



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 06:18 AM EDT

PDB ID : 5GK0  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

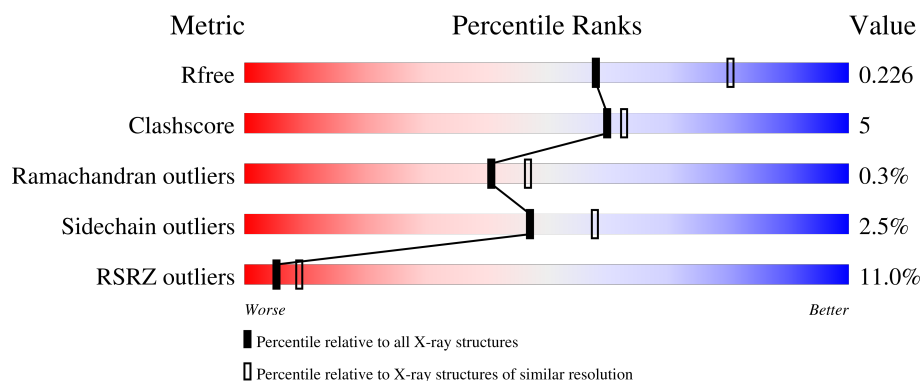
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (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  $\geq 3$ , 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	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </div> </div>
1	B	402	<div> <div>12%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>10%</div> </div> </div>
1	C	402	<div> <div>18%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>6%</div> </div> </div>
1	D	402	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </div> </div>

## 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

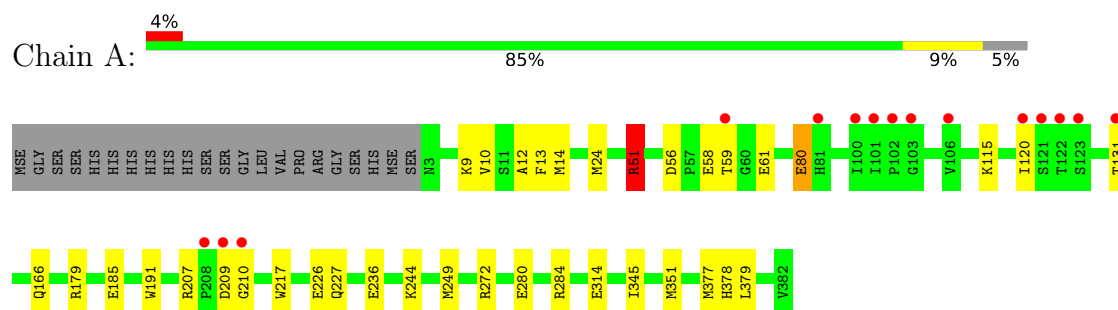
- Molecule 2 is water.

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

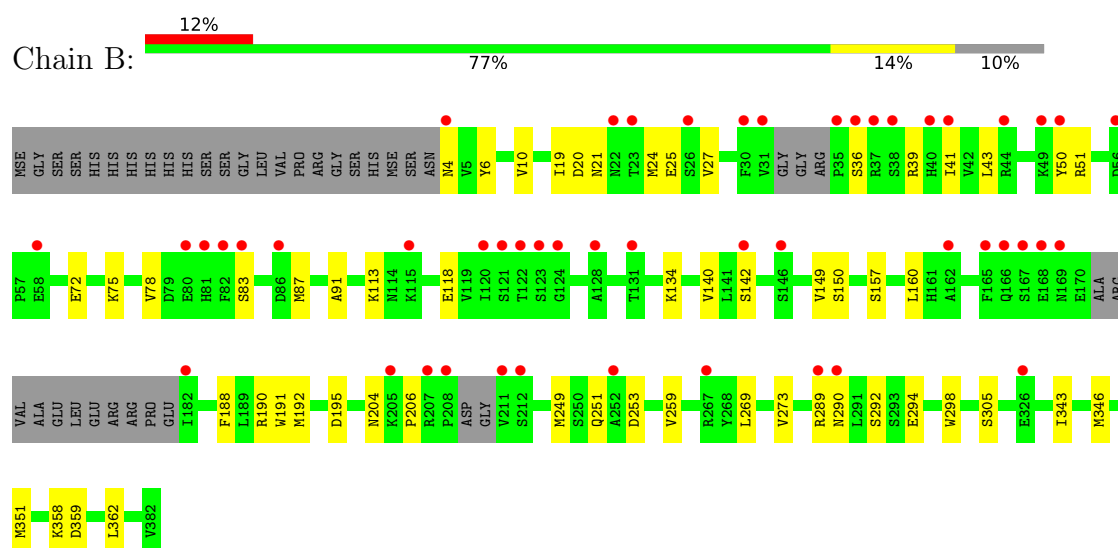
### 3 Residue-property plots [i](#)

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.

