



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:47 AM UTC

PDB ID : 4LU0 / pdb_00004lu0
Title : Crystal structure of 2-Keto-3-deoxy-D-manno-octulosonate-8-phosphate synthase from *Pseudomonas aeruginosa*.
Authors : Asojo, O.A.
Deposited on : 2013-07-24
Resolution : 2.80 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

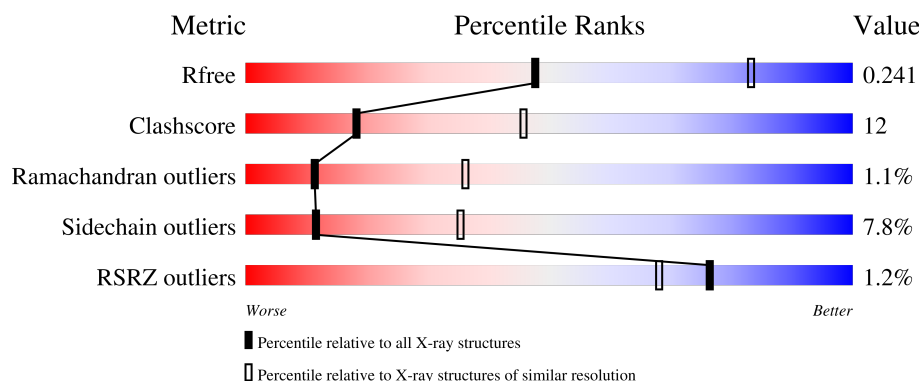
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	287	2% 58% 25% • 14%
1	B	287	% 59% 23% • 14%
1	C	287	% 55% 26% 5% 13%
1	D	287	% 62% 24% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7875 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 2-dehydro-3-deoxyphosphooctonate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1951	1258	330	352	11			
1	B	247	Total	C	N	O	S	0	0	0
			1939	1251	325	352	11			
1	C	250	Total	C	N	O	S	0	0	0
			1967	1267	331	358	11			
1	D	252	Total	C	N	O	S	0	0	0
			1992	1283	336	362	11			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9ZFK4
A	2	HIS	-	expression tag	UNP Q9ZFK4
A	3	HIS	-	expression tag	UNP Q9ZFK4
A	4	HIS	-	expression tag	UNP Q9ZFK4
A	5	HIS	-	expression tag	UNP Q9ZFK4
A	6	HIS	-	expression tag	UNP Q9ZFK4
A	7	HIS	-	expression tag	UNP Q9ZFK4
B	1	MET	-	expression tag	UNP Q9ZFK4
B	2	HIS	-	expression tag	UNP Q9ZFK4
B	3	HIS	-	expression tag	UNP Q9ZFK4
B	4	HIS	-	expression tag	UNP Q9ZFK4
B	5	HIS	-	expression tag	UNP Q9ZFK4
B	6	HIS	-	expression tag	UNP Q9ZFK4
B	7	HIS	-	expression tag	UNP Q9ZFK4
C	1	MET	-	expression tag	UNP Q9ZFK4
C	2	HIS	-	expression tag	UNP Q9ZFK4
C	3	HIS	-	expression tag	UNP Q9ZFK4
C	4	HIS	-	expression tag	UNP Q9ZFK4
C	5	HIS	-	expression tag	UNP Q9ZFK4
C	6	HIS	-	expression tag	UNP Q9ZFK4
C	7	HIS	-	expression tag	UNP Q9ZFK4

