



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:08 AM UTC

PDB ID : 5GK0 / pdb_00005gk0
Title : Crystal structure of selnomethionin-labeled ketosynthase StlD
Authors : Mori, T.; Saito, Y.; Morita, H.; Abe, I.
Deposited on : 2016-07-03
Resolution : 2.33 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

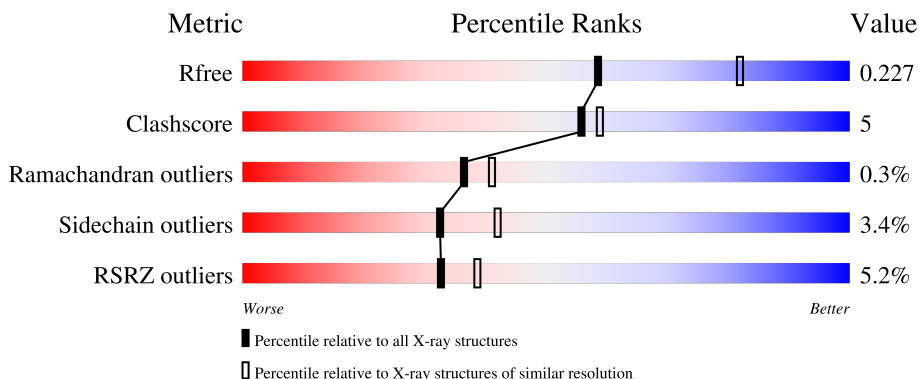
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	402	84% 9% • 5%
1	B	402	8% 76% 14% 10%
1	C	402	9% 77% 15% • 6%
1	D	402	% 85% 9% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12283 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 Ketosynthase StlD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	Se	0	0	0
			2974	1871	511	574	5	13			
1	B	363	Total	C	N	O	S	Se	0	0	0
			2843	1796	481	548	5	13			
1	C	379	Total	C	N	O	S	Se	0	0	0
			2966	1867	509	572	5	13			
1	D	380	Total	C	N	O	S	Se	0	0	0
			2974	1871	511	574	5	13			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	expression tag	UNP Q7N4Z6
A	-18	GLY	-	expression tag	UNP Q7N4Z6
A	-17	SER	-	expression tag	UNP Q7N4Z6
A	-16	SER	-	expression tag	UNP Q7N4Z6
A	-15	HIS	-	expression tag	UNP Q7N4Z6
A	-14	HIS	-	expression tag	UNP Q7N4Z6
A	-13	HIS	-	expression tag	UNP Q7N4Z6
A	-12	HIS	-	expression tag	UNP Q7N4Z6
A	-11	HIS	-	expression tag	UNP Q7N4Z6
A	-10	HIS	-	expression tag	UNP Q7N4Z6
A	-9	SER	-	expression tag	UNP Q7N4Z6
A	-8	SER	-	expression tag	UNP Q7N4Z6
A	-7	GLY	-	expression tag	UNP Q7N4Z6
A	-6	LEU	-	expression tag	UNP Q7N4Z6
A	-5	VAL	-	expression tag	UNP Q7N4Z6
A	-4	PRO	-	expression tag	UNP Q7N4Z6
A	-3	ARG	-	expression tag	UNP Q7N4Z6
A	-2	GLY	-	expression tag	UNP Q7N4Z6
A	-1	SER	-	expression tag	UNP Q7N4Z6
A	0	HIS	-	expression tag	UNP Q7N4Z6
B	-19	MSE	-	expression tag	UNP Q7N4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q7N4Z6
B	-17	SER	-	expression tag	UNP Q7N4Z6
B	-16	SER	-	expression tag	UNP Q7N4Z6
B	-15	HIS	-	expression tag	UNP Q7N4Z6
B	-14	HIS	-	expression tag	UNP Q7N4Z6
B	-13	HIS	-	expression tag	UNP Q7N4Z6
