:F:139:SER:HA	1:F:184:PRO:HD2	1.89	0.54
1:A:98:GLU:HB3	1:A:99:GLU:OE2	2.08	0.54
1:B:42:ASP:OD1	1:B:42:ASP:N	2.39	0.54
1:C:128:LYS:HB2	1:C:175:TYR:CG	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ALA:HB3	1:A:207:HIS:NE2	2.22	0.54
1:F:183:TYR:HE1	1:F:237:GLU:HB3	1.73	0.54
1:B:5:ASP:HA	1:B:30:GLY:O	2.08	0.53
1:E:214:LYS:HB2	1:E:217:GLU:HG3	1.90	0.53
1:F:8:VAL:HG21	1:F:79:PHE:HB2	1.89	0.53
1:A:69:GLN:HG3	1:A:122:TYR:CE1	2.43	0.53
1:F:186:ALA:HB2	1:F:207:HIS:NE2	2.23	0.53
1:B:3:GLN:NE2	2:B:304:HOH:O	2.41	0.53
1:C:68:TRP:O	1:C:72:THR:HG22	2.08	0.53
1:F:166:VAL:HG12	1:F:179:VAL:HG21	1.90	0.53
1:A:220:LYS:HE3	1:B:229:GLY:HA2	1.90	0.53
1:B:66:GLU:HG2	1:B:67:ASP:N	2.24	0.53
1:B:94:PRO:HA	1:B:149:VAL:HG11	1.90	0.53
1:D:207:HIS:CE1	1:D:244:TYR:HB2	2.44	0.52
1:E:3:GLN:HB2	1:E:29:GLU:HG3	1.91	0.52
1:D:128:LYS:HG2	2:D:304:HOH:O	2.09	0.52
1:B:93:THR:HG22	1:B:95:LEU:HD23	1.90	0.52
1:D:175:TYR:HB3	1:D:177:ILE:HD12	1.91	0.52
1:B:94:PRO:O	1:B:95:LEU:HD22	2.10	0.52
1:B:217:GLU:HA	1:B:220:LYS:HE3	1.92	0.52
1:A:232:PHE:HE2	2:B:312:HOH:O	1.92	0.51
1:F:95:LEU:HG	1:F:100:MET:HA	1.92	0.51
1:F:41:GLU:HA	1:F:57:PHE:HE1	1.73	0.51
1:D:146:ASP:OD2	1:D:149:VAL:HG22	2.09	0.51
1:E:166:VAL:HG12	1:E:179:VAL:HG21	1.91	0.51
1:E:141:GLU:O	1:E:153:ASN:ND2	2.44	0.50
1:F:36:PHE:CZ	1:F:57:PHE:HB2	2.46	0.50
1:E:23:ALA:HA	1:E:34:VAL:HG11	1.94	0.50
1:D:92:VAL:HG11	2:D:338:HOH:O	2.10	0.50
1:D:214:LYS:HB2	1:D:217:GLU:HG3	1.94	0.49
1:C:33:GLY:HA2	1:C:54:ARG:O	2.11	0.49
1:E:160:ARG:HH21	1:E:237:GLU:CD	2.20	0.49
1:E:160:ARG:HB2	1:E:183:TYR:OH	2.12	0.49
1:D:22:ILE:HD13	1:D:86:VAL:HG11	1.93	0.49
1:C:204:ILE:HG13	1:C:205:ASP:N	2.27	0.49
1:E:182:ILE:HD13	1:E:238:PHE:HB2	1.95	0.49
1:B:228:ASP:OD1	1:B:228:ASP:N	2.43	0.49
1:F:140:ILE:O	1:F:144:ILE:HG13	2.13	0.48
1:F:139:SER:HB3	1:F:156:LYS:HG3	1.95	0.48
1:E:61:ASP:HB3	1:E:64:LYS:HG2	1.96	0.48
1:A:37:THR:HG22	1:A:58:ILE:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:HD3	2:E:321:HOH:O	2.13	0.48
1:A:139:SER:C	1:A:141:GLU:H	2.22	0.48
1:D:92:VAL:HG23	1:D:152:TYR:HB2	1.95	0.48
1:C:5:ASP:HA	1:C:30:GLY:O	2.14	0.48
1:E:39:ARG:NH2	1:E:61:ASP:OD2	2.45	0.48
1:E:75:VAL:HG11	1:E:82:LEU:HD22	1.95	0.48
1:E:138:SER:HA	1:E:156:LYS:HE2	1.96	0.48
1:A:185:GLY:O	1:A:187:ILE:HG12	2.14	0.48
