



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:45 am BST

PDB ID : 5GK2
Title : The structure of the H302A mutant of StlD
Authors : Mori, T.; Dngfeng, Y.; Morita, H.; Abe, I.
Deposited on : 2016-07-03
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

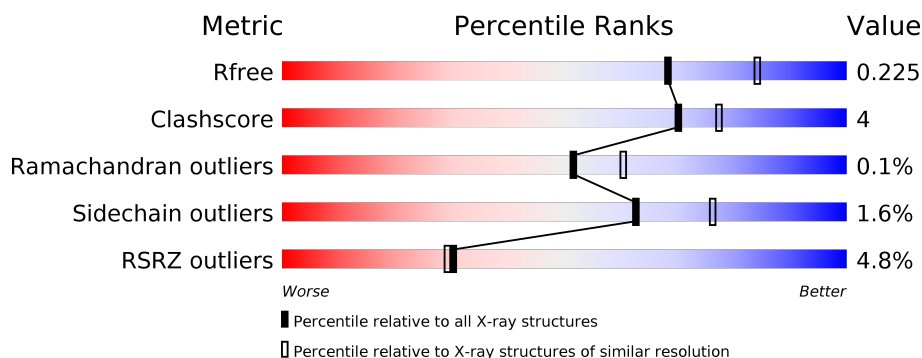
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </div> </div>
1	B	402	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>6%</div> </div> </div>
1	C	402	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>6%</div> </div> </div>
1	D	402	<div> <div>8%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12388 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	0	0	0
			2967	1868	509	572	18			
1	B	379	Total	C	N	O	S	0	0	0
			2959	1864	507	570	18			
1	C	379	Total	C	N	O	S	0	0	0
			2959	1864	507	570	18			
1	D	376	Total	C	N	O	S	0	0	0
			2935	1851	503	563	18			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	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
A	302	ALA	HIS	engineered mutation	UNP Q7N4Z6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP Q7N4Z6
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
B	302	ALA	HIS	engineered mutation	UNP Q7N4Z6
C	-19	MET	-	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
C	302	ALA	HIS	engineered mutation	UNP Q7N4Z6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP Q7N4Z6
D	-18	GLY	-	expression tag	UNP Q7N4Z6
D	-17	SER	-	expression tag	UNP Q7N4Z6
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
D	302	ALA	HIS	engineered mutation	UNP Q7N4Z6

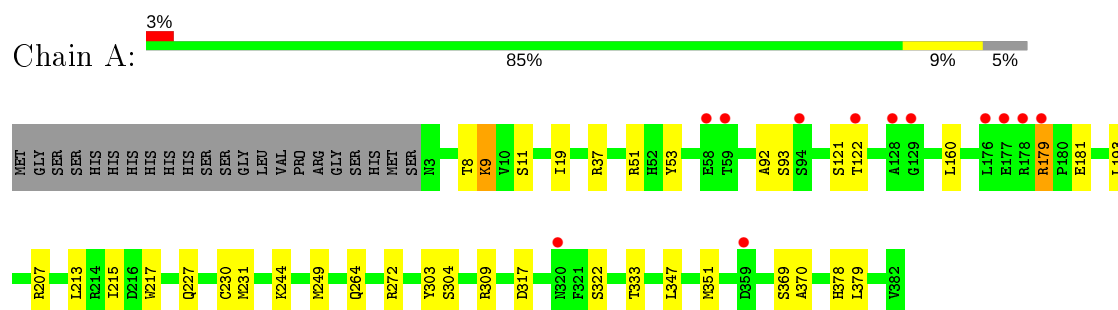
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	163	Total	O	0	0
			163	163		
2	B	179	Total	O	0	0
			179	179		
2	C	123	Total	O	0	0
			123	123		
2	D	103	Total	O	0	0
			103	103		

