



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:10 PM UTC

PDB ID : 8KEM / pdb_00008kem
Title : PKS domains-fused AmpC EC2
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Deposited on : 2023-08-12
Resolution : 2.77 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

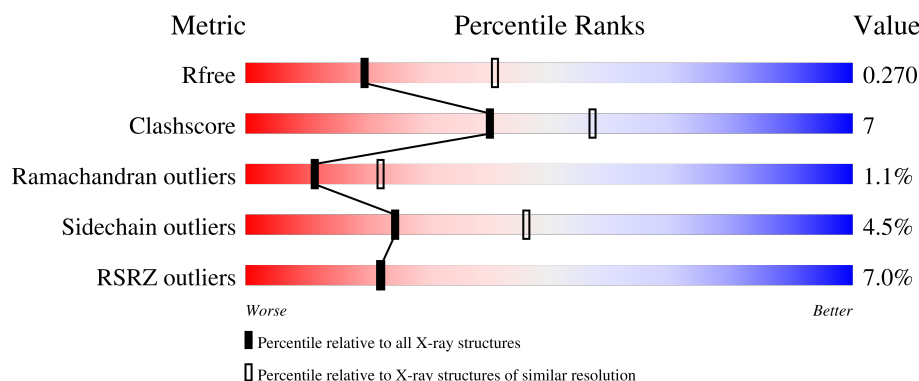
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	428	3% 80% 18% ..
1	B	428	9% 85% 13% ..
1	C	428	8% 72% 19% • 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9464 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 SDR family NAD(P)-dependent oxidoreductase, Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3257	2088	558	603	8			
1	B	424	Total	C	N	O	S	0	0	0
			3203	2046	555	594	8			
1	C	399	Total	C	N	O	S	0	0	0
			3004	1923	521	552	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLY	-	linker	UNP A7Z472
A	34	GLY	-	linker	UNP A7Z472
A	35	GLY	-	linker	UNP A7Z472
A	36	SER	-	linker	UNP A7Z472
A	394	GLY	-	linker	UNP B7SNP8
A	395	GLY	-	linker	UNP B7SNP8
A	396	GLY	-	linker	UNP B7SNP8
A	397	SER	-	linker	UNP B7SNP8
B	33	GLY	-	linker	UNP A7Z472
B	34	GLY	-	linker	UNP A7Z472
B	35	GLY	-	linker	UNP A7Z472
B	36	SER	-	linker	UNP A7Z472
B	394	GLY	-	linker	UNP B7SNP8
B	395	GLY	-	linker	UNP B7SNP8
B	396	GLY	-	linker	UNP B7SNP8
B	397	SER	-	linker	UNP B7SNP8
C	33	GLY	-	linker	UNP A7Z472
C	34	GLY	-	linker	UNP A7Z472
C	35	GLY	-	linker	UNP A7Z472
C	36	SER	-	linker	UNP A7Z472
C	394	GLY	-	linker	UNP B7SNP8
C	395	GLY	-	linker	UNP B7SNP8

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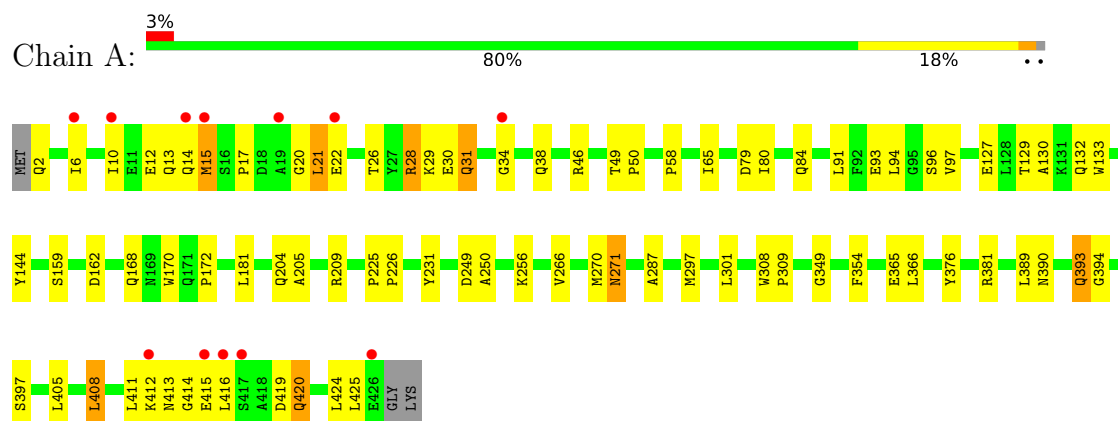
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Chain	Residue	Modelled	Actual	Comment	Reference
C	396	GLY	-	linker	UNP B7SNP8
C	397	SER	-	linker	UNP B7SNP8