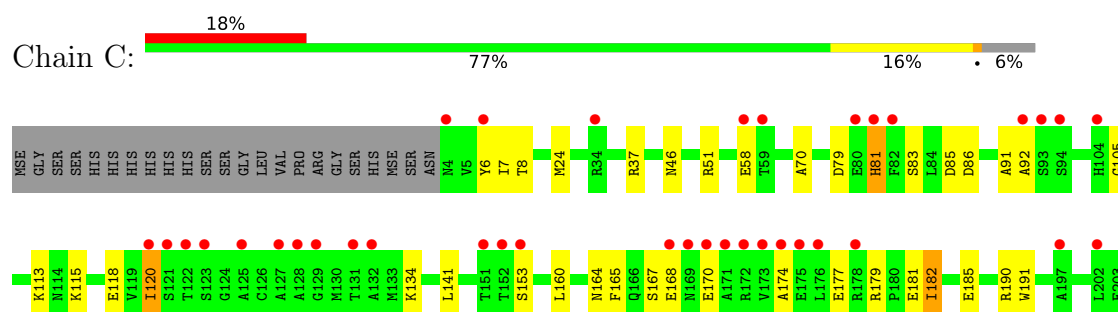
#### • Molecule 1: Ketosynthase StID

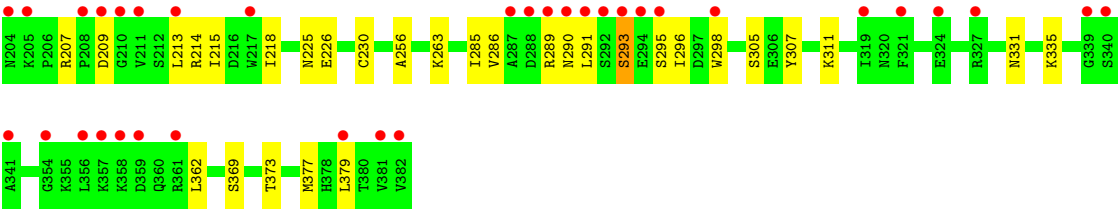


#### • Molecule 1: Ketosynthase StID

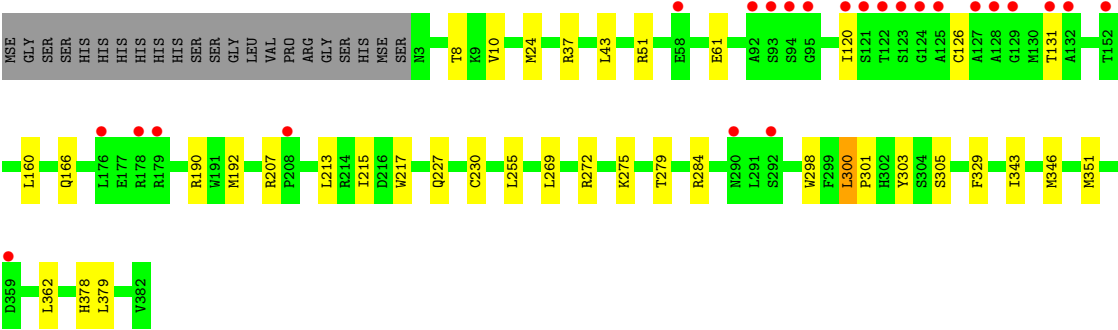
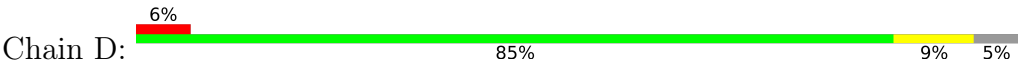


