



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:51 PM UTC

PDB ID : 1IY9 / pdb_00001iy9
Title : Crystal structure of spermidine synthase
Authors : Tan, A.Y.; Smith, P.C.; Shen, J.; Xiao, R.; Acton, T.; Rost, B.; Montelione, G.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2002-07-26
Resolution : 2.30 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

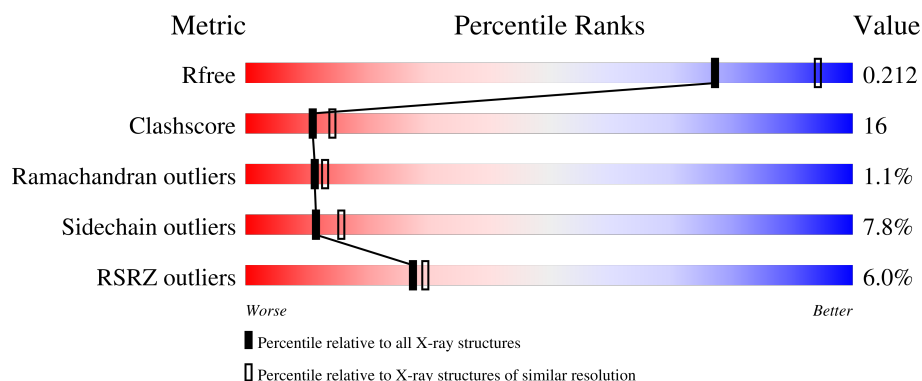
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	275	7% 69% 23% 6%
1	B	275	6% 66% 26% 7%
1	C	275	6% 70% 21% 8%
1	D	275	5% 69% 24% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9099 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 Spermidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2194	1424	347	415	8			
1	B	274	Total	C	N	O	S	0	0	0
			2194	1424	347	415	8			
1	C	274	Total	C	N	O	S	0	0	0
			2194	1424	347	415	8			
1	D	274	Total	C	N	O	S	0	0	0
			2194	1424	347	415	8			

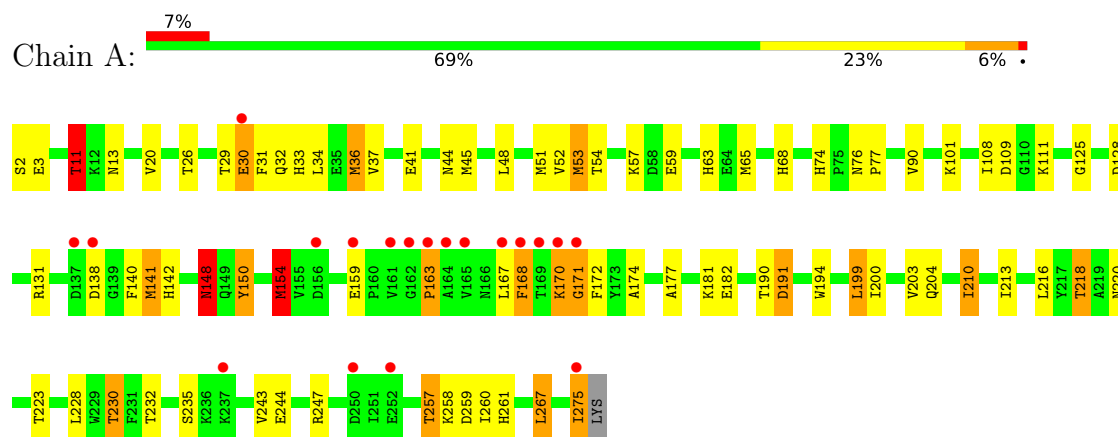
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	92	Total	O	0	0
			92	92		
2	B	79	Total	O	0	0
			79	79		
2	C	66	Total	O	0	0
			66	66		
2	D	86	Total	O	0	0
			86	86		

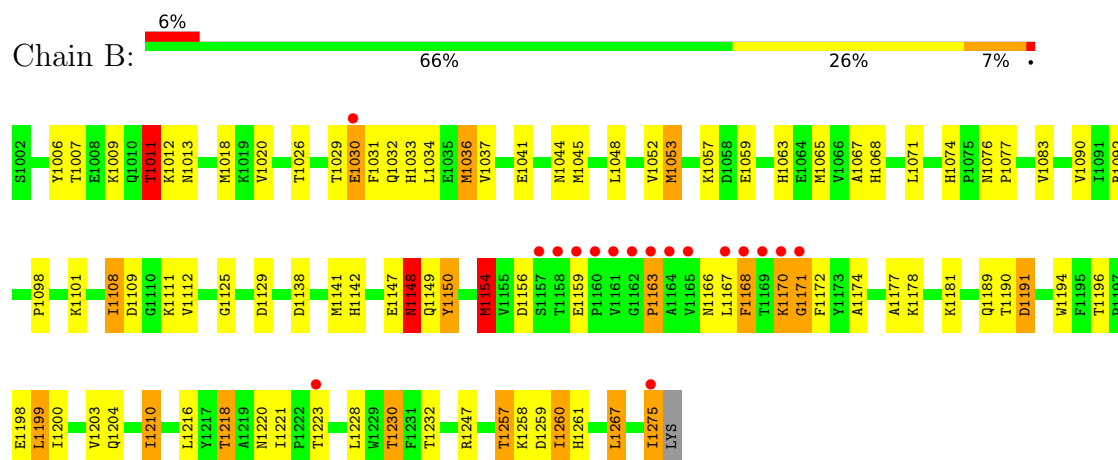
3 Residue-property plots

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.