B	-12	HIS	-	expression tag	UNP Q7N4Z6
B	-11	HIS	-	expression tag	UNP Q7N4Z6
B	-10	HIS	-	expression tag	UNP Q7N4Z6
B	-9	SER	-	expression tag	UNP Q7N4Z6
B	-8	SER	-	expression tag	UNP Q7N4Z6
B	-7	GLY	-	expression tag	UNP Q7N4Z6
B	-6	LEU	-	expression tag	UNP Q7N4Z6
B	-5	VAL	-	expression tag	UNP Q7N4Z6
B	-4	PRO	-	expression tag	UNP Q7N4Z6
B	-3	ARG	-	expression tag	UNP Q7N4Z6
B	-2	GLY	-	expression tag	UNP Q7N4Z6
B	-1	SER	-	expression tag	UNP Q7N4Z6
B	0	HIS	-	expression tag	UNP Q7N4Z6
C	-19	MSE	-	expression tag	UNP Q7N4Z6
C	-18	GLY	-	expression tag	UNP Q7N4Z6
C	-17	SER	-	expression tag	UNP Q7N4Z6
C	-16	SER	-	expression tag	UNP Q7N4Z6
C	-15	HIS	-	expression tag	UNP Q7N4Z6
C	-14	HIS	-	expression tag	UNP Q7N4Z6
C	-13	HIS	-	expression tag	UNP Q7N4Z6
C	-12	HIS	-	expression tag	UNP Q7N4Z6
C	-11	HIS	-	expression tag	UNP Q7N4Z6
C	-10	HIS	-	expression tag	UNP Q7N4Z6
C	-9	SER	-	expression tag	UNP Q7N4Z6
C	-8	SER	-	expression tag	UNP Q7N4Z6
C	-7	GLY	-	expression tag	UNP Q7N4Z6
C	-6	LEU	-	expression tag	UNP Q7N4Z6
C	-5	VAL	-	expression tag	UNP Q7N4Z6
C	-4	PRO	-	expression tag	UNP Q7N4Z6
C	-3	ARG	-	expression tag	UNP Q7N4Z6
C	-2	GLY	-	expression tag	UNP Q7N4Z6
C	-1	SER	-	expression tag	UNP Q7N4Z6
C	0	HIS	-	expression tag	UNP Q7N4Z6
D	-19	MSE	-	expression tag	UNP Q7N4Z6
D	-18	GLY	-	expression tag	UNP Q7N4Z6
D	-17	SER	-	expression tag	UNP Q7N4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q7N4Z6
D	-15	HIS	-	expression tag	UNP Q7N4Z6
D	-14	HIS	-	expression tag	UNP Q7N4Z6
D	-13	HIS	-	expression tag	UNP Q7N4Z6
D	-12	HIS	-	expression tag	UNP Q7N4Z6
D	-11	HIS	-	expression tag	UNP Q7N4Z6
D	-10	HIS	-	expression tag	UNP Q7N4Z6
D	-9	SER	-	expression tag	UNP Q7N4Z6
D	-8	SER	-	expression tag	UNP Q7N4Z6
D	-7	GLY	-	expression tag	UNP Q7N4Z6
D	-6	LEU	-	expression tag	UNP Q7N4Z6
D	-5	VAL	-	expression tag	UNP Q7N4Z6
D	-4	PRO	-	expression tag	UNP Q7N4Z6
D	-3	ARG	-	expression tag	UNP Q7N4Z6
D	-2	GLY	-	expression tag	UNP Q7N4Z6
D	-1	SER	-	expression tag	UNP Q7N4Z6
D	0	HIS	-	expression tag	UNP Q7N4Z6

