



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2018 – 11:47 PM EST

PDB ID : 6EOT
Title : DPP8 - SLRFLYEG, space group 19
Authors : Ross, B.R.; Huber, R.
Deposited on : 2017-10-10
Resolution : 3.50 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

<http://wwpdb.org/validation/2016/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) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

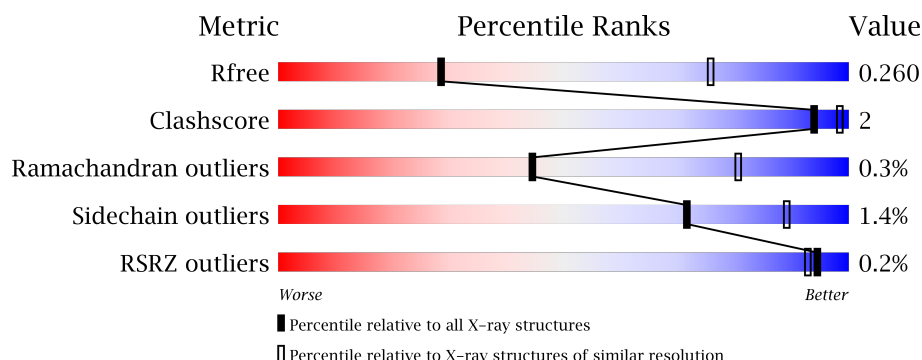
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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. 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	898	
1	B	898	
1	D	898	
1	G	898	
1	I	898	

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Mol	Chain	Length	Quality of chain
1	K	898	<div><div></div><div>87%</div><div>6%7%</div></div>
2	C	8	<div><div></div><div>88%</div><div>13%</div></div>
2	E	8	<div><div></div><div>100%</div><div></div></div>
2	F	8	<div><div></div><div>100%</div><div></div></div>
2	H	8	<div><div></div><div>100%</div><div></div></div>
2	J	8	<div><div></div><div>100%</div><div></div></div>
2	L	8	<div><div></div><div>100%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 41123 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 Dipeptidyl peptidase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	832	Total	C	N	O	S	0	0	0
			6774	4351	1140	1257	26			
1	B	832	Total	C	N	O	S	0	0	0
			6774	4351	1140	1257	26			
1	D	832	Total	C	N	O	S	0	0	0
			6774	4351	1140	1257	26			
1	G	836	Total	C	N	O	S	0	0	0
			6806	4372	1145	1263	26			
1	I	832	Total	C	N	O	S	0	0	0
			6774	4351	1140	1257	26			
1	K	832	Total	C	N	O	S	0	0	0
			6774	4351	1140	1257	26			

- Molecule 2 is a protein called SER-LEU-ARG-PHE-LEU-TYR-GLU-GLY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	8	Total	C	N	O	0	0	0
			69	46	11	12			
2	C	8	Total	C	N	O	0	0	0
			69	46	11	12			
2	E	8	Total	C	N	O	0	0	0
			69	46	11	12			
2	H	8	Total	C	N	O	0	0	0
			69	46	11	12			
2	J	8	Total	C	N	O	0	0	0
			69	46	11	12			
2	L	8	Total	C	N	O	0	0	0
			69	46	11	12			