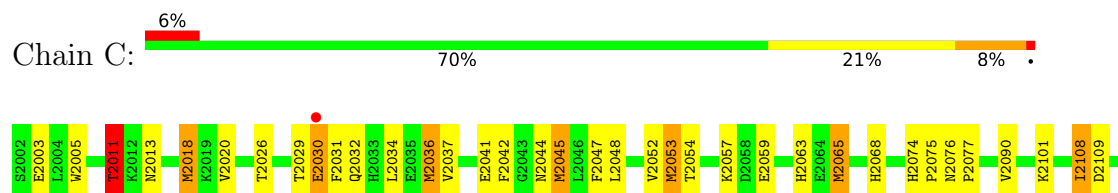
• Molecule 1: Spermidine synthase



• Molecule 1: Spermidine synthase

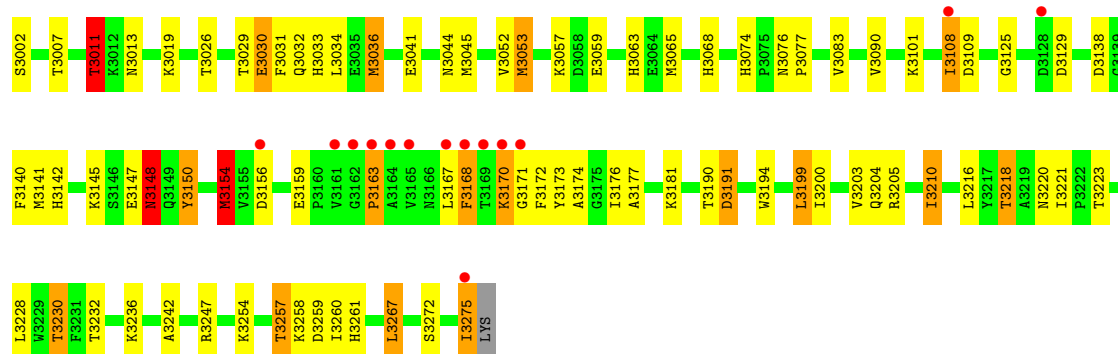


• Molecule 1: Spermidine synthase





● Molecule 1: Spermidine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.10Å 105.80Å 121.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.30 79.87 – 2.30	Depositor EDS
% Data completeness (in resolution range)	78.8 (100.00-2.30) 86.8 (79.87-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 2.29Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.208 , 0.254 (Not available) , 0.212	Depositor DCC
R_{free} test set	2602 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9099	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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	0.84	7/2251 (0.3%)	1.09	9/3055 (0.3%)
1	B	0.81	6/2251 (0.3%)	1.08	14/3055 (0.5%)
1	C	0.82	6/2251 (0.3%)	1.09	16/3055 (0.5%)
1	D	0.81	5/2251 (0.2%)	1.10	15/3055 (0.5%)
All	All	0.82	24/9004 (0.3%)	1.09	54/12220 (0.4%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1036	MET	SD-CE	-10.98	1.52	1.79
1	B	1053	MET	SD-CE	10.92	2.06	1.79
1	D	3036	MET	SD-CE	-10.51	1.53	1.79
1	D	3053	MET	SD-CE	10.43	2.05	1.79
1	C	2036	MET	SD-CE	-10.42	1.53	1.79
1	A	53	MET	SD-CE	10.37	2.05	1.79
1	C	2065	MET	SD-CE	-10.04	1.54	1.79
1	A	36	MET	SD-CE	-9.56	1.55	1.79
1	D	3154	MET	SD-CE	-8.71	1.57	1.79
1	A	65	MET	SD-CE	-8.60	1.58	1.79
1	D	3045	MET	SD-CE	-8.40	1.58	1.79
1	B	1154	MET	SD-CE	-8.18	1.59	1.79
1	B	1065	MET	SD-CE	-8.05	1.59	1.79
1	A	45	MET	SD-CE	-7.60	1.60	1.79
1	C	2053	MET	SD-CE	7.17	1.97	1.79
1	C	2018	MET	SD-CE	-7.12	1.61	1.79
1	B	1045	MET	SD-CE	-7.04	1.61	1.79
1	C	2154	MET	SD-CE	-6.98	1.62	1.79
1	A	141	MET	SD-CE	-6.60	1.63	1.79
1	A	154	MET	SD-CE	-6.56	1.63	1.79
1	B	1018	MET	SD-CE	-6.37	1.63	1.79
1	D	3065	MET	SD-CE	-6.28	1.63	1.79
1	C	2045	MET	SD-CE	-6.13	1.64	1.79
1	A	51	MET	SD-CE	-5.23	1.66	1.79

