



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:23 AM UTC

PDB ID : 1JQB / pdb_00001jqb
Title : Alcohol Dehydrogenase from Clostridium Beijerinckii: Crystal Structure of Mutant with Enhanced Thermal Stability
Authors : Levin, I.; Frolov, F.; Bogin, O.; Peretz, M.; Hacham, Y.; Burstein, Y.
Deposited on : 2001-08-05
Resolution : 1.97 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

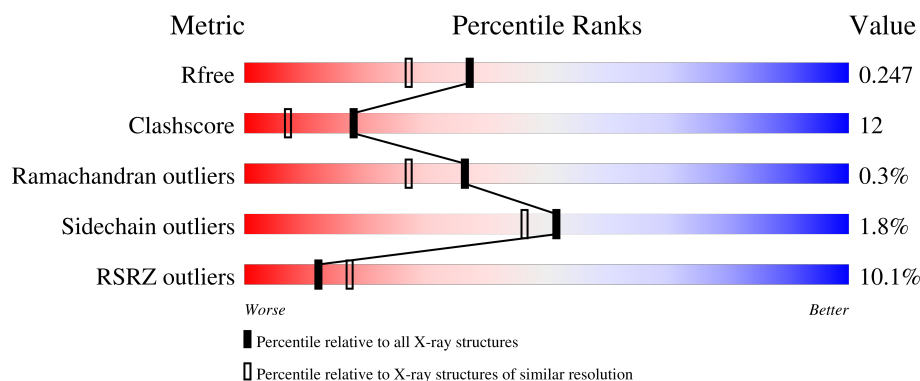
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	351	4% 75% 23% .
1	B	351	11% 75% 23% .
1	C	351	18% 75% 24% .
1	D	351	7% 75% 23% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11004 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 NADP-dependent Alcohol Dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	0	0
			2647	1679	463	483	22			
1	B	351	Total	C	N	O	S	0	0	0
			2647	1679	463	483	22			
1	C	351	Total	C	N	O	S	0	0	0
			2647	1679	463	483	22			
1	D	351	Total	C	N	O	S	0	0	0
			2648	1679	463	484	22			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1154	THR	SER	conflict	UNP P25984
A	1165	GLU	GLN	engineered mutation	UNP P25984
A	1224	GLU	VAL	engineered mutation	UNP P25984
A	1234	LYS	GLU	conflict	UNP P25984
A	1254	LYS	SER	engineered mutation	UNP P25984
A	1304	ARG	MET	engineered mutation	UNP P25984
B	2154	THR	SER	conflict	UNP P25984
B	2165	GLU	GLN	engineered mutation	UNP P25984
B	2224	GLU	VAL	engineered mutation	UNP P25984
B	2234	LYS	GLU	conflict	UNP P25984
B	2254	LYS	SER	engineered mutation	UNP P25984
B	2304	ARG	MET	engineered mutation	UNP P25984
C	3154	THR	SER	conflict	UNP P25984
C	3165	GLU	GLN	engineered mutation	UNP P25984
C	3224	GLU	VAL	engineered mutation	UNP P25984
C	3234	LYS	GLU	conflict	UNP P25984
C	3254	LYS	SER	engineered mutation	UNP P25984
C	3304	ARG	MET	engineered mutation	UNP P25984
D	4154	THR	SER	conflict	UNP P25984
D	4165	GLU	GLN	engineered mutation	UNP P25984
D	4224	GLU	VAL	engineered mutation	UNP P25984

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Chain	Residue	Modelled	Actual	Comment	Reference
D	4234	LYS	GLU	conflict	UNP P25984
D	4254	LYS	SER	engineered mutation	UNP P25984
D	4304	ARG	MET	engineered mutation	UNP P25984

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

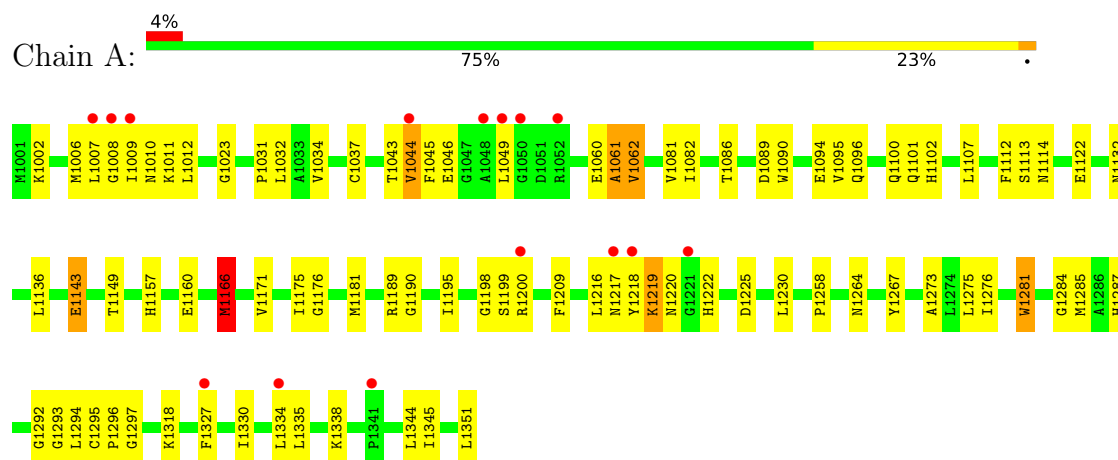
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total	O	0	0
			109	109		
3	B	110	Total	O	0	0
			110	110		
3	C	86	Total	O	0	0
			86	86		
3	D	106	Total	O	0	0
			106	106		