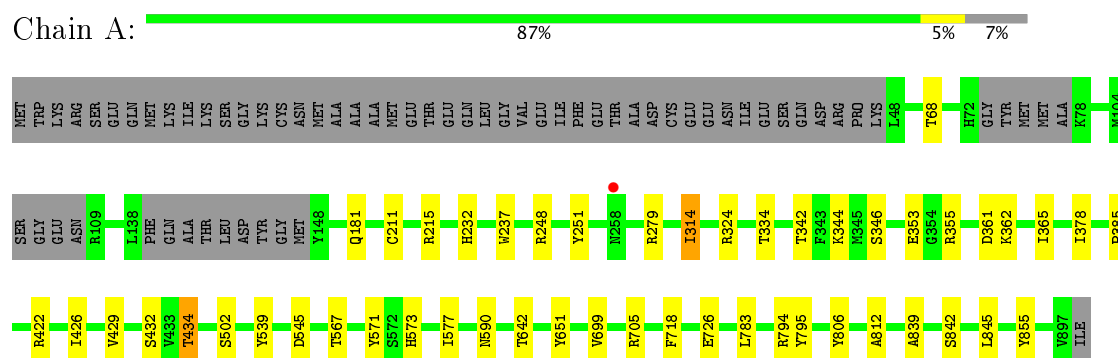
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	6	Total O 6 6	0	0
3	C	1	Total O 1 1	0	0
3	D	6	Total O 6 6	0	0
3	G	4	Total O 4 4	0	0
3	I	5	Total O 5 5	0	0
3	K	3	Total O 3 3	0	0

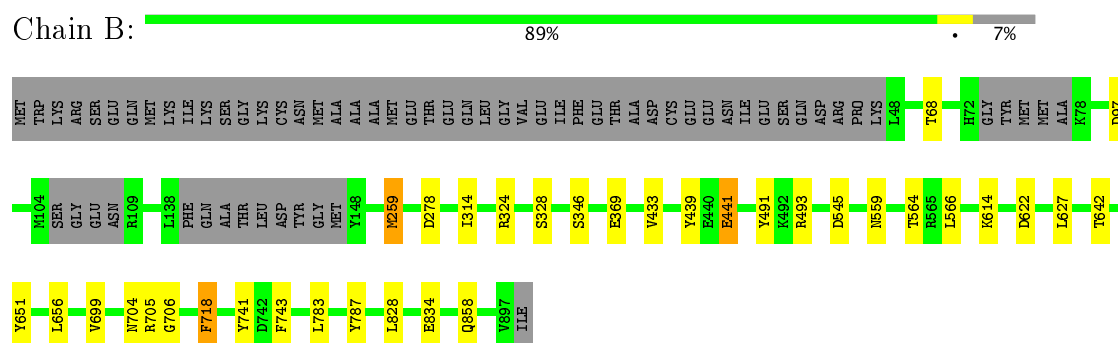
3 Residue-property plots [i](#)

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.

