



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:06 PM UTC

PDB ID : 6EOQ / pdb_00006eoq
Title : DPP9 - Apo
Authors : Ross, B.R.; Huber, R.
Deposited on : 2017-10-10
Resolution : 3.00 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

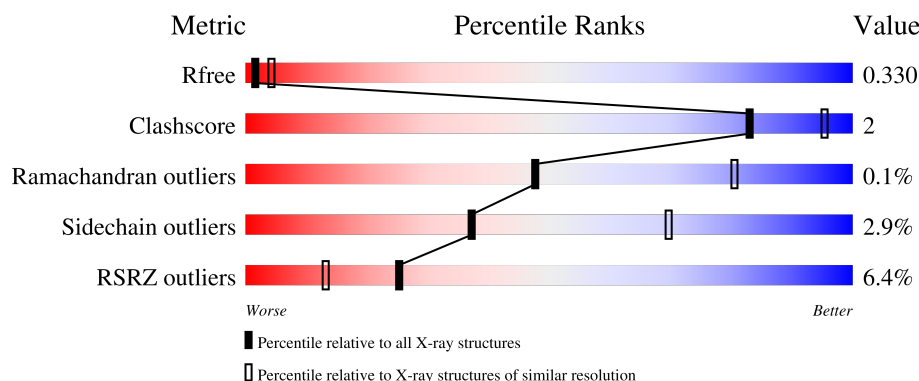
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	869	
1	B	869	
1	C	869	
1	D	869	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24962 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 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	767	Total	C	N	O	S	0	0	0
			6229	4020	1053	1128	28			
1	B	766	Total	C	N	O	S	0	0	0
			6220	4016	1052	1124	28			
1	C	766	Total	C	N	O	S	0	0	0
			6217	4012	1052	1126	27			
1	D	765	Total	C	N	O	S	0	0	0
			6214	4012	1053	1121	28			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	864	HIS	-	expression tag	UNP Q86TI2
A	865	HIS	-	expression tag	UNP Q86TI2
A	866	HIS	-	expression tag	UNP Q86TI2
A	867	HIS	-	expression tag	UNP Q86TI2
A	868	HIS	-	expression tag	UNP Q86TI2
A	869	HIS	-	expression tag	UNP Q86TI2
B	864	HIS	-	expression tag	UNP Q86TI2
B	865	HIS	-	expression tag	UNP Q86TI2
B	866	HIS	-	expression tag	UNP Q86TI2
B	867	HIS	-	expression tag	UNP Q86TI2
B	868	HIS	-	expression tag	UNP Q86TI2
B	869	HIS	-	expression tag	UNP Q86TI2
C	864	HIS	-	expression tag	UNP Q86TI2
C	865	HIS	-	expression tag	UNP Q86TI2
C	866	HIS	-	expression tag	UNP Q86TI2
C	867	HIS	-	expression tag	UNP Q86TI2
C	868	HIS	-	expression tag	UNP Q86TI2
C	869	HIS	-	expression tag	UNP Q86TI2
D	864	HIS	-	expression tag	UNP Q86TI2
D	865	HIS	-	expression tag	UNP Q86TI2
D	866	HIS	-	expression tag	UNP Q86TI2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	867	HIS	-	expression tag	UNP Q86TI2
D	868	HIS	-	expression tag	UNP Q86TI2
D	869	HIS	-	expression tag	UNP Q86TI2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total 15	O 15	0	0
2	B	22	Total 22	O 22	0	0
2	C	19	Total 19	O 19	0	0
2	D	26	Total 26	O 26	0	0

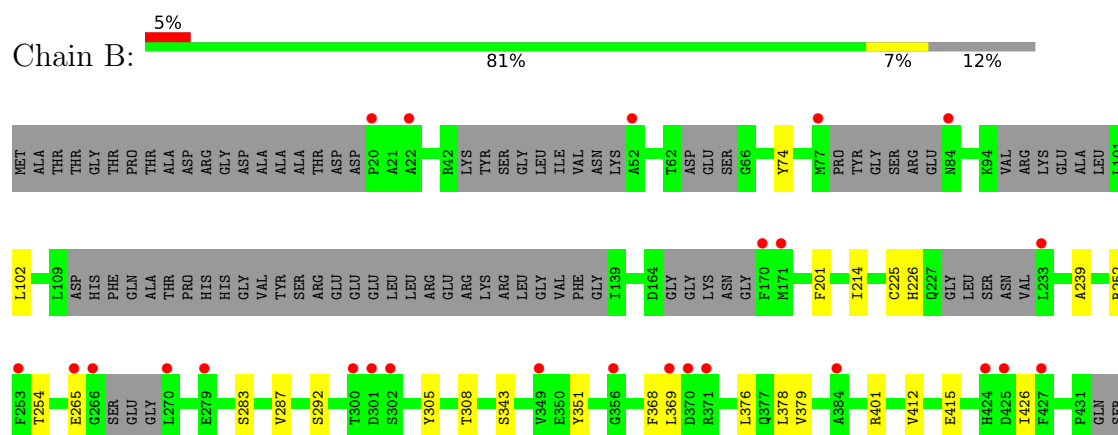
3 Residue-property plots [i](#)