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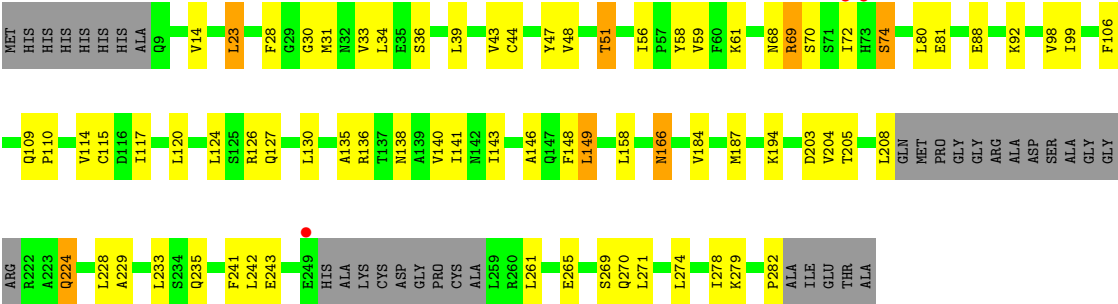
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	expression tag	UNP Q9ZFK4
D	2	HIS	-	expression tag	UNP Q9ZFK4
D	3	HIS	-	expression tag	UNP Q9ZFK4
D	4	HIS	-	expression tag	UNP Q9ZFK4
D	5	HIS	-	expression tag	UNP Q9ZFK4
D	6	HIS	-	expression tag	UNP Q9ZFK4
D	7	HIS	-	expression tag	UNP Q9ZFK4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total O 9 9	0	0
2	B	7	Total O 7 7	0	0
2	C	5	Total O 5 5	0	0
2	D	5	Total O 5 5	0	0



● Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.27Å 95.10Å 145.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.69 – 2.80 57.69 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.5 (57.69-2.80) 95.5 (57.69-2.80)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.56 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.206 , 0.267 (Not available) , 0.241	Depositor DCC
R_{free} test set	1321 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7875	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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](#)

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	0.95	0/1986	1.07	2/2674 (0.1%)
1	B	1.07	2/1972 (0.1%)	1.14	6/2655 (0.2%)
1	C	0.93	0/2002	1.07	4/2697 (0.1%)
1	D	1.08	1/2028 (0.0%)	1.11	5/2732 (0.2%)
All	All	1.01	3/7988 (0.0%)	1.10	17/10758 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	ILE	CA-CB	6.08	1.58	1.54
1	B	56	ILE	N-CA	5.74	1.50	1.45
1	D	166	ASN	CA-C	5.13	1.58	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	GLY	CA-C-N	-7.34	116.46	122.85
1	B	55	GLY	C-N-CA	-7.34	116.46	122.85
1	D	224	GLN	N-CA-C	-6.91	96.08	110.80
1	A	222	ARG	N-CA-C	-6.88	104.36	112.89
1	C	118	ILE	N-CA-C	6.47	117.92	108.53
1	B	182	ASN	N-CA-C	5.72	118.62	110.10
1	C	127	GLN	N-CA-C	5.44	118.11	109.24
1	B	198	TYR	CA-C-N	5.39	125.69	119.93
1	B	198	TYR	C-N-CA	5.39	125.69	119.93
1	D	28	PHE	CA-C-N	-5.37	118.48	122.18
1	D	28	PHE	C-N-CA	-5.37	118.48	122.18
1	C	232	GLY	N-CA-C	-5.35	106.02	112.49
1	B	223	ALA	N-CA-C	-5.33	106.62	113.01
1	D	166	ASN	N-CA-C	5.15	116.70	107.80
1	C	149	LEU	N-CA-C	5.14	117.99	109.46
1	D	114	VAL	CB-CA-C	-5.05	106.64	111.44
1	A	109	GLN	O-C-N	5.05	123.75	120.27