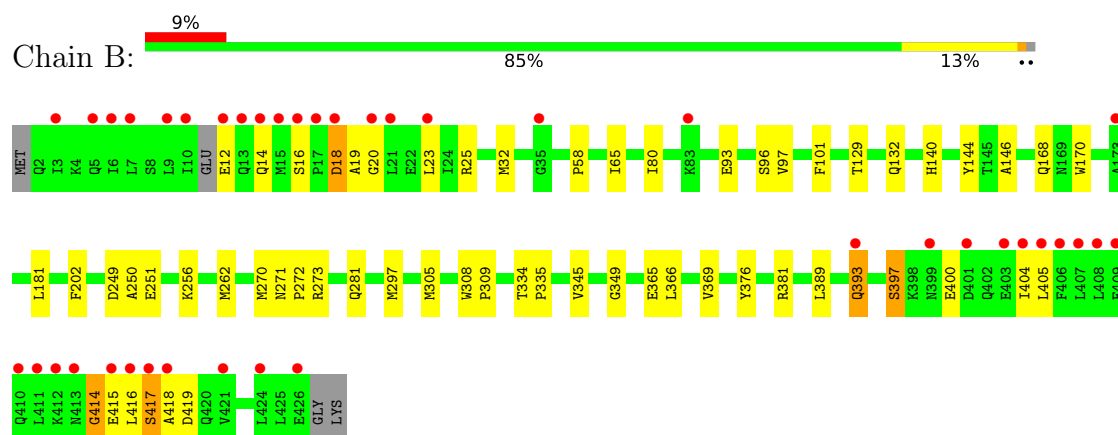
3 Residue-property plots

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.

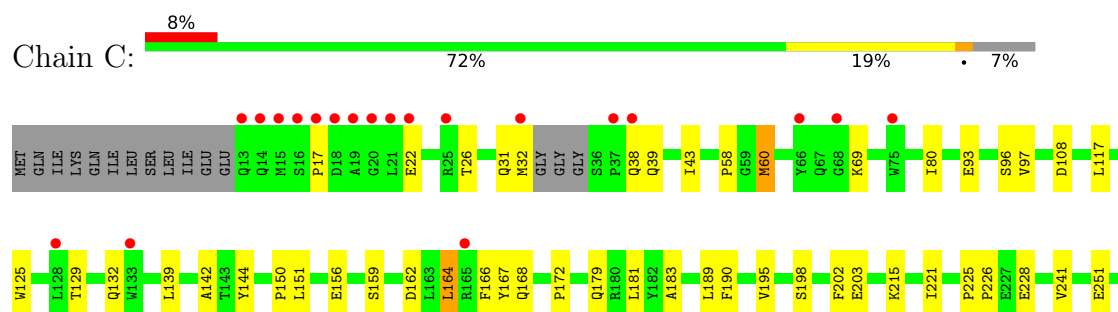
- Molecule 1: SDR family NAD(P)-dependent oxidoreductase,Beta-lactamase

