Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 03:56 PM EDT

PDB ID	:	4FRT
Title	:	Crystal Structure of Pseudomonas aeruginosa OccK7 (OpdD)
Authors	:	Eren, E.; van den Berg, B.
Deposited on	:	2012-06-26
Resolution	:	3.17 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 (i) 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 (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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)	:	2.35

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 3.17 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	Percentile Ranks	Value
Rfree		0.278
Clashscore		12
Ramachandran outliers		2.5%
Sidechain outliers		13.9%
RSRZ outliers		0.7%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
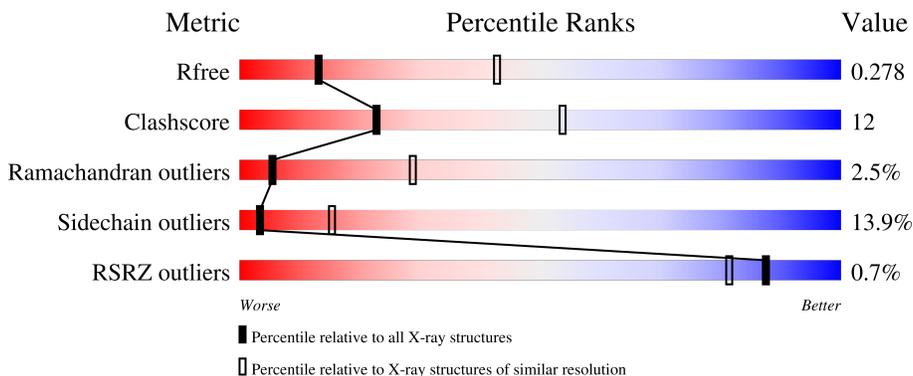
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	400	61% 27% · 8%
1	B	400	.% 64% 24% 6% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5916 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 Probable porin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2944	1857	528	556	3			
1	B	374	Total	C	N	O	S	0	0	0
			2968	1873	528	564	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q9I4U9
A	-4	HIS	-	expression tag	UNP Q9I4U9
A	-3	HIS	-	expression tag	UNP Q9I4U9
A	-2	HIS	-	expression tag	UNP Q9I4U9
A	-1	HIS	-	expression tag	UNP Q9I4U9
A	0	HIS	-	expression tag	UNP Q9I4U9
B	-5	HIS	-	expression tag	UNP Q9I4U9
B	-4	HIS	-	expression tag	UNP Q9I4U9
B	-3	HIS	-	expression tag	UNP Q9I4U9
B	-2	HIS	-	expression tag	UNP Q9I4U9
B	-1	HIS	-	expression tag	UNP Q9I4U9
B	0	HIS	-	expression tag	UNP Q9I4U9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	O	0	0
			2	2		
2	B	2	Total	O	0	0
			2	2		