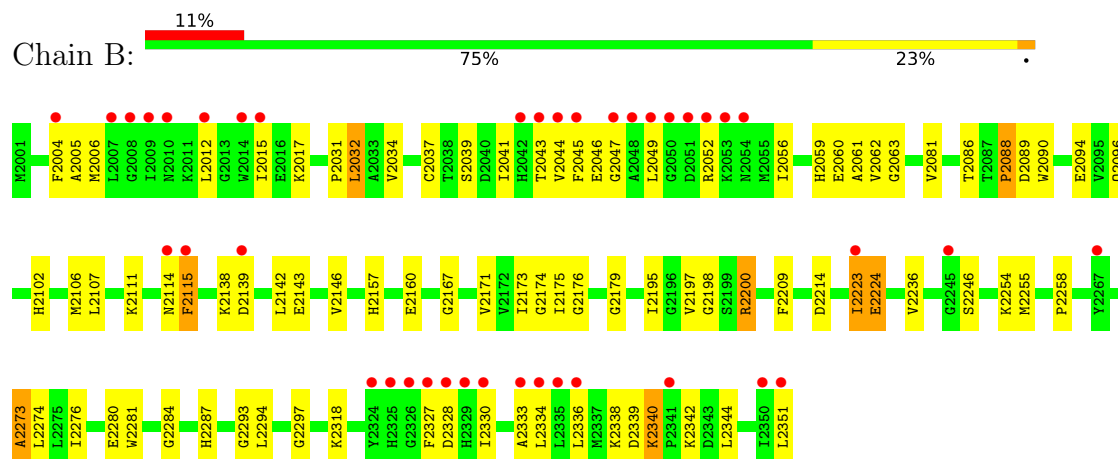
3 Residue-property plots

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.

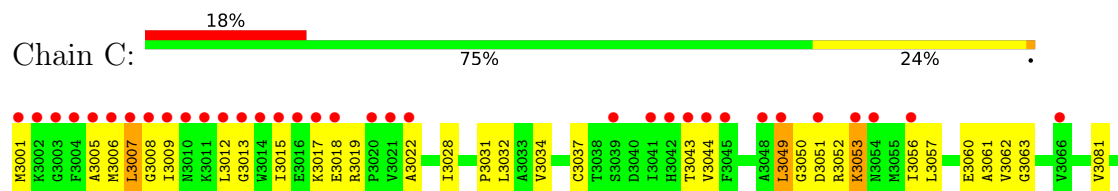
• Molecule 1: NADP-dependent Alcohol Dehydrogenase

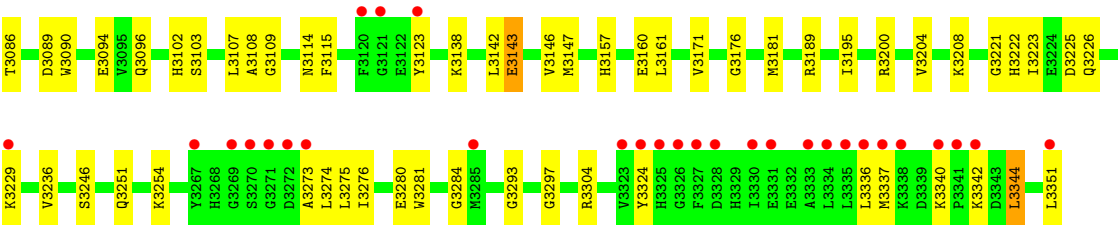


• Molecule 1: NADP-dependent Alcohol Dehydrogenase

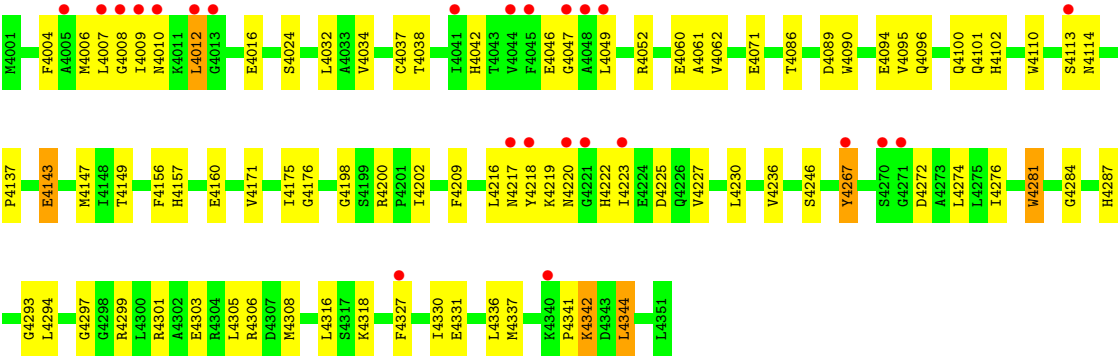
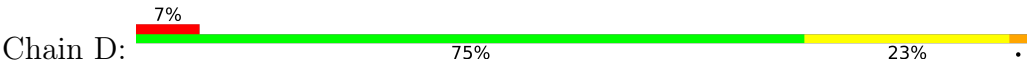


• Molecule 1: NADP-dependent Alcohol Dehydrogenase





● Molecule 1: NADP-dependent Alcohol Dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.70Å 147.80Å 125.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.01 – 1.97 20.01 – 1.97	Depositor EDS
% Data completeness (in resolution range)	97.9 (20.01-1.97) 97.9 (20.01-1.97)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.97Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.247 0.218 , 0.247	Depositor DCC
R_{free} test set	11159 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11004	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	1/2696 (0.0%)	0.95	16/3635 (0.4%)
1	B	0.39	0/2696	0.93	10/3635 (0.3%)
1	C	0.37	0/2696	0.91	6/3635 (0.2%)
1	D	0.37	0/2697	0.94	10/3635 (0.3%)
All	All	0.38	1/10785 (0.0%)	0.93	42/14540 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1166	MET	SD-CE	-6.49	1.63	1.79