- Molecule 2 is water.

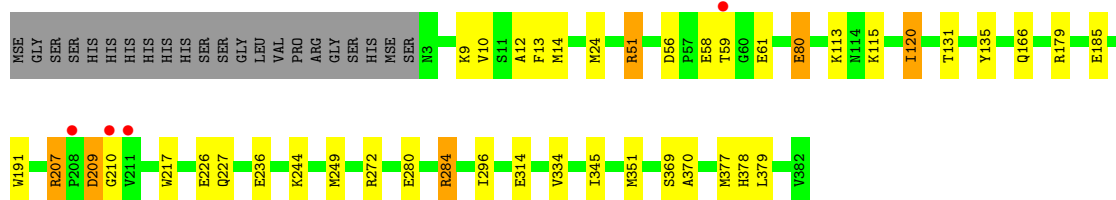
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	193	Total O 193 193	0	0
2	B	72	Total O 72 72	0	0
2	C	84	Total O 84 84	0	0
2	D	177	Total O 177 177	0	0

3 Residue-property plots [i](#)

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

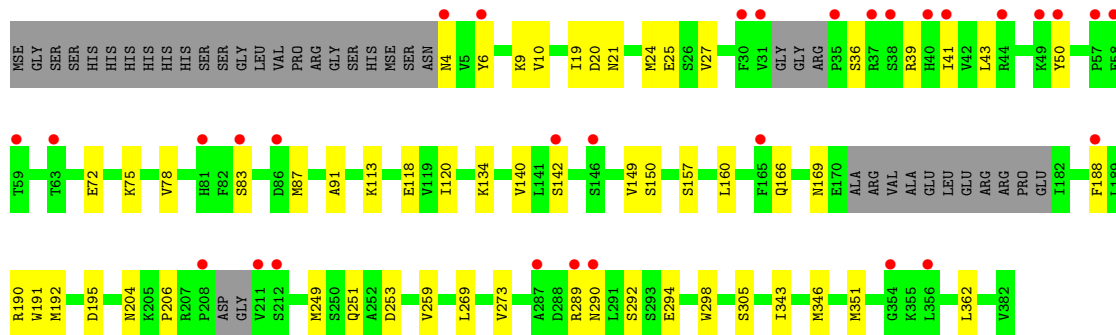
• Molecule 1: Ketosynthase StID

Chain A: 



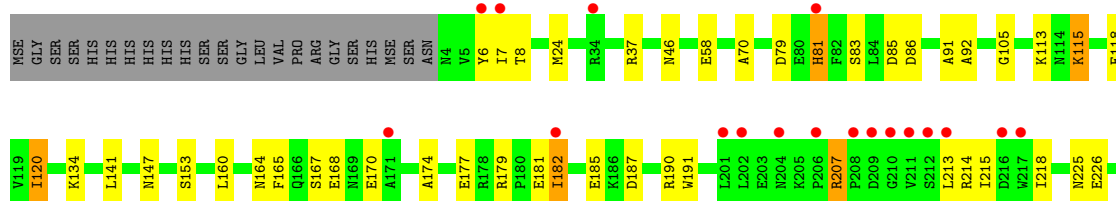
• Molecule 1: Ketosynthase StID

Chain B: 



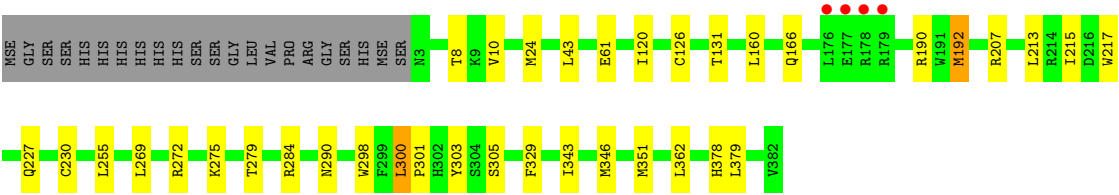
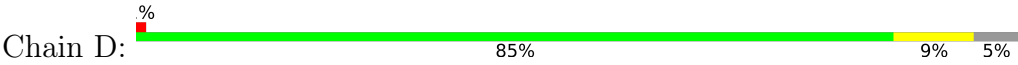
• Molecule 1: Ketosynthase StID

Chain C: 





● Molecule 1: Ketosynthase StID



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.22Å 127.71Å 108.02Å 90.00° 91.39° 90.00°	Depositor
Resolution (Å)	41.73 – 2.33 41.73 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.73-2.33) 99.5 (41.73-2.33)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.22 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.186 , 0.227 0.187 , 0.227	Depositor DCC
R_{free} test set	3637 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12283	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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

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

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	0.40	0/3015	0.58	0/4056
1	B	0.34	0/2880	0.55	0/3870
1	C	0.35	0/3007	0.54	0/4045
1	D	0.40	0/3015	0.56	0/4056
All	All	0.37	0/11917	0.56	0/16027

There are no bond length outliers.

