



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:45 PM UTC

PDB ID : 2AZJ / pdb_00002azj
Title : Crystal structure for the mutant D81C of Sulfolobus solfataricus hexaprenyl pyrophosphate synthase
Authors : Sun, H.Y.; Ko, T.P.; Kuo, C.J.; Guo, R.T.; Chou, C.C.; Liang, P.H.; Wang, A.H.J.
Deposited on : 2005-09-11
Resolution : 2.40 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

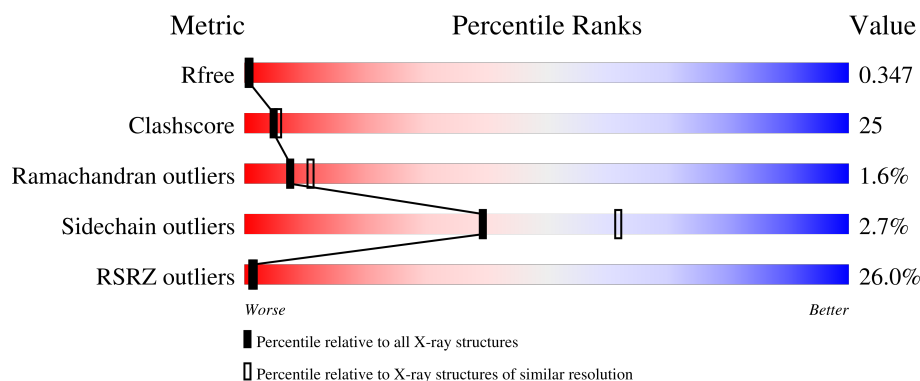
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	289	21% 69% 23% • •
1	B	289	28% 44% 47% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4853 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 Geranylgeranyl pyrophosphate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2237	1443	363	426	5			
1	B	274	Total	C	N	O	S	0	0	0
			2223	1435	361	423	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	GB 15899101
A	-6	ALA	-	expression tag	GB 15899101
A	-5	HIS	-	expression tag	GB 15899101
A	-4	HIS	-	expression tag	GB 15899101
A	-3	HIS	-	expression tag	GB 15899101
A	-2	HIS	-	expression tag	GB 15899101
A	-1	HIS	-	expression tag	GB 15899101
A	0	HIS	-	expression tag	GB 15899101
A	81	CYS	ASP	engineered mutation	GB 15899101
B	-7	MET	-	expression tag	GB 15899101
B	-6	ALA	-	expression tag	GB 15899101
B	-5	HIS	-	expression tag	GB 15899101
B	-4	HIS	-	expression tag	GB 15899101
B	-3	HIS	-	expression tag	GB 15899101
B	-2	HIS	-	expression tag	GB 15899101
B	-1	HIS	-	expression tag	GB 15899101
B	0	HIS	-	expression tag	GB 15899101
B	81	CYS	ASP	engineered mutation	GB 15899101

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	216	Total	O	0	0
			216	216		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	177	Total 177	O 177	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	91.93Å 91.93Å 121.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.37 – 2.40 48.37 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.37-2.40) 97.3 (48.37-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.59 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.317 , 0.347 0.316 , 0.347	Depositor DCC
R_{free} test set	1120 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4853	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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	0.49	0/2279	0.92	5/3077 (0.2%)
1	B	0.37	0/2265	0.85	1/3059 (0.0%)
All	All	0.43	0/4544	0.89	6/6136 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	2	SER	N-CA-C	-10.96	99.92	113.18
1	A	94	LYS	N-CA-C	-6.68	101.71	110.53
1	A	146	ASP	N-CA-C	-5.96	105.97	113.18
1	A	126	ASP	N-CA-C	5.50	117.35	111.36
1	A	124	TYR	N-CA-C	5.25	122.01	114.39
1	B	11	LYS	N-CA-C	-5.16	106.09	112.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	TYR	Sidechain

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	2237	0	2249	75	0
1	B	2223	0	2232	168	2
2	A	216	0	0	7	6
2	B	177	0	0	11	0
All	All	4853	0	4481	227	7

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 25.