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: Probable porin
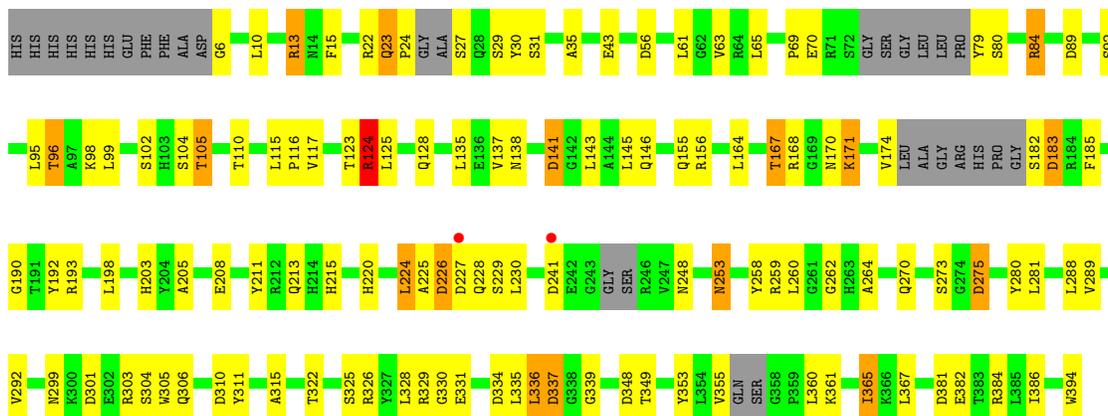
• Molecule 1: Probable porin
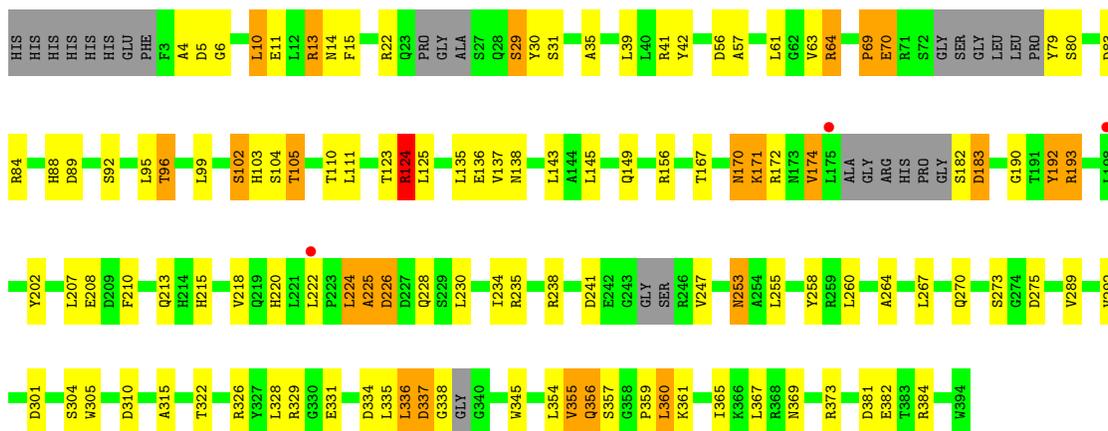
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.25Å 111.15Å 99.93Å 90.00° 123.25° 90.00°	Depositor
Resolution (Å)	14.99 – 3.17 39.65 – 3.17	Depositor EDS
% Data completeness (in resolution range)	97.8 (14.99-3.17) 98.0 (39.65-3.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	3.57 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.210 , 0.269 0.220 , 0.278	Depositor DCC
R_{free} test set	1193 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	76.3	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 56.7	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5916	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.46	0/3008	0.67	0/4060
1	B	0.48	0/3031	0.70	0/4091
All	All	0.47	0/6039	0.69	0/8151

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	2944	0	2796	66	0
1	B	2968	0	2820	69	0
2	A	2	0	0	2	0
2	B	2	0	0	0	0
All	All	5916	0	5616	133	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 12.