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4032	LEU	N-CA-C	-8.00	104.04	113.88
1	D	4114	ASN	N-CA-C	-7.68	101.12	111.96
1	C	3114	ASN	N-CA-C	-7.04	102.49	112.13
1	C	3176	GLY	N-CA-C	-7.04	101.26	112.66
1	B	2176	GLY	N-CA-C	-7.03	101.13	112.31
1	D	4176	GLY	N-CA-C	-6.25	102.37	112.31
1	B	2081	VAL	N-CA-C	6.12	118.72	108.81
1	A	1089	ASP	N-CA-C	-6.05	97.85	108.20
1	A	1149	THR	N-CA-C	6.04	118.66	111.71
1	A	1176	GLY	N-CA-C	-6.04	102.88	112.66
1	D	4062	VAL	N-CA-C	-5.97	99.57	108.46
1	C	3089	ASP	N-CA-C	-5.90	98.11	108.20
1	A	1281	TRP	N-CA-C	-5.80	106.44	112.93
1	B	2032	LEU	N-CA-C	-5.79	106.75	113.88
1	A	1132	ASN	N-CA-C	5.64	119.74	112.41
1	D	4344	LEU	N-CA-C	5.59	118.02	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4281	TRP	N-CA-C	-5.58	106.36	112.72
1	B	2088	PRO	N-CA-C	5.54	119.38	111.13
1	A	1032	LEU	N-CA-C	-5.54	106.66	113.41
1	A	1293	GLY	N-CA-C	5.49	119.30	110.90
1	C	3081	VAL	N-CA-C	5.47	117.98	108.95
1	B	2200	ARG	CA-C-N	5.44	125.52	119.32
1	B	2200	ARG	C-N-CA	5.44	125.52	119.32
1	B	2089	ASP	N-CA-C	-5.43	100.32	108.96
1	C	3109	GLY	N-CA-C	-5.43	107.59	114.16
1	A	1258	PRO	N-CA-C	-5.40	102.72	111.14
1	D	4342	LYS	N-CA-C	5.39	117.16	111.28
1	B	2258	PRO	N-CA-C	-5.36	102.77	111.14
1	A	1200	ARG	CA-C-N	5.32	126.49	119.84
1	A	1200	ARG	C-N-CA	5.32	126.49	119.84
1	B	2273	ALA	N-CA-C	5.31	116.35	108.60
1	D	4149	THR	N-CA-C	5.30	118.53	111.75
1	D	4089	ASP	N-CA-C	-5.26	97.96	107.75
1	A	1062	VAL	N-CA-C	-5.26	100.90	108.48
1	A	1023	GLY	N-CA-C	-5.20	104.24	112.66
1	A	1114	ASN	N-CA-C	-5.16	104.68	111.96
1	A	1044	VAL	N-CA-C	5.15	115.43	110.74
1	A	1061	ALA	N-CA-C	5.14	116.33	108.42
1	D	4293	GLY	N-CA-C	5.11	119.53	110.80
1	C	3062	VAL	N-CA-C	-5.09	100.80	108.12
1	A	1082	ILE	N-CA-C	-5.04	101.16	108.36
1	B	2062	VAL	N-CA-C	-5.04	100.65	108.86