All (227) 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:118:ARG:NH2	1:B:130:ASN:HD22	1.50	1.10
1:B:148:TYR:HA	2:B:445:HOH:O	1.59	1.01
1:A:60:ILE:HD12	1:A:60:ILE:H	1.25	0.99
1:B:70:ILE:HD11	1:B:171:LEU:HD12	1.45	0.96
1:A:1:MET:HG3	1:A:2:SER:H	1.32	0.94
1:A:121:GLN:HG3	1:B:130:ASN:HD21	1.37	0.88
1:B:66:GLY:O	1:B:70:ILE:HG12	1.75	0.86
1:B:248:ILE:HG13	1:B:249:SER:H	1.39	0.86
1:A:3:ILE:HD11	1:A:260:GLU:HB3	1.58	0.85
1:A:118:ARG:HH21	1:B:130:ASN:HD22	1.21	0.83
1:A:83:ILE:HD11	1:A:105:VAL:HG21	1.61	0.83
1:B:16:ARG:HH12	1:B:17:LEU:HD23	1.44	0.81
1:B:204:ASP:HA	1:B:208:LYS:HD3	1.60	0.81
1:B:223:TYR:HB3	1:B:229:LEU:HA	1.64	0.78
1:A:54:VAL:CG2	1:A:60:ILE:HG13	2.14	0.77
1:A:43:ARG:O	1:A:47:THR:HG23	1.87	0.73
1:A:111:TYR:O	1:A:114:PRO:HD2	1.88	0.73
1:B:141:VAL:O	1:B:145:ARG:HG2	1.86	0.73
1:A:54:VAL:HG22	1:A:60:ILE:HG13	1.70	0.73
1:A:60:ILE:HD12	1:A:60:ILE:N	2.04	0.71
1:B:248:ILE:HG13	1:B:249:SER:N	2.04	0.71
1:A:136:TRP:HE1	1:B:110:ASN:HD22	1.37	0.71
1:B:197:GLN:NE2	2:B:428:HOH:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LYS:HA	1:B:231:GLU:CD	2.19	0.68
1:B:238:LEU:O	1:B:242:GLN:HG2	1.93	0.67
1:B:247:LEU:HD22	1:B:251:ILE:HD11	1.75	0.67
1:B:16:ARG:NH1	1:B:17:LEU:HD23	2.08	0.67
1:B:207:THR:C	1:B:208:LYS:HD2	2.20	0.67
1:A:207:THR:HG21	1:A:276:ALA:HB1	1.76	0.67
1:A:121:GLN:HG3	1:B:130:ASN:ND2	2.10	0.66
1:B:181:THR:HA	1:B:184:GLN:HG3	1.77	0.66
1:B:20:GLN:HE21	1:B:20:GLN:HA	1.59	0.66
1:A:30:LEU:HD22	1:B:144:LEU:HD13	1.78	0.66
1:A:33:ILE:HG21	1:A:108:ILE:HG13	1.77	0.65
1:B:54:VAL:C	1:B:56:LEU:H	2.03	0.65
1:B:157:ILE:HD11	1:B:197:GLN:CG	2.27	0.64
1:B:235:SER:O	1:B:239:GLU:HB2	1.98	0.64
1:A:118:ARG:HH22	1:B:130:ASN:HD22	1.41	0.64
1:B:25:ASN:ND2	1:B:111:TYR:OH	2.26	0.64
1:A:183:GLN:NE2	2:A:318:HOH:O	2.30	0.64
1:A:83:ILE:HD11	1:A:105:VAL:CG2	2.28	0.64
1:A:94:LYS:HE2	2:A:451:HOH:O	1.97	0.63
1:B:205:TYR:HB3	1:B:229:LEU:HD21	1.80	0.63
1:B:202:PHE:CD1	1:B:233:VAL:HG21	2.34	0.62
1:A:118:ARG:HH21	1:B:130:ASN:ND2	1.95	0.62
1:A:20:GLN:HA	1:A:20:GLN:NE2	2.14	0.62
1:A:80:LEU:HD11	1:A:109:THR:HG21	1.81	0.62
1:B:199:ILE:HG21	1:B:269:ALA:HA	1.80	0.62
1:A:241:LYS:HE3	2:A:334:HOH:O	1.98	0.61
1:B:183:GLN:HA	1:B:183:GLN:HE21	1.64	0.61
1:B:209:LYS:HB3	1:B:212:GLU:HB2	1.82	0.61
1:B:50:MET:HE2	1:B:60:ILE:HD11	1.82	0.61