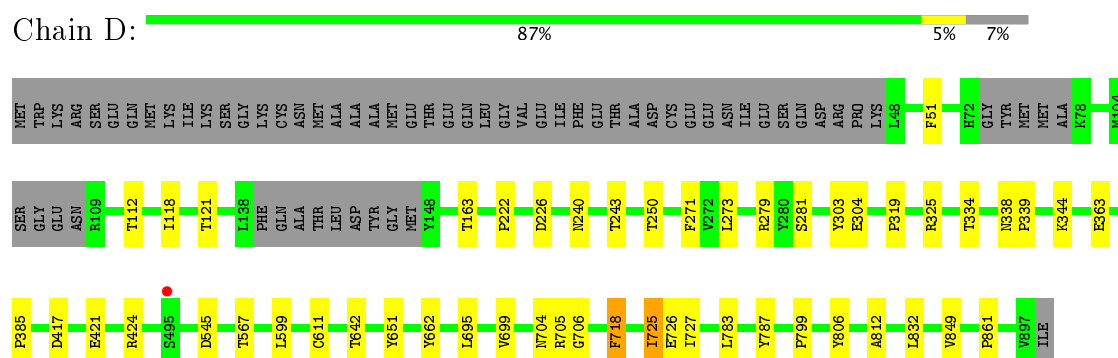
• Molecule 1: Dipeptidyl peptidase 8



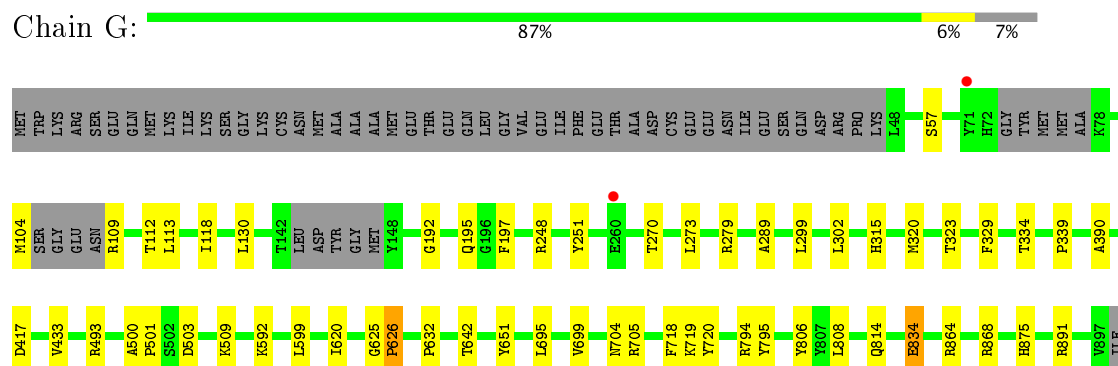
• Molecule 1: Dipeptidyl peptidase 8



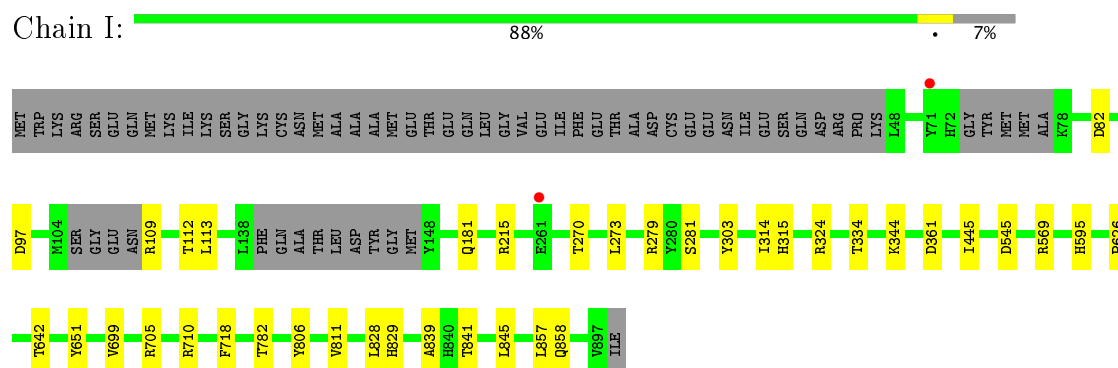
• Molecule 1: Dipeptidyl peptidase 8



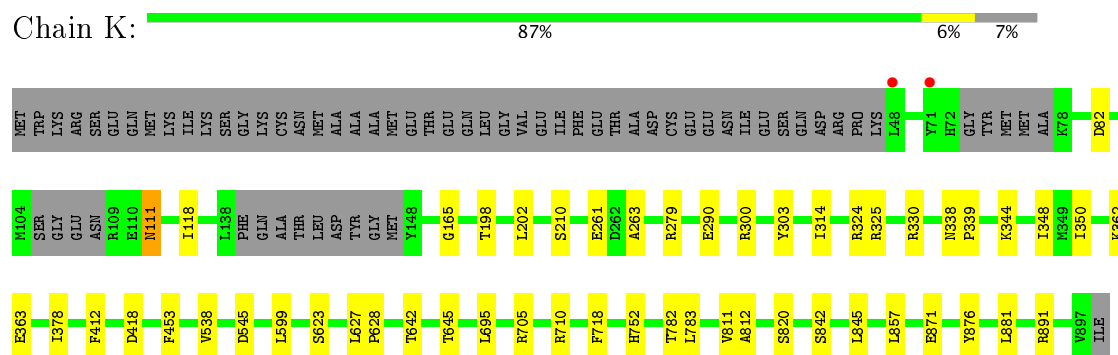
- Molecule 1: Dipeptidyl peptidase 8



- Molecule 1: Dipeptidyl peptidase 8



- Molecule 1: Dipeptidyl peptidase 8

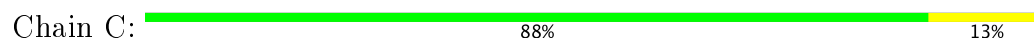


- Molecule 2: SER-LEU-ARG-PHE-LEU-TYR-GLU-GLY



There are no outlier residues recorded for this chain.

