Full wwPDB X-ray Structure Validation Report ⓘ

Jul 18, 2023 – 02:09 PM JST

PDB ID	:	7YKQ
Title	:	Crystal structure of a novel alpha/beta hydrolase mutant from thermomonospora curvata in apo form
Authors	:	Han, X.; Jian, G.; Bornscheuer, U.T.; Wei, R.; Liu, W.
Deposited on	:	2022-07-23
Resolution	:	2.36 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:

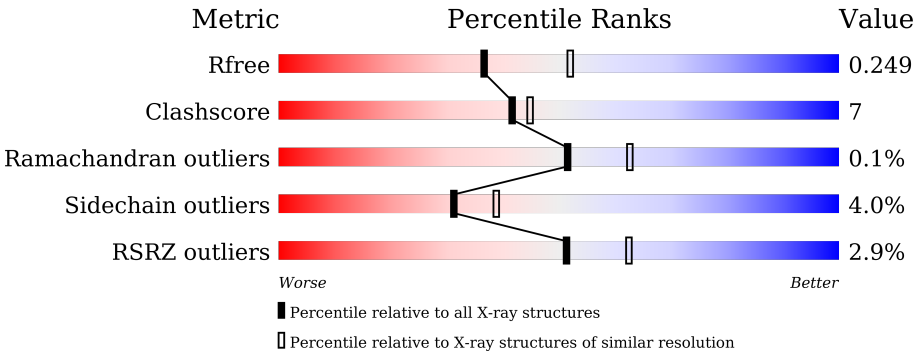
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 <=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	269	3% 79% 16%
1	B	269	6% 75% 19%
1	C	269	% 85% 10%
1	D	269	% 77% 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8231 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 Triacylglycerol lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1989	1252	352	379	6			
1	B	259	Total	C	N	O	S	0	0	0
			1989	1252	352	379	6			
1	C	259	Total	C	N	O	S	0	0	0
			1989	1252	352	379	6			
1	D	259	Total	C	N	O	S	0	0	0
			1989	1252	352	379	6			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASN	-	expression tag	UNP D1A9G5
A	-7	SER	-	expression tag	UNP D1A9G5
A	-6	MET	-	expression tag	UNP D1A9G5
A	-5	HIS	-	expression tag	UNP D1A9G5
A	-4	HIS	-	expression tag	UNP D1A9G5
A	-3	HIS	-	expression tag	UNP D1A9G5
A	-2	HIS	-	expression tag	UNP D1A9G5
A	-1	HIS	-	expression tag	UNP D1A9G5
A	0	HIS	-	expression tag	UNP D1A9G5
A	13	ALA	SER	engineered mutation	UNP D1A9G5
A	14	SER	LEU	engineered mutation	UNP D1A9G5
A	18	PRO	ALA	engineered mutation	UNP D1A9G5
A	41	THR	ARG	engineered mutation	UNP D1A9G5
A	47	ASP	THR	engineered mutation	UNP D1A9G5
A	92	TYR	LEU	engineered mutation	UNP D1A9G5
A	117	ASP	ASN	engineered mutation	UNP D1A9G5
A	141	ARG	LYS	engineered mutation	UNP D1A9G5
A	142	ARG	SER	engineered mutation	UNP D1A9G5
A	144	PRO	THR	engineered mutation	UNP D1A9G5
A	165	THR	ARG	engineered mutation	UNP D1A9G5
A	175	ASN	LEU	engineered mutation	UNP D1A9G5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	185	ALA	SER	engineered mutation	UNP D1A9G5
A	196	THR	ARG	engineered mutation	UNP D1A9G5
A	205	GLY	ASN	engineered mutation	UNP D1A9G5
A	213	THR	PHE	engineered mutation	UNP D1A9G5
A	214	PRO	SER	engineered mutation	UNP D1A9G5
A	224	ALA	SER	engineered mutation	UNP D1A9G5
A	246	PRO	ALA	engineered mutation	UNP D1A9G5
A	247	SER	ILE	engineered mutation	UNP D1A9G5
A	252	GLU	ASP	engineered mutation	UNP D1A9G5
B	-8	ASN	-	expression tag	UNP D1A9G5
B	-7	SER	-	expression tag	UNP D1A9G5
B	-6	MET	-	expression tag	UNP D1A9G5
B	-5	HIS	-	expression tag	UNP D1A9G5
B	-4	HIS	-	expression tag	UNP D1A9G5
B	-3	HIS	-	expression tag	UNP D1A9G5
B	-2	HIS	-	expression tag	UNP D1A9G5
B	-1	HIS	-	expression tag	UNP D1A9G5
B	0	HIS	-	expression tag	UNP D1A9G5
B	13	ALA	SER	engineered mutation	UNP D1A9G5
B	14	SER	LEU	engineered mutation	UNP D1A9G5
B	18	PRO	ALA	engineered mutation	UNP D1A9G5
B	41	THR	ARG	engineered mutation	UNP D1A9G5
B	47	ASP	THR	engineered mutation	UNP D1A9G5
B	92	TYR	LEU	engineered mutation	UNP D1A9G5
B	117	ASP	ASN	engineered mutation	UNP D1A9G5
B	141	ARG	LYS	engineered mutation	UNP D1A9G5
B	142	ARG	SER	engineered mutation	UNP D1A9G5
B	144	PRO	THR	engineered mutation	UNP D1A9G5