1:B:69:ALA:O	1:B:73:LEU:HG	2.00	0.61
1:B:204:ASP:O	1:B:208:LYS:HB2	2.01	0.61
1:B:56:LEU:HD11	1:B:185:MET:HE3	1.81	0.61
1:B:32:ASP:HA	2:B:419:HOH:O	2.00	0.61
1:A:144:LEU:HD22	1:B:28:TRP:CE2	2.37	0.60
1:B:254:GLN:HG2	1:B:255:SER:H	1.67	0.59
1:A:22:LEU:HD21	1:A:38:LEU:HD12	1.83	0.59
1:B:166:LYS:O	1:B:170:VAL:HG12	2.02	0.59
1:B:157:ILE:HG21	1:B:194:ILE:HG23	1.85	0.59
1:A:111:TYR:C	1:A:114:PRO:HD2	2.28	0.58
1:A:118:ARG:NH2	1:B:130:ASN:ND2	2.35	0.58
1:B:220:LEU:HD23	1:B:229:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:CG2	1:A:108:ILE:HG13	2.33	0.58
1:A:26:ARG:HE	1:A:26:ARG:HA	1.69	0.58
1:B:148:TYR:O	1:B:149:ASP:HB2	2.02	0.58
1:B:245:ASP:O	1:B:248:ILE:HG12	2.05	0.57
1:B:157:ILE:HD11	1:B:197:GLN:HG2	1.87	0.57
1:A:182:LYS:HB3	2:A:445:HOH:O	2.03	0.57
1:A:246:GLU:HB3	2:A:463:HOH:O	2.05	0.56
1:B:42:LYS:HB3	1:B:44:PHE:CE2	2.41	0.56
1:B:4:ILE:HG12	1:B:8:LEU:HG	1.87	0.56
1:B:73:LEU:HD21	1:B:116:ALA:HB3	1.86	0.56
1:B:219:GLN:C	1:B:221:PHE:H	2.13	0.56
1:A:147:MET:HE1	1:B:103:ARG:HD3	1.87	0.55
1:B:247:LEU:O	1:B:251:ILE:HG13	2.07	0.55
1:B:16:ARG:NH1	1:B:17:LEU:HA	2.21	0.55
1:B:121:GLN:HG3	1:B:129:LEU:HD22	1.88	0.55
1:A:60:ILE:H	1:A:60:ILE:CD1	1.99	0.55
1:A:91:ARG:O	1:A:91:ARG:HG2	2.07	0.55
1:B:157:ILE:HD11	1:B:197:GLN:HG3	1.88	0.54
1:A:257:TYR:O	1:A:261:ILE:HG13	2.07	0.54
1:B:43:ARG:HD3	1:B:71:GLU:OE1	2.08	0.53
1:B:195:ILE:HA	1:B:198:VAL:HG12	1.90	0.53
1:A:144:LEU:O	1:A:147:MET:HB2	2.09	0.53
1:B:196:TYR:HD1	1:B:268:LEU:HD22	1.74	0.53
1:B:220:LEU:HA	1:B:223:TYR:CD1	2.43	0.53
1:A:1:MET:CG	1:A:2:SER:H	2.06	0.53
1:B:167:LEU:HD11	1:B:171:LEU:HD11	1.90	0.53
1:A:211:GLU:CD	1:A:211:GLU:H	2.17	0.52
1:B:94:LYS:HE2	2:B:294:HOH:O	2.10	0.52
1:B:223:TYR:O	1:B:229:LEU:N	2.42	0.52
1:B:266:GLU:HG3	1:B:270:ASN:ND2	2.24	0.52
1:B:264:LEU:N	1:B:265:PRO:HD2	2.24	0.52
1:B:230:GLU:HG3	2:B:297:HOH:O	2.09	0.52
1:B:157:ILE:CD1	1:B:197:GLN:HG2	2.40	0.51
1:B:192:LEU:O	1:B:195:ILE:HB	2.10	0.51
1:B:190:LYS:O	1:B:194:ILE:HG13	2.10	0.51
1:B:154:ILE:O	1:B:157:ILE:HG22	2.10	0.51
1:B:198:VAL:HG13	1:B:199:ILE:N	2.25	0.51
1:A:39:LYS:HG2	1:A:40:ASP:OD1	2.11	0.51
1:B:3:ILE:HG13	1:B:4:ILE:H	1.74	0.51
1:B:42:LYS:HB3	1:B:44:PHE:CD2	2.46	0.51
1:B:209:LYS:HG3	1:B:211:GLU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:GLU:C	1:B:228:LYS:H	2.19	0.51
1:B:7:TRP:HA	1:B:47:THR:HG21	1.93	0.50