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	2647	0	2685	71	0
1	B	2647	0	2685	74	0
1	C	2647	0	2685	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2648	0	2685	62	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	109	0	0	0	0
3	B	110	0	0	0	0
3	C	86	0	0	5	0
3	D	106	0	0	2	0
All	All	11004	0	10740	261	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (261) 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:2102:HIS:HD2	1:B:2107:LEU:H	1.08	1.02
1:A:1102:HIS:HD2	1:A:1107:LEU:H	1.03	0.94
1:A:1006:MET:HE1	1:A:1043:THR:HG22	1.51	0.92
1:B:2200:ARG:HD2	1:B:2342:LYS:HD3	1.49	0.92
1:B:2336:LEU:HD13	1:B:2344:LEU:HD22	1.54	0.89
1:C:3102:HIS:HD2	1:C:3107:LEU:H	1.19	0.87
1:A:1006:MET:HE2	1:A:1044:VAL:HG22	1.60	0.82
1:D:4006:MET:HE3	1:D:4052:ARG:HB2	1.61	0.82
1:B:2351:LEU:HD23	1:B:2351:LEU:H	1.46	0.80
1:C:3254:LYS:HG2	1:C:3280:GLU:HG2	1.63	0.79
1:C:3007:LEU:HD23	1:C:3007:LEU:H	1.49	0.77
1:A:1217:ASN:HD21	1:A:1219:LYS:HB2	1.50	0.76
1:C:3037:CYS:HB2	1:C:3060:GLU:OE2	1.85	0.76
1:C:3008:GLY:N	3:C:297:HOH:O	2.19	0.74
1:D:4042:HIS:O	1:D:4046:GLU:HB2	1.87	0.74
1:C:3007:LEU:HD21	1:C:3013:GLY:N	2.03	0.74
1:C:3053:LYS:HE3	1:C:3053:LYS:HA	1.70	0.74
1:A:1102:HIS:CD2	1:A:1107:LEU:H	1.96	0.74
1:C:3032:LEU:HG	1:C:3063:GLY:HA2	1.70	0.73
1:C:3053:LYS:HA	3:C:297:HOH:O	1.88	0.73
1:B:2254:LYS:HG2	1:B:2280:GLU:HG2	1.70	0.73
1:C:3006:MET:HB2	1:C:3057:LEU:HD21	1.71	0.73
1:B:2012:LEU:HD21	1:B:2044:VAL:HG21	1.70	0.72
1:C:3007:LEU:HD21	1:C:3012:LEU:C	2.16	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4200:ARG:HH11	1:D:4200:ARG:HB2	1.57	0.70
1:B:2043:THR:HG23	1:B:2049:LEU:HB3	1.72	0.70
1:B:2049:LEU:HD21	1:B:2114:ASN:HA	1.72	0.70
1:A:1216:LEU:HD21	1:A:1230:LEU:HD11	1.73	0.69
1:C:3337:MET:CE	1:C:3344:LEU:HD21	2.22	0.68
1:C:3102:HIS:CD2	1:C:3107:LEU:H	2.07	0.68
1:C:3053:LYS:HE3	3:C:297:HOH:O	1.92	0.67
1:A:1037:CYS:HB2	1:A:1060:GLU:OE2	1.94	0.67
1:A:1007:LEU:HB2	1:A:1011:LYS:HB3	1.76	0.67
1:A:1102:HIS:HE1	1:B:2287:HIS:ND1	1.93	0.67
1:D:4037:CYS:HB2	1:D:4060:GLU:OE2	1.96	0.66
1:B:2111:LYS:HG2	1:B:2115:PHE:CZ	2.31	0.66
1:B:2336:LEU:CD1	1:B:2344:LEU:HD22	2.24	0.65
1:B:2102:HIS:CD2	1:B:2107:LEU:H	2.00	0.64
1:A:1006:MET:HE2	1:A:1044:VAL:CG2	2.28	0.64
1:C:3246:SER:HB2	1:C:3274:LEU:HG	1.80	0.64
1:C:3324:TYR:OH	1:C:3336:LEU:HD11	1.97	0.64
1:B:2034:VAL:HG12	1:B:2061:ALA:HB2	1.80	0.64
1:D:4200:ARG:HD2	1:D:4342:LYS:HA	1.80	0.63
1:B:2209:PHE:CE2	1:B:2318:LYS:HG3	2.33	0.63
1:B:2041:ILE:HD11	1:B:2334:LEU:O	1.98	0.62
1:A:1112:PHE:O	1:A:1113:SER:HB3	1.97	0.62
1:C:3007:LEU:HD23	1:C:3007:LEU:N	2.15	0.62
1:C:3181:MET:HE2	1:C:3181:MET:HA	1.81	0.61
1:C:3015:ILE:HD11	1:C:3017:LYS:HD2	1.83	0.61
1:C:3281:TRP:CE3	1:C:3284:GLY:HA2	2.36	0.60
1:C:3017:LYS:NZ	1:C:3017:LYS:HB3	2.16	0.60
1:C:3043:THR:HB	1:C:3049:LEU:HD13	1.82	0.60
1:C:3225:ASP:O	1:C:3229:LYS:HG3	2.02	0.60
1:A:1101:GLN:HB3	1:A:1294:LEU:HD23	1.84	0.59
1:B:2037:CYS:HB2	1:B:2060:GLU:OE2	2.02	0.59
1:D:4009:ILE:O	1:D:4010:ASN:HB2	2.03	0.59
1:C:3337:MET:HE1	1:C:3344:LEU:HD21	1.82	0.59
1:A:1166:MET:CE	1:D:4308:MET:HE1	2.33	0.58
1:A:1166:MET:HE3	1:A:1166:MET:HA	1.84	0.58
1:C:3157:HIS:HA	1:C:3160:GLU:OE1	2.02	0.58