B	165	THR	ARG	engineered mutation	UNP D1A9G5
B	175	ASN	LEU	engineered mutation	UNP D1A9G5
B	185	ALA	SER	engineered mutation	UNP D1A9G5
B	196	THR	ARG	engineered mutation	UNP D1A9G5
B	205	GLY	ASN	engineered mutation	UNP D1A9G5
B	213	THR	PHE	engineered mutation	UNP D1A9G5
B	214	PRO	SER	engineered mutation	UNP D1A9G5
B	224	ALA	SER	engineered mutation	UNP D1A9G5
B	246	PRO	ALA	engineered mutation	UNP D1A9G5
B	247	SER	ILE	engineered mutation	UNP D1A9G5
B	252	GLU	ASP	engineered mutation	UNP D1A9G5
C	-8	ASN	-	expression tag	UNP D1A9G5
C	-7	SER	-	expression tag	UNP D1A9G5
C	-6	MET	-	expression tag	UNP D1A9G5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	expression tag	UNP D1A9G5
C	-4	HIS	-	expression tag	UNP D1A9G5
C	-3	HIS	-	expression tag	UNP D1A9G5
C	-2	HIS	-	expression tag	UNP D1A9G5
C	-1	HIS	-	expression tag	UNP D1A9G5
C	0	HIS	-	expression tag	UNP D1A9G5
C	13	ALA	SER	engineered mutation	UNP D1A9G5
C	14	SER	LEU	engineered mutation	UNP D1A9G5
C	18	PRO	ALA	engineered mutation	UNP D1A9G5
C	41	THR	ARG	engineered mutation	UNP D1A9G5
C	47	ASP	THR	engineered mutation	UNP D1A9G5
C	92	TYR	LEU	engineered mutation	UNP D1A9G5
C	117	ASP	ASN	engineered mutation	UNP D1A9G5
C	141	ARG	LYS	engineered mutation	UNP D1A9G5
C	142	ARG	SER	engineered mutation	UNP D1A9G5
C	144	PRO	THR	engineered mutation	UNP D1A9G5
C	165	THR	ARG	engineered mutation	UNP D1A9G5
C	175	ASN	LEU	engineered mutation	UNP D1A9G5
C	185	ALA	SER	engineered mutation	UNP D1A9G5
C	196	THR	ARG	engineered mutation	UNP D1A9G5
C	205	GLY	ASN	engineered mutation	UNP D1A9G5
C	213	THR	PHE	engineered mutation	UNP D1A9G5
C	214	PRO	SER	engineered mutation	UNP D1A9G5
C	224	ALA	SER	engineered mutation	UNP D1A9G5
C	246	PRO	ALA	engineered mutation	UNP D1A9G5
C	247	SER	ILE	engineered mutation	UNP D1A9G5
C	252	GLU	ASP	engineered mutation	UNP D1A9G5
D	-8	ASN	-	expression tag	UNP D1A9G5
D	-7	SER	-	expression tag	UNP D1A9G5
D	-6	MET	-	expression tag	UNP D1A9G5
D	-5	HIS	-	expression tag	UNP D1A9G5
D	-4	HIS	-	expression tag	UNP D1A9G5
D	-3	HIS	-	expression tag	UNP D1A9G5
D	-2	HIS	-	expression tag	UNP D1A9G5
D	-1	HIS	-	expression tag	UNP D1A9G5
D	0	HIS	-	expression tag	UNP D1A9G5
D	13	ALA	SER	engineered mutation	UNP D1A9G5
D	14	SER	LEU	engineered mutation	UNP D1A9G5
D	18	PRO	ALA	engineered mutation	UNP D1A9G5
D	41	THR	ARG	engineered mutation	UNP D1A9G5
D	47	ASP	THR	engineered mutation	UNP D1A9G5
D	92	TYR	LEU	engineered mutation	UNP D1A9G5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	117	ASP	ASN	engineered mutation	UNP D1A9G5
D	141	ARG	LYS	engineered mutation	UNP D1A9G5
D	142	ARG	SER	engineered mutation	UNP D1A9G5
D	144	PRO	THR	engineered mutation	UNP D1A9G5
D	165	THR	ARG	engineered mutation	UNP D1A9G5
D	175	ASN	LEU	engineered mutation	UNP D1A9G5
D	185	ALA	SER	engineered mutation	UNP D1A9G5
D	196	THR	ARG	engineered mutation	UNP D1A9G5
D	205	GLY	ASN	engineered mutation	UNP D1A9G5
D	213	THR	PHE	engineered mutation	UNP D1A9G5
D	214	PRO	SER	engineered mutation	UNP D1A9G5
D	224	ALA	SER	engineered mutation	UNP D1A9G5
D	246	PRO	ALA	engineered mutation	UNP D1A9G5
D	247	SER	ILE	engineered mutation	UNP D1A9G5
D	252	GLU	ASP	engineered mutation	UNP D1A9G5