1:A:90:ARG:O	1:A:91:ARG:HB3	2.11	0.50
1:B:183:GLN:NE2	2:B:449:HOH:O	2.44	0.50
1:B:204:ASP:HA	1:B:208:LYS:CD	2.37	0.49
1:A:147:MET:HE1	1:B:107:PHE:HE2	1.77	0.49
1:A:20:GLN:HA	1:A:20:GLN:HE21	1.77	0.49
1:A:33:ILE:HD13	1:A:108:ILE:HG13	1.95	0.49
1:B:78:LEU:O	1:B:81:CYS:HB2	2.13	0.49
1:B:183:GLN:HA	1:B:183:GLN:NE2	2.26	0.49
1:B:268:LEU:O	1:B:272:LEU:HD13	2.13	0.49
1:B:147:MET:HE2	1:B:147:MET:HA	1.95	0.48
1:B:33:ILE:HG13	1:B:108:ILE:HD11	1.93	0.48
1:B:16:ARG:HD2	1:B:16:ARG:C	2.39	0.48
1:B:190:LYS:CE	2:B:429:HOH:O	2.60	0.48
1:B:166:LYS:HE2	1:B:190:LYS:HB2	1.95	0.48
1:B:153:TYR:O	1:B:157:ILE:HB	2.14	0.48
1:B:232:TYR:O	1:B:236:VAL:HG23	2.13	0.48
1:A:153:TYR:N	1:A:219:GLN:HE22	2.12	0.48
1:B:89:THR:O	1:B:89:THR:HG22	2.14	0.48
1:B:154:ILE:HD13	1:B:240:TYR:OH	2.14	0.48
1:A:153:TYR:HB2	1:A:219:GLN:NE2	2.28	0.48
1:B:137:LYS:C	1:B:137:LYS:HD2	2.39	0.47
1:B:228:LYS:HA	1:B:231:GLU:CG	2.45	0.47
1:B:17:LEU:HD11	1:B:64:TYR:CD1	2.50	0.47
1:B:40:ASP:OD1	1:B:40:ASP:C	2.58	0.47
1:B:254:GLN:CG	1:B:255:SER:H	2.26	0.47
1:B:68:LEU:HD12	1:B:68:LEU:O	2.15	0.47
1:A:1:MET:HG3	1:A:2:SER:N	2.14	0.47
1:A:7:TRP:HZ2	1:A:42:LYS:HD2	1.80	0.46
1:B:54:VAL:C	1:B:56:LEU:N	2.71	0.46
1:B:190:LYS:NZ	2:B:429:HOH:O	2.48	0.46
1:B:220:LEU:HA	1:B:223:TYR:HD1	1.80	0.46
1:B:50:MET:HE2	1:B:60:ILE:CD1	2.44	0.46
1:B:60:ILE:HG23	1:B:61:LYS:HD2	1.97	0.46
1:B:224:TYR:HB2	1:B:229:LEU:HD22	1.98	0.46
1:B:260:GLU:O	1:B:263:SER:HB3	2.15	0.46
1:B:219:GLN:C	1:B:221:PHE:N	2.72	0.46
1:B:53:THR:HA	1:B:172:SER:HB2	1.96	0.46
1:B:54:VAL:O	1:B:56:LEU:N	2.49	0.46
1:B:217:ALA:O	1:B:220:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASP:O	1:A:204:ASP:HB2	2.15	0.46
1:A:234:ARG:HD3	2:A:444:HOH:O	2.15	0.46
1:B:22:LEU:HD21	1:B:37:ILE:HG13	1.98	0.46
1:A:105:VAL:HG23	1:A:106:ILE:N	2.30	0.46
1:B:254:GLN:OE1	1:B:257:TYR:HE1	1.99	0.45
1:A:143:ALA:HB1	1:B:107:PHE:CE1	2.51	0.45
1:B:42:LYS:O	1:B:43:ARG:HB2	2.16	0.45
1:B:149:ASP:HB2	2:B:301:HOH:O	2.17	0.45
1:B:149:ASP:O	1:B:150:ASN:C	2.60	0.45
1:B:151:SER:HB2	2:B:331:HOH:O	2.17	0.45
1:B:224:TYR:CD1	1:B:224:TYR:C	2.94	0.45
1:B:224:TYR:HA	1:B:229:LEU:HB2	1.98	0.45
1:A:205:TYR:HA	1:A:213:ILE:HD11	1.98	0.45
1:A:29:ASP:OD2	1:A:29:ASP:N	2.44	0.45
1:B:253:PHE:O	1:B:254:GLN:HB2	2.16	0.45
1:B:11:LYS:HG3	1:B:43:ARG:HB2	1.99	0.44