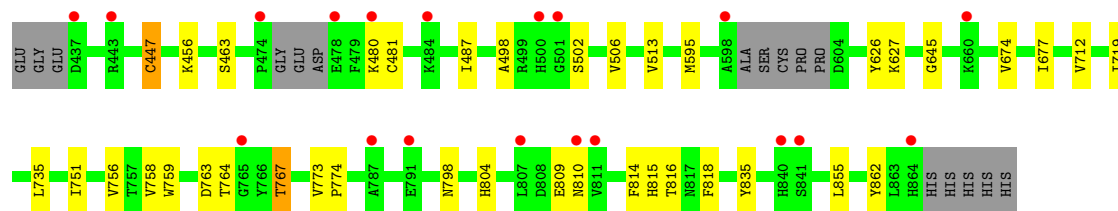
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dipeptidyl peptidase 9

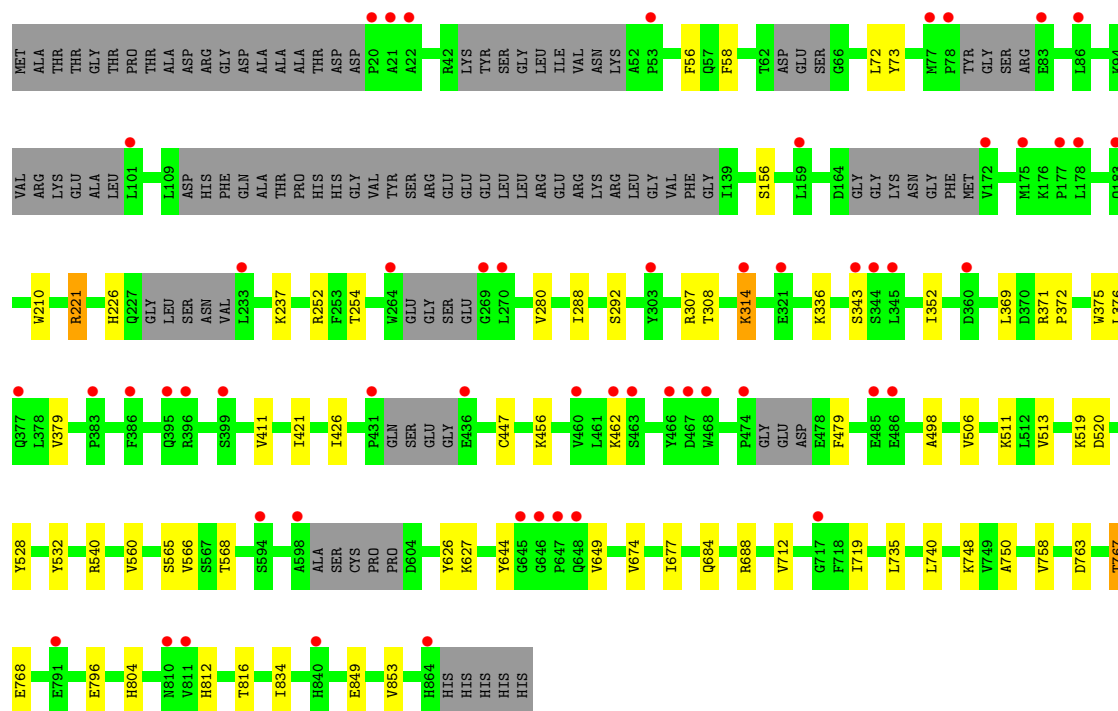
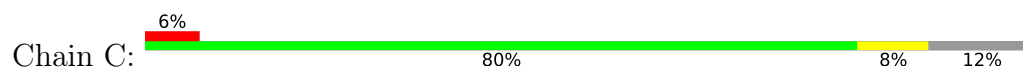


- Molecule 1: Dipeptidyl peptidase 9

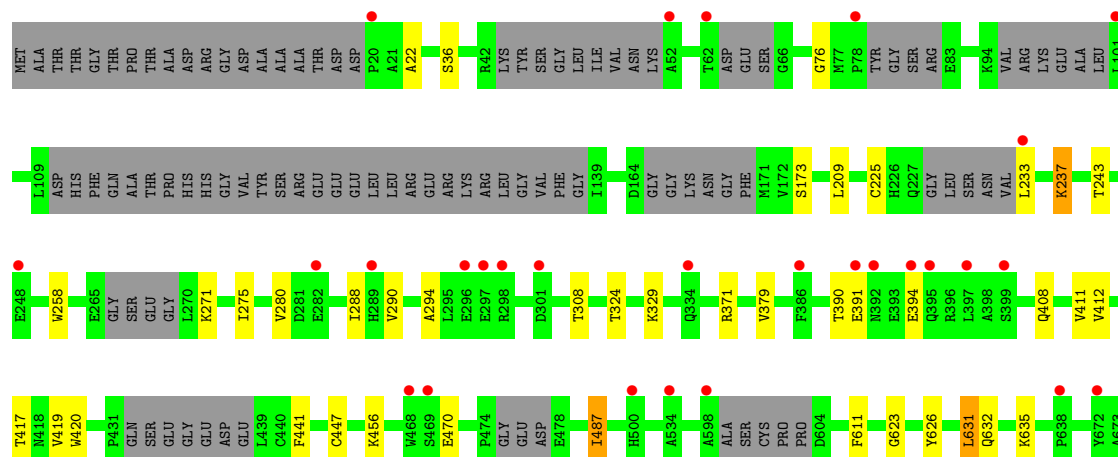
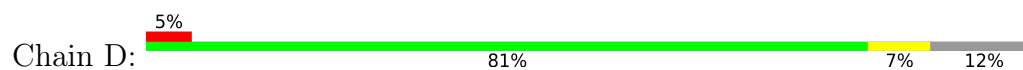