1:F:4:PHE:HA	1:F:7:LYS:HD3	1.96	0.48
1:F:225:VAL:HA	1:F:230:ALA:CB	2.44	0.48
1:C:141:GLU:HG2	1:C:152:TYR:HD2	1.79	0.47
1:D:198:ALA:O	1:D:199:THR:HG23	2.15	0.47
1:F:160:ARG:HD3	1:F:237:GLU:OE1	2.14	0.47
1:A:214:LYS:HD2	1:A:214:LYS:HA	1.57	0.47
1:C:209:MET:HE1	1:D:178:ARG:HG2	1.96	0.47
1:C:175:TYR:N	1:C:175:TYR:CD1	2.81	0.47
1:D:14:GLY:HA3	1:D:36:PHE:HB2	1.97	0.47
1:C:168:LEU:HD11	1:D:247:GLN:HB2	1.95	0.47
1:E:212:LEU:HD22	1:E:212:LEU:HA	1.78	0.47
1:A:104:HIS:HD2	2:A:327:HOH:O	1.96	0.47
1:B:99:GLU:OE1	1:B:99:GLU:N	2.45	0.47
1:F:23:ALA:HB1	1:F:34:VAL:HG11	1.96	0.47
1:A:37:THR:HB	1:A:60:GLN:HB3	1.97	0.47
1:C:20:LEU:HD11	1:C:50:ARG:HH22	1.80	0.47
1:E:139:SER:HA	1:E:184:PRO:HD2	1.96	0.47
1:D:8:VAL:HA	1:D:33:GLY:O	2.15	0.47
1:F:96:GLY:O	1:F:100:MET:N	2.48	0.46
1:D:207:HIS:HE1	1:D:244:TYR:HB2	1.80	0.46
1:B:60:GLN:HG3	1:B:67:ASP:HB3	1.97	0.46
1:B:105:TRP:CE3	1:C:117:MET:HG3	2.51	0.46
1:B:182:ILE:HG12	1:B:238:PHE:HB2	1.96	0.46
1:E:156:LYS:HD2	1:E:156:LYS:N	2.31	0.46
1:A:61:ASP:HB3	1:A:64:LYS:HG2	1.97	0.46
1:D:186:ALA:HB1	1:D:212:LEU:HD22	1.98	0.46
1:A:187:ILE:O	1:A:189:THR:HG23	2.16	0.46
1:F:102:LEU:HD23	1:F:102:LEU:HA	1.70	0.46
1:F:132:GLY:C	1:F:177:ILE:HG23	2.41	0.46
1:B:117:MET:HG3	1:C:105:TRP:CZ3	2.51	0.46
1:C:124:VAL:O	1:C:128:LYS:HB3	2.16	0.46
1:F:12:THR:HG1	1:F:89:ALA:H	1.64	0.46
1:B:93:THR:CG2	1:B:95:LEU:HD23	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:LEU:HD13	1:F:161:LEU:HA	1.78	0.45
1:C:12:THR:HG1	1:C:88:ASN:H	1.63	0.45
1:D:183:TYR:OH	1:D:245:THR:HG21	2.16	0.45
1:E:73:LYS:HE2	1:E:73:LYS:HB2	1.64	0.45
1:B:128:LYS:HD3	1:B:175:TYR:CZ	2.52	0.45
1:B:175:TYR:N	1:B:175:TYR:CD1	2.83	0.45
1:D:93:THR:HB	1:D:104:HIS:NE2	2.32	0.45
1:D:163:THR:HG23	1:D:179:VAL:HG12	1.99	0.45
1:D:182:ILE:HG12	1:D:238:PHE:HB2	1.99	0.45
1:A:39:ARG:HD2	1:E:40:HIS:ND1	2.30	0.45
1:A:69:GLN:O	1:A:73:LYS:HD2	2.17	0.45
1:A:97:ILE:HG21	1:D:166:VAL:HG13	1.98	0.45
1:C:140:ILE:HD12	1:C:144:ILE:HD11	1.98	0.45
1:D:175:TYR:N	1:D:175:TYR:CD1	2.84	0.45
1:F:64:LYS:HA	1:F:64:LYS:HD3	1.60	0.45
1:C:63:SER:HB3	1:C:111:ILE:HD13	1.98	0.45
1:E:45:LYS:HA	1:E:45:LYS:HD2	1.66	0.45
1:A:44:GLY:HA3	1:A:57:PHE:CD1	2.51	0.45
1:A:206:LYS:HB3	1:A:244:TYR:CE2	2.52	0.45
1:B:140:ILE:HD13	1:B:187:ILE:HB	1.99	0.45
1:A:156:LYS:HD2	1:A:156:LYS:HA	1.79	0.45