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2068	HIS	N-CA-C	7.83	120.72	111.71
1	A	68	HIS	N-CA-C	7.80	120.87	111.82
1	B	1068	HIS	N-CA-C	7.62	120.66	111.82
1	D	3068	HIS	N-CA-C	7.50	120.52	111.82
1	D	3168	PHE	N-CA-C	-7.30	100.87	110.43
1	A	168	PHE	N-CA-C	-7.16	101.05	110.43
1	B	1172	PHE	N-CA-C	7.15	119.74	111.02
1	D	3057	LYS	N-CA-C	7.05	119.04	111.36
1	A	172	PHE	N-CA-C	6.97	119.53	111.02
1	C	2168	PHE	N-CA-C	-6.92	101.36	110.43
1	B	1168	PHE	N-CA-C	-6.81	101.50	110.43
1	B	1125	GLY	N-CA-C	6.59	121.72	114.40
1	C	2118	LYS	N-CA-C	6.40	118.34	111.36
1	A	57	LYS	N-CA-C	6.33	118.27	111.36
1	D	3125	GLY	N-CA-C	6.29	121.39	114.40
1	C	2125	GLY	N-CA-C	6.29	121.38	114.40
1	C	2140	PHE	N-CA-C	-6.20	104.60	111.36
1	D	3140	PHE	N-CA-C	-6.13	104.68	111.36
1	C	2057	LYS	N-CA-C	6.09	118.00	111.36
1	D	3221	ILE	CA-C-N	6.09	125.77	119.56
1	D	3221	ILE	C-N-CA	6.09	125.77	119.56
1	A	125	GLY	N-CA-C	6.02	121.08	114.40
1	B	1057	LYS	N-CA-C	5.95	117.85	111.36
1	C	2221	ILE	CA-C-N	5.93	125.61	119.56
1	C	2221	ILE	C-N-CA	5.93	125.61	119.56
1	D	3011	THR	N-CA-C	-5.81	99.91	108.79
1	A	140	PHE	N-CA-C	-5.79	105.05	111.36
1	C	2129	ASP	CA-C-N	5.69	125.54	119.28
1	C	2129	ASP	C-N-CA	5.69	125.54	119.28
1	B	1129	ASP	CA-C-N	5.62	125.46	119.28
1	B	1129	ASP	C-N-CA	5.62	125.46	119.28
1	B	1267	LEU	N-CA-C	5.56	117.08	110.07
1	C	2172	PHE	N-CA-C	5.54	120.45	111.37
1	A	11	THR	N-CA-C	-5.53	100.32	108.79
1	D	3129	ASP	CA-C-N	5.46	125.29	119.28
1	D	3129	ASP	C-N-CA	5.46	125.29	119.28
1	B	1221	ILE	N-CA-C	-5.44	102.76	108.15
1	B	1150	TYR	N-CA-C	5.38	118.17	109.40
1	A	150	TYR	N-CA-C	5.36	118.13	109.40
1	D	3267	LEU	N-CA-C	5.33	116.79	110.07
1	D	3172	PHE	N-CA-C	5.31	120.08	111.37
1	B	1011	THR	N-CA-C	-5.28	100.71	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3108	ILE	CB-CA-C	-5.27	103.73	112.26
1	D	3036	MET	N-CA-C	-5.25	101.14	109.96
1	D	3150	TYR	N-CA-C	5.22	117.90	109.40
1	A	267	LEU	N-CA-C	5.15	117.39	110.29
1	C	2108	ILE	CB-CA-C	-5.14	103.93	112.26
1	B	1108	ILE	CB-CA-C	-5.13	103.95	112.26
1	C	2267	LEU	N-CA-C	5.12	116.52	110.07
1	B	1112	VAL	N-CA-C	-5.11	105.56	110.72
1	C	2042	PHE	N-CA-C	5.11	119.47	112.88
1	C	2150	TYR	N-CA-C	5.10	117.71	109.40
1	C	2011	THR	N-CA-C	-5.07	101.03	108.79
1	B	1189	GLN	N-CA-C	-5.03	103.41	110.50

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	2194	0	2167	75	0
1	B	2194	0	2167	83	0
1	C	2194	0	2167	69	0
1	D	2194	0	2167	75	0
2	A	92	0	0	13	0
2	B	79	0	0	16	0
2	C	66	0	0	9	0
2	D	86	0	0	16	0
All	All	9099	0	8668	286	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 16.