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	1951	0	1994	44	0
1	B	1939	0	1981	56	0
1	C	1967	0	2000	61	0
1	D	1992	0	2030	44	0
2	A	9	0	0	2	0
2	B	7	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
All	All	7875	0	8005	192	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 (192) 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:102:VAL:HG23	1:A:134:MET:HE2	1.33	1.09
1:B:232:GLY:O	1:B:237:LEU:HD23	1.53	1.06
1:A:144:LYS:NZ	1:A:172:CYS:SG	2.31	1.04
1:B:120:LEU:HD13	1:B:134:MET:HE1	1.49	0.94
1:B:144:LYS:NZ	1:B:172:CYS:SG	2.41	0.94
1:A:203:ASP:HA	1:A:241:PHE:HB2	1.55	0.89
1:B:59:VAL:HG22	1:B:97:PRO:HG2	1.59	0.82
1:B:284:ILE:HG12	1:D:270:GLN:HE22	1.43	0.82
1:A:147:GLN:HG2	2:A:305:HOH:O	1.79	0.81
1:C:63:SER:HB3	1:C:101:ASP:OD1	1.82	0.79
1:C:203:ASP:HA	1:C:241:PHE:HB3	1.65	0.78
1:D:203:ASP:HA	1:D:241:PHE:HB2	1.66	0.77
1:B:232:GLY:O	1:B:237:LEU:CD2	2.36	0.73
1:B:203:ASP:HA	1:B:241:PHE:HB3	1.70	0.71
1:A:194:LYS:HE2	1:A:236:LYS:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LYS:NZ	1:C:243:GLU:OE2	2.25	0.68
1:A:102:VAL:CG2	1:A:134:MET:HE2	2.18	0.68
1:A:132:VAL:O	1:A:136:ARG:HG2	1.92	0.68
1:B:277:LEU:HD12	1:B:281:PHE:CZ	2.29	0.68
1:A:101:ASP:HB3	1:A:119:GLN:HB3	1.75	0.67
1:D:241:PHE:O	1:D:242:LEU:HD12	1.95	0.67
1:B:222:ARG:HG3	1:B:223:ALA:H	1.58	0.67
1:A:231:ALA:HB2	1:C:235:GLN:NE2	2.12	0.65
1:D:51:THR:HG23	1:D:56:ILE:O	1.97	0.65
1:C:102:VAL:HG13	1:C:134:MET:HE2	1.79	0.64
1:C:275:ASP:OD1	1:C:279:LYS:NZ	2.28	0.64
1:D:146:ALA:HB3	1:D:149:LEU:HD22	1.79	0.64
1:A:148:PHE:CD1	1:A:149:LEU:HD13	2.32	0.64
1:C:49:ARG:CZ	1:C:49:ARG:HB3	2.27	0.63
1:B:17:ILE:HG12	1:B:57:PRO:HB3	1.80	0.63
1:A:228:LEU:HD22	1:C:188:LEU:HD21	1.81	0.63
1:B:120:LEU:HD13	1:B:134:MET:CE	2.26	0.62
1:C:69:ARG:HE	1:C:70:SER:H	1.45	0.62
1:B:11:ILE:HG12	1:B:23:LEU:HD11	1.82	0.61
1:D:44:CYS:O	1:D:48:VAL:HG23	2.00	0.61
1:B:84:MET:HE3	1:B:111:VAL:HG22	1.82	0.61
1:B:47:TYR:O	1:B:51:THR:OG1	2.17	0.60
1:B:119:GLN:NE2	1:B:144:LYS:HE2	2.15	0.60
1:D:59:VAL:HG12	1:D:99:ILE:HG22	1.83	0.60
1:D:135:ALA:HA	1:D:141:ILE:HD11	1.82	0.60
1:B:51:THR:HG22	1:B:56:ILE:HB	1.83	0.60
1:C:8:ALA:O	1:C:197:GLU:HG2	2.02	0.60
1:A:275:ASP:OD1	1:A:279:LYS:NZ	2.35	0.59