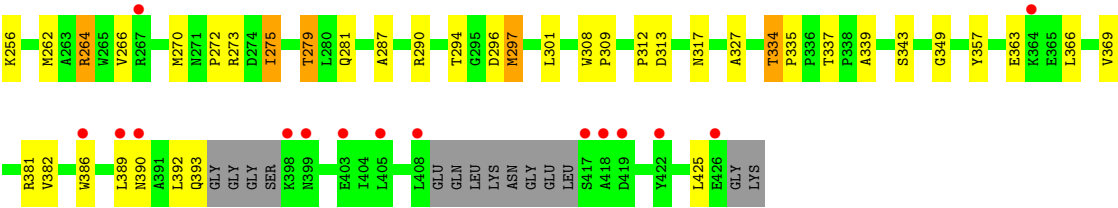


- Molecule 1: SDR family NAD(P)-dependent oxidoreductase,Beta-lactamase



- Molecule 1: SDR family NAD(P)-dependent oxidoreductase,Beta-lactamase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.47Å 248.86Å 153.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.37 – 2.77 29.37 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.37-2.77) 99.8 (29.37-2.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.76Å)	Xtriage
Refinement program	phenix.refine 1.10.1_2155, PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.229 , 0.266 0.232 , 0.270	Depositor DCC
R_{free} test set	2655 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	80.3	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9464	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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	0.14	0/3343	0.37	0/4563
1	B	0.14	0/3287	0.37	0/4487
1	C	0.13	0/3082	0.36	1/4211 (0.0%)
All	All	0.14	0/9712	0.37	1/13261 (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	C	17	PRO	N-CA-CB	5.73	109.58	103.39