- Molecule 2: SER-LEU-ARG-PHE-LEU-TYR-GLU-GLY





- Molecule 2: SER-LEU-ARG-PHE-LEU-TYR-GLU-GLY

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: SER-LEU-ARG-PHE-LEU-TYR-GLU-GLY

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: SER-LEU-ARG-PHE-LEU-TYR-GLU-GLY

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: SER-LEU-ARG-PHE-LEU-TYR-GLU-GLY

Chain L:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	148.16Å 264.68Å 268.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.87 – 3.50 43.87 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.87-3.50) 99.9 (43.87-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.35	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.205 , 0.262 0.209 , 0.260	Depositor DCC
R_{free} test set	6671 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	41123	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.42	0/6960	0.68	0/9439
1	B	0.42	0/6960	0.68	0/9439
1	D	0.43	0/6960	0.68	0/9439
1	G	0.43	0/6993	0.68	0/9484
1	I	0.42	0/6960	0.68	0/9439
1	K	0.43	0/6960	0.67	0/9439
2	C	0.48	0/70	0.60	0/92
2	E	0.58	0/70	0.70	0/92
2	F	0.55	0/70	0.67	0/92
2	H	0.52	0/70	0.64	0/92
2	J	0.54	0/70	0.64	0/92
2	L	0.52	0/70	0.64	0/92
All	All	0.43	0/42213	0.68	0/57231

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 [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	6774	0	6602	26	0
1	B	6774	0	6602	15	0
1	D	6774	0	6602	25	0
1	G	6806	0	6631	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	6774	0	6602	22	0
1	K	6774	0	6602	28	0
2	C	69	0	66	1	0
2	E	69	0	66	0	0
2	F	69	0	66	0	0
2	H	69	0	66	0	0
2	J	69	0	66	0	0
2	L	69	0	66	0	0
3	A	8	0	0	0	0
3	B	6	0	0	0	0
3	C	1	0	0	0	0
3	D	6	0	0	0	0
3	G	4	0	0	1	0
3	I	5	0	0	1	0
3	K	3	0	0	0	0
All	All	41123	0	40037	130	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 2.