1:C:197:GLU:O	1:C:198:TYR:HB2	2.01	0.58
1:D:98:VAL:HG23	1:D:115:CYS:SG	2.43	0.58
1:C:119:GLN:NE2	1:C:144:LYS:HG3	2.19	0.58
1:A:59:VAL:HG22	1:A:97:PRO:HB2	1.86	0.58
1:C:170:ILE:HG12	1:C:199:PRO:HB2	1.85	0.58
1:B:201:PHE:CE2	1:B:239:GLY:HA3	2.38	0.57
1:A:102:VAL:HG23	1:A:134:MET:CE	2.20	0.57
1:C:23:LEU:O	1:C:279:LYS:HE2	2.04	0.57
1:A:221:ARG:HG3	1:A:222:ARG:H	1.68	0.57
1:B:222:ARG:HG3	1:B:223:ALA:N	2.21	0.56
1:C:14:VAL:O	1:C:16:ASP:N	2.38	0.56
1:A:23:LEU:O	1:A:279:LYS:HE2	2.05	0.56
1:A:66:LYS:H	1:A:76:ARG:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:LYS:HG3	1:C:154:MET:SD	2.46	0.56
1:C:226:THR:HA	1:C:267:PHE:HE1	1.70	0.56
1:C:147:GLN:HE21	1:C:147:GLN:H	1.52	0.56
1:D:127:GLN:HE21	1:D:130:LEU:HB2	1.71	0.55
1:B:181:ASN:HB3	2:B:307:HOH:O	2.06	0.54
1:C:10:LYS:HB2	1:C:198:TYR:H	1.71	0.54
1:A:277:LEU:HD22	1:C:277:LEU:HD12	1.89	0.54
1:D:148:PHE:CE1	1:D:149:LEU:HD13	2.42	0.54
1:C:72:ILE:C	1:C:74:SER:H	2.16	0.54
1:D:69:ARG:HD2	1:D:70:SER:H	1.73	0.53
1:A:130:LEU:O	1:A:134:MET:HG3	2.08	0.53
1:D:274:LEU:O	1:D:278:ILE:HG12	2.08	0.53
1:D:88:GLU:OE2	1:D:88:GLU:HA	2.09	0.53
1:A:224:GLN:HE21	1:C:188:LEU:HD22	1.73	0.53
1:C:144:LYS:NZ	1:C:172:CYS:SG	2.82	0.53
1:A:137:THR:O	1:A:139:ALA:N	2.42	0.52
1:B:187:MET:HE3	1:D:187:MET:HG3	1.90	0.52
1:A:45:GLU:HG3	1:A:94:PHE:HE1	1.74	0.52
1:C:37:ARG:HD2	1:C:89:GLU:OE2	2.08	0.52
1:B:120:LEU:CD1	1:B:134:MET:HE1	2.32	0.52
1:C:245:HIS:H	1:C:260:ARG:HG2	1.75	0.52
1:D:148:PHE:CD1	1:D:149:LEU:HD13	2.45	0.52
1:B:36:SER:OG	1:B:39:LEU:HB2	2.10	0.51
1:C:226:THR:HG22	1:C:267:PHE:CD1	2.46	0.51
1:D:14:VAL:CG2	1:D:140:VAL:HG21	2.41	0.51
1:D:126:ARG:HE	1:D:149:LEU:HD11	1.76	0.50
1:B:51:THR:HG21	1:B:58:TYR:HB2	1.94	0.50
1:B:234:SER:HA	1:B:278:ILE:HG13	1.94	0.50
1:B:235:GLN:HB2	1:B:237:LEU:HD21	1.93	0.50
1:B:13:ARG:NH1	1:B:13:ARG:HB2	2.26	0.49
1:A:27:LEU:HD11	1:A:242:LEU:HD12	1.93	0.49
1:A:137:THR:C	1:A:139:ALA:H	2.20	0.49
1:B:54:LEU:HD23	1:B:56:ILE:HD11	1.94	0.49
1:B:78:PRO:O	1:B:82:GLU:HB3	2.12	0.49
1:C:119:GLN:HE21	1:C:144:LYS:HG3	1.77	0.49
1:C:277:LEU:HD22	1:C:281:PHE:CZ	2.48	0.49
1:B:18:GLN:HB3	1:B:23:LEU:HD13	1.95	0.49
1:B:149:LEU:HG	1:B:153:GLU:HG2	1.95	0.49
1:C:72:ILE:HG22	1:C:73:HIS:H	1.79	0.48
1:A:117:ILE:HG12	1:A:140:VAL:HG13	1.96	0.48