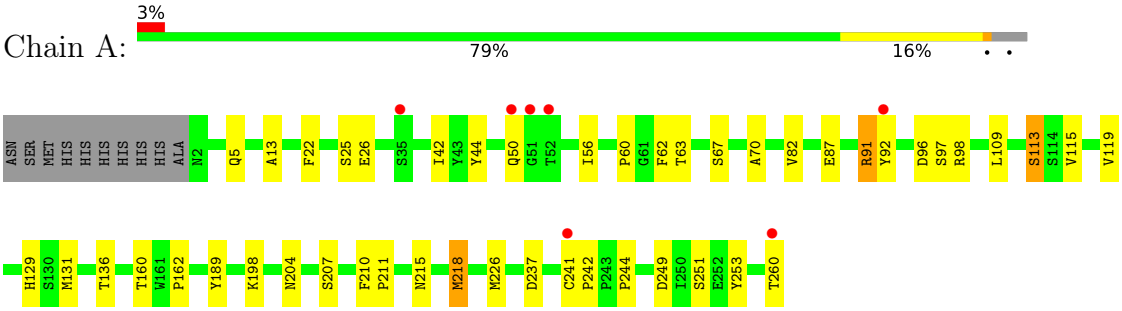
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	79	Total O 79 79	0	0
2	B	64	Total O 64 64	0	0
2	C	62	Total O 62 62	0	0
2	D	70	Total O 70 70	0	0

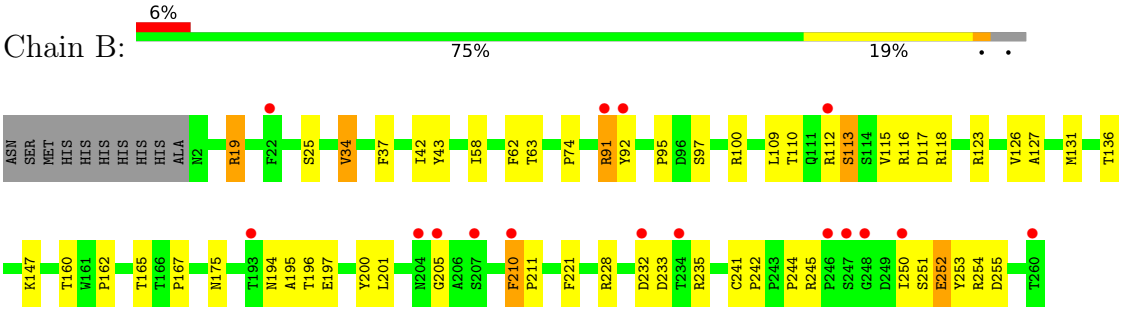
3 Residue-property plots (i)

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.

