



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:44 PM UTC

PDB ID : 6QZW / pdb_00006qzw
Title : DPP8 bound to a dipeptide (MP) from the N-terminus of BRCA2
Authors : Ross, B.; Geiss-Friedlander, R.; Huber, R.
Deposited on : 2019-03-12
Resolution : 3.20 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 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

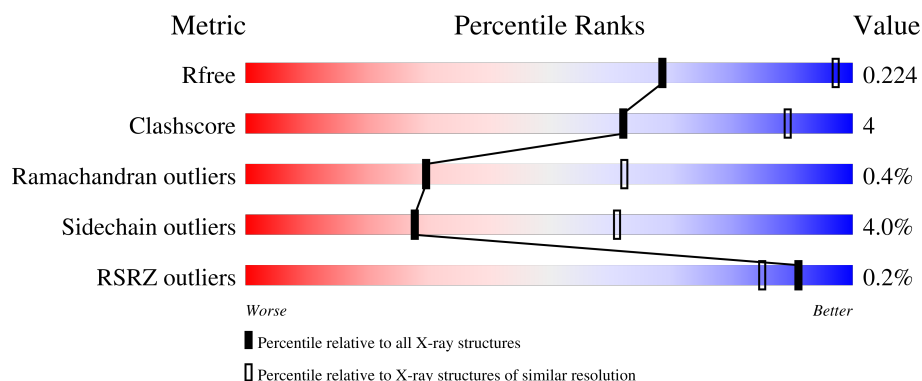
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 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	898	 80% 12% • 7%
1	B	898	 79% 13% • 7%
1	C	898	 80% 12% • 7%
2	D	2	 50% 50%
2	E	2	 50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 20409 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	C	833	Total	C	N	O	S	0	0	0
			6780	4354	1141	1259	26			
1	A	833	Total	C	N	O	S	0	0	0
			6780	4354	1141	1259	26			
1	B	833	Total	C	N	O	S	0	0	0
			6780	4354	1141	1259	26			

- Molecule 2 is a protein called MET-PRO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O	S	0	0	0
			16	10	2	3	1			
2	E	2	Total	C	N	O	S	0	0	0
			16	10	2	3	1			
2	F	2	Total	C	N	O	S	0	0	0
			16	10	2	3	1			

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

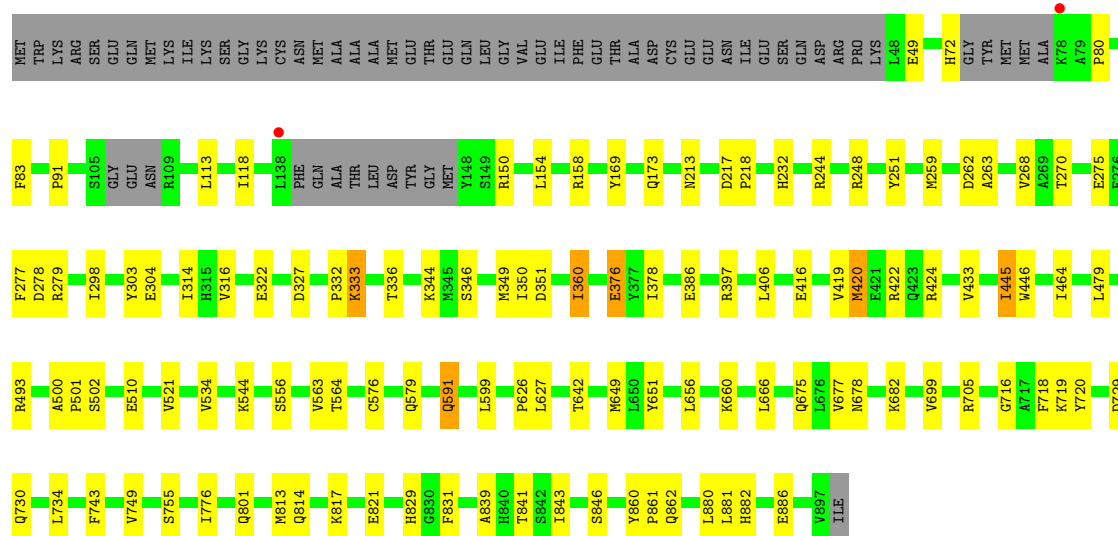
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	8	Total	O	0	0
			8	8		
4	A	6	Total	O	0	0
			6	6		
4	B	6	Total	O	0	0
			6	6		

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.