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	3257	0	3174	43	0
1	B	3203	0	3067	31	0
1	C	3004	0	2874	50	0
All	All	9464	0	9115	123	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 (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LYS:HB2	1:A:394:GLY:HA2	1.64	0.77
1:C:117:LEU:HB3	1:C:139:LEU:HB2	1.69	0.75
1:C:386:TRP:O	1:C:390:ASN:HB2	1.90	0.72
1:B:366:LEU:HG	1:B:389:LEU:HD22	1.73	0.70
1:A:366:LEU:HG	1:A:389:LEU:HD22	1.75	0.69
1:B:335:PRO:HD3	1:C:139:LEU:HD22	1.79	0.65
1:B:397:SER:HB3	1:B:400:GLU:HB2	1.83	0.61
1:A:132:GLN:NE2	1:A:170:TRP:O	2.34	0.60
1:B:96:SER:HB2	1:B:349:GLY:HA2	1.83	0.59
1:B:129:THR:H	1:B:168:GLN:HE22	1.48	0.59
1:A:414:GLY:O	1:A:416:LEU:N	2.36	0.59
1:A:129:THR:H	1:A:168:GLN:HE22	1.51	0.58
1:B:417:SER:O	1:B:419:ASP:N	2.37	0.58
1:C:225:PRO:HA	1:C:228:GLU:HG2	1.84	0.58
1:A:65:ILE:HG21	1:A:270:MET:HE1	1.87	0.57
1:A:93:GLU:HG2	1:A:256:LYS:HD2	1.87	0.57
1:A:376:TYR:CE2	1:A:381:ARG:HG2	2.40	0.57
1:C:313:ASP:O	1:C:317:ASN:ND2	2.35	0.56
1:A:96:SER:HB2	1:A:349:GLY:HA2	1.88	0.56
1:B:308:TRP:CD2	1:B:309:PRO:HA	2.41	0.55
1:C:386:TRP:O	1:C:390:ASN:CB	2.53	0.55
1:A:6:ILE:HG23	1:A:15:MET:HE1	1.88	0.55
1:B:132:GLN:NE2	1:B:170:TRP:O	2.39	0.55
1:B:58:PRO:HB3	1:B:80:ILE:HD11	1.88	0.55
1:A:130:ALA:HB3	1:A:133:TRP:HD1	1.71	0.54
1:B:101:PHE:HZ	1:B:262:MET:HE1	1.73	0.54
1:C:290:ARG:NH2	1:C:343:SER:OG	2.41	0.54
1:B:376:TYR:CE2	1:B:381:ARG:HG2	2.43	0.54
1:C:272:PRO:HB2	1:C:281:GLN:HG3	1.89	0.54
1:C:312:PRO:HB3	1:C:386:TRP:CE2	2.43	0.53
1:C:349:GLY:O	1:C:381:ARG:NH1	2.40	0.53
1:C:159:SER:H	1:C:162:ASP:HB2	1.73	0.53
1:C:108:ASP:OD1	1:C:279:THR:OG1	2.26	0.53
1:C:97:VAL:HG23	1:C:349:GLY:HA3	1.90	0.52
1:B:18:ASP:O	1:B:20:GLY:N	2.42	0.52
1:B:101:PHE:CZ	1:B:262:MET:HE1	2.45	0.52
1:A:420:GLN:O	1:A:424:LEU:HG	2.11	0.51
1:A:132:GLN:HB2	1:A:172:PRO:HG3	1.93	0.51
1:C:39:GLN:O	1:C:43:ILE:HG22	2.11	0.51
1:A:159:SER:H	1:A:162:ASP:HB2	1.75	0.51
1:C:308:TRP:HZ3	1:C:386:TRP:HZ3	1.59	0.51
1:B:97:VAL:HG23	1:B:349:GLY:HA3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:SER:HB2	1:C:349:GLY:HA2	1.92	0.50
1:A:144:TYR:HB3	1:A:181:LEU:O	2.12	0.50
1:C:287:ALA:HA	1:C:301:LEU:HB2	1.93	0.50
1:A:28:ARG:HA	1:A:31:GLN:HB2	1.93	0.50
1:A:30:GLU:HA	1:A:34:GLY:HA2	1.94	0.50
1:C:181:LEU:HD13	1:C:327:ALA:HB2	1.94	0.50
1:C:132:GLN:HG3	1:C:172:PRO:HD3	1.93	0.49
1:C:357:TYR:CZ	1:C:382:VAL:HG22	2.47	0.49
1:A:10:ILE:HD13	1:A:408:LEU:HG	1.94	0.49
1:B:271:ASN:HD21	1:B:365:GLU:CD	2.17	0.49
1:A:91:LEU:HB2	1:A:231:TYR:HA	1.93	0.49
1:B:262:MET:HB3	1:B:369:VAL:HG11	1.96	0.48
1:A:271:ASN:ND2	1:A:365:GLU:OE2	2.46	0.48
1:A:79:ASP:HB3	1:A:84:GLN:HB3	1.96	0.48
1:A:390:ASN:ND2	1:A:393:GLN:OE1	2.46	0.47
1:B:414:GLY:O	1:B:416:LEU:N	2.48	0.47
1:C:296:ASP:OD1	1:C:296:ASP:N	2.41	0.46
1:C:366:LEU:HG	1:C:389:LEU:HD22	1.98	0.46
1:B:249:ASP:OD1	1:B:250:ALA:N	2.48	0.46