#### • Molecule 1: Ketosynthase StID





● Molecule 1: Ketosynthase StId



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 99.6 (41.73-2.33)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.22 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, $R_{free}$	0.186 , 0.227 0.186 , 0.226	Depositor DCC
$R_{free}$ test set	3637 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.9	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.44	0/3015	0.62	1/4056 (0.0%)
1	B	0.38	0/2880	0.56	0/3870
1	C	0.40	0/3007	0.55	0/4045
1	D	0.43	0/3015	0.58	0/4056
All	All	0.41	0/11917	0.58	1/16027 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	ARG	NE-CZ-NH2	-6.43	117.09	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	24	0
1	B	2843	0	2778	32	0
1	C	2966	0	2900	39	0
1	D	2974	0	2906	18	0
2	A	193	0	0	2	0
2	B	72	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	84	0	0	0	0
2	D	177	0	0	0	0
All	All	12283	0	11490	107	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 (107) 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: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:C:160:LEU:HD22	1:C:190:ARG:HA	1.85	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:A:80:GLU:H	1:A:80:GLU:CD	2.10	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:13:PHE:C	1:A:14:MSE:HE2	2.29	0.53
1:A:120:ILE:HG13	1:D:131:THR:HB	1.91	0.53
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:B:157:SER:OG	1:B:195:ASP:OD2	2.19	0.50
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: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:C:168:GLU:HB2	1:C:256:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:182:ILE:O	1:C:182:ILE:HG13	2.18	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: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: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:B:358:LYS:O	1:B:359:ASP:HB2	2.21	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%)	41	47
1	B	354/402 (88%)	331 (94%)	21 (6%)	2 (1%)	25	26
1	C	376/402 (94%)	355 (94%)	21 (6%)	0	100	100
1	D	377/402 (94%)	366 (97%)	10 (3%)	1 (0%)	41	47
All	All	1484/1608 (92%)	1415 (95%)	65 (4%)	4 (0%)	41	47

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%)	314 (98%)	7 (2%)	52	63
1	B	309/325 (95%)	304 (98%)	5 (2%)	62	74
1	C	320/325 (98%)	307 (96%)	13 (4%)	30	38
1	D	321/325 (99%)	314 (98%)	7 (2%)	52	63
All	All	1271/1300 (98%)	1239 (98%)	32 (2%)	47	58

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	80	GLU
1	A	115	LYS
1	A	166	GLN
1	A	179	ARG
1	A	185	GLU
1	A	314	GLU
1	B	4	ASN
1	B	41	ILE
1	B	51	ARG
1	B	289	ARG
1	B	305	SER
1	C	37	ARG
1	C	51	ARG
1	C	58	GLU
1	C	81	HIS
1	C	113	LYS
1	C	120	ILE
1	C	182	ILE
1	C	185	GLU
1	C	209	ASP
1	C	263	LYS
1	C	293	SER
1	C	295	SER
1	C	373	THR
1	D	37	ARG
1	D	51	ARG
1	D	61	GLU
1	D	166	GLN
1	D	255	LEU
1	D	284	ARG
1	D	300	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
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	D	126	1	3,7,8	0.66	0	1,8,10	2.49	1 (100%)
1	CSD	C	126	1	3,7,8	0.73	0	1,8,10	0.50	0
1	CSD	A	126	1	3,7,8	0.58	0	1,8,10	1.50	0
1	CSD	B	126	1	3,7,8	0.65	0	1,8,10	0.32	0

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	D	126	1	-	1/2/6/8	-
1	CSD	C	126	1	-	1/2/6/8	-
1	CSD	A	126	1	-	1/2/6/8	-
1	CSD	B	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	2.49	110.27	105.54