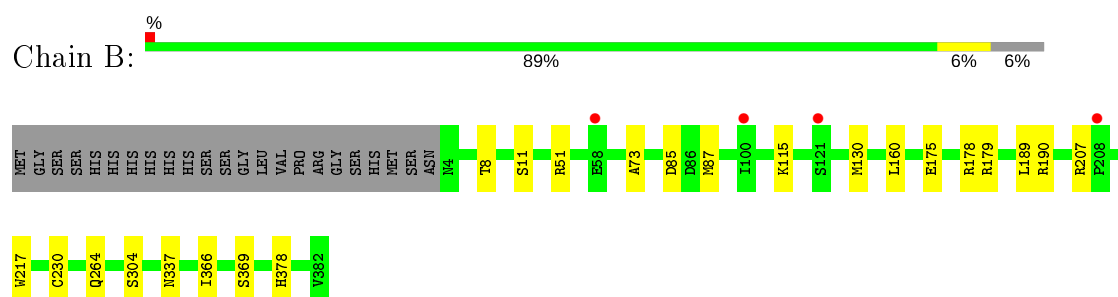
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

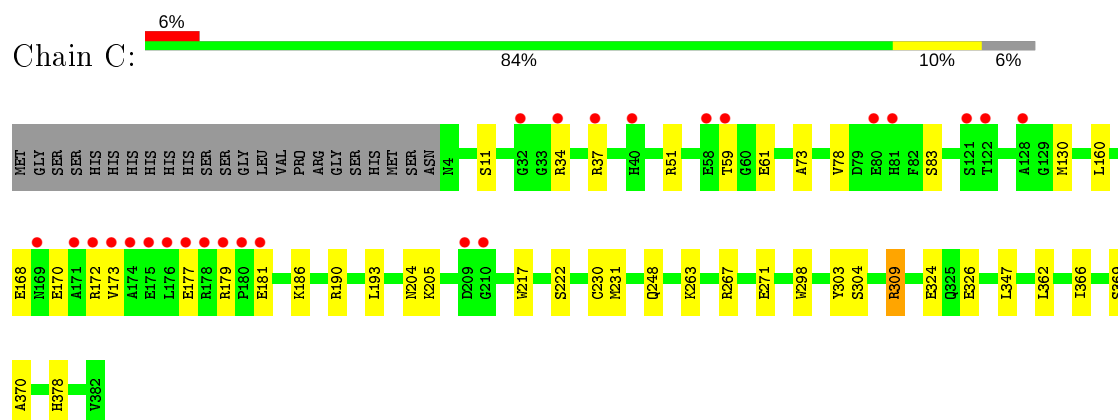
• Molecule 1: Ketosynthase StlD



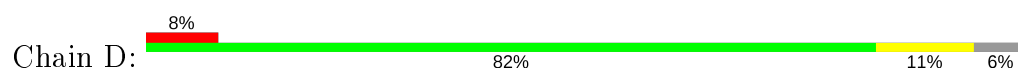
• Molecule 1: Ketosynthase StlD

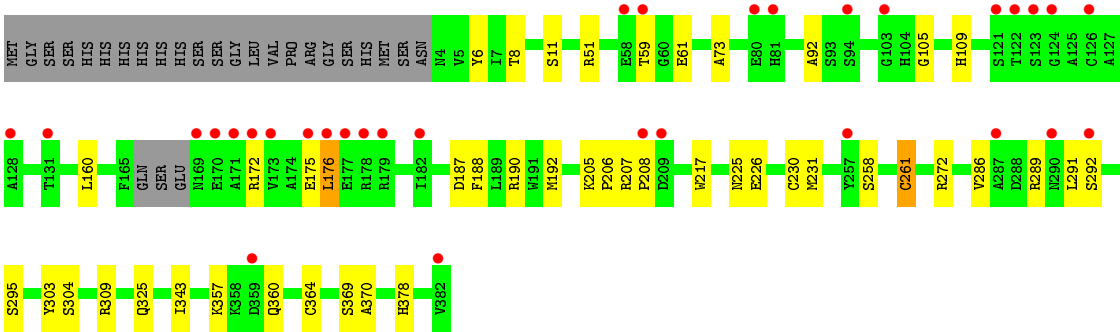


• Molecule 1: Ketosynthase StlD



• Molecule 1: Ketosynthase StlD





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.17Å 127.92Å 108.15Å 90.00° 91.08° 90.00°	Depositor
Resolution (Å)	41.70 – 2.20 41.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (41.70-2.20) 99.7 (41.70-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.174 , 0.224 0.174 , 0.225	Depositor DCC
R_{free} test set	4334 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12388	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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	0.43	1/3028 (0.0%)	0.58	0/4095
1	B	0.43	0/3020	0.59	0/4084
1	C	0.42	0/3020	0.59	1/4084 (0.0%)
1	D	0.40	0/2995	0.58	1/4049 (0.0%)
All	All	0.42	1/12063 (0.0%)	0.58	2/16312 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	ARG	C-N	7.57	1.48	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	37	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	D	176	LEU	CA-CB-CG	5.07	126.95	115.30