All (130) 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:324:ARG:HB2	1:B:314:ILE:HD11	1.39	1.03
1:A:324:ARG:CB	1:B:314:ILE:HD11	2.20	0.69
1:D:725:ILE:O	1:D:727:ILE:N	2.26	0.68
1:D:319:PRO:HA	1:D:832:LEU:HD21	1.77	0.67
1:D:718:PHE:HB3	1:D:725:ILE:HD11	1.76	0.67
1:I:324:ARG:C	1:K:314:ILE:HD11	2.15	0.67
1:D:273:LEU:HD13	1:D:279:ARG:HH21	1.64	0.63
1:I:315:HIS:HB2	1:K:325:ARG:HA	1.84	0.59
1:I:324:ARG:CB	1:K:314:ILE:HD11	2.33	0.59
1:G:433:VAL:O	1:G:493:ARG:NH2	2.36	0.59
1:D:279:ARG:NH2	1:D:304:GLU:OE2	2.37	0.58
1:B:566:LEU:O	1:B:614:LYS:HD3	2.03	0.58
1:I:782:THR:HA	1:I:811:VAL:HG22	1.86	0.58
1:I:324:ARG:O	1:K:314:ILE:HD11	2.04	0.56
1:I:324:ARG:HB2	1:K:314:ILE:HD11	1.87	0.56
1:G:719:LYS:HE2	1:G:720:TYR:CE2	2.41	0.56
1:K:642:THR:HG21	1:K:705:ARG:NH1	2.20	0.56
1:D:279:ARG:NH1	1:D:281:SER:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:VAL:O	1:B:493:ARG:NH2	2.40	0.54
1:G:500:ALA:HB1	1:G:501:PRO:CD	2.38	0.54
1:K:752:HIS:NE2	1:K:876:TYR:OH	2.36	0.54
1:A:344:LYS:NZ	1:A:361:ASP:OD2	2.38	0.54
1:K:198:THR:HG21	1:K:202:LEU:HD21	1.89	0.53
1:D:334:THR:HG21	1:D:806:TYR:OH	2.08	0.53
1:G:302:LEU:HD22	1:G:390:ALA:HB1	1.91	0.53
1:K:348:ILE:HG22	1:K:350:ILE:HD11	1.91	0.52
1:G:130:LEU:HD12	1:G:620:ILE:HG12	1.90	0.52
1:D:325:ARG:HA	1:G:315:HIS:HB2	1.90	0.52
1:D:783:LEU:HD13	1:D:812:ALA:HB3	1.93	0.51
1:I:334:THR:HG21	1:I:806:TYR:OH	2.12	0.50
1:B:706:GLY:HA3	1:B:718:PHE:CE2	2.46	0.50
1:B:787:TYR:HH	2:C:10:SER:N	2.09	0.50
1:G:270:THR:HG21	1:G:339:PRO:HG3	1.92	0.50
1:D:642:THR:HG21	1:D:705:ARG:NH2	2.27	0.50
1:G:270:THR:HG21	1:G:339:PRO:CG	2.42	0.50
1:I:828:LEU:HD23	1:I:858:GLN:HB2	1.94	0.49
1:A:334:THR:HG21	1:A:806:TYR:OH	2.12	0.49
1:K:290:GLU:OE2	1:K:300:ARG:NH2	2.43	0.49
1:K:782:THR:HA	1:K:811:VAL:HG22	1.95	0.49
1:A:794:ARG:HD2	1:A:795:TYR:CZ	2.47	0.49
1:A:248:ARG:HD3	1:A:251:TYR:CE1	2.48	0.48
1:B:651:TYR:HB2	1:B:699:VAL:HB	1.95	0.48
1:B:439:TYR:CZ	1:B:441:GLU:HG2	2.49	0.48
1:D:799:PRO:HA	1:D:806:TYR:CE2	2.49	0.48
1:I:273:LEU:HD13	1:I:279:ARG:HH21	1.79	0.48
1:I:324:ARG:HB2	1:K:314:ILE:CD1	2.43	0.48
1:B:642:THR:HG21	1:B:705:ARG:NH1	2.29	0.47
1:A:211:CYS:HB3	1:A:232:HIS:CE1	2.49	0.47
1:A:651:TYR:HB2	1:A:699:VAL:HB	1.96	0.47
1:B:741:TYR:HB3	1:B:743:PHE:CZ	2.51	0.46
1:I:642:THR:HG21	1:I:705:ARG:NH1	2.29	0.46
1:G:320:MET:O	1:G:323:THR:OG1	2.34	0.46
1:G:334:THR:HG21	1:G:806:TYR:OH	2.15	0.46
1:I:303:TYR:OH	1:I:344:LYS:NZ	2.37	0.46
1:D:118:ILE:HD12	1:D:599:LEU:CD2	2.46	0.46
1:G:642:THR:HG21	1:G:705:ARG:CZ	2.46	0.46
1:A:353:GLU:HB2	1:A:355:ARG:HG2	1.97	0.46
1:G:592:LYS:HD2	1:G:632:PRO:HG3	1.97	0.46
1:K:111:ASN:HB3	1:K:165:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:645:THR:O	1:K:710:ARG:NH2	2.49	0.46
1:A:539:TYR:HB2	1:A:577:ILE:HD13	1.98	0.45
1:I:181:GLN:NE2	1:I:215:ARG:O	2.49	0.45
1:D:338:ASN:HB3	1:D:339:PRO:CD	2.46	0.45
1:G:834:GLU:OE2	1:G:864:ARG:NE	2.49	0.45
1:A:432:SER:O	1:A:434:THR:HG22	2.16	0.45
1:G:248:ARG:HD3	1:G:251:TYR:CE2	2.52	0.45
1:G:118:ILE:HD12	1:G:599:LEU:CD2	2.47	0.45
1:K:362:LYS:HB3	1:K:412:PHE:HB3	1.98	0.45
1:K:118:ILE:HD12	1:K:599:LEU:CD2	2.46	0.45
1:G:625:GLY:O	1:G:626:PRO:C	2.54	0.45
1:B:259:MET:HG2	1:B:328:SER:HB2	1.97	0.45