1:D:4110:TRP:HZ2	3:D:99:HOH:O	1.85	0.58
1:D:4113:SER:HB3	3:D:99:HOH:O	2.03	0.58
1:D:4008:GLY:HA2	1:D:4052:ARG:O	2.04	0.58
1:D:4217:ASN:OD1	1:D:4219:LYS:HB2	2.03	0.58
1:D:4049:LEU:HG	1:D:4267:TYR:OH	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4101:GLN:HB3	1:D:4294:LEU:HD23	1.86	0.57
1:B:2045:PHE:CE2	1:B:2338:LYS:HD3	2.39	0.57
1:D:4157:HIS:HA	1:D:4160:GLU:OE1	2.04	0.57
1:B:2086:THR:HB	1:B:2297:GLY:HA3	1.87	0.56
1:D:4171:VAL:HG23	1:D:4236:VAL:HG11	1.86	0.56
1:D:4009:ILE:HD12	1:D:4047:GLY:HA3	1.87	0.56
1:D:4219:LYS:C	1:D:4220:ASN:HD22	2.13	0.56
1:D:4341:PRO:HD2	1:D:4344:LEU:HD23	1.87	0.56
1:C:3204:VAL:HG12	1:C:3208:LYS:HE3	1.86	0.56
1:A:1209:PHE:CE2	1:A:1318:LYS:HG3	2.40	0.56
1:C:3102:HIS:HE1	1:D:4287:HIS:ND1	2.03	0.56
1:D:4200:ARG:HB2	1:D:4200:ARG:NH1	2.21	0.56
1:C:3006:MET:HE2	1:C:3052:ARG:HB2	1.87	0.55
1:C:3006:MET:CE	1:C:3052:ARG:HB2	2.36	0.55
1:D:4216:LEU:HD21	1:D:4230:LEU:HD11	1.88	0.55
1:D:4012:LEU:HD23	1:D:4012:LEU:N	2.22	0.55
1:C:3049:LEU:H	1:C:3049:LEU:CD2	2.20	0.55
1:D:4281:TRP:CE3	1:D:4284:GLY:HA2	2.42	0.54
1:A:1086:THR:HB	1:A:1297:GLY:HA3	1.89	0.54
1:B:2015:ILE:HD11	1:B:2017:LYS:HD2	1.88	0.54
1:C:3009:ILE:HD11	1:C:3051:ASP:HA	1.90	0.54
1:A:1287:HIS:ND1	1:B:2102:HIS:HE1	2.05	0.54
1:A:1034:VAL:HG12	1:A:1061:ALA:HB2	1.88	0.54
1:C:3034:VAL:HG12	1:C:3061:ALA:HB2	1.90	0.54
1:B:2039:SER:OG	1:B:2059:HIS:HE1	1.91	0.53
1:C:3337:MET:HE2	1:C:3344:LEU:HD21	1.90	0.53
1:C:3171:VAL:HG22	1:C:3195:ILE:HB	1.91	0.53
1:D:4218:TYR:H	1:D:4218:TYR:HD1	1.56	0.53
1:B:2031:PRO:HG2	1:B:2351:LEU:HD11	1.91	0.53
1:D:4246:SER:HB2	1:D:4274:LEU:HG	1.90	0.53
1:C:3017:LYS:HB3	1:C:3017:LYS:HZ3	1.73	0.52
1:D:4094:GLU:HG2	1:D:4102:HIS:O	2.09	0.52
1:C:3049:LEU:H	1:C:3049:LEU:HD23	1.74	0.52
1:C:3094:GLU:HG2	1:C:3102:HIS:O	2.09	0.52
1:B:2223:ILE:HG23	1:B:2255:MET:CE	2.40	0.52
1:A:1285:MET:HE3	1:B:2294:LEU:HA	1.92	0.52
1:C:3226:GLN:HA	1:C:3229:LYS:HD2	1.91	0.52
1:A:1275:LEU:C	1:A:1275:LEU:HD23	2.35	0.52
1:B:2043:THR:HG23	1:B:2049:LEU:CB	2.39	0.52
1:D:4090:TRP:HA	1:D:4095:VAL:HG21	1.90	0.52
1:A:1031:PRO:O	1:A:1351:LEU:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1334:LEU:C	1:A:1334:LEU:HD23	2.35	0.52
1:C:3275:LEU:N	1:C:3275:LEU:HD12	2.25	0.52
1:B:2138:LYS:HE3	1:B:2139:ASP:OD2	2.10	0.51
1:A:1002:LYS:HG2	1:A:1122:GLU:OE1	2.09	0.51
1:A:1334:LEU:HD23	1:A:1334:LEU:O	2.10	0.51
1:B:2032:LEU:HG	1:B:2063:GLY:HA2	1.92	0.51
1:D:4222:HIS:HB2	1:D:4225:ASP:OD2	2.10	0.51
1:A:1094:GLU:HG2	1:A:1102:HIS:O	2.10	0.51
1:C:3022:ALA:HB2	1:C:3028:ILE:HG12	1.93	0.51
1:A:1222:HIS:HB2	1:A:1225:ASP:OD2	2.11	0.51
1:A:1096:GLN:HG2	1:C:3090:TRP:CZ3	2.46	0.51
1:A:1166:MET:HE1	1:D:4308:MET:HE1	1.92	0.50
1:A:1276:ILE:O	1:B:2273:ALA:HB1	2.12	0.50
1:B:2327:PHE:CD1	1:B:2351:LEU:HD13	2.46	0.50
1:A:1009:ILE:N	1:A:1009:ILE:HD12	2.26	0.50
1:D:4327:PHE:CE1	1:D:4330:ILE:HD12	2.46	0.50
1:B:2096:GLN:HG2	1:D:4090:TRP:CZ3	2.46	0.50
1:D:4301:ARG:O	1:D:4305:LEU:HG	2.12	0.50
1:D:4004:PHE:CZ	1:D:4331:GLU:HG3	2.47	0.49
1:A:1344:LEU:HD12	1:A:1345:ILE:H	1.77	0.49
1:C:3007:LEU:HD11	1:C:3012:LEU:O	2.13	0.49
1:A:1166:MET:HE3	1:A:1190:GLY:HA3	1.93	0.49
1:A:1287:HIS:CE1	1:B:2293:GLY:HA3	2.48	0.49