1:B:12:THR:O	1:B:88:ASN:HB3	2.17	0.44
1:E:184:PRO:HA	1:E:240:VAL:HG23	1.98	0.44
1:A:134:ILE:HB	1:A:179:VAL:HG13	1.99	0.44
1:D:139:SER:C	2:D:311:HOH:O	2.59	0.44
1:F:164:LYS:HZ3	1:F:237:GLU:HG2	1.82	0.44
1:E:117:MET:HE3	1:E:117:MET:HB3	1.90	0.44
1:F:4:PHE:HD2	1:F:31:ALA:HB2	1.83	0.44
1:F:117:MET:HE3	1:F:117:MET:HB3	1.92	0.44
1:A:105:TRP:CE3	1:D:117:MET:HG3	2.53	0.44
1:B:97:ILE:HG22	1:C:169:GLU:CD	2.43	0.44
1:E:27:LEU:HA	2:E:304:HOH:O	2.17	0.44
1:F:225:VAL:HA	1:F:230:ALA:HB3	1.99	0.44
1:B:85:ILE:HG13	1:B:127:MET:HE2	2.00	0.43
1:B:161:LEU:HB3	1:C:153:ASN:HB3	2.00	0.43
1:F:143:MET:HE3	1:F:143:MET:HB3	1.84	0.43
1:A:70:ASN:CA	1:A:73:LYS:HD2	2.41	0.43
1:D:212:LEU:HD22	1:D:212:LEU:HA	1.88	0.43
1:E:110:ALA:HA	1:E:114:THR:HB	2.00	0.43
1:F:143:MET:HA	1:F:160:ARG:HH22	1.83	0.43
1:D:84:ALA:HA	1:D:133:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:TRP:HB3	1:F:122:TYR:CD2	2.54	0.43
1:B:101:THR:OG1	1:B:104:HIS:HB2	2.18	0.43
1:B:169:GLU:CD	1:C:97:ILE:HG22	2.43	0.43
1:B:72:THR:HG21	1:B:122:TYR:HB3	2.01	0.43
1:B:149:VAL:HG23	1:B:152:TYR:HB3	2.01	0.43
1:E:28:LYS:HE2	1:E:28:LYS:HB2	1.28	0.43
1:F:182:ILE:HD11	1:F:225:VAL:CG1	2.44	0.43
1:A:40:HIS:CD2	1:E:39:ARG:HG3	2.54	0.43
1:C:128:LYS:HD3	1:C:129:GLU:HG3	2.01	0.43
1:F:139:SER:HA	1:F:184:PRO:HD3	1.99	0.43
1:B:134:ILE:HB	1:B:179:VAL:HG13	2.01	0.42
1:A:216:GLU:H	1:A:216:GLU:CD	2.28	0.42
1:C:168:LEU:O	1:C:172:GLU:N	2.52	0.42
1:A:127:MET:HE1	1:A:133:ALA:O	2.19	0.42
1:A:150:PRO:HD2	2:A:303:HOH:O	2.19	0.42
1:C:160:ARG:HG3	1:C:183:TYR:OH	2.18	0.42
1:D:44:GLY:HA3	1:D:57:PHE:CD1	2.54	0.42
1:E:102:LEU:HD23	1:E:102:LEU:HA	1.71	0.42
1:A:141:GLU:O	1:A:153:ASN:ND2	2.51	0.42
1:A:206:LYS:HD3	1:A:206:LYS:HA	1.67	0.42
1:B:241:ASP:HA	2:B:312:HOH:O	2.20	0.42
1:C:25:LEU:HD23	1:C:223:VAL:HB	2.02	0.42
1:C:214:LYS:HB3	1:C:216:GLU:OE1	2.20	0.42
1:F:135:VAL:HG22	1:F:225:VAL:HG22	2.02	0.42
1:A:117:MET:HG3	1:D:105:TRP:CZ3	2.55	0.42
1:A:221:MET:HE2	1:A:221:MET:HB2	1.78	0.41
1:E:95:LEU:HD21	1:E:101:THR:HG23	2.02	0.41
1:A:124:VAL:HG11	1:D:98:GLU:HB2	2.02	0.41
1:B:98:GLU:OE1	1:C:173:LYS:NZ	2.34	0.41
1:F:101:THR:HG23	1:F:104:HIS:H	1.85	0.41
1:E:68:TRP:CD1	1:E:118:LEU:HB3	2.54	0.41
1:A:70:ASN:HA	1:A:73:LYS:CD	2.42	0.41
1:E:220:LYS:HE2	1:E:220:LYS:HB2	1.84	0.41
1:D:162:LEU:O	1:D:166:VAL:HG23	2.20	0.41