1:I:112:THR:HG22	1:I:113:LEU:N	2.31	0.45
1:A:642:THR:HG21	1:A:705:ARG:NH1	2.32	0.44
1:B:491:TYR:HE2	1:B:493:ARG:HG3	1.81	0.44
1:D:240:ASN:ND2	1:D:243:THR:OG1	2.50	0.44
1:K:348:ILE:HG22	1:K:350:ILE:CD1	2.47	0.44
1:K:783:LEU:HD13	1:K:812:ALA:HB3	2.00	0.44
1:A:365:ILE:HD12	1:A:429:VAL:HG21	1.99	0.44
1:K:695:LEU:HD13	1:K:881:LEU:HD11	2.00	0.44
1:A:783:LEU:HD13	1:A:812:ALA:HB3	2.01	0.43
1:D:706:GLY:HA3	1:D:718:PHE:CE2	2.53	0.43
1:D:334:THR:OG1	1:D:787:TYR:O	2.28	0.43
1:G:651:TYR:HB2	1:G:699:VAL:HB	1.99	0.43
1:G:808:LEU:O	1:G:814:GLN:NE2	2.51	0.43
1:I:279:ARG:NH1	1:I:281:SER:O	2.51	0.43
1:D:849:VAL:HA	1:G:875:HIS:CD2	2.53	0.43
1:G:273:LEU:HD13	1:G:279:ARG:NH2	2.34	0.43
1:G:289:ALA:HB2	1:G:299:LEU:HD23	2.01	0.43
1:A:726:GLU:N	1:A:726:GLU:OE1	2.52	0.43
1:G:192:GLY:HA2	1:G:197:PHE:CE1	2.54	0.43
1:A:839:ALA:HA	1:A:842:SER:OG	2.20	0.42
1:D:421:GLU:OE2	1:D:424:ARG:NH2	2.53	0.42
1:I:344:LYS:NZ	1:I:361:ASP:OD2	2.35	0.42
1:K:279:ARG:NH1	1:K:378:ILE:O	2.48	0.42
1:A:344:LYS:HD2	1:A:362:LYS:O	2.19	0.42
1:K:263:ALA:HB2	1:K:330:ARG:NH2	2.34	0.42
1:A:181:GLN:NE2	1:A:215:ARG:O	2.52	0.42
1:I:841:THR:O	1:I:845:LEU:HG	2.19	0.42
1:G:112:THR:HG22	1:G:113:LEU:N	2.34	0.42
1:A:314:ILE:HD11	1:B:324:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:651:TYR:HB2	1:D:699:VAL:HB	2.02	0.42
1:I:845:LEU:HD11	1:I:857:LEU:HD22	2.01	0.42
1:K:338:ASN:HB3	1:K:339:PRO:HD2	2.01	0.42
1:G:109:ARG:NH2	3:G:901:HOH:O	2.53	0.42
1:B:314:ILE:HA	1:B:314:ILE:HD12	1.73	0.41
1:I:839:ALA:HB3	1:K:324:ARG:HG2	2.02	0.41
1:A:571:TYR:HD1	1:A:590:ASN:HB3	1.84	0.41
1:I:109:ARG:N	3:I:901:HOH:O	2.52	0.41
1:D:226:ASP:HB3	1:D:240:ASN:OD1	2.20	0.41
1:G:329:PHE:CZ	1:G:834:GLU:HB2	2.56	0.41
1:G:794:ARG:HD2	1:G:795:TYR:CZ	2.55	0.41
1:A:567:THR:HB	1:A:573:HIS:CD2	2.56	0.41
1:A:794:ARG:HD2	1:A:795:TYR:CE1	2.55	0.41
1:D:334:THR:HG22	1:D:799:PRO:HD3	2.03	0.41
1:D:344:LYS:HD2	1:D:363:GLU:HA	2.03	0.41
1:K:344:LYS:HD2	1:K:363:GLU:HA	2.02	0.41
1:I:314:ILE:HD11	1:K:324:ARG:HB2	2.02	0.41
1:D:271:PHE:C	1:D:271:PHE:CD1	2.95	0.40
1:G:642:THR:HG21	1:G:705:ARG:NH1	2.36	0.40
1:B:828:LEU:HD23	1:B:858:GLN:HB2	2.03	0.40
1:D:303:TYR:CE1	1:D:344:LYS:HB2	2.57	0.40
1:A:232:HIS:HB3	1:A:237:TRP:CD1	2.57	0.40
1:D:51:PHE:CD2	1:D:662:TYR:CE1	3.09	0.40
1:I:651:TYR:HB2	1:I:699:VAL:HB	2.03	0.40
1:K:303:TYR:CE1	1:K:344:LYS:HB2	2.56	0.40
1:K:627:LEU:HD12	1:K:628:PRO:HD2	2.04	0.40
1:A:845:LEU:HD22	1:A:855:TYR:CE2	2.57	0.40
1:K:845:LEU:HD11	1:K:857:LEU:HD22	2.04	0.40
1:A:279:ARG:NH1	1:A:378:ILE:O	2.55	0.40
1:A:422:ARG:O	1:A:426:ILE:HG13	2.22	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	824/898 (92%)	764 (93%)	59 (7%)	1 (0%)	55	88
1	B	824/898 (92%)	772 (94%)	49 (6%)	3 (0%)	38	77
1	D	824/898 (92%)	750 (91%)	69 (8%)	5 (1%)	28	70
1	G	828/898 (92%)	762 (92%)	64 (8%)	2 (0%)	51	85
1	I	824/898 (92%)	765 (93%)	56 (7%)	3 (0%)	38	77
1	K	824/898 (92%)	768 (93%)	53 (6%)	3 (0%)	38	77
2	C	6/8 (75%)	6 (100%)	0	0	100	100
2	E	6/8 (75%)	6 (100%)	0	0	100	100
2	F	6/8 (75%)	3 (50%)	3 (50%)	0	100	100
2	H	6/8 (75%)	3 (50%)	3 (50%)	0	100	100
2	J	6/8 (75%)	6 (100%)	0	0	100	100
2	L	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
All	All	4984/5436 (92%)	4610 (92%)	357 (7%)	17 (0%)	44	80