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	2967	0	2904	18	0
1	B	2959	0	2898	10	0
1	C	2959	0	2898	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2935	0	2878	28	0
2	A	163	0	0	3	0
2	B	179	0	0	0	0
2	C	123	0	0	1	0
2	D	103	0	0	1	0
All	All	12388	0	11578	85	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 4.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:PHE:O	1:D:192:MET:HG3	1.84	0.77
1:D:286:VAL:HA	1:D:291:LEU:HD13	1.67	0.76
1:C:172:ARG:NH1	1:C:181:GLU:O	2.19	0.75
1:C:177:GLU:HG3	1:C:179:ARG:H	1.53	0.72
1:D:289:ARG:HB2	1:D:291:LEU:HD11	1.70	0.71
1:D:172:ARG:HA	1:D:175:GLU:HG2	1.72	0.71
1:C:34:ARG:HH22	1:C:181:GLU:CD	1.97	0.68
1:C:78:VAL:HG13	1:C:83:SER:HA	1.74	0.67
1:D:289:ARG:HB2	1:D:291:LEU:CD1	2.25	0.65
1:D:59:THR:HG21	1:D:61:GLU:HG3	1.82	0.61
1:D:172:ARG:HD2	1:D:172:ARG:N	2.17	0.60
1:A:303:TYR:OH	1:A:309:ARG:NH1	2.35	0.59
1:C:204:ASN:O	1:C:205:LYS:HG2	2.03	0.58
1:D:230:CYS:HB3	1:D:369:SER:O	2.03	0.58
1:D:258:SER:HB2	1:D:261:CYS:SG	2.44	0.58
1:D:59:THR:CG2	1:D:61:GLU:HG3	2.34	0.57
1:D:225:ASN:ND2	1:D:226:GLU:HG3	2.20	0.56
1:C:168:GLU:O	1:C:172:ARG:HG3	2.04	0.56
1:C:303:TYR:OH	1:C:309:ARG:NH1	2.39	0.56
1:D:175:GLU:HG3	1:D:176:LEU:N	2.22	0.55
1:D:8:THR:HB	1:D:207:ARG:HG3	1.89	0.55
1:C:34:ARG:NH2	1:C:181:GLU:OE2	2.36	0.55
1:C:130:MET:HG3	1:C:366:ILE:HD13	1.89	0.55
1:D:6:TYR:CE2	1:D:206:PRO:HD3	2.43	0.54
1:C:222:SER:OG	1:D:109:HIS:HD2	1.91	0.54
1:C:179:ARG:NH2	1:C:181:GLU:HB2	2.24	0.53
1:D:292:SER:O	1:D:295:SER:OG	2.22	0.53
1:C:177:GLU:HG3	1:C:179:ARG:N	2.22	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:TRP:CZ2	1:D:378:HIS:HB2	2.45	0.51
1:B:8:THR:HB	1:B:207:ARG:HG2	1.92	0.51
1:B:175:GLU:O	1:B:175:GLU:HG3	2.10	0.51
1:B:160:LEU:HD13	1:B:190:ARG:HA	1.93	0.50
1:D:160:LEU:HD22	1:D:190:ARG:HA	1.93	0.50
1:C:179:ARG:HH21	1:C:181:GLU:HB2	1.74	0.50
1:D:11:SER:OG	1:D:73:ALA:O	2.30	0.50
1:D:217:TRP:CE2	1:D:378:HIS:HB2	2.47	0.49
1:C:217:TRP:CZ2	1:C:378:HIS:HB2	2.48	0.48
1:A:37:ARG:NH1	1:A:181:GLU:OE2	2.43	0.47
1:A:213:LEU:HD11	1:A:351:MET:HG3	1.95	0.47
1:C:324:GLU:HG3	1:C:326:GLU:HG3	1.97	0.47
1:A:230:CYS:HB3	1:A:369:SER:O	2.15	0.46
1:C:186:LYS:HG2	1:C:263:LYS:HG2	1.97	0.46
1:B:85:ASP:O	1:B:115:LYS:HE2	2.15	0.46
1:D:261:CYS:HB2	2:D:457:HOH:O	2.14	0.46
1:B:130:MET:HG3	1:B:366:ILE:HD13	1.97	0.46