1:E:145:GLY:HA2	1:E:153:ASN:ND2	2.35	0.41
1:F:221:MET:O	1:F:225:VAL:HG12	2.20	0.41
1:A:91:ILE:HD12	1:E:43:GLU:HG2	2.03	0.41
1:A:92:VAL:HG13	1:A:152:TYR:CG	2.55	0.41
1:D:155:ALA:O	1:D:159:VAL:HG23	2.19	0.41
1:E:140:ILE:O	1:E:144:ILE:HG13	2.21	0.41
1:F:8:VAL:HB	1:F:81:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:HB2	1:D:147:PRO:HB3	2.02	0.41
1:B:197:ASP:N	2:B:308:HOH:O	2.53	0.41
1:C:27:LEU:HD11	1:C:51:LEU:HD13	2.03	0.41
1:C:127:MET:HE2	1:C:127:MET:HB2	1.64	0.41
1:C:230:ALA:HB1	1:C:233:SER:HB2	2.02	0.41
1:D:36:PHE:CZ	1:D:57:PHE:HB2	2.56	0.41
1:E:183:TYR:CD1	1:E:183:TYR:N	2.89	0.41
1:F:143:MET:HA	1:F:160:ARG:NH2	2.35	0.41
1:B:93:THR:HG22	1:B:104:HIS:CE1	2.56	0.41
1:F:138:SER:N	1:F:182:ILE:O	2.54	0.41
1:D:85:ILE:HD12	1:D:123:GLY:HA2	2.04	0.40
1:E:12:THR:HB	1:E:89:ALA:HB2	2.04	0.40
1:E:142:GLY:HA3	1:E:156:LYS:HB3	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	244/247 (99%)	235 (96%)	9 (4%)	0	100	100
1	B	242/247 (98%)	235 (97%)	7 (3%)	0	100	100
1	C	235/247 (95%)	228 (97%)	7 (3%)	0	100	100
1	D	228/247 (92%)	221 (97%)	7 (3%)	0	100	100
1	E	232/247 (94%)	227 (98%)	5 (2%)	0	100	100
1	F	226/247 (92%)	224 (99%)	2 (1%)	0	100	100
All	All	1407/1482 (95%)	1370 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	180/190 (95%)	170 (94%)	10 (6%)	19	22
1	B	186/190 (98%)	183 (98%)	3 (2%)	55	70
1	C	167/190 (88%)	156 (93%)	11 (7%)	15	17
1	D	174/190 (92%)	159 (91%)	15 (9%)	10	9
1	E	175/190 (92%)	134 (77%)	41 (23%)	1	0
1	F	156/190 (82%)	110 (70%)	46 (30%)	0	0
All	All	1038/1140 (91%)	912 (88%)	126 (12%)	5	4

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	43	GLU
1	A	53	GLU
1	A	92	VAL
1	A	101	THR
1	A	175	TYR
1	A	191	LEU
1	A	192	ILE
1	A	206	LYS
1	A	220	LYS
1	B	42	ASP
1	B	138	SER
1	B	139	SER
1	C	73	LYS
1	C	127	MET
1	C	128	LYS
1	C	129	GLU
1	C	130	HIS
1	C	175	TYR
1	C	189	THR
1	C	199	THR
1	C	204	ILE

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Mol	Chain	Res	Type
1	C	211	ARG
1	C	228	ASP
1	D	15	THR
1	D	20	LEU
1	D	37	THR
1	D	42	ASP
1	D	55	SER
1	D	63	SER
1	D	137	ILE
1	D	175	TYR
1	D	191	LEU
1	D	192	ILE
1	D	193	ASP
1	D	205	ASP
1	D	206	LYS
1	D	209	MET
1	D	212	LEU
1	E	16	LYS
1	E	18	ILE
1	E	25	LEU
1	E	28	LYS
1	E	29	GLU
1	E	37	THR
1	E	41	GLU
1	E	45	LYS
1	E	48	GLN
1	E	50	ARG
1	E	53	GLU