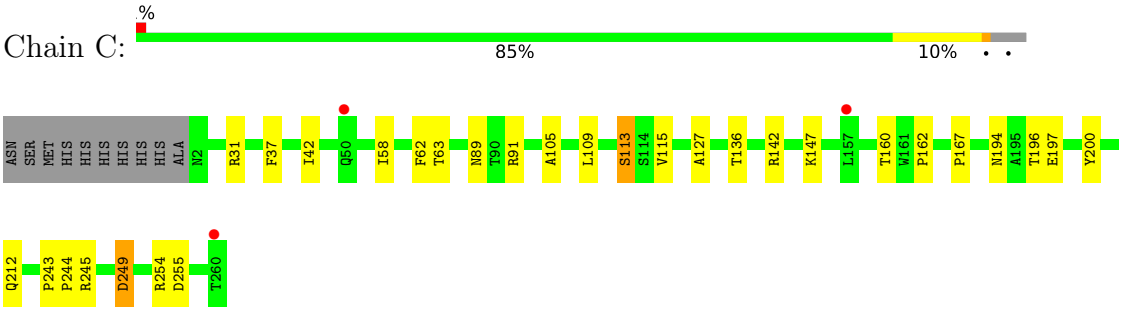
• Molecule 1: Triacylglycerol lipase



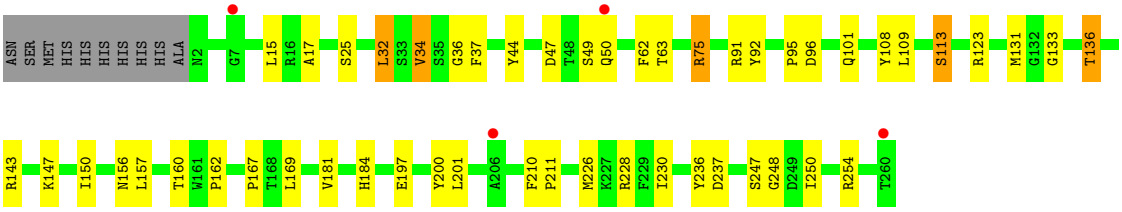
• Molecule 1: Triacylglycerol lipase



• Molecule 1: Triacylglycerol lipase



• Molecule 1: Triacylglycerol lipase


ASN SER MET HIS HIS HIS HIS HIS HIS ALA N2 G7 L15 R16 A17 S25 L32 S33 V34 S35 G36 F37 Y44 D47 T48 S49 Q50 F62 T63 R75 R91 Y92 P95 D96 Q101 Y108 L109 S113 R123 M131 G132 G133 T136
R143 K147 I150 N156 L157 T160 W161 P162 P167 T168 L169 V181 H184 E197 Y200 L201 A206 F210 P211 M226 K227 R228 P229 I230 Y236 D237 S247 G248 D249 I250 R254 T260

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.25Å 63.59Å 91.54Å 90.00° 97.80° 90.00°	Depositor
Resolution (Å)	45.34 – 2.36 46.22 – 2.36	Depositor EDS
% Data completeness (in resolution range)	97.7 (45.34-2.36) 93.2 (46.22-2.36)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.208 , 0.246 0.214 , 0.249	Depositor DCC
R_{free} test set	2013 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8231	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.34	0/2046	0.55	0/2794
1	B	0.32	0/2046	0.57	0/2794
1	C	0.30	0/2046	0.54	0/2794
1	D	0.32	0/2046	0.57	0/2794
All	All	0.32	0/8184	0.56	0/11176

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	1989	0	1918	27	0
1	B	1989	0	1918	34	0
1	C	1989	0	1918	17	0
1	D	1989	0	1918	32	0
2	A	79	0	0	1	0
2	B	64	0	0	2	0
2	C	62	0	0	2	0
2	D	70	0	0	1	0
All	All	8231	0	7672	109	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 7.