1:B:304:SER:HB2	1:B:337:ASN:ND2	2.31	0.46
1:A:244:LYS:NZ	2:A:404:HOH:O	2.48	0.45
1:D:309:ARG:NH1	1:D:325:GLN:OE1	2.47	0.45
1:C:160:LEU:HD22	1:C:190:ARG:HA	1.98	0.45
1:D:231:MET:HB3	1:D:370:ALA:HA	1.99	0.45
1:C:179:ARG:HH21	1:C:181:GLU:CD	2.20	0.45
1:C:298:TRP:HB2	1:C:362:LEU:HG	1.98	0.44
1:C:181:GLU:OE1	1:C:181:GLU:N	2.50	0.44
1:C:248:GLN:NE2	2:C:403:HOH:O	2.45	0.44
1:A:179:ARG:NH2	2:A:402:HOH:O	2.46	0.43
1:B:230:CYS:HB3	1:B:369:SER:O	2.18	0.43
1:D:357:LYS:N	1:D:360:GLN:OE1	2.39	0.43
1:C:177:GLU:HG2	1:C:179:ARG:O	2.18	0.43
1:C:267:ARG:O	1:C:271:GLU:HG3	2.18	0.43
1:A:217:TRP:CZ2	1:A:378:HIS:HB2	2.54	0.43
1:D:192:MET:HB3	1:D:192:MET:HE3	1.90	0.43
1:C:11:SER:OG	1:C:73:ALA:O	2.34	0.43
1:A:8:THR:HB	1:A:207:ARG:HG2	2.01	0.43
1:A:9:LYS:HD3	2:A:415:HOH:O	2.18	0.43
1:C:170:GLU:HA	1:C:173:VAL:HG22	2.00	0.43
1:C:160:LEU:HD11	1:C:193:LEU:HB2	1.99	0.42
1:C:324:GLU:HG3	1:C:326:GLU:H	1.84	0.42
1:D:343:ILE:HD11	1:D:364:CYS:HB3	2.01	0.42
1:A:244:LYS:HD3	1:A:249:MET:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:SER:HB3	1:A:122:THR:OG1	2.20	0.42
1:D:205:LYS:HA	1:D:205:LYS:HD3	1.94	0.42
1:B:189:LEU:HD11	1:B:264:GLN:HB2	2.02	0.41
1:B:11:SER:OG	1:B:73:ALA:O	2.37	0.41
1:C:230:CYS:HB3	1:C:369:SER:O	2.20	0.41
1:A:231:MET:HB3	1:A:370:ALA:HA	2.02	0.41
1:A:92:ALA:O	1:A:121:SER:HA	2.20	0.41
1:C:231:MET:HB3	1:C:370:ALA:HA	2.01	0.41
1:B:217:TRP:CZ2	1:B:378:HIS:HB2	2.55	0.41
1:C:59:THR:HB	1:C:61:GLU:H	1.85	0.41
1:A:227:GLN:OE1	1:A:272:ARG:HD3	2.21	0.40
1:A:160:LEU:HD11	1:A:193:LEU:HB2	2.03	0.40
1:A:215:ILE:HA	1:A:379:LEU:HD23	2.04	0.40
1:A:317:ASP:OD1	1:A:322:SER:OG	2.27	0.40
1:A:19:ILE:HD12	1:A:53:TYR:HD2	1.87	0.40
1:D:92:ALA:HB3	1:D:105:GLY:HA2	2.03	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	378/402 (94%)	366 (97%)	12 (3%)	0	100	100
1	B	377/402 (94%)	365 (97%)	12 (3%)	0	100	100
1	C	377/402 (94%)	362 (96%)	15 (4%)	0	100	100
1	D	372/402 (92%)	354 (95%)	17 (5%)	1 (0%)	41	46
All	All	1504/1608 (94%)	1447 (96%)	56 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	208	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	321/340 (94%)	314 (98%)	7 (2%)	52	65
1	B	320/340 (94%)	316 (99%)	4 (1%)	69	81
1	C	320/340 (94%)	316 (99%)	4 (1%)	69	81
1	D	317/340 (93%)	311 (98%)	6 (2%)	57	71
All	All	1278/1360 (94%)	1257 (98%)	21 (2%)	62	76