1	E	56	LEU
1	E	60	GLN
1	E	69	GLN
1	E	78	LYS
1	E	85	ILE
1	E	91	ILE
1	E	93	THR
1	E	102	LEU
1	E	103	ASP
1	E	112	ASP
1	E	130	HIS
1	E	143	MET
1	E	144	ILE
1	E	156	LYS

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Mol	Chain	Res	Type
1	E	162	LEU
1	E	173	LYS
1	E	182	ILE
1	E	189	THR
1	E	201	GLN
1	E	203	TYR
1	E	204	ILE
1	E	205	ASP
1	E	206	LYS
1	E	207	HIS
1	E	211	ARG
1	E	212	LEU
1	E	228	ASP
1	E	231	SER
1	E	240	VAL
1	E	247	GLN
1	F	16	LYS
1	F	20	LEU
1	F	25	LEU
1	F	28	LYS
1	F	29	GLU
1	F	32	LYS
1	F	34	VAL
1	F	37	THR
1	F	40	HIS
1	F	41	GLU
1	F	56	LEU
1	F	58	ILE
1	F	59	THR
1	F	60	GLN
1	F	62	VAL
1	F	64	LYS
1	F	70	ASN
1	F	75	VAL
1	F	78	LYS
1	F	79	PHE
1	F	85	ILE
1	F	91	ILE
1	F	92	VAL
1	F	93	THR
1	F	98	GLU
1	F	102	LEU

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Mol	Chain	Res	Type
1	F	121	LYS
1	F	128	LYS
1	F	129	GLU
1	F	143	MET
1	F	144	ILE
1	F	149	VAL
1	F	160	ARG
1	F	161	LEU
1	F	162	LEU
1	F	164	LYS
1	F	173	LYS
1	F	177	ILE
1	F	189	THR
1	F	206	LYS
1	F	218	VAL
1	F	225	VAL
1	F	228	ASP
1	F	233	SER
1	F	239	VAL
1	F	240	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	B	130	HIS
1	B	201	GLN
1	C	6	ASN
1	E	69	GLN
1	E	87	ASN
1	E	106	ASN
1	E	153	ASN
1	F	48	GLN
1	F	70	ASN
1	F	87	ASN
1	F	88	ASN
1	F	153	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	246/247 (99%)	0.43	12 (4%) 35 31	34, 48, 95, 125	0
1	B	244/247 (98%)	0.46	13 (5%) 32 29	35, 51, 73, 92	0
1	C	239/247 (96%)	0.84	19 (7%) 18 16	39, 59, 94, 132	0
1	D	234/247 (94%)	0.86	21 (8%) 15 13	41, 61, 109, 134	0
1	E	236/247 (95%)	1.15	33 (13%) 6 5	42, 59, 89, 121	0
1	F	230/247 (93%)	1.62	65 (28%) 1 1	44, 72, 105, 120	0
All	All	1429/1482 (96%)	0.89	163 (11%) 10 8	34, 58, 96, 134	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	14	GLY	5.4
1	C	197	ASP	4.7
1	F	175	TYR	4.5
1	F	184	PRO	4.4
1	D	191	LEU	4.3
1	A	203	TYR	4.3
1	F	142	GLY	4.3
1	F	176	ALA	4.0
1	E	79	PHE	3.9
1	F	39	ARG	3.9
1	E	142	GLY	3.8
1	F	132	GLY	3.7
1	C	207	HIS	3.6
1	C	53	GLU	3.5
1	D	205	ASP	3.5
1	F	82	LEU	3.4
1	C	188	ALA	3.3
1	D	194	HIS	3.3
1	D	246	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	232	PHE	3.3
1	E	203	TYR	3.3
1	C	190	PRO	3.3
1	F	22	ILE	3.3
1	F	60	GLN	3.3
1	E	143	MET	3.2
1	B	142	GLY	3.2
1	C	186	ALA	3.2
1	F	212	LEU	3.2
1	F	51	LEU	3.2
1	C	187	ILE	3.2
1	D	192	ILE	3.2