1:B:2034:VAL:HG12	1:B:2061:ALA:CB	2.42	0.49
1:D:4137:PRO:HD3	1:D:4306:ARG:HD2	1.94	0.49
1:B:2004:PHE:HE2	1:B:2334:LEU:HD23	1.77	0.49
1:A:1062:VAL:HG11	1:A:1136:LEU:HD22	1.94	0.49
1:B:2142:LEU:O	1:B:2146:VAL:HG23	2.13	0.49
1:B:2224:GLU:HG2	1:B:2254:LYS:HB2	1.95	0.48
1:B:2006:MET:CE	1:B:2052:ARG:H	2.26	0.48
1:B:2090:TRP:CZ3	1:D:4096:GLN:HG2	2.49	0.48
1:C:3293:GLY:HA3	1:D:4287:HIS:CE1	2.48	0.48
1:B:2086:THR:HG22	1:B:2088:PRO:HD3	1.94	0.48
1:C:3138:LYS:HE2	3:C:330:HOH:O	2.13	0.48
1:B:2327:PHE:HD1	1:B:2351:LEU:HD13	1.78	0.48
1:D:4267:TYR:CD1	1:D:4267:TYR:C	2.91	0.48
1:A:1143:GLU:CD	1:A:1143:GLU:H	2.20	0.48
1:C:3009:ILE:HD11	1:C:3050:GLY:O	2.13	0.48
1:C:3031:PRO:O	1:C:3351:LEU:HD12	2.13	0.48
1:D:4218:TYR:C	1:D:4219:LYS:HG3	2.38	0.48
1:A:1012:LEU:HD21	1:A:1044:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2096:GLN:HG2	1:D:4090:TRP:CH2	2.49	0.48
1:B:2223:ILE:HG23	1:B:2255:MET:HE1	1.96	0.48
1:B:2041:ILE:HG23	1:B:2045:PHE:HD2	1.78	0.48
1:C:3142:LEU:O	1:C:3146:VAL:HG23	2.13	0.47
1:B:2106:MET:HG2	1:B:2107:LEU:HD12	1.96	0.47
1:C:3007:LEU:H	1:C:3007:LEU:CD2	2.16	0.47
1:D:4086:THR:HB	1:D:4297:GLY:HA3	1.97	0.47
1:A:1009:ILE:HD12	1:A:1009:ILE:H	1.78	0.47
1:A:1175:ILE:HG12	1:A:1198:GLY:HA3	1.96	0.47
1:B:2094:GLU:HG2	1:B:2102:HIS:O	2.15	0.47
1:C:3340:LYS:NZ	1:C:3340:LYS:HB3	2.30	0.47
1:D:4006:MET:CE	1:D:4052:ARG:HB2	2.40	0.47
1:D:4009:ILE:CD1	1:D:4047:GLY:HA3	2.44	0.46
1:A:1006:MET:C	1:A:1008:GLY:H	2.22	0.46
1:B:2006:MET:HE1	1:B:2052:ARG:H	1.81	0.46
1:D:4006:MET:HE3	1:D:4052:ARG:CB	2.40	0.46
1:A:1090:TRP:CH2	1:C:3096:GLN:HG2	2.51	0.46
1:B:2200:ARG:NH2	1:B:2344:LEU:O	2.49	0.46
1:A:1327:PHE:HA	1:A:1351:LEU:HD22	1.98	0.46
1:B:2246:SER:HB2	1:B:2274:LEU:HG	1.98	0.46
1:C:3342:LYS:N	1:C:3342:LYS:HD2	2.30	0.46
1:D:4299:ARG:O	1:D:4303:GLU:HG3	2.15	0.46
1:C:3049:LEU:HD23	1:C:3050:GLY:N	2.31	0.45
1:A:1327:PHE:O	1:A:1330:ILE:HG13	2.16	0.45
1:B:2333:ALA:O	1:B:2336:LEU:HB3	2.17	0.45
1:A:1327:PHE:HD1	1:A:1351:LEU:CD2	2.28	0.45
1:B:2171:VAL:HG23	1:B:2236:VAL:HG11	1.98	0.45
1:B:2173:ILE:HA	1:B:2197:VAL:HB	1.97	0.45
1:C:3086:THR:HB	1:C:3297:GLY:HA3	1.98	0.45
1:D:4223:ILE:O	1:D:4227:VAL:HG23	2.17	0.45
1:A:1219:LYS:O	1:A:1220:ASN:ND2	2.49	0.45
1:C:3001:MET:HE1	1:C:3123:TYR:O	2.17	0.45
1:A:1009:ILE:H	1:A:1009:ILE:CD1	2.30	0.44
1:B:2175:ILE:HG12	1:B:2198:GLY:HA3	1.99	0.44
1:C:3276:ILE:HD11	1:D:4276:ILE:HD11	2.00	0.44
1:A:1218:TYR:C	1:A:1220:ASN:H	2.26	0.44
1:B:2328:ASP:C	1:B:2330:ILE:H	2.26	0.44
1:C:3102:HIS:HD2	1:C:3107:LEU:N	1.99	0.44
1:A:1090:TRP:CZ3	1:C:3096:GLN:HG2	2.53	0.44
1:B:2004:PHE:CZ	1:B:2012:LEU:HB3	2.52	0.44
1:C:3171:VAL:HG23	1:C:3236:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4156:PHE:O	1:D:4160:GLU:HG3	2.17	0.44
1:A:1006:MET:HG2	1:A:1008:GLY:H	1.83	0.44
1:B:2047:GLY:C	1:B:2049:LEU:H	2.25	0.44
1:A:1007:LEU:N	1:A:1007:LEU:HD12	2.33	0.43
1:A:1189:ARG:HA	1:A:1189:ARG:HD2	1.85	0.43
1:B:2086:THR:O	1:B:2297:GLY:HA3	2.17	0.43
1:B:2157:HIS:HA	1:B:2160:GLU:OE1	2.17	0.43
1:A:1090:TRP:HA	1:A:1095:VAL:HG21	1.99	0.43
1:A:1344:LEU:HD12	1:A:1345:ILE:N	2.33	0.43
1:C:3274:LEU:N	1:C:3274:LEU:HD12	2.34	0.43
1:C:3147:MET:HE2	1:C:3147:MET:HA	2.01	0.43