All (286) 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:D:3053:MET:SD	1:D:3053:MET:CE	2.05	1.45
1:B:1053:MET:SD	1:B:1053:MET:CE	2.06	1.42
1:A:53:MET:SD	1:A:53:MET:CE	2.05	1.41
1:B:1190:THR:HG23	1:B:1230:THR:HG22	1.42	1.02
1:A:190:THR:HG23	1:A:230:THR:HG22	1.42	1.00
1:D:3190:THR:HG23	1:D:3230:THR:HG22	1.43	1.00
1:C:2190:THR:HG23	1:C:2230:THR:HG22	1.41	1.00
1:A:11:THR:HG22	1:A:13:ASN:H	1.27	1.00
1:C:2011:THR:HG22	1:C:2013:ASN:H	1.28	0.97
1:D:3011:THR:HG22	1:D:3013:ASN:H	1.26	0.96
1:B:1011:THR:HG22	1:B:1013:ASN:H	1.28	0.95
1:D:3216:LEU:HD11	1:D:3230:THR:HG23	1.50	0.93
1:D:3029:THR:HG22	1:D:3031:PHE:H	1.34	0.93
1:C:2029:THR:HG22	1:C:2031:PHE:H	1.34	0.92
1:A:29:THR:HG22	1:A:31:PHE:H	1.34	0.91
1:C:2037:VAL:HB	2:C:4034:HOH:O	1.70	0.90
1:B:1029:THR:HG22	1:B:1031:PHE:H	1.36	0.90
1:B:1216:LEU:HD11	1:B:1230:THR:HG23	1.53	0.89
1:A:216:LEU:HD11	1:A:230:THR:HG23	1.54	0.88
1:B:1257:THR:HG22	1:B:1259:ASP:H	1.38	0.88
1:C:2216:LEU:HD11	1:C:2230:THR:HG23	1.59	0.85
1:A:257:THR:HG22	1:A:259:ASP:H	1.43	0.83
1:B:1011:THR:HG21	1:C:2041:GLU:OE1	1.80	0.81
1:D:3257:THR:HG22	1:D:3259:ASP:H	1.47	0.80
1:A:190:THR:HG23	1:A:230:THR:CG2	2.13	0.79
1:C:2257:THR:HG22	1:C:2259:ASP:H	1.48	0.79
1:D:3029:THR:HG21	1:D:3109:ASP:OD2	1.82	0.79
1:D:3190:THR:HG23	1:D:3230:THR:CG2	2.13	0.79
1:B:1052:VAL:HG11	1:B:1223:THR:CG2	2.14	0.78
1:C:2190:THR:HG23	1:C:2230:THR:CG2	2.14	0.78
1:D:3191:ASP:O	1:D:3230:THR:HB	1.84	0.78
1:A:191:ASP:O	1:A:230:THR:HB	1.85	0.77
1:D:3052:VAL:HG11	1:D:3223:THR:CG2	2.15	0.77
1:A:128:ASP:HB3	2:A:4189:HOH:O	1.84	0.76
1:B:1177:ALA:HB2	1:B:1210:ILE:HD11	1.66	0.76
1:B:1216:LEU:HD11	1:B:1230:THR:CG2	2.15	0.76
1:B:1190:THR:HG23	1:B:1230:THR:CG2	2.15	0.76
1:A:29:THR:HG21	1:A:109:ASP:OD2	1.85	0.76
1:A:111:LYS:HD3	2:A:4027:HOH:O	1.84	0.76
1:B:1041:GLU:OE1	1:C:2011:THR:HG21	1.86	0.75
1:D:3216:LEU:HD11	1:D:3230:THR:CG2	2.15	0.75
1:C:2191:ASP:O	1:C:2230:THR:HB	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:THR:HG21	1:D:3041:GLU:OE1	1.88	0.74
1:B:1191:ASP:O	1:B:1230:THR:HB	1.87	0.74
1:D:3272:SER:HB2	2:D:4074:HOH:O	1.87	0.74
1:D:3177:ALA:HB2	1:D:3210:ILE:HD11	1.70	0.74
1:A:52:VAL:HG11	1:A:223:THR:CG2	2.17	0.74
1:A:216:LEU:HD11	1:A:230:THR:CG2	2.18	0.74
1:C:2029:THR:HG21	1:C:2109:ASP:OD2	1.87	0.74
1:B:1029:THR:HG21	1:B:1109:ASP:OD2	1.88	0.73
1:C:2052:VAL:HG11	1:C:2223:THR:CG2	2.19	0.73
1:C:2177:ALA:HB2	1:C:2210:ILE:HD11	1.71	0.72
1:C:2216:LEU:HD11	1:C:2230:THR:CG2	2.18	0.72
1:C:2138:ASP:HB3	1:C:2141:MET:HB2	1.71	0.72
2:B:4051:HOH:O	1:C:2257:THR:HG21	1.90	0.72
1:A:36:MET:HE1	1:A:44:ASN:HB3	1.72	0.71
1:D:3170:LYS:HE2	1:D:3170:LYS:HA	1.72	0.71
1:A:177:ALA:HB2	1:A:210:ILE:HD11	1.73	0.70
1:D:3002:SER:HB3	2:D:4018:HOH:O	1.90	0.70
1:A:41:GLU:OE1	1:D:3011:THR:HG21	1.91	0.70
1:B:1052:VAL:HG11	1:B:1223:THR:HG22	1.73	0.70
1:A:170:LYS:HA	1:A:170:LYS:HE2	1.74	0.69
1:C:2190:THR:CG2	1:C:2230:THR:HG22	2.20	0.69
1:D:3036:MET:HE1	1:D:3044:ASN:HB3	1.73	0.69
1:C:2174:ALA:HA	1:C:2210:ILE:HD13	1.75	0.69
1:A:33:HIS:HD2	2:B:4276:HOH:O	1.76	0.68
1:B:1257:THR:HG22	1:B:1259:ASP:N	2.07	0.68
1:D:3052:VAL:HG11	1:D:3223:THR:HG22	1.76	0.68
1:B:1190:THR:CG2	1:B:1230:THR:HG22	2.22	0.67
1:C:2170:LYS:HE2	1:C:2170:LYS:HA	1.74	0.67
1:D:3204:GLN:HG2	1:D:3275:ILE:HB	1.77	0.67
1:B:1170:LYS:HE2	1:B:1170:LYS:HA	1.74	0.67
1:A:54:THR:HG22	2:A:4036:HOH:O	1.95	0.67
1:D:3254:LYS:HE2	2:D:4238:HOH:O	1.95	0.67
1:B:1142:HIS:HD2	2:B:4247:HOH:O	1.77	0.67
1:B:1138:ASP:HB3	1:B:1141:MET:HB2	1.76	0.66
1:C:2148:ASN:HB2	1:C:2181:LYS:HA	1.76	0.66
1:D:3190:THR:CG2	1:D:3230:THR:HG22	2.23	0.66
1:D:3141:MET:SD	1:D:3163:PRO:HB2	2.35	0.66
1:A:174:ALA:HA	1:A:210:ILE:HD13	1.76	0.66
1:A:74:HIS:HD2	1:A:76:ASN:H	1.43	0.66
1:D:3148:ASN:HB2	1:D:3181:LYS:HA	1.78	0.66
1:A:138:ASP:HB3	1:A:141:MET:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1148:ASN:HB2	1:B:1181:LYS:HA	1.77	0.65
1:B:1074:HIS:HD2	1:B:1076:ASN:H	1.45	0.65
1:B:1204:GLN:HG2	1:B:1275:ILE:HB	1.77	0.65
1:B:1036:MET:HE1	1:B:1044:ASN:HB3	1.79	0.65
1:D:3142:HIS:HD2	2:D:4075:HOH:O	1.78	0.64
1:D:3074:HIS:HD2	1:D:3076:ASN:H	1.46	0.64
1:D:3138:ASP:HB3	1:D:3141:MET:HB2	1.79	0.64
1:A:190:THR:CG2	1:A:230:THR:HG22	2.23	0.64
1:D:3052:VAL:HG11	1:D:3223:THR:HG21	1.79	0.64
1:D:3174:ALA:HA	1:D:3210:ILE:HD13	1.79	0.64
1:C:2052:VAL:HG11	1:C:2223:THR:HG22	1.80	0.64
1:A:182:GLU:HG2	2:A:4008:HOH:O	1.96	0.64
1:C:2074:HIS:HD2	1:C:2076:ASN:H	1.45	0.64