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	11	SER
1	A	51	ARG
1	A	264	GLN
1	A	304	SER
1	A	333	THR
1	A	347	LEU
1	B	51	ARG
1	B	87	MET
1	B	178	ARG
1	B	179	ARG
1	C	51	ARG
1	C	304	SER
1	C	309	ARG
1	C	347	LEU
1	D	51	ARG
1	D	187	ASP
1	D	261	CYS
1	D	272	ARG
1	D	303	TYR
1	D	304	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	270	ASN
1	D	109	HIS
1	D	164	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 carbohydrates 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	380/402 (94%)	-0.07	12 (3%) 47 45	21, 33, 52, 81	0
1	B	379/402 (94%)	-0.35	4 (1%) 80 79	22, 30, 46, 73	0
1	C	379/402 (94%)	0.09	25 (6%) 18 17	26, 38, 70, 102	0
1	D	376/402 (93%)	0.31	32 (8%) 10 9	24, 41, 64, 86	0
All	All	1514/1608 (94%)	-0.01	73 (4%) 30 29	21, 35, 61, 102	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	176	LEU	8.2
1	A	178	ARG	6.8
1	A	179	ARG	6.6
1	A	176	LEU	6.2
1	C	178	ARG	6.0
1	D	176	LEU	5.9
1	C	174	ALA	5.3
1	D	209	ASP	4.5
1	D	173	VAL	4.4
1	D	171	ALA	4.4
1	C	175	GLU	4.2
1	D	175	GLU	3.8
1	D	169	ASN	3.7
1	D	59	THR	3.6
1	C	181	GLU	3.5
1	D	178	ARG	3.4
1	C	173	VAL	3.4
1	C	210	GLY	3.3
1	D	179	ARG	3.3
1	D	382	VAL	3.3
1	D	122	THR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	177	GLU	3.3
1	D	81	HIS	3.1
1	A	177	GLU	3.1
1	D	172	ARG	3.1
1	C	34	ARG	3.0
1	C	32	GLY	3.0
1	D	290	ASN	2.9
1	C	37	ARG	2.9
1	D	170	GLU	2.7
1	D	128	ALA	2.7
1	D	292	SER	2.7
1	C	171	ALA	2.7
1	A	128	ALA	2.7
1	C	40	HIS	2.7
1	C	58	GLU	2.6
1	D	94	SER	2.6
1	D	123	SER	2.6
1	B	208	PRO	2.6
1	D	182	ILE	2.6
1	D	58	GLU	2.5
1	C	179	ARG	2.5
1	D	287	ALA	2.5
1	C	81	HIS	2.4
1	C	128	ALA	2.4
1	D	121	SER	2.4
1	B	121	SER	2.4
1	C	172	ARG	2.4
1	C	59	THR	2.4
1	D	257	TYR	2.3
1	A	59	THR	2.3
1	A	129	GLY	2.3
1	D	359	ASP	2.3
1	D	80	GLU	2.3
1	C	180	PRO	2.2
1	D	124	GLY	2.2
1	B	100	ILE	2.2
1	A	359	ASP	2.1
1	A	94	SER	2.1
1	D	103	GLY	2.1
1	D	131	THR	2.1
1	A	320	ASN	2.1
1	C	122	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	121	SER	2.1
1	D	177	GLU	2.1
1	D	208	PRO	2.1
1	D	126	CYS	2.1
1	A	58	GLU	2.1
1	B	58	GLU	2.1
1	C	80	GLU	2.1
1	C	169	ASN	2.0
1	C	209	ASP	2.0
1	A	122	THR	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 carbohydrates 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.