1:C:148:PHE:CE1	1:C:149:LEU:HD22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:GLY:HA3	1:D:61:LYS:O	2.13	0.48
1:B:120:LEU:HB2	1:B:134:MET:HE1	1.96	0.47
1:C:98:VAL:HG23	1:C:115:CYS:HA	1.96	0.47
1:B:270:GLN:HE21	1:D:282:PRO:HD2	1.79	0.47
1:D:127:GLN:O	1:D:127:GLN:HG3	2.14	0.47
1:A:148:PHE:CE1	1:A:149:LEU:HD13	2.50	0.47
1:B:59:VAL:HG22	1:B:97:PRO:CG	2.39	0.47
1:A:10:LYS:HA	1:A:197:GLU:O	2.15	0.47
1:C:14:VAL:HG23	1:C:17:ILE:HB	1.97	0.47
1:A:72:ILE:HG23	1:A:73:HIS:H	1.79	0.47
1:B:76:ARG:NH1	1:C:128:THR:HB	2.30	0.47
1:C:205:THR:HG23	1:C:242:LEU:HD12	1.97	0.46
1:B:119:GLN:HE22	1:B:144:LYS:HE2	1.81	0.46
1:C:72:ILE:O	1:C:74:SER:N	2.49	0.46
1:A:40:ALA:HB1	1:A:90:ILE:HD11	1.98	0.45
1:A:233:LEU:HD12	1:A:271:LEU:HD22	1.98	0.45
1:D:204:VAL:HG11	1:D:229:ALA:HB2	1.97	0.45
1:B:13:ARG:HB2	1:B:13:ARG:HH11	1.80	0.45
1:A:109:GLN:N	1:A:110:PRO:HD2	2.32	0.45
1:C:117:ILE:HG12	1:C:140:VAL:CG1	2.47	0.45
1:C:152:GLN:H	1:C:152:GLN:CD	2.25	0.45
1:C:267:PHE:CZ	1:C:271:LEU:HD11	2.52	0.45
1:D:36:SER:OG	1:D:39:LEU:HD13	2.17	0.45
1:C:154:MET:HA	1:C:154:MET:HE2	1.99	0.44
1:B:158:LEU:HD11	1:B:171:LEU:HD11	1.98	0.44
1:C:18:GLN:HB3	1:C:23:LEU:CD2	2.48	0.44
1:C:49:ARG:HB3	1:C:49:ARG:NH1	2.31	0.44
1:A:94:PHE:O	1:A:95:LYS:C	2.60	0.44
1:B:275:ASP:OD1	1:B:279:LYS:HE2	2.17	0.44
1:C:78:PRO:HB2	1:C:82:GLU:HB3	1.99	0.44
1:A:123:PHE:HE2	1:D:126:ARG:HD2	1.83	0.44
1:A:234:SER:HA	1:A:278:ILE:HG13	2.00	0.44
1:D:135:ALA:O	1:D:166:ASN:HB2	2.17	0.44
1:D:47:TYR:HB3	1:D:58:TYR:CZ	2.52	0.43
1:C:72:ILE:H	1:C:72:ILE:HG13	1.56	0.43
1:C:222:ARG:C	1:C:224:GLN:H	2.27	0.43
1:B:204:VAL:HG11	1:B:229:ALA:HB2	2.00	0.43
1:C:102:VAL:HG23	1:C:107:GLN:HG3	2.00	0.43
1:C:274:LEU:O	1:C:278:ILE:HG12	2.18	0.43
1:A:60:PHE:HB3	1:A:98:VAL:HG12	2.01	0.43
1:A:122:ALA:HB1	1:A:146:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:GLU:O	1:D:269:SER:HB2	2.18	0.43
1:A:19:ILE:HG12	1:A:26:VAL:HG21	2.00	0.43
1:A:15:GLY:HA3	2:A:304:HOH:O	2.19	0.42
1:C:197:GLU:O	1:C:198:TYR:CB	2.67	0.42
1:D:117:ILE:HG12	1:D:140:VAL:HB	2.01	0.42
1:D:208:LEU:HD21	1:D:228:LEU:HD12	2.00	0.42
1:A:155:LYS:HA	1:A:158:LEU:HD12	1.99	0.42
1:D:205:THR:HG21	1:D:243:GLU:H	1.83	0.42
1:A:45:GLU:HG3	1:A:94:PHE:CE1	2.51	0.42