1:B:45:ARG:HG3	1:B:45:ARG:HH11	1.82	0.44
1:A:26:ARG:O	1:A:28:TRP:N	2.50	0.44
1:B:260:GLU:OE1	1:B:260:GLU:N	2.50	0.44
1:A:1:MET:CG	1:A:2:SER:N	2.76	0.44
1:B:207:THR:OG1	1:B:276:ALA:HB1	2.17	0.44
1:A:161:THR:OG1	1:A:197:GLN:NE2	2.50	0.44
1:B:169:THR:OG1	1:B:170:VAL:N	2.51	0.44
1:A:54:VAL:HG21	1:A:60:ILE:HG13	1.97	0.43
1:B:183:GLN:HE21	1:B:183:GLN:CA	2.27	0.43
1:B:10:ALA:C	1:B:12:ALA:N	2.71	0.43
1:B:11:LYS:HD2	1:B:42:LYS:O	2.17	0.43
1:B:172:SER:O	1:B:176:SER:N	2.35	0.43
1:B:20:GLN:HA	1:B:20:GLN:NE2	2.30	0.43
1:B:70:ILE:CD1	1:B:171:LEU:HD12	2.32	0.43
1:B:162:GLY:O	1:B:165:PHE:N	2.49	0.43
1:A:151:SER:O	1:A:152:ASP:HB2	2.18	0.43
1:A:264:LEU:N	1:A:265:PRO:CD	2.82	0.43
1:B:72:ILE:HG23	1:B:112:LEU:HD22	2.01	0.43
1:B:87:ASP:O	1:B:88:ALA:HB3	2.19	0.43
1:B:242:GLN:HA	1:B:242:GLN:NE2	2.34	0.43
1:B:23:ASN:C	1:B:25:ASN:H	2.26	0.43
1:B:244:TYR:O	1:B:248:ILE:HG23	2.18	0.43
1:B:247:LEU:CD2	1:B:251:ILE:HD11	2.47	0.42
1:A:256:LYS:HE3	1:A:257:TYR:CE1	2.53	0.42
1:B:45:ARG:HG3	1:B:45:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ILE:CG1	1:B:249:SER:N	2.80	0.42
1:A:46:GLY:O	1:A:49:ASN:HB3	2.19	0.42
1:A:91:ARG:NH2	2:A:456:HOH:O	2.52	0.42
1:B:153:TYR:HB2	1:B:219:GLN:NE2	2.34	0.42
1:A:137:LYS:O	1:A:141:VAL:HG23	2.20	0.42
1:B:3:ILE:HG13	1:B:4:ILE:N	2.34	0.42
1:B:170:VAL:CG2	1:B:186:LEU:HG	2.49	0.42
1:B:196:TYR:CD1	1:B:268:LEU:HD22	2.54	0.42
1:A:203:VAL:HG22	1:A:273:LEU:HD23	2.01	0.42
1:B:152:ASP:OD2	1:B:152:ASP:C	2.63	0.42
1:A:144:LEU:HB2	1:B:28:TRP:CH2	2.55	0.42
1:B:40:ASP:O	1:B:43:ARG:NH2	2.53	0.42
1:B:204:ASP:OD1	1:B:208:LYS:HG2	2.20	0.42
1:B:240:TYR:CD1	1:B:243:LYS:HD2	2.55	0.42
1:B:247:LEU:HA	1:B:250:ASN:HD22	1.85	0.42
1:B:51:PHE:HZ	1:B:260:GLU:HG2	1.84	0.41
1:B:87:ASP:OD2	1:B:87:ASP:N	2.53	0.41
1:B:33:ILE:HG23	1:B:34:SER:N	2.36	0.41
1:B:70:ILE:CD1	1:B:167:LEU:HG	2.50	0.41
1:B:55:ALA:O	1:B:56:LEU:HD23	2.20	0.41
1:B:212:GLU:O	1:B:213:ILE:C	2.63	0.41
1:A:108:ILE:HA	1:B:144:LEU:HD11	2.02	0.41
1:A:113:ILE:HB	1:A:114:PRO:HD3	2.02	0.41
1:B:32:ASP:OD2	1:B:104:LYS:HE3	2.21	0.41
1:B:229:LEU:HB3	2:B:322:HOH:O	2.20	0.41
1:A:54:VAL:HG12	1:A:257:TYR:CZ	2.55	0.41
1:B:100:TYR:CZ	1:B:104:LYS:HD2	2.56	0.41
1:B:16:ARG:HD2	1:B:16:ARG:O	2.20	0.41
1:B:164:LEU:HD12	1:B:164:LEU:HA	1.84	0.41
1:A:14:ILE:HG21	1:A:71:GLU:HG3	2.03	0.41
1:A:3:ILE:HD11	1:A:260:GLU:CB	2.39	0.40