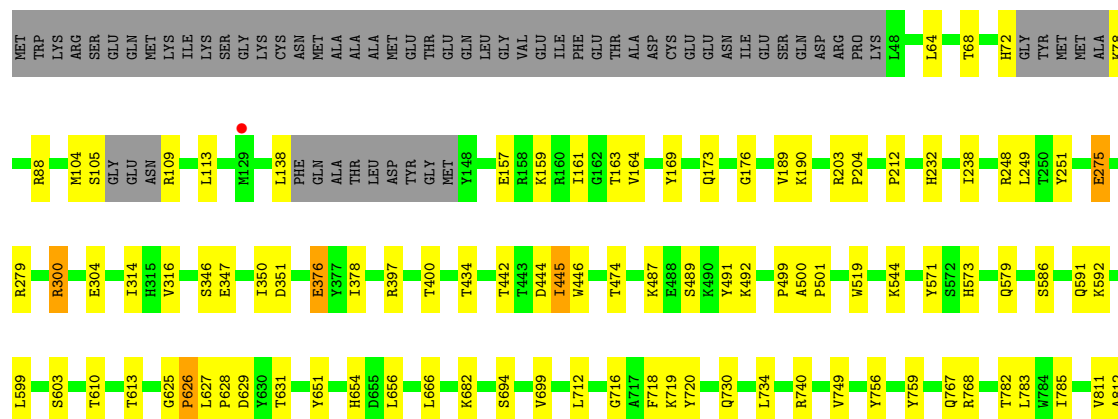
• Molecule 1: Dipeptidyl peptidase 8

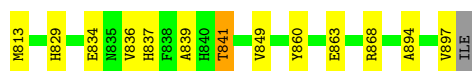
Chain C: 



• Molecule 1: Dipeptidyl peptidase 8

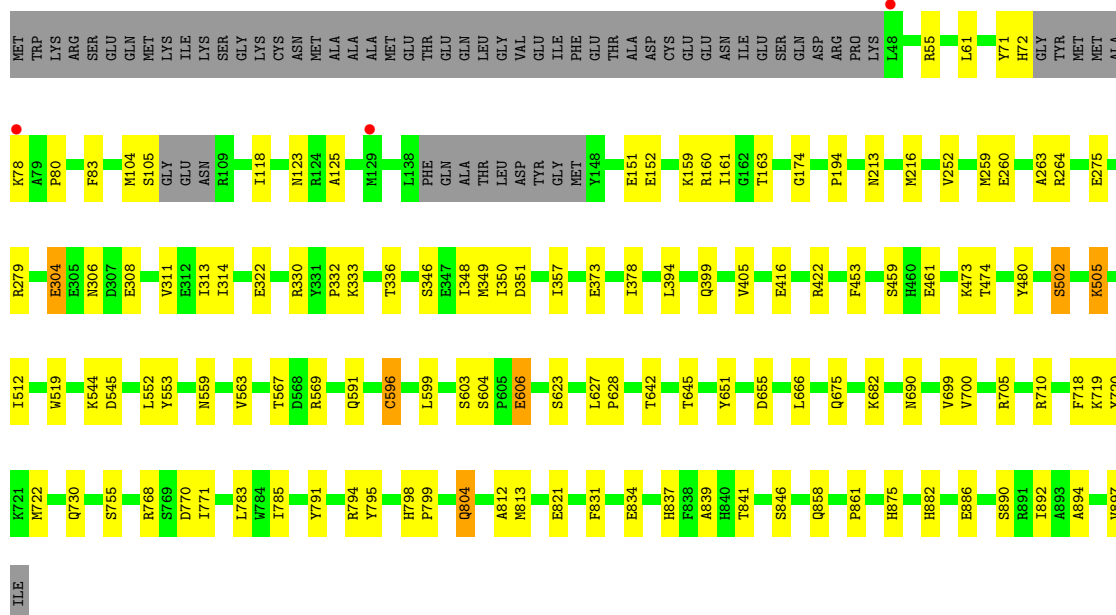
Chain A: 