All (109) 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:95:PRO:HG3	1:D:131:MET:HG2	1.59	0.84
1:C:160:THR:HG22	1:C:162:PRO:HD3	1.60	0.81
1:B:160:THR:HG22	1:B:162:PRO:HD3	1.67	0.76
1:B:95:PRO:HG3	1:B:131:MET:HG2	1.69	0.74
1:B:63:THR:HA	1:B:91:ARG:HB2	1.67	0.74
1:D:17:ALA:O	1:D:75:ARG:NH1	2.23	0.71
1:D:49:SER:OG	1:D:50:GLN:OE1	2.04	0.71
1:A:42:ILE:HG21	1:A:115:VAL:HG21	1.72	0.71
1:B:19:ARG:NH1	2:B:301:HOH:O	2.24	0.70
1:D:123:ARG:HB3	1:D:147:LYS:HD2	1.74	0.70
1:C:142:ARG:NH2	2:C:302:HOH:O	2.26	0.69
1:C:245:ARG:NH1	2:C:303:HOH:O	2.26	0.68
1:C:109:LEU:HA	1:C:113:SER:HB3	1.77	0.67
1:C:62:PHE:O	1:C:63:THR:HG22	1.95	0.66
1:B:109:LEU:HA	1:B:113:SER:HB3	1.78	0.65
1:D:160:THR:HG22	1:D:162:PRO:HD3	1.80	0.63
1:D:109:LEU:HA	1:D:113:SER:HB3	1.82	0.61
1:D:200:TYR:HB3	1:D:254:ARG:HB2	1.81	0.61
1:A:160:THR:HG22	1:A:162:PRO:HD3	1.82	0.61
1:A:25:SER:HB2	1:A:44:TYR:CZ	2.37	0.59
1:D:34:VAL:HG23	1:D:108:TYR:CD2	2.39	0.58
1:B:62:PHE:CE1	1:B:92:TYR:HA	2.39	0.58
1:B:42:ILE:HG21	1:B:115:VAL:HG21	1.86	0.58
1:B:165:THR:HA	1:B:194:ASN:O	2.06	0.55
1:D:47:ASP:OD1	1:D:50:GLN:NE2	2.35	0.55
1:D:34:VAL:HG21	1:D:37:PHE:CZ	2.41	0.55
1:B:200:TYR:HB3	1:B:254:ARG:HB2	1.87	0.55
1:B:201:LEU:HD11	1:B:250:ILE:HG12	1.87	0.55
1:B:117:ASP:OD2	1:B:117:ASP:N	2.41	0.54
1:A:62:PHE:O	1:A:63:THR:HG22	2.08	0.53
1:C:167:PRO:HA	1:C:197:GLU:O	2.09	0.53
1:C:200:TYR:HD2	1:C:254:ARG:HG3	1.74	0.53
1:A:82:VAL:HG21	1:A:119:VAL:HG22	1.91	0.53
1:D:150:ILE:HD13	1:D:169:LEU:HB3	1.91	0.53
1:B:126:VAL:HG23	1:B:136:THR:HG23	1.91	0.52
1:B:244:PRO:HD2	1:B:253:TYR:CD2	2.45	0.51
1:D:226:MET:O	1:D:230:ILE:HB	2.11	0.51
1:D:201:LEU:HD11	1:D:250:ILE:HG12	1.93	0.51
1:B:195:ALA:O	1:B:196:THR:OG1	2.25	0.50
1:A:241:CYS:HA	1:A:242:PRO:C	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ARG:HG2	1:B:147:LYS:HE2	1.95	0.49
1:D:147:LYS:O	1:D:167:PRO:HD2	2.13	0.49
1:D:247:SER:OG	1:D:248:GLY:N	2.46	0.49
1:A:109:LEU:HA	1:A:113:SER:HB3	1.94	0.48
1:B:100:ARG:NE	2:B:309:HOH:O	2.46	0.48
1:D:167:PRO:HA	1:D:197:GLU:O	2.12	0.48
1:A:22:PHE:HE2	1:A:50:GLN:HG3	1.78	0.47
1:D:15:LEU:HD21	1:D:236:TYR:HE2	1.79	0.47
1:D:34:VAL:HG21	1:D:37:PHE:CE1	2.48	0.47
1:A:204:ASN:HD22	1:A:251:SER:HB3	1.78	0.47
1:B:244:PRO:HD2	1:B:253:TYR:CE2	2.49	0.47
1:A:56:ILE:HG21	1:A:226:MET:HE3	1.97	0.47
1:A:60:PRO:O	1:A:98:ARG:NH1	2.47	0.47
1:A:189:TYR:CE1	1:A:198:LYS:HD2	2.50	0.46
1:D:62:PHE:CD2	1:D:63:THR:HG23	2.50	0.46
1:A:67:SER:HA	1:A:70:ALA:HB2	1.98	0.46
1:B:62:PHE:CD2	1:B:63:THR:HG23	2.51	0.46