1:A:148:ASN:HB2	1:A:181:LYS:HA	1.80	0.63
1:B:1196:THR:HA	2:B:4305:HOH:O	1.97	0.63
1:C:2074:HIS:HB3	1:C:2077:PRO:HG3	1.80	0.63
1:A:257:THR:HG22	1:A:259:ASP:N	2.12	0.63
1:A:52:VAL:HG11	1:A:223:THR:HG21	1.79	0.63
1:A:257:THR:HG21	2:D:4142:HOH:O	1.97	0.63
1:D:3257:THR:HG22	1:D:3259:ASP:N	2.12	0.63
1:A:52:VAL:HG11	1:A:223:THR:HG22	1.80	0.62
1:A:204:GLN:HG2	1:A:275:ILE:HB	1.81	0.62
1:B:1098:PRO:HD2	2:B:4132:HOH:O	1.98	0.62
1:B:1052:VAL:HG11	1:B:1223:THR:HG21	1.81	0.62
1:C:2036:MET:HE1	1:C:2044:ASN:HB3	1.81	0.62
1:B:1174:ALA:HA	1:B:1210:ILE:HD13	1.81	0.61
1:D:3030:GLU:H	1:D:3030:GLU:CD	2.06	0.61
1:C:2052:VAL:HG11	1:C:2223:THR:HG21	1.82	0.61
1:C:2030:GLU:CD	1:C:2030:GLU:H	2.09	0.60
1:B:1141:MET:SD	1:B:1163:PRO:HB2	2.41	0.60
1:D:3074:HIS:HB3	1:D:3077:PRO:HG3	1.83	0.60
1:C:2204:GLN:HG2	1:C:2275:ILE:HB	1.83	0.60
1:D:3053:MET:SD	2:D:4213:HOH:O	2.56	0.60
1:A:29:THR:HG21	1:A:109:ASP:CG	2.27	0.60
1:A:194:TRP:HE1	1:D:3220:ASN:HD21	1.49	0.60
1:C:2258:LYS:O	1:C:2261:HIS:HB3	2.02	0.60
1:D:3218:THR:HG23	1:D:3228:LEU:HD11	1.83	0.60
1:B:1030:GLU:CD	1:B:1030:GLU:H	2.10	0.59
1:B:1220:ASN:HD21	1:C:2194:TRP:HE1	1.49	0.59
1:C:2257:THR:HG22	1:C:2259:ASP:N	2.17	0.59
1:B:1059:GLU:OE1	1:B:1063:HIS:HD2	1.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3029:THR:HG21	1:D:3109:ASP:CG	2.28	0.59
1:C:2029:THR:HG21	1:C:2109:ASP:CG	2.28	0.59
1:A:30:GLU:CD	1:A:30:GLU:H	2.10	0.58
1:B:1177:ALA:HB2	1:B:1210:ILE:CD1	2.33	0.58
1:B:1071:LEU:HD12	2:B:4067:HOH:O	2.04	0.58
1:B:1074:HIS:HB3	1:B:1077:PRO:HG3	1.85	0.58
1:D:3205:ARG:HD3	2:D:4094:HOH:O	2.01	0.58
1:A:74:HIS:HB3	1:A:77:PRO:HG3	1.85	0.58
1:B:1029:THR:HG21	1:B:1109:ASP:CG	2.28	0.58
1:A:247:ARG:HG3	2:A:4177:HOH:O	2.02	0.57
1:A:2:SER:HA	1:B:1006:TYR:OH	2.04	0.57
1:B:1111:LYS:HD3	2:B:4215:HOH:O	2.03	0.57
1:C:2045:MET:HB3	2:C:4034:HOH:O	2.05	0.57
1:C:2011:THR:HG22	1:C:2013:ASN:N	2.11	0.57
1:D:3108:ILE:HG23	1:D:3138:ASP:HA	1.86	0.57
1:A:220:ASN:HD21	1:D:3194:TRP:HE1	1.53	0.56
1:B:1220:ASN:ND2	1:C:2194:TRP:HE1	2.04	0.56
1:D:3247:ARG:O	1:D:3247:ARG:HD3	2.06	0.56
1:B:1149:GLN:HG2	2:B:4234:HOH:O	2.05	0.56
1:B:1108:ILE:HG23	1:B:1138:ASP:HA	1.88	0.56
1:B:1198:GLU:HG2	2:B:4305:HOH:O	2.05	0.56
1:D:3258:LYS:HG2	2:D:4029:HOH:O	2.06	0.56
1:C:2142:HIS:HE1	1:C:2150:TYR:OH	1.89	0.56
1:A:194:TRP:HE1	1:D:3220:ASN:ND2	2.03	0.56
1:C:2108:ILE:HG23	1:C:2138:ASP:HA	1.87	0.55
1:D:3059:GLU:OE1	1:D:3063:HIS:HD2	1.89	0.55
1:C:2218:THR:HG23	1:C:2228:LEU:HD11	1.87	0.55
1:C:2059:GLU:OE1	1:C:2063:HIS:HD2	1.90	0.55
1:B:1011:THR:HG22	1:B:1013:ASN:N	2.11	0.55
1:A:108:ILE:HG23	1:A:138:ASP:HA	1.89	0.55
1:A:131:ARG:HG3	2:A:4244:HOH:O	2.07	0.54
1:C:2141:MET:SD	1:C:2163:PRO:HB2	2.48	0.54
1:A:59:GLU:OE1	1:A:63:HIS:HD2	1.90	0.54
1:A:11:THR:HG22	1:A:13:ASN:N	2.10	0.54
1:B:1218:THR:HG23	1:B:1228:LEU:HD11	1.88	0.54
1:A:142:HIS:HE1	1:A:150:TYR:OH	1.91	0.54
1:B:1247:ARG:O	1:B:1247:ARG:HD3	2.07	0.54
1:A:74:HIS:HE1	2:A:4230:HOH:O	1.90	0.53
1:D:3258:LYS:O	1:D:3261:HIS:HB3	2.07	0.53
1:A:29:THR:HG22	1:A:30:GLU:N	2.23	0.53
1:B:1142:HIS:HE1	1:B:1150:TYR:OH	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1257:THR:HG21	2:C:4033:HOH:O	2.08	0.53
1:B:1258:LYS:HE2	2:B:4212:HOH:O	2.08	0.53
1:B:1011:THR:HG23	2:C:4147:HOH:O	2.07	0.53
1:C:2177:ALA:HB2	1:C:2210:ILE:CD1	2.39	0.53
1:D:3199:LEU:HD22	1:D:3203:VAL:HG23	1.91	0.52
1:C:2247:ARG:O	1:C:2247:ARG:HD3	2.10	0.52
1:A:220:ASN:ND2	1:D:3194:TRP:HE1	2.07	0.52
1:B:1190:THR:HG21	1:B:1232:THR:OG1	2.10	0.52
1:D:3142:HIS:HE1	1:D:3150:TYR:OH	1.93	0.52
1:A:3:GLU:HB2	1:B:1007:THR:O	2.10	0.51
1:C:2054:THR:HG22	2:C:4120:HOH:O	2.10	0.51
1:A:247:ARG:O	1:A:247:ARG:HD3	2.10	0.51
2:C:4254:HOH:O	1:D:3033:HIS:HD2	1.93	0.51
1:A:199:LEU:HD22	1:A:203:VAL:HG23	1.91	0.51
1:C:2223:THR:HG22	1:C:2223:THR:O	2.11	0.51
1:B:1194:TRP:HE1	1:C:2220:ASN:HD21	1.59	0.51
1:C:2047:PHE:HE1	2:C:4034:HOH:O	1.92	0.51
1:D:3223:THR:HG22	1:D:3223:THR:O	2.11	0.51
1:A:29:THR:CG2	1:A:30:GLU:N	2.73	0.51
1:B:1199:LEU:HD22	1:B:1203:VAL:HG23	1.92	0.51
1:B:1200:ILE:O	1:B:1204:GLN:HB2	2.11	0.51
1:D:3242:ALA:HB3	2:D:4068:HOH:O	2.11	0.51
1:A:142:HIS:HD2	2:A:4013:HOH:O	1.93	0.50
1:D:3029:THR:HG22	1:D:3030:GLU:N	2.26	0.50
1:D:3218:THR:CG2	1:D:3228:LEU:HD11	2.41	0.50
1:C:2199:LEU:HD22	1:C:2203:VAL:HG23	1.93	0.50
1:A:218:THR:HG23	1:A:228:LEU:HD11	1.92	0.50
1:C:2029:THR:HG22	1:C:2030:GLU:N	2.26	0.50
1:D:3029:THR:CG2	1:D:3030:GLU:N	2.75	0.49