1:B:151:SER:O	1:B:152:ASP:C	2.63	0.40
1:A:149:ASP:O	1:A:150:ASN:C	2.64	0.40
1:A:106:ILE:HD12	1:B:83:ILE:HD13	2.04	0.40
1:B:201:ASP:CG	1:B:217:ALA:HB2	2.46	0.40
1:B:257:TYR:CD1	1:B:257:TYR:N	2.90	0.40
1:A:148:TYR:C	1:A:150:ASN:H	2.29	0.40
1:B:10:ALA:O	1:B:13:THR:N	2.54	0.40
1:B:223:TYR:CB	1:B:229:LEU:HA	2.41	0.40
1:B:198:VAL:CG1	1:B:199:ILE:N	2.84	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:284:HOH:O	2:A:284:HOH:O[5_555]	0.50	1.70
2:A:283:HOH:O	2:A:283:HOH:O[4_556]	0.75	1.45
2:A:282:HOH:O	2:A:282:HOH:O[4_556]	0.85	1.35
1:B:249:SER:CB	1:B:249:SER:CB[6_555]	2.06	0.14
2:A:355:HOH:O	2:A:480:HOH:O[4_556]	2.07	0.13
1:B:211:GLU:OE2	2:A:374:HOH:O[6_655]	2.13	0.07
2:A:361:HOH:O	2:A:447:HOH:O[5_565]	2.18	0.02

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	274/289 (95%)	254 (93%)	16 (6%)	4 (2%)	8	12
1	B	272/289 (94%)	218 (80%)	49 (18%)	5 (2%)	6	9
All	All	546/578 (94%)	472 (86%)	65 (12%)	9 (2%)	7	11

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	39	LYS
1	B	149	ASP
1	B	213	ILE
1	B	253	PHE
1	B	55	ALA
1	A	91	ARG
1	A	149	ASP
1	B	147	MET

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	242/254 (95%)	237 (98%)	5 (2%)	47	69
1	B	240/254 (94%)	232 (97%)	8 (3%)	33	55
All	All	482/508 (95%)	469 (97%)	13 (3%)	39	62

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ILE
1	A	90	ARG
1	A	108	ILE
1	A	109	THR
1	A	147	MET
1	B	40	ASP
1	B	87	ASP
1	B	109	THR
1	B	185	MET
1	B	239	GLU
1	B	247	LEU
1	B	257	TYR
1	B	260	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	25	ASN
1	A	49	ASN
1	A	102	ASN
1	A	110	ASN
1	A	121	GLN
1	A	130	ASN
1	A	178	HIS
1	A	183	GLN

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Mol	Chain	Res	Type
1	A	197	GLN
1	A	242	GLN
1	B	20	GLN
1	B	23	ASN
1	B	25	ASN
1	B	110	ASN
1	B	130	ASN
1	B	183	GLN
1	B	184	GLN
1	B	197	GLN
1	B	219	GLN
1	B	242	GLN
1	B	250	ASN
1	B	270	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	276/289 (95%)	1.40	62 (22%)	2 2	20, 37, 68, 88	0
1	B	274/289 (94%)	1.66	81 (29%)	1 1	28, 66, 109, 115	0
All	All	550/578 (95%)	1.53	143 (26%)	1 1	20, 49, 103, 115	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	TRP	5.4
1	B	3	ILE	4.5
1	A	4	ILE	4.5
1	B	244	TYR	4.4
1	B	148	TYR	4.3
1	B	55	ALA	4.3
1	B	205	TYR	4.2
1	B	276	ALA	4.2
1	B	253	PHE	4.1
1	B	247	LEU	4.0
1	B	194	ILE	4.0