1:D:147:LYS:HD3	1:D:230:ILE:HA	1.98	0.46
1:A:5:GLN:NE2	2:A:312:HOH:O	2.48	0.46
1:A:215:ASN:HB3	1:A:218:MET:HE3	1.98	0.46
1:A:96:ASP:OD2	1:A:97:SER:N	2.48	0.46
1:C:162:PRO:O	1:C:194:ASN:ND2	2.47	0.45
1:A:13:ALA:H	1:B:118:ARG:HH12	1.64	0.45
1:B:123:ARG:HA	1:B:147:LYS:HG3	1.98	0.45
1:B:34:VAL:HG21	1:B:37:PHE:CZ	2.52	0.45
1:B:228:ARG:O	1:B:228:ARG:NH1	2.48	0.45
1:B:167:PRO:HA	1:B:197:GLU:O	2.17	0.45
1:A:129:HIS:CD2	1:A:211:PRO:HG2	2.52	0.45
1:B:210:PHE:CD1	1:B:211:PRO:HD3	2.52	0.45
1:A:160:THR:CG2	1:A:162:PRO:HD3	2.45	0.44
1:A:62:PHE:CE2	1:A:92:TYR:HA	2.52	0.44
1:D:123:ARG:CB	1:D:147:LYS:HD2	2.46	0.44
1:B:58:ILE:HA	1:B:127:ALA:O	2.17	0.44
1:C:91:ARG:H	1:C:91:ARG:HG2	1.53	0.44
1:C:42:ILE:HG21	1:C:115:VAL:HG21	1.99	0.44
1:C:58:ILE:HA	1:C:127:ALA:O	2.18	0.44
1:B:175:ASN:ND2	1:B:205:GLY:HA2	2.33	0.43
1:A:62:PHE:HB2	1:A:131:MET:SD	2.58	0.43
1:D:63:THR:HA	1:D:91:ARG:HB3	2.00	0.43
1:C:31:ARG:NH2	1:C:89:ASN:O	2.45	0.43
1:D:34:VAL:HG11	1:D:37:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:VAL:HG21	1:B:37:PHE:CE1	2.54	0.43
1:B:233:ASP:OD1	1:B:235:ARG:HG3	2.19	0.43
1:C:37:PHE:CE1	1:C:105:ALA:HA	2.53	0.43
1:B:43:TYR:CE2	1:B:74:PRO:HD3	2.54	0.43
1:D:32:LEU:H	1:D:32:LEU:HD22	1.84	0.43
1:A:87:GLU:HB3	1:A:91:ARG:HH22	1.84	0.42
1:D:133:GLY:HA2	1:D:136:THR:HG23	2.01	0.42
1:A:244:PRO:HG2	1:A:253:TYR:CG	2.55	0.42
1:A:207:SER:O	1:A:210:PHE:HD2	2.02	0.42
1:D:181:VAL:HG22	2:D:329:HOH:O	2.19	0.42
1:A:218:MET:HB2	1:A:218:MET:HE2	1.91	0.42
1:D:25:SER:HB2	1:D:44:TYR:CZ	2.55	0.42
1:A:26:GLU:HA	1:A:42:ILE:O	2.20	0.42
1:B:100:ARG:HE	1:B:100:ARG:HB3	1.54	0.41
1:B:241:CYS:HA	1:B:242:PRO:C	2.40	0.41
1:C:212:GLN:H	1:C:212:GLN:HG2	1.72	0.41
1:B:110:THR:O	1:B:116:ARG:HB2	2.20	0.41
1:B:221:PHE:CE2	1:B:244:PRO:HG2	2.55	0.41
1:D:15:LEU:HD21	1:D:236:TYR:CE2	2.55	0.41
1:C:243:PRO:HA	1:C:244:PRO:HD3	1.96	0.41
1:C:249:ASP:OD1	1:C:249:ASP:N	2.50	0.41
1:A:22:PHE:CE2	1:A:50:GLN:HG3	2.55	0.41
1:C:147:LYS:HE2	1:C:147:LYS:HB3	1.79	0.41
1:D:36:GLY:O	1:D:101:GLN:HG2	2.21	0.41
1:D:156:ASN:H	1:D:184:HIS:HD2	1.69	0.41
1:B:252:GLU:HG3	1:B:253:TYR:N	2.35	0.41
1:D:62:PHE:CE1	1:D:92:TYR:HA	2.56	0.41
1:D:210:PHE:CG	1:D:211:PRO:HD3	2.56	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	257/269 (96%)	253 (98%)	4 (2%)	0	100	100
1	B	257/269 (96%)	252 (98%)	5 (2%)	0	100	100
1	C	257/269 (96%)	253 (98%)	4 (2%)	0	100	100
1	D	257/269 (96%)	251 (98%)	5 (2%)	1 (0%)	34	38
All	All	1028/1076 (96%)	1009 (98%)	18 (2%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	228	ARG