All (133) 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:B:224:LEU:HD12	1:B:228:GLN:HG3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ALA:HB3	1:B:310:ASP:HB2	1.68	0.75
1:A:23:GLN:HB3	1:A:24:PRO:HD3	1.74	0.69
1:B:56:ASP:HB2	1:B:96:THR:HG23	1.73	0.68
1:A:141:ASP:OD1	1:A:141:ASP:N	2.26	0.66
1:B:35:ALA:HB1	1:B:125:LEU:HD22	1.78	0.64
1:A:248:ASN:HB3	1:A:275:ASP:HB2	1.80	0.63
1:B:145:LEU:HD23	1:B:190:GLY:HA3	1.80	0.63
1:B:355:VAL:HG11	1:B:361:LYS:HB2	1.80	0.63
1:A:35:ALA:HB1	1:A:125:LEU:HD22	1.81	0.62
1:A:23:GLN:HB3	1:A:27:SER:HB3	1.81	0.62
1:A:225:ALA:O	1:A:227:ASP:N	2.34	0.60
1:A:198:LEU:HD13	1:A:220:HIS:HD2	1.66	0.60
1:A:56:ASP:HB2	1:A:96:THR:HG23	1.85	0.59
1:A:264:ALA:HB3	1:A:310:ASP:HB2	1.84	0.59
1:A:15:PHE:CZ	1:A:124:ARG:HD2	2.38	0.58
1:B:360:LEU:C	1:B:361:LYS:HG2	2.23	0.58
1:A:171:LYS:HB3	1:A:299:ASN:HB3	1.84	0.58
1:B:15:PHE:CZ	1:B:124:ARG:HD2	2.38	0.58
1:B:13:ARG:NH1	1:B:124:ARG:O	2.37	0.57
1:B:354:LEU:O	1:B:356:GLN:N	2.36	0.57
1:A:301:ASP:OD2	1:A:334:ASP:HB2	2.04	0.57
1:A:228:GLN:OE1	1:A:258:TYR:OH	2.23	0.56
1:A:335:LEU:O	1:A:337:ASP:N	2.38	0.56
1:B:335:LEU:O	1:B:337:ASP:N	2.38	0.56
1:B:329:ARG:NH1	1:B:331:GLU:OE1	2.38	0.56
1:A:259:ARG:NH2	2:A:402:HOH:O	2.37	0.56
1:B:301:ASP:OD2	1:B:334:ASP:HB2	2.06	0.56
1:B:69:PRO:HA	1:B:83:ASP:HA	1.88	0.55
1:B:104:SER:OG	1:B:137:VAL:HG23	2.07	0.54
1:A:182:SER:OG	1:A:183:ASP:N	2.39	0.54
1:A:224:LEU:HD11	1:A:258:TYR:HE1	1.73	0.54
1:A:84:ARG:NH2	2:A:401:HOH:O	2.36	0.54
1:B:105:THR:O	1:B:135:LEU:HD12	2.07	0.54
1:A:198:LEU:HD13	1:A:220:HIS:CD2	2.42	0.54
1:B:360:LEU:HD22	1:B:360:LEU:N	2.23	0.54
1:A:22:ARG:NH2	1:A:381:ASP:OD2	2.40	0.53
1:B:360:LEU:HD22	1:B:360:LEU:H	1.74	0.53
1:B:360:LEU:O	1:B:361:LYS:HG2	2.08	0.53
1:A:270:GLN:HB3	1:A:304:SER:OG	2.07	0.53
1:B:123:THR:O	1:B:124:ARG:HD3	2.08	0.53
1:B:182:SER:OG	1:B:183:ASP:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ARG:HB2	1:A:156:ARG:HD2	1.90	0.53
1:A:253:ASN:HB2	1:A:289:VAL:HG22	1.89	0.53
1:B:224:LEU:N	1:B:225:ALA:HB2	2.24	0.53
1:B:15:PHE:CE2	1:B:124:ARG:HD2	2.44	0.52
1:B:220:HIS:CE1	1:B:222:LEU:HB2	2.43	0.52
1:B:359:PRO:HB2	1:B:360:LEU:HD13	1.91	0.52
1:B:105:THR:HG22	1:B:136:GLU:HG3	1.91	0.52
1:A:211:TYR:CE2	1:A:213:GLN:HB2	2.45	0.52
1:B:29:SER:HB2	1:B:70:GLU:HB2	1.92	0.52
1:A:6:GLY:O	1:A:394:TRP:NE1	2.28	0.51
1:B:270:GLN:HB3	1:B:304:SER:OG	2.10	0.51
1:A:185:PHE:CD1	1:A:281:LEU:HD21	2.46	0.51
1:B:220:HIS:HE1	1:B:222:LEU:HB2	1.75	0.51
1:A:95:LEU:HD22	1:B:79:TYR:HD2	1.77	0.50
1:A:137:VAL:HG13	1:A:145:LEU:HB2	1.93	0.50
1:B:102:SER:OG	1:B:103:HIS:N	2.43	0.50
1:B:22:ARG:NH2	1:B:381:ASP:OD2	2.44	0.50
1:B:137:VAL:HG13	1:B:145:LEU:HB2	1.92	0.50
1:B:172:ARG:HB3	1:B:174:VAL:HG12	1.93	0.49
1:A:224:LEU:HD11	1:A:258:TYR:CE1	2.48	0.48
1:A:123:THR:O	1:A:124:ARG:HD3	2.14	0.48
1:A:30:TYR:O	1:A:69:PRO:HD2	2.14	0.48
1:B:235:ARG:HB2	1:B:253:ASN:ND2	2.29	0.47
1:B:253:ASN:HB3	1:B:270:GLN:HG3	1.96	0.47
1:B:258:TYR:OH	1:B:260:LEU:HD12	2.15	0.47
1:A:258:TYR:CE2	1:A:260:LEU:HB2	2.49	0.47