1	B	210	VAL	3.9
1	B	4	ILE	3.8
1	B	221	PHE	3.8
1	A	276	ALA	3.5
1	B	6	PHE	3.5
1	A	274	LYS	3.5
1	B	240	TYR	3.4
1	B	264	LEU	3.4
1	B	268	LEU	3.3
1	B	251	ILE	3.3
1	A	270	ASN	3.2
1	B	92	GLY	3.2
1	B	7	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	227	GLY	3.2
1	B	257	TYR	3.1
1	B	237	TYR	3.0
1	A	60	ILE	3.0
1	A	149	ASP	3.0
1	A	233	VAL	2.9
1	A	173	ALA	2.9
1	A	263	SER	2.9
1	B	88	ALA	2.9
1	B	220	LEU	2.9
1	B	258	LEU	2.9
1	B	149	ASP	2.9
1	B	215	GLY	2.9
1	B	248	ILE	2.9
1	B	52	PHE	2.9
1	B	225	ARG	2.8
1	B	207	THR	2.8
1	B	254	GLN	2.8
1	B	144	LEU	2.8
1	B	236	VAL	2.8
1	A	203	VAL	2.7
1	A	225	ARG	2.7
1	B	141	VAL	2.7
1	B	175	ALA	2.7
1	B	195	ILE	2.7
1	A	31	VAL	2.7
1	B	192	LEU	2.6
1	A	212	GLU	2.6
1	B	53	THR	2.6
1	B	269	ALA	2.6
1	B	265	PRO	2.6
1	A	195	ILE	2.6
1	A	237	TYR	2.6
1	B	124	TYR	2.6
1	A	214	ASP	2.5
1	A	147	MET	2.5
1	B	224	TYR	2.5
1	A	238	LEU	2.5
1	B	86	LEU	2.5
1	A	262	ARG	2.5
1	A	33	ILE	2.5
1	B	206	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	193	GLY	2.4
1	B	226	GLU	2.4
1	A	224	TYR	2.4
1	A	265	PRO	2.4
1	A	37	ILE	2.4
1	B	273	LEU	2.4
1	B	150	ASN	2.4
1	B	227	GLY	2.4
1	B	204	ASP	2.4
1	B	238	LEU	2.4
1	B	233	VAL	2.4
1	B	189	GLY	2.4
1	B	154	ILE	2.4
1	B	80	LEU	2.4
1	A	148	TYR	2.4
1	A	153	TYR	2.4
1	A	88	ALA	2.4
1	B	203	VAL	2.3
1	A	226	GLU	2.3
1	A	273	LEU	2.3
1	B	202	PHE	2.3
1	B	179	TYR	2.3
1	A	275	GLU	2.3
1	A	207	THR	2.3
1	A	25	ASN	2.3
1	B	87	ASP	2.3
1	B	222	LYS	2.3
1	A	210	VAL	2.3
1	A	106	ILE	2.2
1	A	259	SER	2.2
1	B	8	LEU	2.2
1	B	267	PHE	2.2
1	B	196	TYR	2.2
1	A	41	GLY	2.2
1	A	258	LEU	2.2
1	B	120	ILE	2.2
1	A	93	ASP	2.2
1	A	188	VAL	2.2
1	A	151	SER	2.2
1	B	263	SER	2.2
1	A	260	GLU	2.2
1	B	96	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	2.2
1	A	191	TYR	2.2
1	B	213	ILE	2.2
1	A	235	SER	2.2
1	B	234	ARG	2.2
1	B	28	TRP	2.2
1	B	44	PHE	2.2
1	A	269	ALA	2.1
1	B	250	ASN	2.1
1	A	30	LEU	2.1
1	A	196	TYR	2.1
1	B	232	TYR	2.1
1	A	132	SER	2.1
1	A	57	GLY	2.1
1	A	142	GLY	2.1
1	A	9	GLU	2.1
1	A	146	ASP	2.1
1	B	255	SER	2.1
1	A	58	GLY	2.1
1	A	215	GLY	2.1
1	B	186	LEU	2.1
1	B	155	ARG	2.1
1	A	257	TYR	2.1
1	A	126	ASP	2.1
1	B	245	ASP	2.1
1	B	256	LYS	2.1
1	B	10	ALA	2.1
1	A	47	THR	2.1
1	B	191	TYR	2.1
1	B	147	MET	2.1
1	A	213	ILE	2.0
1	A	174	TYR	2.0
1	B	64	TYR	2.0
1	A	216	SER	2.0
1	A	103	ARG	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.