- Molecule 1: Dipeptidyl peptidase 8

Chain B: 79% 13% 7%



- Molecule 2: MET-PRO

Chain D: 50% 50%



- Molecule 2: MET-PRO

Chain E: 50% 50%



- Molecule 2: MET-PRO

Chain F: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	162.73Å 246.07Å 261.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.58 – 3.20 44.58 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.58-3.20) 99.9 (44.58-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.184 , 0.225 0.187 , 0.224	Depositor DCC
R_{free} test set	4323 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	89.5	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20409	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.98	0/6966	1.08	1/9447 (0.0%)
1	B	1.00	0/6966	1.08	0/9447
1	C	0.99	0/6966	1.08	1/9447 (0.0%)
2	D	0.61	0/16	0.62	0/19
2	E	0.51	0/16	0.71	0/19
2	F	0.54	0/16	0.67	0/19
All	All	0.99	0/20946	1.08	2/28398 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	860	TYR	CB-CA-C	6.08	116.98	110.65
1	C	860	TYR	CB-CA-C	5.94	116.82	110.65

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	6780	0	6607	56	0
1	B	6780	0	6607	59	0
1	C	6780	0	6607	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	16	0	18	1	0
2	E	16	0	18	1	0
2	F	16	0	18	1	0
3	C	1	0	0	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	C	8	0	0	0	0
All	All	20409	0	19875	165	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 (165) 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:591:GLN:HE22	1:B:682:LYS:HG2	1.52	0.74
1:C:419:VAL:HG13	1:C:420:MET:HE3	1.71	0.73
1:A:591:GLN:HE22	1:A:682:LYS:HG2	1.57	0.69
1:C:642:THR:HG21	1:C:705:ARG:NH1	2.09	0.68
1:A:654:HIS:ND1	1:A:694:SER:HA	2.11	0.66
1:B:627:LEU:HD12	1:B:628:PRO:HD2	1.79	0.65
1:A:627:LEU:HD12	1:A:628:PRO:HD2	1.79	0.65
1:A:275:GLU:OE1	2:D:1:MET:N	2.32	0.62
1:A:279:ARG:HH22	1:A:304:GLU:CD	2.06	0.62
1:C:445:ILE:O	1:C:719:LYS:NZ	2.24	0.62
1:A:445:ILE:HD12	1:A:712:LEU:HG	1.83	0.61
1:B:804:GLN:HE21	1:B:804:GLN:HA	1.65	0.60
1:B:279:ARG:HH22	1:B:304:GLU:CD	2.09	0.60
1:C:656:LEU:HD11	1:C:743:PHE:CD2	2.37	0.60
1:C:420:MET:HA	1:C:420:MET:HE2	1.83	0.59
1:A:783:LEU:HD13	1:A:812:ALA:HB3	1.86	0.58
1:A:445:ILE:O	1:A:719:LYS:NZ	2.37	0.58
1:C:591:GLN:HE22	1:C:682:LYS:HG2	1.69	0.57