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	MET
1	D	725	ILE
1	K	111	ASN
1	G	503	ASP
1	D	611	CYS
1	D	861	PRO
1	I	595	HIS
1	B	656	LEU
1	K	418	ASP
1	D	726	GLU
1	G	626	PRO
1	I	626	PRO
1	K	453	PHE
1	B	278	ASP
1	D	385	PRO
1	A	385	PRO
1	I	445	ILE

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	740/795 (93%)	732 (99%)	8 (1%)	78	91
1	B	740/795 (93%)	726 (98%)	14 (2%)	62	85
1	D	740/795 (93%)	729 (98%)	11 (2%)	70	88
1	G	743/795 (94%)	732 (98%)	11 (2%)	70	88
1	I	740/795 (93%)	732 (99%)	8 (1%)	78	91
1	K	740/795 (93%)	729 (98%)	11 (2%)	70	88
2	C	7/7 (100%)	7 (100%)	0	100	100
2	E	7/7 (100%)	7 (100%)	0	100	100
2	F	7/7 (100%)	7 (100%)	0	100	100
2	H	7/7 (100%)	7 (100%)	0	100	100
2	J	7/7 (100%)	7 (100%)	0	100	100
2	L	7/7 (100%)	7 (100%)	0	100	100
All	All	4485/4812 (93%)	4422 (99%)	63 (1%)	71	89