1:A:29:THR:HB	1:A:32:GLN:O	2.13	0.49
1:C:2029:THR:CG2	1:C:2030:GLU:N	2.76	0.49
1:C:2003:GLU:HB2	1:D:3007:THR:O	2.12	0.49
1:B:1067:ALA:HB1	2:B:4067:HOH:O	2.13	0.49
1:D:3011:THR:HG22	1:D:3013:ASN:N	2.09	0.49
1:D:3177:ALA:HB2	1:D:3210:ILE:CD1	2.38	0.49
1:D:3200:ILE:O	1:D:3204:GLN:HB2	2.14	0.48
1:A:190:THR:HG21	1:A:232:THR:OG1	2.13	0.48
1:A:177:ALA:HB2	1:A:210:ILE:CD1	2.41	0.48
1:C:2190:THR:HG21	1:C:2232:THR:OG1	2.13	0.48
1:A:223:THR:HG22	1:A:223:THR:O	2.13	0.48
1:A:258:LYS:O	1:A:261:HIS:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2029:THR:HB	1:C:2032:GLN:O	2.14	0.48
1:D:3190:THR:HG21	1:D:3232:THR:OG1	2.14	0.48
1:B:1194:TRP:HE1	1:C:2220:ASN:ND2	2.12	0.48
1:D:3029:THR:HB	1:D:3032:GLN:O	2.14	0.48
2:A:4293:HOH:O	1:B:1033:HIS:HD2	1.97	0.48
1:B:1170:LYS:HB3	2:B:4301:HOH:O	2.13	0.48
1:D:3257:THR:HG23	2:D:4029:HOH:O	2.13	0.48
1:B:1029:THR:HG22	1:B:1030:GLU:N	2.29	0.47
1:A:204:GLN:HE21	1:A:275:ILE:HD12	1.79	0.47
1:D:3145:LYS:HB2	2:D:4082:HOH:O	2.15	0.47
1:B:1258:LYS:O	1:B:1261:HIS:HB3	2.14	0.47
1:B:1029:THR:HB	1:B:1032:GLN:O	2.14	0.47
1:C:2074:HIS:HE1	2:C:4107:HOH:O	1.97	0.47
1:D:3168:PHE:HB2	1:D:3174:ALA:HB3	1.97	0.47
1:D:3176:ILE:HB	2:D:4083:HOH:O	2.14	0.47
1:A:244:GLU:HG2	2:A:4146:HOH:O	2.15	0.46
1:D:3019:LYS:HE3	2:D:4113:HOH:O	2.14	0.46
1:B:1223:THR:HG22	1:B:1223:THR:O	2.15	0.46
1:B:1178:LYS:HE3	2:B:4144:HOH:O	2.14	0.46
1:D:3216:LEU:CD1	1:D:3230:THR:HG23	2.35	0.45
1:C:2168:PHE:O	1:C:2171:GLY:N	2.50	0.45
1:B:1029:THR:CG2	1:B:1030:GLU:N	2.78	0.45
1:B:1218:THR:CG2	1:B:1228:LEU:HD11	2.46	0.45
1:A:200:ILE:O	1:A:204:GLN:HB2	2.16	0.45
1:D:3168:PHE:CB	1:D:3174:ALA:HB3	2.46	0.45
1:C:2090:VAL:HG11	1:C:2154:MET:HG3	1.97	0.45
1:C:2168:PHE:HB2	1:C:2174:ALA:HB3	1.99	0.45
1:A:258:LYS:HG2	2:A:4311:HOH:O	2.17	0.45
1:B:1260:ILE:HD13	1:B:1260:ILE:HA	1.83	0.45
1:C:2218:THR:CG2	1:C:2228:LEU:HD11	2.47	0.45
1:D:3173:TYR:HA	2:D:4083:HOH:O	2.16	0.44
1:C:2168:PHE:CB	1:C:2174:ALA:HB3	2.47	0.44
1:B:1020:VAL:HG13	1:B:1037:VAL:HG13	2.00	0.44
1:C:2200:ILE:O	1:C:2204:GLN:HB2	2.18	0.44
1:B:1168:PHE:CB	1:B:1174:ALA:HB3	2.47	0.44
1:C:2020:VAL:HG13	1:C:2037:VAL:HG13	2.00	0.44
1:D:3142:HIS:CD2	2:D:4075:HOH:O	2.62	0.44
1:B:1168:PHE:HB2	1:B:1174:ALA:HB3	1.99	0.44
1:C:2075:PRO:HB3	2:C:4133:HOH:O	2.18	0.43
1:B:1216:LEU:CD1	1:B:1230:THR:HG23	2.36	0.43
1:D:3147:GLU:O	1:D:3148:ASN:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:PHE:CB	1:A:174:ALA:HB3	2.48	0.43
1:A:218:THR:CG2	1:A:228:LEU:HD11	2.49	0.43
1:D:3077:PRO:HD3	1:D:3247:ARG:NH2	2.33	0.43
1:D:3090:VAL:HG11	1:D:3154:MET:HG3	2.01	0.43
1:D:3236:LYS:HG2	2:D:4078:HOH:O	2.18	0.43
1:D:3204:GLN:HE21	1:D:3275:ILE:HD12	1.84	0.42
1:A:168:PHE:HB2	1:A:174:ALA:HB3	2.00	0.42
1:B:1059:GLU:CD	1:B:1092:ARG:HH22	2.27	0.42
1:B:1168:PHE:O	1:B:1171:GLY:N	2.51	0.42
1:A:216:LEU:CD1	1:A:230:THR:HG23	2.39	0.42
1:B:1009:LYS:HD2	1:C:2005:TRP:CH2	2.55	0.42
1:D:3218:THR:HG23	1:D:3228:LEU:CD1	2.49	0.42
1:B:1048:LEU:HD12	1:B:1053:MET:HE3	2.00	0.42
1:B:1142:HIS:CD2	2:B:4247:HOH:O	2.60	0.42
1:A:141:MET:SD	1:A:163:PRO:HB2	2.59	0.42
1:B:1083:VAL:O	1:B:1156:ASP:HB2	2.19	0.42
1:B:1147:GLU:O	1:B:1148:ASN:C	2.62	0.42
1:B:1166:ASN:O	1:B:1171:GLY:HA3	2.19	0.42
1:C:2216:LEU:CD1	1:C:2230:THR:HG23	2.41	0.42
1:A:77:PRO:HD3	1:A:247:ARG:NH2	2.35	0.42
1:A:90:VAL:HG11	1:A:154:MET:HG3	2.02	0.42
1:B:1012:LYS:HG3	2:B:4208:HOH:O	2.19	0.42
1:B:1077:PRO:HD3	1:B:1247:ARG:NH2	2.35	0.42
1:B:1218:THR:HG21	2:B:4052:HOH:O	2.20	0.42
1:D:3083:VAL:O	1:D:3156:ASP:HB2	2.21	0.41
1:A:20:VAL:HG13	1:A:37:VAL:HG13	2.02	0.41
1:A:168:PHE:O	1:A:171:GLY:N	2.52	0.41
1:A:48:LEU:HD12	1:A:53:MET:HE3	2.02	0.41
1:C:2170:LYS:HE2	1:C:2170:LYS:CA	2.48	0.41
1:A:54:THR:CG2	2:A:4036:HOH:O	2.63	0.41
1:C:2018:MET:HE3	1:C:2047:PHE:HZ	1.86	0.41
1:C:2065:MET:HB3	1:C:2065:MET:HE3	1.91	0.41
1:C:2159:GLU:HA	1:C:2160:PRO:HD2	1.96	0.41
1:A:213:ILE:HB	1:A:235:SER:HB3	2.02	0.40
1:A:243:VAL:HB	2:A:4035:HOH:O	2.21	0.40
1:C:2048:LEU:HD12	1:C:2053:MET:HE3	2.03	0.40
1:B:1090:VAL:HG11	1:B:1154:MET:HG3	2.02	0.40
1:B:1247:ARG:HD3	1:B:1247:ARG:C	2.47	0.40
1:C:2204:GLN:HE21	1:C:2275:ILE:HD12	1.87	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	272/275 (99%)	256 (94%)	13 (5%)	3 (1%)	11	13
1	B	272/275 (99%)	255 (94%)	14 (5%)	3 (1%)	11	13
1	C	272/275 (99%)	257 (94%)	12 (4%)	3 (1%)	11	13
1	D	272/275 (99%)	255 (94%)	14 (5%)	3 (1%)	11	13
All	All	1088/1100 (99%)	1023 (94%)	53 (5%)	12 (1%)	11	13