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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	366/402 (91%)	-0.03	15 (4%) 37 48	14, 25, 44, 68	0
1	B	349/402 (86%)	0.72	49 (14%) 2 4	20, 41, 62, 74	0
1	C	365/402 (90%)	0.96	71 (19%) 1 2	18, 41, 66, 78	0
1	D	366/402 (91%)	0.27	24 (6%) 18 26	12, 26, 47, 82	0
All	All	1446/1608 (89%)	0.48	159 (10%) 5 9	12, 32, 61, 82	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	TRP	6.7
1	B	37	ARG	6.6
1	C	209	ASP	5.5
1	D	178	ARG	5.4
1	B	40	HIS	5.2
1	C	122	THR	4.7
1	B	81	HIS	4.7
1	B	31	VAL	4.6
1	B	38	SER	4.6
1	C	80	GLU	4.4
1	C	6	TYR	4.4
1	B	182	ILE	4.3
1	C	290	ASN	4.3
1	B	86	ASP	4.3
1	B	58	GLU	4.3
1	C	128	ALA	4.2
1	C	354	GLY	4.2
1	D	176	LEU	4.1
1	C	289	ARG	4.0
1	C	287	ALA	4.0
1	B	290	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	59	THR	3.8
1	B	169	ASN	3.8
1	C	81	HIS	3.6
1	B	207	ARG	3.6
1	C	204	ASN	3.5
1	B	121	SER	3.5
1	C	298	TRP	3.4
1	C	176	LEU	3.4
1	C	324	GLU	3.4
1	B	26	SER	3.4
1	B	82	PHE	3.4
1	D	125	ALA	3.4
1	B	165	PHE	3.4
1	C	4	ASN	3.4
1	D	122	THR	3.3
1	B	80	GLU	3.3
1	C	178	ARG	3.3
1	C	358	LYS	3.3
1	B	22	ASN	3.2
1	B	211	VAL	3.2
1	C	120	ILE	3.2
1	C	152	THR	3.2
1	C	382	VAL	3.2
1	D	179	ARG	3.2
1	A	100	ILE	3.1
1	B	146	SER	3.1
1	B	36	SER	3.1
1	C	175	GLU	3.1
1	C	294	GLU	3.1
1	C	293	SER	3.1
1	C	321	PHE	3.1
1	C	131	THR	3.1
1	D	128	ALA	3.1
1	D	132	ALA	3.1
1	C	292	SER	3.0
1	A	208	PRO	3.0
1	B	44	ARG	3.0
1	C	82	PHE	2.9
1	B	122	THR	2.9
1	B	41	ILE	2.9
1	D	290	ASN	2.9
1	B	30	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	125	ALA	2.9
1	B	128	ALA	2.9
1	B	212	SER	2.8
1	D	124	GLY	2.8
1	B	83	SER	2.8
1	C	121	SER	2.8
1	D	95	GLY	2.8
1	B	208	PRO	2.8
1	C	208	PRO	2.8
1	C	127	ALA	2.8
1	C	202	LEU	2.8
1	B	123	SER	2.8
1	C	129	GLY	2.8
1	C	211	VAL	2.8
1	B	4	ASN	2.7
1	A	210	GLY	2.7
1	B	252	ALA	2.7
1	B	166	GLN	2.7
1	D	123	SER	2.7
1	B	120	ILE	2.7
1	C	357	LYS	2.7
1	C	123	SER	2.7
1	B	205	LYS	2.6
1	C	92	ALA	2.6
1	A	103	GLY	2.6
1	A	102	PRO	2.6
1	D	129	GLY	2.6
1	A	121	SER	2.6
1	B	167	SER	2.6
1	A	106	VAL	2.6
1	C	172	ARG	2.5
1	D	359	ASP	2.5
1	D	131	THR	2.5
1	C	173	VAL	2.5
1	D	127	ALA	2.5
1	C	153	SER	2.5
1	B	49	LYS	2.5
1	A	122	THR	2.5
1	C	58	GLU	2.5
1	A	209	ASP	2.5
1	B	35	PRO	2.5
1	D	120	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	131	THR	2.4
1	C	205	LYS	2.4
1	C	93	SER	2.4
1	C	361	ARG	2.4
1	A	101	ILE	2.4
1	C	168	GLU	2.4
1	B	142	SER	2.4
1	C	288	ASP	2.4
1	C	94	SER	2.4
1	C	340	SER	2.4
1	C	171	ALA	2.4
1	C	210	GLY	2.3
1	C	169	ASN	2.3
1	C	341	ALA	2.3
1	C	291	LEU	2.3
1	C	356	LEU	2.3
1	D	94	SER	2.3
1	B	168	GLU	2.3
1	C	174	ALA	2.3
1	D	208	PRO	2.3
1	A	120	ILE	2.3
1	A	123	SER	2.3
1	D	121	SER	2.3
1	D	58	GLU	2.2
1	D	93	SER	2.2
1	C	132	ALA	2.2
1	B	56	ASP	2.2
1	B	162	ALA	2.2
1	C	339	GLY	2.2
1	A	59	THR	2.2
1	A	81	HIS	2.2
1	D	92	ALA	2.2
1	C	327	ARG	2.2
1	B	124	GLY	2.2
1	B	267	ARG	2.2
1	B	289	ARG	2.1
1	C	381	VAL	2.1
1	C	197	ALA	2.1
1	D	152	THR	2.1
1	C	151	THR	2.1
1	C	34	ARG	2.1
1	A	131	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	50	TYR	2.1
1	C	295	SER	2.1
1	D	292	SER	2.1
1	B	23	THR	2.1
1	C	104	HIS	2.0
1	B	326	GLU	2.0
1	C	379	LEU	2.0
1	C	359	ASP	2.0
1	C	170	GLU	2.0
1	C	213	LEU	2.0
1	C	319	ILE	2.0
1	B	115	LYS	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CSD	C	126	8/9	0.97	0.23	28,31,33,44	0
1	CSD	D	126	8/9	0.97	0.22	18,18,25,37	0
1	CSD	A	126	8/9	0.98	0.18	14,18,22,25	0
1	CSD	B	126	8/9	0.98	0.17	21,24,31,40	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.