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	THR
1	A	314	ILE
1	A	342	THR
1	A	346	SER
1	A	434	THR
1	A	502	SER
1	A	545	ASP
1	A	718	PHE
1	B	68	THR
1	B	97	ASP
1	B	346	SER
1	B	369	GLU
1	B	441	GLU
1	B	545	ASP

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Mol	Chain	Res	Type
1	B	559	ASN
1	B	564	THR
1	B	622	ASP
1	B	627	LEU
1	B	704	ASN
1	B	718	PHE
1	B	783	LEU
1	B	834	GLU
1	D	112	THR
1	D	121	THR
1	D	163	THR
1	D	222	PRO
1	D	250	THR
1	D	417	ASP
1	D	545	ASP
1	D	567	THR
1	D	695	LEU
1	D	704	ASN
1	D	718	PHE
1	G	57	SER
1	G	104	MET
1	G	195	GLN
1	G	417	ASP
1	G	509	LYS
1	G	695	LEU
1	G	704	ASN
1	G	718	PHE
1	G	834	GLU
1	G	868	ARG
1	G	891	ARG
1	I	82	ASP
1	I	97	ASP
1	I	270	THR
1	I	545	ASP
1	I	569	ARG
1	I	710	ARG
1	I	718	PHE
1	I	829	HIS
1	K	82	ASP
1	K	210	SER
1	K	261	GLU
1	K	538	VAL

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Mol	Chain	Res	Type
1	K	545	ASP
1	K	623	SER
1	K	718	PHE
1	K	820	SER
1	K	842	SER
1	K	871	GLU
1	K	891	ARG

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

Mol	Chain	Res	Type
1	B	709	HIS
1	D	837	HIS
1	I	181	GLN

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	832/898 (92%)	-0.25	1 (0%) 95 94	48, 69, 97, 137	0
1	B	832/898 (92%)	-0.32	0 100 100	44, 65, 93, 127	0
1	D	832/898 (92%)	-0.20	1 (0%) 95 94	54, 81, 110, 135	0
1	G	836/898 (93%)	-0.30	2 (0%) 94 93	45, 67, 99, 149	0
1	I	832/898 (92%)	-0.30	2 (0%) 94 93	46, 69, 100, 134	0
1	K	832/898 (92%)	-0.26	2 (0%) 94 93	44, 71, 102, 132	0
2	C	8/8 (100%)	-0.16	0 100 100	71, 76, 103, 111	0
2	E	8/8 (100%)	-0.15	0 100 100	79, 85, 114, 115	0
2	F	8/8 (100%)	-0.04	0 100 100	69, 80, 92, 103	0
2	H	8/8 (100%)	-0.15	0 100 100	69, 75, 92, 104	0
2	J	8/8 (100%)	-0.30	0 100 100	63, 70, 91, 97	0
2	L	8/8 (100%)	-0.22	0 100 100	68, 75, 89, 90	0
All	All	5044/5436 (92%)	-0.27	8 (0%) 94 93	44, 70, 102, 149	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	71	TYR	2.8
1	A	258	ASN	2.7
1	D	495	SER	2.3
1	G	71	TYR	2.3
1	I	71	TYR	2.3
1	I	261	GLU	2.2
1	G	260	GLU	2.0
1	K	48	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 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.