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	GLY
1	B	1171	GLY
1	C	2171	GLY
1	D	3171	GLY
1	A	148	ASN
1	B	1148	ASN
1	C	2148	ASN
1	D	3148	ASN
1	D	3163	PRO
1	A	163	PRO
1	B	1163	PRO
1	C	2163	PRO

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	244/245 (100%)	225 (92%)	19 (8%)	11	16
1	B	244/245 (100%)	225 (92%)	19 (8%)	11	16
1	C	244/245 (100%)	225 (92%)	19 (8%)	11	16
1	D	244/245 (100%)	225 (92%)	19 (8%)	11	16
All	All	976/980 (100%)	900 (92%)	76 (8%)	11	16

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	26	THR
1	A	30	GLU
1	A	34	LEU
1	A	101	LYS
1	A	148	ASN
1	A	154	MET
1	A	159	GLU
1	A	167	LEU
1	A	170	LYS
1	A	191	ASP
1	A	199	LEU
1	A	210	ILE
1	A	218	THR
1	A	230	THR
1	A	257	THR
1	A	260	ILE
1	A	267	LEU
1	A	275	ILE
1	B	1011	THR
1	B	1026	THR
1	B	1030	GLU
1	B	1034	LEU
1	B	1101	LYS
1	B	1148	ASN
1	B	1154	MET
1	B	1159	GLU
1	B	1167	LEU
1	B	1170	LYS
1	B	1191	ASP
1	B	1199	LEU
1	B	1210	ILE
1	B	1218	THR