There are no bond angle outliers.

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	2974	0	2906	26	0
1	B	2843	0	2778	31	0
1	C	2966	0	2900	41	0
1	D	2974	0	2906	18	0
2	A	193	0	0	2	0
2	B	72	0	0	0	0
2	C	84	0	0	0	0
2	D	177	0	0	0	0
All	All	12283	0	11490	110	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 5.

All (110) 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:C:218:ILE:HG12	1:C:377:MSE:HG3	1.53	0.88
1:B:249:MSE:HE1	1:B:259:VAL:HG21	1.67	0.76
1:B:24:MSE:HE3	1:B:191:TRP:CE3	2.24	0.73
1:B:251:GLN:HG3	1:C:164:ASN:ND2	2.07	0.69
1:B:87:MSE:HE2	1:B:149:VAL:HG21	1.76	0.67
1:B:36:SER:HB3	1:B:39:ARG:HB2	1.81	0.63
1:A:226:GLU:HB2	2:A:559:HOH:O	2.00	0.62
1:C:286:VAL:HA	1:C:291:LEU:HD12	1.82	0.61
1:B:160:LEU:HD22	1:B:190:ARG:HA	1.81	0.61
1:B:157:SER:OG	1:B:195:ASP:OD2	2.19	0.60
1:A:10:VAL:HG21	1:A:351:MSE:HE1	1.84	0.59
1:A:236:GLU:HG2	1:A:249:MSE:HE1	1.84	0.59
1:B:10:VAL:HG21	1:B:351:MSE:HE1	1.85	0.59
1:D:343:ILE:HA	1:D:346:MSE:HE3	1.85	0.59
1:C:298:TRP:HB2	1:C:362:LEU:HG	1.83	0.59
1:A:80:GLU:H	1:A:80:GLU:CD	2.10	0.58
1:C:160:LEU:HD22	1:C:190:ARG:HA	1.85	0.58
1:A:13:PHE:C	1:A:14:MSE:HE2	2.29	0.58
1:B:134:LYS:NZ	1:C:118:GLU:OE1	2.32	0.57
1:C:177:GLU:OE1	1:C:179:ARG:NH2	2.35	0.57
1:B:24:MSE:HE3	1:B:191:TRP:HE3	1.70	0.57
1:C:70:ALA:HB2	1:C:153:SER:HB3	1.87	0.56
1:A:56:ASP:OD1	1:A:58:GLU:HG2	2.05	0.56
1:B:249:MSE:CE	1:B:259:VAL:HG21	2.36	0.56
1:A:227:GLN:OE1	1:A:272:ARG:HD3	2.06	0.55
1:C:6:TYR:CD2	1:C:214:ARG:HB2	2.40	0.55
1:B:118:GLU:OE1	1:C:134:LYS:NZ	2.39	0.55
1:C:6:TYR:HD2	1:C:214:ARG:HB2	1.72	0.55
1:A:14:MSE:HE1	1:A:345:ILE:HG12	1.88	0.55
1:B:249:MSE:HE1	1:B:259:VAL:CG2	2.35	0.55
1:C:79:ASP:OD2	1:C:207:ARG:NH2	2.40	0.54
1:C:230:CYS:HB3	1:C:369:SER:O	2.07	0.54
1:B:6:TYR:CE2	1:B:206:PRO:HG3	2.43	0.54
1:A:59:THR:HG23	1:A:61:GLU:HG2	1.89	0.53
1:D:213:LEU:HD11	1:D:351:MSE:HE2	1.91	0.53
1:B:269:LEU:HD12	1:B:273:VAL:HB	1.91	0.53
1:A:120:ILE:HG13	1:D:131:THR:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:TYR:CZ	1:C:311:LYS:HE3	2.44	0.52
1:C:81:HIS:HB2	1:C:207:ARG:NH2	2.25	0.52
1:A:244:LYS:O	1:A:249:MSE:HE3	2.10	0.52
1:C:289:ARG:HG3	1:C:290:ASN:H	1.74	0.52
1:C:167:SER:HB2	1:C:170:GLU:HB2	1.93	0.51
1:C:85:ASP:HB3	1:C:115:LYS:HD3	1.92	0.51
1:C:165:PHE:HE2	1:C:182:ILE:HD13	1.76	0.51
1:C:285:ILE:HG22	1:C:291:LEU:HD11	1.93	0.49
1:A:131:THR:HB	1:D:120:ILE:HG13	1.93	0.49
1:B:142:SER:HB2	1:C:141:LEU:HD23	1.94	0.49
1:C:83:SER:HB3	1:C:86:ASP:OD2	2.12	0.49
1:A:209:ASP:OD1	1:A:209:ASP:N	2.45	0.49
1:B:19:ILE:HD13	1:B:27:VAL:HG21	1.95	0.49
1:C:293:SER:HA	1:C:296:ILE:HD13	1.95	0.49
1:B:78:VAL:HG13	1:B:83:SER:HA	1.94	0.49
1:B:343:ILE:HA	1:B:346:MSE:HE3	1.95	0.49
1:B:249:MSE:HE3	1:B:253:ASP:HB3	1.95	0.48
1:D:227:GLN:OE1	1:D:272:ARG:HD3	2.14	0.48