1:A:116:PRO:HG2	1:A:203:HIS:ND1	2.30	0.47
1:B:207:LEU:HD23	1:B:210:PHE:HD2	1.80	0.47
1:B:4:ALA:O	1:B:6:GLY:N	2.49	0.46
1:B:253:ASN:HB2	1:B:289:VAL:HG22	1.97	0.46
1:B:258:TYR:CE2	1:B:260:LEU:HB2	2.51	0.46
1:B:171:LYS:HD3	1:B:171:LYS:HA	1.57	0.46
1:B:305:TRP:O	1:B:328:LEU:HA	2.15	0.46
1:B:171:LYS:HD2	1:B:336:LEU:HD12	1.97	0.45
1:A:105:THR:O	1:A:135:LEU:HD12	2.16	0.45
1:A:43:GLU:HA	1:A:56:ASP:OD1	2.15	0.45
1:B:336:LEU:C	1:B:338:GLY:H	2.19	0.45
1:A:171:LYS:HD3	1:A:171:LYS:HA	1.56	0.45
1:A:13:ARG:NH1	1:A:124:ARG:O	2.49	0.45
1:A:79:TYR:HD2	1:B:95:LEU:HD22	1.82	0.45
1:A:211:TYR:HE2	1:A:213:GLN:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:HD12	1:A:185:PHE:HB2	1.99	0.45
1:B:225:ALA:HA	1:B:228:GLN:O	2.16	0.45
1:A:253:ASN:HB3	1:A:270:GLN:HG3	1.99	0.45
1:A:305:TRP:O	1:A:328:LEU:HA	2.17	0.45
1:B:124:ARG:HB2	1:B:156:ARG:HD2	1.98	0.45
1:A:382:GLU:OE1	1:A:384:ARG:NE	2.48	0.44
1:A:167:THR:OG1	1:A:280:TYR:O	2.36	0.44
1:B:170:ASN:O	1:B:171:LYS:HD3	2.17	0.44
1:A:292:VAL:HG21	1:A:328:LEU:HD13	1.98	0.44
1:A:117:VAL:HB	1:A:205:ALA:HB2	2.00	0.43
1:A:128:GLN:NE2	1:A:155:GLN:OE1	2.50	0.43
1:B:64:ARG:NH1	1:B:88:HIS:CG	2.86	0.43
1:A:258:TYR:OH	1:A:260:LEU:HD12	2.19	0.43
1:B:11:GLU:HB3	1:B:39:LEU:HB2	2.00	0.43
1:B:336:LEU:O	1:B:338:GLY:N	2.46	0.43
1:A:355:VAL:HG11	1:A:361:LYS:HB2	2.00	0.43
1:A:270:GLN:NE2	1:A:288:LEU:HD13	2.33	0.43
1:A:365:ILE:HA	1:A:386:ILE:O	2.19	0.42
1:A:168:ARG:HA	1:A:174:VAL:HB	2.01	0.42
1:A:303:ARG:O	1:A:330:GLY:HA2	2.19	0.42
1:B:10:LEU:H	1:B:10:LEU:HD12	1.85	0.42
1:B:359:PRO:HA	1:B:361:LYS:H	1.84	0.42
1:A:104:SER:OG	1:A:137:VAL:HG23	2.20	0.42
1:A:224:LEU:HG	1:A:229:SER:HA	2.02	0.42
1:B:29:SER:HA	1:B:70:GLU:HA	2.01	0.42
1:B:192:TYR:HD1	1:B:193:ARG:N	2.17	0.42
1:B:228:GLN:OE1	1:B:258:TYR:OH	2.30	0.41
1:B:183:ASP:N	1:B:183:ASP:OD1	2.53	0.41
1:B:356:GLN:HA	1:B:357:SER:HA	1.61	0.41
1:B:30:TYR:O	1:B:69:PRO:HD2	2.21	0.41
1:B:382:GLU:OE1	1:B:384:ARG:NH2	2.50	0.41
1:A:56:ASP:CG	1:A:98:LYS:HE2	2.41	0.41
1:A:145:LEU:HD23	1:A:190:GLY:HA3	2.03	0.41
1:A:227:ASP:N	1:A:227:ASP:OD1	2.53	0.41
1:A:262:GLY:O	1:A:311:TYR:HA	2.20	0.41
1:A:325:SER:HA	1:A:348:ASP:O	2.21	0.41
1:A:329:ARG:NH1	1:A:331:GLU:OE1	2.48	0.41
1:B:42:TYR:HB3	1:B:57:ALA:HB3	2.02	0.41
1:A:306:GLN:NE2	1:A:326:ARG:HD2	2.36	0.41
1:B:110:THR:O	1:B:111:LEU:HD23	2.21	0.41
1:B:218:VAL:HG13	1:B:234:ILE:HB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:VAL:HG12	1:B:326:ARG:CZ	2.51	0.40
1:A:115:LEU:HD21	1:A:146:GLN:HG2	2.03	0.40
1:B:202:TYR:CD2	1:B:202:TYR:C	2.94	0.40
1:B:213:GLN:HA	1:B:238:ARG:O	2.20	0.40
1:A:96:THR:HG22	1:A:110:THR:HB	2.04	0.40
1:A:185:PHE:CZ	1:A:205:ALA:HB1	2.56	0.40
1:A:334:ASP:OD1	1:A:336:LEU:N	2.33	0.40
1:B:255:LEU:HD12	1:B:267:LEU:O	2.22	0.40
1:B:345:TRP:CZ2	1:B:373:ARG:HG3	2.56	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	358/400 (90%)	317 (88%)	33 (9%)	8 (2%)	6	32
1	B	362/400 (90%)	321 (89%)	31 (9%)	10 (3%)	5	26
All	All	720/800 (90%)	638 (89%)	64 (9%)	18 (2%)	5	29