1:A:376:GLU:HG3	1:A:397:ARG:HB2	1.85	0.57
1:B:783:LEU:HD13	1:B:812:ALA:HB3	1.86	0.57
1:B:348:ILE:HG22	1:B:350:ILE:HD11	1.87	0.56
1:A:894:ALA:O	1:A:897:VAL:HG22	2.05	0.56
1:C:705:ARG:NH1	1:C:729:ASP:OD1	2.38	0.56
1:B:651:TYR:HB2	1:B:699:VAL:HB	1.88	0.56
1:B:798:HIS:ND1	1:B:799:PRO:HD2	2.22	0.55
1:B:894:ALA:O	1:B:897:VAL:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:LYS:HG2	1:A:720:TYR:CD2	2.42	0.55
1:B:666:LEU:HD21	1:B:730:GLN:HE21	1.73	0.54
1:A:189:VAL:CG1	1:A:204:PRO:HA	2.38	0.54
1:B:552:LEU:HB3	1:B:567:THR:HG23	1.89	0.54
1:A:350:ILE:HG22	1:A:351:ASP:O	2.08	0.53
1:A:625:GLY:O	1:A:626:PRO:C	2.52	0.53
1:B:279:ARG:NH1	1:B:378:ILE:O	2.42	0.53
1:C:279:ARG:NH1	1:C:378:ILE:O	2.41	0.52
1:B:642:THR:HG21	1:B:705:ARG:NH1	2.23	0.52
1:B:160:ARG:NH2	1:B:275:GLU:OE1	2.42	0.52
1:C:500:ALA:HB1	1:C:501:PRO:HD2	1.92	0.52
1:C:675:GLN:HG2	1:C:678:ASN:HD22	1.75	0.52
1:B:350:ILE:HD12	1:B:350:ILE:N	2.25	0.52
1:B:104:MET:HE1	1:B:163:THR:HG22	1.92	0.51
1:C:446:TRP:CH2	1:C:716:GLY:HA2	2.46	0.51
1:A:767:GLN:O	1:A:768:ARG:HD2	2.11	0.51
1:B:260:GLU:HG3	1:B:313:ILE:HD13	1.92	0.51
1:A:591:GLN:HE22	1:A:682:LYS:CG	2.24	0.51
1:A:400:THR:O	1:A:442:THR:HA	2.12	0.50
1:C:150:ARG:NH1	1:C:327:ASP:OD2	2.45	0.50
1:A:113:LEU:HD21	1:A:169:TYR:CD1	2.46	0.49
1:B:399:GLN:OE1	1:B:794:ARG:NH1	2.45	0.49
1:B:858:GLN:HE22	1:B:875:HIS:HE1	1.59	0.49
1:C:814:GLN:HE21	1:C:817:LYS:NZ	2.10	0.49
1:C:651:TYR:HB2	1:C:699:VAL:HB	1.94	0.49
1:A:837:HIS:HD2	1:A:839:ALA:H	1.60	0.49
1:A:176:GLY:O	1:A:190:LYS:HA	2.13	0.49
1:C:433:VAL:O	1:C:493:ARG:NH2	2.46	0.49
1:A:782:THR:HA	1:A:811:VAL:HG22	1.93	0.49
1:A:500:ALA:HB1	1:A:501:PRO:CD	2.43	0.49
1:A:631:THR:HB	1:A:654:HIS:HE2	1.78	0.49
1:A:64:LEU:C	1:A:64:LEU:HD23	2.39	0.48
1:C:666:LEU:HD21	1:C:730:GLN:HE21	1.78	0.48
1:B:722:MET:HE3	1:B:795:TYR:CB	2.43	0.48
1:B:890:SER:OG	1:B:892:ILE:HG22	2.14	0.48
1:C:303:TYR:CZ	1:C:344:LYS:HB2	2.49	0.48
1:C:719:LYS:HG2	1:C:720:TYR:CD2	2.48	0.48
1:B:78:LYS:HD2	1:B:163:THR:HG21	1.95	0.48
1:C:406:LEU:HD11	1:C:464:ILE:HD13	1.96	0.48
1:A:64:LEU:O	1:A:68:THR:HG23	2.14	0.48
1:B:72:HIS:CE1	1:B:627:LEU:HD21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:831:PHE:HB3	1:C:861:PRO:HA	1.96	0.47