1:B:31:MET:HE3	1:B:43:VAL:HG21	2.02	0.42
1:B:194:LYS:NZ	1:B:236:LYS:HB3	2.33	0.42
1:D:33:VAL:HG22	1:D:34:LEU:N	2.34	0.42
1:C:128:THR:O	1:C:132:VAL:HG23	2.18	0.42
1:B:44:CYS:O	1:B:48:VAL:HG23	2.19	0.42
1:C:117:ILE:HG12	1:C:140:VAL:HG13	2.02	0.42
1:D:23:LEU:O	1:D:279:LYS:NZ	2.43	0.42
1:B:173:GLU:HB2	1:B:193:MET:HE1	2.02	0.42
1:D:120:LEU:HD23	1:D:143:ILE:HG23	2.01	0.42
1:D:92:LYS:HE3	1:D:92:LYS:HB2	1.83	0.41
1:A:126:ARG:HB3	1:D:68:ASN:HB2	2.02	0.41
1:B:25:PHE:HB2	1:B:239:GLY:HA2	2.01	0.41
1:B:26:VAL:HG13	1:B:57:PRO:HB2	2.02	0.41
1:B:123:PHE:HB3	1:C:123:PHE:O	2.19	0.41
1:B:284:ILE:HG12	1:D:270:GLN:NE2	2.23	0.41
1:C:87:PHE:HD1	1:C:98:VAL:HG11	1.85	0.41
1:B:60:PHE:HB3	1:B:98:VAL:HG12	2.02	0.41
1:C:242:LEU:HG	1:C:243:GLU:N	2.35	0.41
1:A:221:ARG:HG3	1:A:222:ARG:N	2.34	0.41
1:D:194:LYS:NZ	1:D:235:GLN:O	2.51	0.41
1:B:60:PHE:CD2	1:B:60:PHE:C	2.98	0.41
1:B:149:LEU:HD12	1:B:149:LEU:HA	1.90	0.41
1:C:104:GLU:O	1:C:107:GLN:HG2	2.20	0.41
1:C:155:LYS:HD2	1:C:155:LYS:HA	1.84	0.41
1:C:195:GLN:C	1:C:197:GLU:H	2.29	0.41
1:D:106:PHE:CD1	1:D:106:PHE:C	2.98	0.41
1:B:119:GLN:HE21	1:B:144:LYS:HG3	1.85	0.41
1:C:137:THR:O	1:C:138:ASN:C	2.64	0.41
1:D:233:LEU:HD12	1:D:271:LEU:HD22	2.01	0.41
1:A:78:PRO:HB2	1:A:82:GLU:HB3	2.03	0.41
1:A:145:LYS:NZ	1:A:149:LEU:O	2.48	0.41
1:B:47:TYR:HB3	1:B:58:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ILE:HD11	1:B:73:HIS:CE1	2.56	0.41
1:B:184:VAL:HG11	1:D:184:VAL:HG11	2.02	0.41
1:C:201:PHE:CE2	1:C:239:GLY:HA3	2.56	0.41
1:D:31:MET:HE2	1:D:33:VAL:O	2.21	0.41
1:D:43:VAL:HA	1:D:261:LEU:HD11	2.03	0.41
1:D:99:ILE:HB	1:D:117:ILE:HB	2.03	0.41
1:B:109:GLN:O	1:B:110:PRO:C	2.61	0.40
1:C:19:ILE:HA	2:C:304:HOH:O	2.21	0.40
1:C:199:PRO:HB3	1:C:238:ALA:CB	2.51	0.40
1:C:233:LEU:HD23	1:C:233:LEU:HA	1.91	0.40
1:B:109:GLN:O	1:B:113:GLU:HG2	2.22	0.40
1:C:50:VAL:HG11	1:C:265:GLU:HA	2.03	0.40
1:D:109:GLN:HB3	1:D:110:PRO:CD	2.51	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	241/287 (84%)	224 (93%)	13 (5%)	4 (2%)	7	25
1	B	241/287 (84%)	230 (95%)	10 (4%)	1 (0%)	30	60
1	C	244/287 (85%)	223 (91%)	17 (7%)	4 (2%)	7	27
1	D	246/287 (86%)	226 (92%)	18 (7%)	2 (1%)	16	44
All	All	972/1148 (85%)	903 (93%)	58 (6%)	11 (1%)	11	36