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	ASP
1	A	337	ASP
1	B	355	VAL
1	A	124	ARG
1	A	339	GLY
1	B	5	ASP
1	B	69	PRO
1	B	124	ARG
1	B	337	ASP

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Mol	Chain	Res	Type
1	A	23	GLN
1	A	336	LEU
1	B	336	LEU
1	A	102	SER
1	B	225	ALA
1	B	226	ASP
1	B	315	ALA
1	A	315	ALA
1	B	102	SER

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	301/329 (92%)	261 (87%)	40 (13%)	4	17
1	B	304/329 (92%)	260 (86%)	44 (14%)	3	14
All	All	605/658 (92%)	521 (86%)	84 (14%)	3	15

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	13	ARG
1	A	29	SER
1	A	31	SER
1	A	61	LEU
1	A	63	VAL
1	A	65	LEU
1	A	70	GLU
1	A	80	SER
1	A	84	ARG
1	A	89	ASP
1	A	92	SER
1	A	96	THR
1	A	99	LEU

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Mol	Chain	Res	Type
1	A	105	THR
1	A	124	ARG
1	A	138	ASN
1	A	141	ASP
1	A	143	LEU
1	A	167	THR
1	A	170	ASN
1	A	171	LYS
1	A	183	ASP
1	A	192	TYR
1	A	193	ARG
1	A	208	GLU
1	A	215	HIS
1	A	224	LEU
1	A	226	ASP
1	A	230	LEU
1	A	241	ASP
1	A	253	ASN
1	A	273	SER
1	A	275	ASP
1	A	322	THR
1	A	349	THR
1	A	353	TYR
1	A	360	LEU
1	A	365	ILE
1	A	367	LEU
1	B	10	LEU
1	B	13	ARG
1	B	14	ASN
1	B	29	SER
1	B	31	SER
1	B	41	ARG
1	B	61	LEU
1	B	63	VAL
1	B	64	ARG
1	B	70	GLU
1	B	80	SER
1	B	84	ARG
1	B	89	ASP
1	B	92	SER
1	B	96	THR
1	B	99	LEU

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Mol	Chain	Res	Type
1	B	105	THR
1	B	124	ARG
1	B	138	ASN
1	B	143	LEU
1	B	149	GLN
1	B	167	THR
1	B	170	ASN
1	B	171	LYS
1	B	174	VAL
1	B	183	ASP
1	B	192	TYR
1	B	193	ARG
1	B	208	GLU
1	B	215	HIS
1	B	224	LEU
1	B	226	ASP
1	B	230	LEU
1	B	241	ASP
1	B	247	VAL
1	B	253	ASN
1	B	273	SER
1	B	275	ASP
1	B	322	THR
1	B	356	GLN
1	B	360	LEU
1	B	365	ILE
1	B	367	LEU
1	B	369	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	HIS
1	A	290	ASN
1	A	306	GLN
1	B	14	ASN
1	B	220	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data (i)

6.1   Protein, DNA and RNA chains (i)

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	370/400 (92%)	-0.29	2 (0%)	91	86	48, 78, 114, 148	0
1	B	374/400 (93%)	-0.27	3 (0%)	86	78	49, 76, 115, 152	0
All	All	744/800 (93%)	-0.28	5 (0%)	87	81	48, 77, 115, 152	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	LEU	3.8
1	A	227	ASP	2.9
1	B	222	LEU	2.5
1	A	241	ASP	2.1
1	B	198	LEU	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.