1:C:118:ILE:HD12	1:C:599:LEU:CD2	2.45	0.47
1:A:654:HIS:ND1	1:A:694:SER:CA	2.78	0.47
1:B:645:THR:O	1:B:710:ARG:NH1	2.40	0.47
1:C:649:MET:HG3	1:C:677:VAL:HG22	1.97	0.47
1:C:298:ILE:HG12	1:C:349:MET:HG3	1.97	0.47
1:B:627:LEU:HD12	1:B:628:PRO:CD	2.44	0.47
1:A:159:LYS:HD3	1:A:161:ILE:HD11	1.96	0.47
1:B:348:ILE:HG22	1:B:350:ILE:CD1	2.44	0.47
1:C:72:HIS:CE1	1:C:627:LEU:HD21	2.50	0.46
1:C:277:PHE:O	1:C:278:ASP:C	2.58	0.46
1:A:571:TYR:HB2	1:A:573:HIS:CE1	2.50	0.46
1:B:123:ASN:HD21	1:B:125:ALA:HB3	1.80	0.46
1:C:213:ASN:H	1:C:232:HIS:HE1	1.64	0.46
1:A:573:HIS:HD2	1:A:586:SER:OG	1.98	0.46
1:B:263:ALA:HB2	1:B:330:ARG:HH21	1.80	0.46
1:A:666:LEU:HD21	1:A:730:GLN:HE21	1.80	0.45
1:C:248:ARG:HD3	1:C:251:TYR:CE2	2.52	0.45
1:A:519:TRP:CG	1:A:544:LYS:HA	2.51	0.45
1:B:519:TRP:CG	1:B:544:LYS:HA	2.51	0.45
1:B:553:TYR:HB3	1:B:563:VAL:HG12	1.97	0.45
1:A:829:HIS:HD2	1:A:841:THR:OG1	2.00	0.45
1:A:173:GLN:NE2	1:A:579:GLN:HE22	2.15	0.45
1:B:118:ILE:HD12	1:B:599:LEU:CD2	2.47	0.45
1:B:55:ARG:HD2	1:B:892:ILE:CG2	2.47	0.45
1:B:308:GLU:HA	1:B:311:VAL:HG23	1.99	0.45
1:B:351:ASP:HA	1:B:357:ILE:HD11	1.98	0.45
1:B:666:LEU:HD12	1:B:700:VAL:O	2.16	0.45
1:B:473:LYS:HG3	1:B:480:TYR:CZ	2.52	0.44
1:C:350:ILE:HG22	1:C:351:ASP:O	2.17	0.44
1:A:863:GLU:HA	1:A:863:GLU:OE1	2.17	0.44
1:B:80:PRO:HB2	1:B:83:PHE:CZ	2.53	0.44
1:B:416:GLU:O	1:B:422:ARG:HD2	2.16	0.44
1:C:49:GLU:O	1:C:660:LYS:HA	2.18	0.44
1:C:154:LEU:O	1:C:158:ARG:HG2	2.17	0.44
1:C:262:ASP:O	1:C:263:ALA:HB3	2.17	0.44
1:B:596:CYS:SG	1:B:623:SER:HB2	2.58	0.44
1:C:734:LEU:HD21	1:C:749:VAL:HG11	1.99	0.44
1:A:104:MET:O	1:A:105:SER:C	2.59	0.44
1:C:173:GLN:NE2	1:C:579:GLN:HE22	2.16	0.44
1:A:300:ARG:NH1	1:A:347:GLU:OE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:GLU:H	1:B:606:GLU:HG2	1.65	0.43
1:A:719:LYS:HG2	1:A:720:TYR:CE2	2.53	0.43
1:B:569:ARG:NH1	1:B:569:ARG:HB3	2.33	0.43
1:B:152:GLU:HG3	1:B:216:MET:HE1	2.00	0.43
1:B:768:ARG:C	1:B:770:ASP:H	2.26	0.43
1:B:882:HIS:CE1	1:B:886:GLU:HG3	2.52	0.43
1:B:333:LYS:HG3	1:B:785:ILE:O	2.18	0.43
1:C:544:LYS:HE2	1:C:563:VAL:HB	2.01	0.43
1:B:755:SER:OG	2:E:2:PRO:HB2	2.18	0.43
1:C:479:LEU:HG	1:C:521:VAL:HG21	2.01	0.43
1:B:78:LYS:CD	1:B:163:THR:HG21	2.49	0.43
1:B:104:MET:O	1:B:105:SER:C	2.62	0.43