1:B:305:MET:HG3	1:B:345:VAL:HG22	1.98	0.46
1:B:262:MET:HE2	1:B:262:MET:HA	1.98	0.45
1:A:58:PRO:HB3	1:A:80:ILE:HD11	1.97	0.45
1:A:97:VAL:HG23	1:A:349:GLY:HA3	1.98	0.45
1:C:290:ARG:HB2	1:C:337:THR:HB	1.97	0.45
1:A:266:VAL:HG12	1:A:270:MET:HE2	1.99	0.45
1:C:308:TRP:CD2	1:C:309:PRO:HA	2.52	0.45
1:A:93:GLU:HB2	1:A:354:PHE:CG	2.52	0.44
1:C:129:THR:N	1:C:168:GLN:OE1	2.38	0.44
1:C:297:MET:HE3	1:C:297:MET:HB3	1.83	0.44
1:A:12:GLU:O	1:A:14:GLN:N	2.51	0.44
1:A:94:LEU:HB3	1:A:97:VAL:HB	1.98	0.44
1:B:144:TYR:HB3	1:B:181:LEU:O	2.18	0.44
1:B:93:GLU:HG2	1:B:256:LYS:HD2	1.99	0.44
1:A:12:GLU:C	1:A:14:GLN:H	2.25	0.44
1:A:393:GLN:O	1:A:393:GLN:HG2	2.17	0.44
1:C:60:MET:HE2	1:C:60:MET:HB2	1.88	0.44
1:A:205:ALA:O	1:A:209:ARG:HB2	2.17	0.44
1:B:297:MET:HE3	1:B:297:MET:HB3	1.93	0.44
1:C:273:ARG:HD2	1:C:281:GLN:NE2	2.33	0.44
1:C:151:LEU:HA	1:C:183:ALA:HA	2.00	0.44
1:C:202:PHE:CE1	1:C:251:GLU:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ILE:HG21	1:B:270:MET:HE1	1.99	0.43
1:C:225:PRO:N	1:C:226:PRO:HD2	2.34	0.43
1:A:127:GLU:OE1	1:A:127:GLU:N	2.39	0.43
1:C:58:PRO:HB3	1:C:80:ILE:HD11	2.00	0.43
1:A:21:LEU:HD12	1:A:405:LEU:HG	2.01	0.43
1:A:287:ALA:HA	1:A:301:LEU:HB2	2.01	0.43
1:C:215:LYS:HB2	1:C:264:ARG:NH1	2.33	0.43
1:C:251:GLU:OE1	1:C:251:GLU:N	2.50	0.43
1:A:10:ILE:HD11	1:A:20:GLY:HA3	2.01	0.43
1:A:308:TRP:CD2	1:A:309:PRO:HA	2.54	0.43
1:C:203:GLU:HA	1:C:221:ILE:HD12	2.01	0.43
1:C:266:VAL:HG12	1:C:270:MET:HE2	2.01	0.42
1:B:272:PRO:HB2	1:B:281:GLN:HG3	2.00	0.42
1:C:142:ALA:HB2	1:C:190:PHE:CD1	2.54	0.42
1:C:334:THR:HA	1:C:335:PRO:HA	1.86	0.42
1:A:93:GLU:HB2	1:A:354:PHE:CD1	2.55	0.42
1:C:22:GLU:O	1:C:26:THR:HG23	2.19	0.42
1:A:10:ILE:HG13	1:A:15:MET:HE3	2.01	0.42
1:B:12:GLU:C	1:B:14:GLN:H	2.27	0.42
1:C:195:VAL:O	1:C:198:SER:OG	2.34	0.42
1:A:249:ASP:OD1	1:A:250:ALA:N	2.53	0.41
1:C:144:TYR:HB3	1:C:181:LEU:O	2.20	0.41
1:C:39:GLN:H	1:C:39:GLN:HG3	1.66	0.41
1:C:272:PRO:HA	1:C:275:ILE:HD13	2.01	0.41
1:A:17:PRO:HB3	1:A:408:LEU:HB3	2.02	0.41
1:B:25:ARG:NH1	1:B:393:GLN:HE22	2.18	0.41
1:A:49:THR:HB	1:A:50:PRO:HD3	2.03	0.41
1:B:140:HIS:HB3	1:B:146:ALA:HA	2.03	0.41
1:C:167:TYR:CE2	1:C:189:LEU:HD22	2.55	0.41
1:C:262:MET:HB3	1:C:369:VAL:HG11	2.02	0.41
1:C:150:PRO:HG3	1:C:166:PHE:HZ	1.86	0.41
1:C:156:GLU:H	1:C:156:GLU:CD	2.29	0.41
1:C:202:PHE:CZ	1:C:251:GLU:HG3	2.56	0.41
1:A:297:MET:HE3	1:A:297:MET:HB3	1.87	0.41
1:B:400:GLU:O	1:B:404:ILE:HB	2.20	0.41
1:C:93:GLU:HG2	1:C:256:LYS:HD2	2.03	0.40
1:C:125:TRP:CZ2	1:C:164:LEU:HG	2.56	0.40
1:B:12:GLU:N	1:B:12:GLU:OE1	2.54	0.40
1:A:225:PRO:N	1:A:226:PRO:HD2	2.36	0.40
1:B:202:PHE:CE1	1:B:251:GLU:HG3	2.57	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	423/428 (99%)	401 (95%)	18 (4%)	4 (1%)	14	28
1	B	420/428 (98%)	397 (94%)	15 (4%)	8 (2%)	6	12
1	C	391/428 (91%)	380 (97%)	10 (3%)	1 (0%)	36	56
All	All	1234/1284 (96%)	1178 (96%)	43 (4%)	13 (1%)	11	22