1:C:331:ASN:HB2	1:C:335:LYS:HG2	1.96	0.48
1:B:72:GLU:OE2	1:B:75:LYS:NZ	2.39	0.48
1:A:51:ARG:HD3	2:A:557:HOH:O	2.14	0.48
1:C:165:PHE:CE2	1:C:182:ILE:HD13	2.49	0.47
1:B:188:PHE:CZ	1:B:192:MSE:HE3	2.49	0.47
1:C:46:ASN:HA	1:C:305:SER:OG	2.14	0.47
1:C:24:MSE:HE2	1:C:191:TRP:HE3	1.80	0.47
1:B:20:ASP:HB3	1:B:50:TYR:CE1	2.49	0.47
1:D:217:TRP:CZ2	1:D:378:HIS:HB2	2.50	0.47
1:A:236:GLU:HG2	1:A:249:MSE:CE	2.45	0.46
1:C:7:ILE:N	1:C:213:LEU:O	2.48	0.46
1:B:292:SER:HB3	1:B:294:GLU:OE2	2.16	0.46
1:A:9:LYS:HD3	1:A:207:ARG:HH22	1.81	0.45
1:B:298:TRP:HB2	1:B:362:LEU:HG	1.99	0.45
1:C:182:ILE:HD11	1:C:187:ASP:CG	2.41	0.45
1:D:24:MSE:SE	1:D:43:LEU:HD21	2.67	0.44
1:A:12:ALA:HB1	1:A:14:MSE:CE	2.47	0.44
1:A:369:SER:O	1:A:370:ALA:C	2.61	0.44
1:C:168:GLU:HB2	1:C:256:ALA:HA	1.99	0.44
1:A:280:GLU:OE1	1:A:284:ARG:NH2	2.51	0.44
1:A:10:VAL:CG2	1:A:351:MSE:HE1	2.46	0.44
1:D:192:MSE:HB3	1:D:192:MSE:HE3	1.56	0.44
1:D:300:LEU:HD22	1:D:329:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:ARG:CG	1:C:290:ASN:H	2.30	0.43
1:B:25:GLU:OE2	1:B:36:SER:N	2.49	0.43
1:D:303:TYR:O	1:D:305:SER:N	2.48	0.43
1:C:377:MSE:SE	1:C:379:LEU:HD21	2.68	0.43
1:D:275:LYS:HA	1:D:279:THR:OG1	2.18	0.43
1:D:351:MSE:HE3	1:D:351:MSE:HB2	1.58	0.43
1:B:21:ASN:HB3	1:B:43:LEU:HD13	2.00	0.42
1:A:244:LYS:HB3	1:A:249:MSE:HE2	2.01	0.42
1:C:92:ALA:HB3	1:C:105:GLY:HA2	2.01	0.42
1:A:135:TYR:C	1:A:135:TYR:CD1	2.98	0.42
1:B:91:ALA:O	1:B:150:SER:HA	2.20	0.42
1:B:192:MSE:HE2	1:B:192:MSE:HB2	1.82	0.42
1:C:91:ALA:HA	1:C:120:ILE:HG13	2.02	0.42
1:B:140:VAL:CG1	1:B:204:ASN:HB3	2.50	0.41
1:C:215:ILE:HA	1:C:379:LEU:HD23	2.02	0.41
1:D:8:THR:HB	1:D:207:ARG:HG2	2.02	0.41
1:B:21:ASN:O	1:B:39:ARG:NH1	2.53	0.41
1:C:8:THR:HB	1:C:207:ARG:HD3	2.01	0.41
1:C:174:ALA:HB2	1:C:181:GLU:HB3	2.02	0.41
1:A:24:MSE:HE3	1:A:51:ARG:HD2	2.01	0.41
1:D:230:CYS:SG	1:D:269:LEU:HB2	2.60	0.41
1:C:294:GLU:H	1:C:294:GLU:CD	2.28	0.41
1:A:217:TRP:CZ2	1:A:378:HIS:HB2	2.56	0.41
1:C:225:ASN:ND2	1:C:226:GLU:HG2	2.36	0.41
1:D:10:VAL:HG21	1:D:351:MSE:HE1	2.02	0.41
1:C:331:ASN:OD1	1:C:331:ASN:N	2.52	0.41
1:D:160:LEU:HD22	1:D:190:ARG:HA	2.02	0.41
1:A:24:MSE:HE2	1:A:191:TRP:HE3	1.85	0.40
1:D:215:ILE:HA	1:D:379:LEU:HD23	2.03	0.40
1:D:298:TRP:HB2	1:D:362:LEU:HG	2.03	0.40
1:A:377:MSE:SE	1:A:379:LEU:HD21	2.72	0.40
1:C:147:ASN:OD1	1:C:147:ASN:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	377/402 (94%)	363 (96%)	13 (3%)	1 (0%)	36	41
1	B	354/402 (88%)	331 (94%)	21 (6%)	2 (1%)	21	22
1	C	376/402 (94%)	355 (94%)	21 (6%)	0	100	100
1	D	377/402 (94%)	366 (97%)	10 (3%)	1 (0%)	36	41
All	All	1484/1608 (92%)	1415 (95%)	65 (4%)	4 (0%)	36	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	290	ASN
1	B	113	LYS
1	A	210	GLY
1	D	301	PRO