1	E	204	ILE	3.2
1	A	202	PHE	3.1
1	F	218	VAL	3.1
1	C	204	ILE	3.1
1	C	203	TYR	3.1
1	A	192	ILE	3.1
1	A	198	ALA	3.1
1	F	10	LEU	3.1
1	E	2	GLY	3.1
1	E	202	PHE	3.1
1	F	205	ASP	3.1
1	E	177	ILE	3.0
1	F	211	ARG	3.0
1	F	4	PHE	3.0
1	C	198	ALA	3.0
1	F	231	SER	3.0
1	F	34	VAL	3.0
1	E	82	LEU	2.9
1	E	207	HIS	2.9
1	D	211	ARG	2.9
1	F	89	ALA	2.9
1	F	143	MET	2.9
1	A	39	ARG	2.9
1	D	198	ALA	2.9
1	F	9	ALA	2.9
1	F	177	ILE	2.9
1	A	186	ALA	2.8
1	E	8	VAL	2.8
1	F	223	VAL	2.8
1	C	130	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	131	GLY	2.8
1	E	175	TYR	2.8
1	F	50	ARG	2.8
1	B	104	HIS	2.8
1	B	144	ILE	2.8
1	F	97	ILE	2.8
1	F	145	GLY	2.8
1	A	197	ASP	2.7
1	E	109	ILE	2.7
1	F	36	PHE	2.7
1	E	56	LEU	2.7
1	F	27	LEU	2.7
1	F	133	ALA	2.6
1	F	240	VAL	2.6
1	F	185	GLY	2.6
1	F	54	ARG	2.6
1	D	147	PRO	2.6
1	F	91	ILE	2.6
1	C	201	GLN	2.6
1	E	210	GLY	2.6
1	B	91	ILE	2.6
1	D	208	PRO	2.6
1	A	191	LEU	2.5
1	D	39	ARG	2.5
1	D	212	LEU	2.5
1	C	205	ASP	2.5
1	E	205	ASP	2.5
1	F	71	ALA	2.5
1	B	207	HIS	2.5
1	D	15	THR	2.5
1	E	139	SER	2.5
1	F	233	SER	2.5
1	F	244	TYR	2.5
1	E	190	PRO	2.5
1	D	189	THR	2.4
1	B	244	TYR	2.4
1	F	188	ALA	2.4
1	B	2	GLY	2.4
1	F	13	GLY	2.4
1	F	166	VAL	2.4
1	F	20	LEU	2.4
1	A	38	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	224	PHE	2.4
1	F	144	ILE	2.4
1	F	44	GLY	2.4
1	D	199	THR	2.4
1	E	91	ILE	2.4
1	F	210	GLY	2.3
1	E	31	ALA	2.3
1	E	240	VAL	2.3
1	E	230	ALA	2.3
1	C	199	THR	2.3
1	D	148	THR	2.3
1	F	92	VAL	2.3
1	A	195	LEU	2.3
1	B	82	LEU	2.3
1	F	120	CYS	2.3
1	D	190	PRO	2.3
1	E	229	GLY	2.3
1	B	143	MET	2.3
1	D	206	LYS	2.3
1	F	109	ILE	2.3
1	C	57	PHE	2.2
1	D	10	LEU	2.2
1	E	25	LEU	2.2
1	F	62	VAL	2.3
1	F	141	GLU	2.2
1	E	225	VAL	2.2
1	F	75	VAL	2.2
1	F	247	GLN	2.2
1	B	35	ALA	2.2
1	B	148	THR	2.2
1	F	162	LEU	2.2
1	D	75	VAL	2.2
1	F	83	ASP	2.2
1	E	81	GLN	2.2
1	E	161	LEU	2.2
1	F	56	LEU	2.2
1	C	202	PHE	2.2
1	D	79	PHE	2.2
1	E	120	CYS	2.2
1	C	189	THR	2.2
1	E	62	VAL	2.1
1	E	186	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	140	ILE	2.1
1	F	18	ILE	2.1
1	F	128	LYS	2.1
1	A	194	HIS	2.1
1	F	37	THR	2.1
1	E	168	LEU	2.1
1	E	94	PRO	2.1
1	F	8	VAL	2.1
1	F	113	LEU	2.1
1	B	204	ILE	2.1
1	F	16	LYS	2.0
1	D	91	ILE	2.0
1	F	47	VAL	2.0
1	F	80	GLY	2.0
1	F	79	PHE	2.0
1	A	199	THR	2.0
1	C	55	SER	2.0
1	F	40	HIS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.