5.3.2 Protein sidechains (i)

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	211/220 (96%)	204 (97%)	7 (3%)	38	46
1	B	211/220 (96%)	198 (94%)	13 (6%)	18	19
1	C	211/220 (96%)	206 (98%)	5 (2%)	49	59
1	D	211/220 (96%)	202 (96%)	9 (4%)	29	35
All	All	844/880 (96%)	810 (96%)	34 (4%)	31	39

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ARG
1	A	113	SER
1	A	136	THR
1	A	218	MET
1	A	237	ASP
1	A	249	ASP
1	A	260	THR
1	B	19	ARG
1	B	25	SER
1	B	34	VAL

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Mol	Chain	Res	Type
1	B	91	ARG
1	B	97	SER
1	B	112	ARG
1	B	113	SER
1	B	210	PHE
1	B	232	ASP
1	B	245	ARG
1	B	251	SER
1	B	252	GLU
1	B	255	ASP
1	C	113	SER
1	C	136	THR
1	C	196	THR
1	C	249	ASP
1	C	255	ASP
1	D	32	LEU
1	D	34	VAL
1	D	75	ARG
1	D	96	ASP
1	D	113	SER
1	D	136	THR
1	D	143	ARG
1	D	157	LEU
1	D	237	ASP

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	5	GLN
1	A	50	GLN
1	A	204	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 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^{th} 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	259/269 (96%)	0.40	7 (2%) 54 64	24, 34, 44, 60	0
1	B	259/269 (96%)	0.53	16 (6%) 20 29	24, 32, 44, 60	0
1	C	259/269 (96%)	0.35	3 (1%) 79 86	22, 30, 39, 60	0
1	D	259/269 (96%)	0.39	4 (1%) 73 81	24, 32, 43, 54	0
All	All	1036/1076 (96%)	0.42	30 (2%) 51 62	22, 32, 43, 60	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	SER	5.9
1	B	260	THR	5.8
1	A	260	THR	5.4
1	C	260	THR	5.3
1	A	51	GLY	4.0
1	B	248	GLY	3.5
1	A	50	GLN	3.5
1	B	22	PHE	3.1
1	D	7	GLY	2.9
1	D	50	GLN	2.9
1	D	206	ALA	2.8
1	B	91	ARG	2.8
1	B	205	GLY	2.7
1	D	260	THR	2.7
1	B	112	ARG	2.7
1	B	204	ASN	2.6
1	B	92	TYR	2.5
1	A	35	SER	2.4
1	B	250	ILE	2.3
1	B	232	ASP	2.3
1	B	210	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	207	SER	2.2
1	C	157	LEU	2.2
1	A	92	TYR	2.1
1	A	52	THR	2.1
1	B	193	THR	2.1
1	C	50	GLN	2.1
1	B	246	PRO	2.1
1	B	234	THR	2.1
1	A	241	CYS	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 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.