1:D:4209:PHE:CE2	1:D:4318:LYS:HG3	2.54	0.43
1:A:1335:LEU:O	1:A:1338:LYS:HB3	2.19	0.43
1:D:4143:GLU:CD	1:D:4143:GLU:H	2.27	0.43
1:D:4336:LEU:HB3	1:D:4344:LEU:HD22	2.01	0.43
1:A:1007:LEU:HD13	1:A:1012:LEU:C	2.44	0.43
1:C:3143:GLU:CD	1:C:3143:GLU:H	2.26	0.43
1:C:3189:ARG:HD2	1:C:3189:ARG:HA	1.90	0.43
1:A:1009:ILE:HG22	1:A:1010:ASN:ND2	2.34	0.43
1:A:1045:PHE:O	1:A:1046:GLU:HG3	2.19	0.43
1:A:1264:ASN:O	1:A:1292:GLY:HA2	2.19	0.43
1:A:1281:TRP:CE3	1:A:1284:GLY:HA2	2.53	0.43
1:D:4200:ARG:HG2	1:D:4202:ILE:HG22	2.01	0.43
1:B:2015:ILE:CD1	1:B:2017:LYS:HD2	2.48	0.42
1:A:1217:ASN:ND2	1:A:1219:LYS:HB2	2.27	0.42
1:B:2209:PHE:CD2	1:B:2318:LYS:HG3	2.53	0.42
1:D:4341:PRO:HD2	1:D:4344:LEU:CD2	2.48	0.42
1:A:1049:LEU:HG	1:A:1267:TYR:OH	2.19	0.42
1:B:2171:VAL:HG22	1:B:2195:ILE:HB	2.02	0.42
1:B:2090:TRP:CH2	1:D:4096:GLN:HG2	2.55	0.42
1:B:2224:GLU:CD	1:B:2224:GLU:H	2.25	0.42
1:B:2281:TRP:CE3	1:B:2284:GLY:HA2	2.55	0.42
1:C:3221:GLY:O	1:C:3222:HIS:C	2.62	0.42
1:D:4209:PHE:CD2	1:D:4318:LYS:HG3	2.54	0.42
1:B:2005:ALA:HB2	1:B:2056:ILE:HA	2.01	0.42
1:D:4147:MET:HB2	1:D:4316:LEU:HD13	2.02	0.42
1:A:1181:MET:HE2	1:A:1181:MET:HA	2.01	0.42
1:C:3053:LYS:HE3	1:C:3053:LYS:CA	2.47	0.42
1:B:2006:MET:HE2	1:B:2052:ARG:HB2	2.02	0.42
1:B:2200:ARG:HG3	1:B:2200:ARG:HH11	1.85	0.42
1:B:2195:ILE:HG12	1:B:2214:ASP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4034:VAL:HG12	1:D:4061:ALA:HB2	2.01	0.42
1:D:4086:THR:O	1:D:4297:GLY:HA3	2.20	0.42
1:B:2209:PHE:CE1	1:B:2318:LYS:HE2	2.55	0.41
1:C:3018:GLU:O	1:C:3019:ARG:C	2.63	0.41
1:C:3108:ALA:HA	1:C:3115:PHE:HE2	1.84	0.41
1:B:2167:GLY:HA3	1:C:3304:ARG:HB3	2.00	0.41
1:D:4024:SER:OG	1:D:4071:GLU:HG2	2.20	0.41
1:A:1062:VAL:HG13	1:A:1081:VAL:O	2.21	0.41
1:A:1273:ALA:HB1	1:B:2276:ILE:O	2.20	0.41
1:B:2006:MET:HG3	1:B:2044:VAL:HG22	2.02	0.41
1:B:2339:ASP:O	1:B:2340:LYS:C	2.64	0.41
1:A:1295:CYS:HA	1:A:1296:PRO:HD3	1.93	0.41
1:C:3273:ALA:HB1	1:D:4276:ILE:O	2.21	0.41
1:A:1171:VAL:HG22	1:A:1195:ILE:HB	2.03	0.41
1:C:3223:ILE:HD11	1:C:3251:GLN:OE1	2.20	0.41
1:D:4217:ASN:C	1:D:4219:LYS:H	2.29	0.41
1:A:1006:MET:C	1:A:1008:GLY:N	2.79	0.41
1:C:3043:THR:HA	1:C:3049:LEU:HD22	2.02	0.41
1:D:4038:THR:HG23	1:D:4337:MET:HE3	2.03	0.41
1:C:3138:LYS:HA	3:C:384:HOH:O	2.20	0.41
1:A:1199:SER:HB3	1:A:1217:ASN:OD1	2.20	0.41
1:C:3086:THR:O	1:C:3297:GLY:HA3	2.21	0.41
1:A:1102:HIS:CE1	1:B:2287:HIS:ND1	2.82	0.41
1:C:3005:ALA:HB2	1:C:3056:ILE:HA	2.03	0.41
1:C:3005:ALA:CB	1:C:3056:ILE:HA	2.51	0.41
1:D:4175:ILE:HG12	1:D:4198:GLY:HA3	2.02	0.41
1:A:1157:HIS:HA	1:A:1160:GLU:OE1	2.21	0.40
1:B:2174:GLY:O	1:B:2179:GLY:HA3	2.21	0.40
1:C:3094:GLU:HB2	1:C:3103:SER:HA	2.02	0.40
1:A:1276:ILE:HD11	1:B:2276:ILE:HD11	2.03	0.40
1:A:1327:PHE:HD1	1:A:1351:LEU:HD21	1.86	0.40
1:C:3200:ARG:O	1:C:3204:VAL:HG23	2.20	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	349/351 (99%)	330 (95%)	18 (5%)	1 (0%)	36	27
1	B	349/351 (99%)	333 (95%)	14 (4%)	2 (1%)	21	12
1	C	349/351 (99%)	323 (93%)	25 (7%)	1 (0%)	36	27
1	D	349/351 (99%)	329 (94%)	20 (6%)	0	100	100
All	All	1396/1404 (99%)	1315 (94%)	77 (6%)	4 (0%)	36	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2115	PHE
1	A	1219	LYS
1	C	3044	VAL
1	B	2340	LYS