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	PHE
1	A	138	ASN

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Mol	Chain	Res	Type
1	C	15	GLY
1	C	73	HIS
1	A	34	LEU
1	D	74	SER
1	C	68	ASN
1	D	138	ASN
1	B	71	SER
1	C	198	TYR
1	A	72	ILE

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	213/241 (88%)	196 (92%)	17 (8%)	11	34
1	B	210/241 (87%)	195 (93%)	15 (7%)	13	39
1	C	214/241 (89%)	191 (89%)	23 (11%)	6	21
1	D	218/241 (90%)	206 (94%)	12 (6%)	19	51
All	All	855/964 (89%)	788 (92%)	67 (8%)	11	35

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	46	GLU
1	A	70	SER
1	A	76	ARG
1	A	93	THR
1	A	102	VAL
1	A	140	VAL
1	A	149	LEU
1	A	153	GLU
1	A	174	ARG
1	A	204	VAL
1	A	206	HIS

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Mol	Chain	Res	Type
1	A	208	LEU
1	A	240	LEU
1	A	243	GLU
1	A	261	LEU
1	A	262	ASN
1	B	9	GLN
1	B	14	VAL
1	B	39	LEU
1	B	51	THR
1	B	54	LEU
1	B	56	ILE
1	B	149	LEU
1	B	152	GLN
1	B	153	GLU
1	B	188	LEU
1	B	204	VAL
1	B	233	LEU
1	B	237	LEU
1	B	277	LEU
1	B	284	ILE
1	C	23	LEU
1	C	27	LEU
1	C	33	VAL
1	C	39	LEU
1	C	46	GLU
1	C	49	ARG
1	C	66	LYS
1	C	68	ASN
1	C	72	ILE
1	C	82	GLU
1	C	95	LYS
1	C	102	VAL
1	C	127	GLN
1	C	140	VAL
1	C	147	GLN
1	C	149	LEU
1	C	172	CYS
1	C	204	VAL
1	C	240	LEU
1	C	260	ARG
1	C	262	ASN
1	C	272	LYS

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Mol	Chain	Res	Type
1	C	277	LEU
1	D	23	LEU
1	D	51	THR
1	D	69	ARG
1	D	72	ILE
1	D	74	SER
1	D	80	LEU
1	D	81	GLU
1	D	124	LEU
1	D	136	ARG
1	D	149	LEU
1	D	158	LEU
1	D	224	GLN

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	119	GLN
1	A	142	ASN
1	A	224	GLN
1	A	245	HIS
1	A	273	GLN
1	B	119	GLN
1	B	181	ASN
1	B	182	ASN
1	B	206	HIS
1	B	224	GLN
1	B	270	GLN
1	C	119	GLN
1	C	147	GLN
1	C	224	GLN
1	C	273	GLN
1	D	127	GLN
1	D	181	ASN
1	D	195	GLN
1	D	270	GLN

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	247/287 (86%)	-0.01	5 (2%) 65 56	19, 41, 73, 117	0
1	B	247/287 (86%)	-0.10	2 (0%) 82 75	21, 39, 65, 82	0
1	C	250/287 (87%)	-0.02	2 (0%) 82 75	21, 44, 73, 98	0
1	D	252/287 (87%)	-0.05	3 (1%) 76 68	17, 39, 68, 113	0
All	All	996/1148 (86%)	-0.04	12 (1%) 76 68	17, 41, 70, 117	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	SER	4.0
1	A	73	HIS	3.1
1	B	209	GLN	2.7
1	A	126	ARG	2.6
1	A	127	GLN	2.6
1	B	123	PHE	2.3
1	C	15	GLY	2.3
1	C	8	ALA	2.2
1	D	73	HIS	2.1
1	D	72	ILE	2.0
1	D	249	GLU	2.0
1	A	206	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.