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	321/325 (99%)	307 (96%)	14 (4%)	25	33
1	B	309/325 (95%)	301 (97%)	8 (3%)	40	53
1	C	320/325 (98%)	306 (96%)	14 (4%)	25	33
1	D	321/325 (99%)	314 (98%)	7 (2%)	45	58
All	All	1271/1300 (98%)	1228 (97%)	43 (3%)	32	42

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	80	GLU

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Mol	Chain	Res	Type
1	A	113	LYS
1	A	115	LYS
1	A	120	ILE
1	A	166	GLN
1	A	179	ARG
1	A	185	GLU
1	A	207	ARG
1	A	209	ASP
1	A	284	ARG
1	A	296	ILE
1	A	314	GLU
1	A	334	VAL
1	B	4	ASN
1	B	9	LYS
1	B	41	ILE
1	B	120	ILE
1	B	166	GLN
1	B	169	ASN
1	B	289	ARG
1	B	305	SER
1	C	37	ARG
1	C	58	GLU
1	C	81	HIS
1	C	113	LYS
1	C	115	LYS
1	C	120	ILE
1	C	182	ILE
1	C	185	GLU
1	C	207	ARG
1	C	263	LYS
1	C	293	SER
1	C	295	SER
1	C	331	ASN
1	C	373	THR
1	D	61	GLU
1	D	166	GLN
1	D	192	MSE
1	D	255	LEU
1	D	284	ARG
1	D	290	ASN
1	D	300	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
1	B	99	GLN
1	C	164	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSD	C	126	1	4,7,8	0.81	0	1,8,10	0.55	0
1	CSD	B	126	1	4,7,8	1.01	0	1,8,10	0.30	0
1	CSD	A	126	1	4,7,8	0.86	0	1,8,10	1.51	0
1	CSD	D	126	1	4,7,8	1.11	0	1,8,10	2.54	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	C	126	1	-	1/2/6/8	-
1	CSD	B	126	1	-	1/2/6/8	-
1	CSD	A	126	1	-	1/2/6/8	-
1	CSD	D	126	1	-	1/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	126	CSD	OD1-SG-CB	2.54	110.27	105.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	126	CSD	CA-CB-SG-OD1
1	B	126	CSD	CA-CB-SG-OD1
1	C	126	CSD	CA-CB-SG-OD1
1	D	126	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