1:B:791:TYR:O	1:B:795:TYR:HD1	2.01	0.43
1:C:776:ILE:HD13	1:C:880:LEU:HD12	2.00	0.43
1:B:719:LYS:HG3	1:B:720:TYR:CD2	2.54	0.43
1:A:212:PRO:HD2	1:A:232:HIS:CE1	2.54	0.43
1:A:279:ARG:NH1	1:A:378:ILE:O	2.52	0.43
1:B:159:LYS:HD3	1:B:161:ILE:HD11	2.00	0.43
1:C:113:LEU:HD21	1:C:169:TYR:CD1	2.54	0.42
1:A:434:THR:HG21	1:A:489:SER:HB2	2.01	0.42
1:B:174:GLY:O	1:B:194:PRO:HD3	2.19	0.42
1:C:416:GLU:O	1:C:422:ARG:HD2	2.19	0.42
1:C:882:HIS:CE1	1:C:886:GLU:HG3	2.54	0.42
1:C:839:ALA:O	1:C:843:ILE:HG22	2.19	0.42
1:B:349:MET:C	1:B:350:ILE:HD12	2.45	0.42
1:B:502:SER:HA	1:B:505:LYS:HG3	2.01	0.42
1:B:831:PHE:HB3	1:B:861:PRO:HA	2.01	0.42
1:A:157:GLU:OE2	1:A:868:ARG:NH1	2.51	0.42
1:A:651:TYR:HB2	1:A:699:VAL:HB	2.02	0.42
1:A:829:HIS:HE1	1:A:836:VAL:O	2.03	0.42
1:B:279:ARG:NH2	1:B:304:GLU:OE2	2.49	0.42
1:A:105:SER:HB2	1:A:109:ARG:HD3	2.02	0.42
1:B:837:HIS:HD2	1:B:839:ALA:H	1.67	0.42
1:C:80:PRO:HB2	1:C:83:PHE:CZ	2.55	0.41
1:C:333:LYS:HG2	1:C:336:THR:HG23	2.02	0.41
1:A:238:ILE:HG12	1:A:249:LEU:HD21	2.00	0.41
1:A:491:TYR:CD2	1:A:499:PRO:HB3	2.55	0.41
1:A:78:LYS:HD2	1:A:163:THR:CG2	2.50	0.41
1:C:464:ILE:O	1:C:464:ILE:HG23	2.20	0.41
1:A:189:VAL:HG13	1:A:204:PRO:HA	2.02	0.41
1:C:755:SER:OG	2:F:2:PRO:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:VAL:HG12	1:B:264:ARG:HB3	2.01	0.41
1:A:628:PRO:O	1:A:629:ASP:HB2	2.20	0.41
1:A:719:LYS:HE2	1:A:720:TYR:CZ	2.55	0.41
1:C:719:LYS:HE2	1:C:720:TYR:CE2	2.56	0.41
1:C:829:HIS:HD2	1:C:841:THR:OG1	2.04	0.41
1:A:734:LEU:HD21	1:A:749:VAL:HG11	2.02	0.41
1:A:756:TYR:O	1:A:759:TYR:HB3	2.21	0.41
1:A:446:TRP:CH2	1:A:716:GLY:HA2	2.56	0.41
1:A:248:ARG:HD3	1:A:251:TYR:CE1	2.56	0.41
1:C:244:ARG:HD2	1:A:720:TYR:CD2	2.56	0.40
1:A:627:LEU:HD12	1:A:628:PRO:CD	2.47	0.40
1:C:217:ASP:N	1:C:218:PRO:CD	2.85	0.40
1:C:275:GLU:HA	1:C:275:GLU:OE1	2.22	0.40
1:C:349:MET:HE1	1:C:360:ILE:HD11	2.03	0.40
1:C:376:GLU:HG3	1:C:397:ARG:HB2	2.02	0.40
1:B:394:LEU:HD12	1:B:405:VAL:HG21	2.03	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	825/898 (92%)	779 (94%)	44 (5%)	2 (0%)	43	73
1	B	825/898 (92%)	779 (94%)	44 (5%)	2 (0%)	43	73
1	C	825/898 (92%)	771 (94%)	49 (6%)	5 (1%)	21	56
All	All	2475/2694 (92%)	2329 (94%)	137 (6%)	9 (0%)	30	62