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Mol	Chain	Res	Type
1	B	1230	THR
1	B	1257	THR
1	B	1260	ILE
1	B	1267	LEU
1	B	1275	ILE
1	C	2011	THR
1	C	2026	THR
1	C	2030	GLU
1	C	2034	LEU
1	C	2101	LYS
1	C	2148	ASN
1	C	2154	MET
1	C	2159	GLU
1	C	2167	LEU
1	C	2170	LYS
1	C	2191	ASP
1	C	2199	LEU
1	C	2210	ILE
1	C	2218	THR
1	C	2230	THR
1	C	2257	THR
1	C	2260	ILE
1	C	2267	LEU
1	C	2275	ILE
1	D	3011	THR
1	D	3026	THR
1	D	3030	GLU
1	D	3034	LEU
1	D	3101	LYS
1	D	3148	ASN
1	D	3154	MET
1	D	3159	GLU
1	D	3167	LEU
1	D	3170	LYS
1	D	3191	ASP
1	D	3199	LEU
1	D	3210	ILE
1	D	3218	THR
1	D	3230	THR
1	D	3257	THR
1	D	3260	ILE
1	D	3267	LEU

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Mol	Chain	Res	Type
1	D	3275	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	33	HIS
1	A	63	HIS
1	A	74	HIS
1	A	135	GLN
1	A	142	HIS
1	A	148	ASN
1	A	166	ASN
1	A	204	GLN
1	A	220	ASN
1	B	1033	HIS
1	B	1063	HIS
1	B	1074	HIS
1	B	1135	GLN
1	B	1142	HIS
1	B	1166	ASN
1	B	1204	GLN
1	B	1220	ASN
1	C	2033	HIS
1	C	2063	HIS
1	C	2074	HIS
1	C	2079	HIS
1	C	2135	GLN
1	C	2142	HIS
1	C	2166	ASN
1	C	2204	GLN
1	C	2220	ASN
1	D	3032	GLN
1	D	3033	HIS
1	D	3063	HIS
1	D	3074	HIS
1	D	3135	GLN
1	D	3142	HIS
1	D	3166	ASN
1	D	3204	GLN
1	D	3220	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](#)

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	274/275 (99%)	0.46	19 (6%) 23 25	19, 31, 57, 101	0
1	B	274/275 (99%)	0.33	17 (6%) 26 28	18, 32, 56, 101	0
1	C	274/275 (99%)	0.36	16 (5%) 29 31	18, 32, 56, 101	0
1	D	274/275 (99%)	0.38	14 (5%) 33 35	19, 32, 56, 100	0
All	All	1096/1100 (99%)	0.38	66 (6%) 27 29	18, 32, 59, 101	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	LYS	9.5
1	A	168	PHE	7.9
1	A	169	THR	7.3
1	C	2169	THR	7.0
1	D	3170	LYS	5.4
1	D	3164	ALA	5.4
1	A	171	GLY	5.3
1	B	1169	THR	5.2
1	A	164	ALA	4.9
1	D	3163	PRO	4.9
1	C	2164	ALA	4.8
1	B	1164	ALA	4.7
1	A	167	LEU	4.6
1	D	3168	PHE	4.5
1	C	2168	PHE	4.5
1	B	1167	LEU	4.4
1	C	2170	LYS	4.4
1	B	1170	LYS	4.0
1	B	1168	PHE	3.9
1	A	163	PRO	3.9
1	D	3167	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	2160	PRO	3.8
1	A	250	ASP	3.7
1	C	2163	PRO	3.7
1	A	165	VAL	3.7
1	C	2167	LEU	3.6
1	A	161	VAL	3.6
1	B	1163	PRO	3.6
1	B	1275	ILE	3.5
1	D	3169	THR	3.3
1	C	2165	VAL	3.3
1	D	3161	VAL	3.2
1	B	1161	VAL	3.2
1	D	3171	GLY	3.1
1	C	2161	VAL	3.1
1	A	162	GLY	3.0
1	D	3156	ASP	3.0
1	A	275	ILE	3.0
1	A	159	GLU	3.0
1	B	1160	PRO	3.0
1	D	3165	VAL	2.9
1	C	2162	GLY	2.8
1	D	3128	ASP	2.7
1	D	3162	GLY	2.7
1	A	156	ASP	2.7
1	B	1030	GLU	2.7
1	B	1165	VAL	2.6
1	D	3275	ILE	2.6
1	C	2156	ASP	2.6
1	A	137	ASP	2.6
1	B	1171	GLY	2.5
1	C	2128	ASP	2.5
1	C	2148	ASN	2.5
1	C	2159	GLU	2.4
1	A	30	GLU	2.4
1	B	1223	THR	2.3
1	A	252	GLU	2.3
1	C	2275	ILE	2.3
1	B	1159	GLU	2.2
1	B	1162	GLY	2.2
1	B	1157	SER	2.2
1	A	138	ASP	2.1
1	C	2030	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1158	THR	2.1
1	A	237	LYS	2.1
1	D	3108	ILE	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.