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	366/402 (91%)	-0.29	4 (1%) 78 81	14, 25, 44, 68	0
1	B	349/402 (86%)	0.56	31 (8%) 15 18	20, 41, 62, 74	0
1	C	365/402 (90%)	0.65	36 (9%) 13 15	18, 41, 66, 78	0
1	D	366/402 (91%)	-0.24	4 (1%) 78 81	12, 26, 47, 82	0
All	All	1446/1608 (89%)	0.17	75 (5%) 33 39	12, 32, 61, 82	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	TRP	5.7
1	B	290	ASN	4.7
1	B	208	PRO	4.3
1	D	176	LEU	4.3
1	B	40	HIS	3.5
1	B	86	ASP	3.2
1	B	211	VAL	3.1
1	B	41	ILE	3.1
1	B	289	ARG	3.0
1	C	216	ASP	3.0
1	A	210	GLY	2.9
1	C	286	VAL	2.9
1	C	209	ASP	2.9
1	C	321	PHE	2.9
1	B	38	SER	2.8
1	B	30	PHE	2.8
1	D	179	ARG	2.8
1	B	83	SER	2.8
1	C	212	SER	2.7
1	C	289	ARG	2.7
1	C	362	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	142	SER	2.7
1	B	4	ASN	2.7
1	C	211	VAL	2.6
1	B	44	ARG	2.6
1	A	211	VAL	2.6
1	B	35	PRO	2.6
1	C	381	VAL	2.6
1	C	202	LEU	2.6
1	D	178	ARG	2.6
1	A	59	THR	2.6
1	C	213	LEU	2.5
1	C	300	LEU	2.5
1	C	379	LEU	2.5
1	C	208	PRO	2.5
1	C	182	ILE	2.5
1	C	382	VAL	2.4
1	B	6	TYR	2.4
1	B	57	PRO	2.4
1	C	6	TYR	2.4
1	B	37	ARG	2.4
1	B	31	VAL	2.4
1	C	354	GLY	2.4
1	C	292	SER	2.4
1	B	58	GLU	2.4
1	B	354	GLY	2.3
1	B	81	HIS	2.3
1	C	34	ARG	2.3
1	C	206	PRO	2.3
1	B	212	SER	2.3
1	B	50	TYR	2.3
1	C	287	ALA	2.3
1	D	177	GLU	2.3
1	C	290	ASN	2.2
1	C	210	GLY	2.2
1	C	298	TRP	2.2
1	B	356	LEU	2.2
1	C	378	HIS	2.2
1	B	188	PHE	2.2
1	B	146	SER	2.2
1	C	7	ILE	2.1
1	B	287	ALA	2.1
1	C	201	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	291	LEU	2.1
1	C	314	GLU	2.1
1	C	81	HIS	2.1
1	B	63	THR	2.1
1	C	295	SER	2.1
1	C	204	ASN	2.1
1	B	49	LYS	2.0
1	B	59	THR	2.0
1	C	171	ALA	2.0
1	C	319	ILE	2.0
1	A	208	PRO	2.0
1	B	165	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	CSD	C	126	8/9	0.96	0.08	28,31,33,44	0
1	CSD	B	126	8/9	0.97	0.06	21,24,31,40	0
1	CSD	A	126	8/9	0.97	0.06	14,18,22,25	0
1	CSD	D	126	8/9	0.97	0.06	18,18,25,37	0

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.