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	259	MET

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Mol	Chain	Res	Type
1	A	626	PRO
1	A	445	ILE
1	C	91	PRO
1	C	626	PRO
1	C	445	ILE
1	B	453	PHE
1	C	332	PRO
1	B	332	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	741/795 (93%)	713 (96%)	28 (4%)	29	62
1	B	741/795 (93%)	706 (95%)	35 (5%)	23	57
1	C	741/795 (93%)	714 (96%)	27 (4%)	31	63
2	D	2/2 (100%)	2 (100%)	0	100	100
2	E	2/2 (100%)	2 (100%)	0	100	100
2	F	2/2 (100%)	2 (100%)	0	100	100
All	All	2229/2391 (93%)	2139 (96%)	90 (4%)	28	61

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	268	VAL
1	C	270	THR
1	C	304	GLU
1	C	314	ILE
1	C	316	VAL
1	C	322	GLU
1	C	333	LYS
1	C	346	SER
1	C	360	ILE
1	C	376	GLU

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Mol	Chain	Res	Type
1	C	386	GLU
1	C	420	MET
1	C	424	ARG
1	C	502	SER
1	C	510	GLU
1	C	534	VAL
1	C	556	SER
1	C	564	THR
1	C	576	CYS
1	C	591	GLN
1	C	718	PHE
1	C	801	GLN
1	C	813	MET
1	C	821	GLU
1	C	846	SER
1	C	862	GLN
1	C	881	LEU
1	A	72	HIS
1	A	88	ARG
1	A	138	LEU
1	A	164	VAL
1	A	203	ARG
1	A	275	GLU
1	A	300	ARG
1	A	314	ILE
1	A	316	VAL
1	A	346	SER
1	A	376	GLU
1	A	444	ASP
1	A	474	THR
1	A	487	LYS
1	A	492	LYS
1	A	592	LYS
1	A	599	LEU
1	A	603	SER
1	A	610	THR
1	A	613	THR
1	A	656	LEU
1	A	718	PHE
1	A	740	ARG
1	A	785	ILE
1	A	813	MET

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Mol	Chain	Res	Type
1	A	834	GLU
1	A	841	THR
1	A	849	VAL
1	B	61	LEU
1	B	71	TYR
1	B	151	GLU
1	B	213	ASN
1	B	259	MET
1	B	304	GLU
1	B	306	ASN
1	B	314	ILE
1	B	322	GLU
1	B	336	THR
1	B	346	SER
1	B	373	GLU
1	B	459	SER
1	B	461	GLU
1	B	474	THR
1	B	502	SER
1	B	505	LYS
1	B	512	ILE
1	B	545	ASP
1	B	559	ASN
1	B	596	CYS
1	B	603	SER
1	B	604	SER
1	B	606	GLU
1	B	655	ASP
1	B	675	GLN
1	B	690	ASN
1	B	718	PHE
1	B	771	ILE
1	B	804	GLN
1	B	813	MET
1	B	821	GLU
1	B	834	GLU
1	B	841	THR
1	B	846	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	60	GLN
1	C	72	HIS
1	C	173	GLN
1	C	188	HIS
1	C	199	GLN
1	C	213	ASN
1	C	232	HIS
1	C	258	ASN
1	C	274	GLN
1	C	403	GLN
1	C	573	HIS
1	C	591	GLN
1	C	673	GLN
1	C	675	GLN
1	C	690	ASN
1	C	704	ASN
1	C	730	GLN
1	C	814	GLN
1	C	829	HIS
1	C	837	HIS
1	C	858	GLN
1	C	875	HIS
1	C	882	HIS
1	A	89	ASN
1	A	123	ASN
1	A	199	GLN
1	A	232	HIS
1	A	253	HIS
1	A	254	ASN
1	A	403	GLN
1	A	573	HIS
1	A	579	GLN
1	A	580	HIS
1	A	591	GLN
1	A	657	GLN
1	A	704	ASN
1	A	709	HIS
1	A	724	GLN
1	A	730	GLN
1	A	814	GLN
1	A	829	HIS
1	A	837	HIS
1	A	858	GLN

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Mol	Chain	Res	Type
1	A	879	HIS
1	B	89	ASN
1	B	188	HIS
1	B	195	GLN
1	B	199	GLN
1	B	200	GLN
1	B	232	HIS
1	B	306	ASN
1	B	423	GLN
1	B	573	HIS
1	B	591	GLN
1	B	593	ASN
1	B	657	GLN
1	B	675	GLN
1	B	690	ASN
1	B	704	ASN
1	B	709	HIS
1	B	730	GLN
1	B	804	GLN
1	B	814	GLN
1	B	829	HIS
1	B	837	HIS
1	B	858	GLN
1	B	882	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	833/898 (92%)	-0.27	1 (0%) 92 89	58, 85, 131, 179	0
1	B	833/898 (92%)	-0.22	3 (0%) 88 79	61, 89, 132, 183	0
1	C	833/898 (92%)	-0.25	2 (0%) 91 85	61, 86, 130, 184	0
2	D	2/2 (100%)	0.35	0 100 100	102, 102, 102, 115	0
2	E	2/2 (100%)	0.67	0 100 100	112, 112, 112, 118	0
2	F	2/2 (100%)	0.77	0 100 100	99, 99, 99, 118	0
All	All	2505/2700 (92%)	-0.25	6 (0%) 91 85	58, 87, 131, 184	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	48	LEU	2.7
1	A	129	MET	2.5
1	B	78	LYS	2.3
1	C	138	LEU	2.3
1	C	78	LYS	2.3
1	B	129	MET	2.2

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NA	C	901	1/1	0.92	0.06	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.