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	279/279 (100%)	276 (99%)	3 (1%)	65	61
1	B	279/279 (100%)	275 (99%)	4 (1%)	59	54
1	C	279/279 (100%)	273 (98%)	6 (2%)	45	38
1	D	279/279 (100%)	272 (98%)	7 (2%)	42	33
All	All	1116/1116 (100%)	1096 (98%)	20 (2%)	51	46

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1100	GLN
1	A	1143	GLU

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Mol	Chain	Res	Type
1	A	1166	MET
1	B	2046	GLU
1	B	2143	GLU
1	B	2223	ILE
1	B	2224	GLU
1	C	3007	LEU
1	C	3049	LEU
1	C	3053	LYS
1	C	3143	GLU
1	C	3161	LEU
1	C	3344	LEU
1	D	4007	LEU
1	D	4012	LEU
1	D	4016	GLU
1	D	4100	GLN
1	D	4143	GLU
1	D	4267	TYR
1	D	4272	ASP

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

Mol	Chain	Res	Type
1	A	1010	ASN
1	A	1102	HIS
1	A	1217	ASN
1	A	1220	ASN
1	A	1251	GLN
1	A	1325	HIS
1	A	1329	HIS
1	B	2010	ASN
1	B	2102	HIS
1	B	2232	ASN
1	B	2312	ASN
1	C	3102	HIS
1	C	3220	ASN
1	C	3232	ASN
1	C	3329	HIS
1	D	4220	ASN
1	D	4232	ASN
1	D	4251	GLN
1	D	4312	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [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	351/351 (100%)	0.25	15 (4%) 40 49	15, 25, 51, 59	0
1	B	351/351 (100%)	0.33	40 (11%) 10 13	12, 23, 58, 70	0
1	C	351/351 (100%)	0.71	63 (17%) 3 4	14, 29, 64, 70	0
1	D	351/351 (100%)	0.33	24 (6%) 23 31	16, 26, 51, 61	0
All	All	1404/1404 (100%)	0.40	142 (10%) 12 17	12, 26, 58, 70	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4008	GLY	6.5
1	C	3013	GLY	5.6
1	C	3049	LEU	5.6
1	D	4218	TYR	5.4
1	C	3015	ILE	5.3
1	B	2049	LEU	5.2
1	B	2330	ILE	5.1
1	C	3327	PHE	5.0
1	C	3004	PHE	4.8
1	C	3009	ILE	4.7
1	A	1008	GLY	4.6
1	D	4009	ILE	4.4
1	C	3003	GLY	4.4
1	D	4049	LEU	4.4
1	C	3014	TRP	4.4
1	C	3008	GLY	4.3
1	C	3006	MET	4.3
1	A	1049	LEU	4.2
1	B	2267	TYR	4.1
1	D	4012	LEU	4.1
1	C	3005	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	4007	LEU	4.0
1	A	1009	ILE	3.9
1	C	3043	THR	3.8
1	C	3267	TYR	3.8
1	C	3021	VAL	3.8
1	B	2012	LEU	3.7
1	A	1048	ALA	3.7
1	A	1218	TYR	3.7
1	B	2333	ALA	3.6
1	C	3336	LEU	3.6
1	C	3044	VAL	3.6
1	B	2048	ALA	3.5
1	B	2007	LEU	3.5
1	C	3012	LEU	3.5
1	B	2324	TYR	3.4
1	C	3054	ASN	3.4
1	C	3053	LYS	3.4
1	C	3340	LYS	3.4
1	C	3334	LEU	3.4
1	C	3002	LYS	3.3
1	C	3042	HIS	3.3
1	D	4220	ASN	3.3
1	B	2004	PHE	3.3
1	B	2327	PHE	3.3
1	C	3328	ASP	3.3
1	C	3331	GLU	3.2
1	B	2326	GLY	3.2
1	C	3333	ALA	3.2
1	B	2335	LEU	3.2
1	B	2334	LEU	3.1
1	B	2042	HIS	3.1
1	D	4270	SER	3.1
1	B	2045	PHE	3.1
1	C	3048	ALA	3.1
1	D	4048	ALA	3.1
1	A	1050	GLY	3.0
1	B	2050	GLY	3.0
1	B	2336	LEU	2.9
1	C	3335	LEU	2.9
1	C	3326	GLY	2.9
1	B	2043	THR	2.9
1	D	4223	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	4221	GLY	2.8
1	C	3016	GLU	2.8
1	C	3337	MET	2.8
1	C	3045	PHE	2.8
1	B	2329	HIS	2.8
1	C	3007	LEU	2.8
1	B	2014	TRP	2.8
1	C	3272	ASP	2.8
1	C	3010	ASN	2.7
1	D	4217	ASN	2.7
1	B	2328	ASP	2.7
1	B	2053	LYS	2.7
1	C	3066	VAL	2.7
1	C	3123	TYR	2.6
1	A	1327	PHE	2.6
1	B	2341	PRO	2.6
1	A	1044	VAL	2.6
1	D	4340	LYS	2.6
1	B	2008	GLY	2.6
1	B	2010	ASN	2.6
1	A	1007	LEU	2.6
1	B	2047	GLY	2.6
1	B	2115	PHE	2.5
1	A	1334	LEU	2.5
1	C	3017	LYS	2.5
1	C	3269	GLY	2.5
1	A	1200	ARG	2.5
1	C	3341	PRO	2.5
1	D	4271	GLY	2.5
1	D	4010	ASN	2.5
1	B	2052	ARG	2.5
1	C	3273	ALA	2.5
1	C	3323	VAL	2.5
1	D	4044	VAL	2.5
1	C	3271	GLY	2.5
1	B	2114	ASN	2.5
1	C	3011	LYS	2.5
1	C	3229	LYS	2.5
1	C	3324	TYR	2.4
1	C	3056	ILE	2.4
1	B	2325	HIS	2.4
1	B	2351	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	3285	MET	2.4
1	C	3120	PHE	2.4
1	A	1217	ASN	2.4
1	C	3121	GLY	2.4
1	C	3325	HIS	2.4
1	D	4267	TYR	2.4
1	B	2009	ILE	2.4
1	B	2223	ILE	2.4
1	D	4045	PHE	2.3
1	A	1341	PRO	2.3
1	D	4047	GLY	2.3
1	C	3022	ALA	2.3
1	C	3330	ILE	2.3
1	C	3351	LEU	2.3
1	A	1221	GLY	2.3
1	C	3041	ILE	2.3
1	D	4013	GLY	2.2
1	B	2044	VAL	2.2
1	C	3018	GLU	2.2
1	B	2015	ILE	2.2
1	B	2051	ASP	2.2
1	C	3039	SER	2.2
1	C	3270	SER	2.2
1	D	4005	ALA	2.2
1	C	3001	MET	2.2
1	C	3051	ASP	2.2
1	D	4113	SER	2.2
1	A	1052	ARG	2.2
1	B	2054	ASN	2.1
1	D	4327	PHE	2.1
1	D	4041	ILE	2.1
1	B	2139	ASP	2.1
1	C	3020	PRO	2.1
1	C	3342	LYS	2.0
1	C	3338	LYS	2.0
1	B	2350	ILE	2.0
1	B	2245	GLY	2.0

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

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

6.3 Carbohydrates [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($\text{\AA}^2$)	Q<0.9
2	ZN	B	2353	1/1	0.94	0.05	41,41,41,41	0
2	ZN	A	1353	1/1	0.97	0.04	35,35,35,35	0
2	ZN	C	3353	1/1	0.97	0.05	41,41,41,41	0
2	ZN	D	4353	1/1	0.98	0.04	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.