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	ASN
1	A	415	GLU
1	B	18	ASP
1	B	19	ALA
1	B	415	GLU
1	B	418	ALA
1	B	32	MET
1	B	397	SER
1	C	339	ALA
1	A	13	GLN
1	A	397	SER
1	B	417	SER
1	B	414	GLY

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	330/350 (94%)	312 (94%)	18 (6%)	19	37
1	B	315/350 (90%)	309 (98%)	6 (2%)	50	70
1	C	295/350 (84%)	277 (94%)	18 (6%)	17	31
All	All	940/1050 (90%)	898 (96%)	42 (4%)	24	46

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	15	MET
1	A	21	LEU
1	A	22	GLU
1	A	26	THR
1	A	28	ARG
1	A	31	GLN
1	A	38	GLN
1	A	46	ARG
1	A	204	GLN
1	A	271	ASN
1	A	393	GLN
1	A	408	LEU
1	A	411	LEU
1	A	412	LYS
1	A	419	ASP
1	A	420	GLN
1	A	425	LEU
1	B	16	SER
1	B	23	LEU
1	B	273	ARG
1	B	334	THR
1	B	393	GLN
1	B	405	LEU
1	C	31	GLN
1	C	32	MET
1	C	38	GLN
1	C	60	MET
1	C	69	LYS
1	C	164	LEU
1	C	179	GLN
1	C	241	VAL
1	C	264	ARG
1	C	275	ILE

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Mol	Chain	Res	Type
1	C	279	THR
1	C	294	THR
1	C	297	MET
1	C	334	THR
1	C	363	GLU
1	C	392	LEU
1	C	393	GLN
1	C	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	271	ASN
1	B	171	GLN
1	B	179	GLN
1	B	285	GLN
1	C	38	GLN
1	C	179	GLN
1	C	218	HIS
1	C	271	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 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	425/428 (99%)	0.27	12 (2%) 55 53	51, 67, 112, 131	0
1	B	424/428 (99%)	0.56	40 (9%) 14 13	50, 69, 120, 141	0
1	C	399/428 (93%)	0.70	35 (8%) 15 15	58, 84, 139, 151	0
All	All	1248/1284 (97%)	0.51	87 (6%) 22 22	50, 73, 123, 151	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	408	LEU	7.3
1	B	407	LEU	6.5
1	B	421	VAL	5.4
1	B	411	LEU	4.8
1	B	14	GLN	4.7
1	B	404	ILE	4.4
1	B	13	GLN	4.2
1	C	13	GLN	4.1
1	B	412	LYS	3.8
1	B	405	LEU	3.8
1	B	21	LEU	3.8
1	C	20	GLY	3.8
1	B	15	MET	3.7
1	C	405	LEU	3.5
1	B	417	SER	3.4
1	B	10	ILE	3.4
1	A	426	GLU	3.4
1	B	426	GLU	3.3
1	B	418	ALA	3.3
1	C	19	ALA	3.3
1	C	14	GLN	3.2
1	C	426	GLU	3.2
1	B	424	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	14	GLN	3.1
1	C	418	ALA	3.1
1	B	16	SER	3.1
1	C	17	PRO	3.1
1	C	165	ARG	3.1
1	C	21	LEU	3.0
1	C	408	LEU	3.0
1	C	22	GLU	3.0
1	B	399	ASN	2.9
1	C	398	LYS	2.9
1	C	417	SER	2.9
1	C	389	LEU	2.9
1	B	9	LEU	2.9
1	B	403	GLU	2.8
1	A	15	MET	2.8
1	B	35	GLY	2.8
1	C	37	PRO	2.7
1	B	401	ASP	2.7
1	B	17	PRO	2.7
1	B	6	ILE	2.7
1	B	416	LEU	2.7
1	B	20	GLY	2.7
1	C	25	ARG	2.6
1	B	409	GLU	2.6
1	B	18	ASP	2.6
1	B	410	GLN	2.6
1	B	413	ASN	2.6
1	C	386	TRP	2.5
1	A	417	SER	2.5
1	A	416	LEU	2.5
1	A	22	GLU	2.5
1	B	393	GLN	2.5
1	A	412	LYS	2.4
1	A	34	GLY	2.4
1	B	12	GLU	2.4
1	C	419	ASP	2.4
1	B	5	GLN	2.4
1	A	19	ALA	2.4
1	B	7	LEU	2.4
1	C	390	ASN	2.4
1	B	23	LEU	2.3
1	B	415	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	32	MET	2.3
1	C	422	TYR	2.3
1	C	38	GLN	2.3
1	C	75	TRP	2.3
1	B	173	ALA	2.3
1	C	133	TRP	2.3
1	A	10	ILE	2.2
1	C	403	GLU	2.2
1	C	399	ASN	2.2
1	C	66	TYR	2.2
1	C	364	LYS	2.2
1	C	267	ARG	2.1
1	B	406	PHE	2.1
1	C	15	MET	2.1
1	B	3	ILE	2.1
1	C	18	ASP	2.0
1	A	415	GLU	2.0
1	B	83	LYS	2.0
1	C	68	GLY	2.0
1	C	16	SER	2.0
1	C	128	LEU	2.0
1	A	6	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.