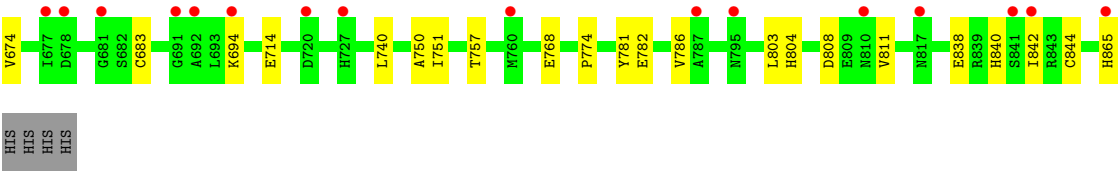


• Molecule 1: Dipeptidyl peptidase 9



• Molecule 1: Dipeptidyl peptidase 9





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.37Å 118.02Å 164.46Å 90.00° 105.49° 90.00°	Depositor
Resolution (Å)	49.26 – 3.00 49.26 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.26-3.00) 99.8 (49.26-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.55	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.273 , 0.334 0.274 , 0.330	Depositor DCC
R_{free} test set	4443 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.741	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24962	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0125e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.71	0/6414	0.90	2/8698 (0.0%)
1	B	0.69	0/6404	0.89	4/8685 (0.0%)
1	C	0.69	0/6401	0.91	1/8683 (0.0%)
1	D	0.70	0/6399	0.89	6/8680 (0.1%)
All	All	0.70	0/25618	0.90	13/34746 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	408	GLN	N-CA-C	6.86	114.18	108.07
1	D	840	HIS	N-CA-C	6.18	120.28	112.87
1	B	835	TYR	CA-C-N	5.93	125.61	119.56
1	B	835	TYR	C-N-CA	5.93	125.61	119.56
1	D	76	GLY	N-CA-C	5.76	118.90	110.38
1	A	85	SER	N-CA-C	5.53	117.37	109.14
1	A	643	VAL	N-CA-C	5.32	115.31	107.75
1	B	369	LEU	N-CA-C	5.23	118.09	109.72
1	C	421	ILE	CB-CA-C	-5.23	106.26	111.80
1	D	842	ILE	N-CA-C	5.12	113.97	106.55
1	D	290	VAL	CA-C-N	5.10	125.39	119.93
1	D	290	VAL	C-N-CA	5.10	125.39	119.93
1	B	764	THR	CB-CA-C	-5.08	102.67	110.81

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	6229	0	6029	34	0
1	B	6220	0	6026	26	0
1	C	6217	0	6021	33	0
1	D	6214	0	6024	25	0
2	A	15	0	0	0	0
2	B	22	0	0	2	0
2	C	19	0	0	1	0
2	D	26	0	0	0	0
All	All	24962	0	24100	116	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 (116) 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:314:LYS:HA	1:A:314:LYS:HE3	1.64	0.78
1:C:314:LYS:HA	1:C:314:LYS:HE2	1.74	0.70
1:C:565:SER:HG	1:C:568:THR:HG1	1.43	0.65
1:B:368:PHE:CE2	1:B:379:VAL:HG11	2.31	0.64
1:A:308:THR:HG21	1:A:781:TYR:OH	1.97	0.63
1:B:815:HIS:CD2	2:B:902:HOH:O	2.51	0.62
1:A:310:SER:O	1:A:371:ARG:NH2	2.33	0.61
1:D:308:THR:HG21	1:D:781:TYR:OH	2.01	0.60
1:A:74:TYR:HH	1:A:105:TRP:CD1	2.19	0.60
1:A:712:VAL:HG12	1:A:719:ILE:HD12	1.84	0.59
1:D:308:THR:HG22	1:D:774:PRO:HD3	1.84	0.59
1:A:373:GLN:OE1	1:A:769:ARG:NH1	2.40	0.55
1:A:410:TYR:HB3	1:A:481:CYS:SG	2.47	0.54
1:A:565:SER:OG	1:A:568:THR:HG22	2.08	0.54
1:B:415:GLU:HB3	1:B:447:CYS:SG	2.48	0.53
1:C:308:THR:HG21	1:C:767:THR:HB	1.90	0.53
1:B:426:ILE:HD12	1:B:498:ALA:HB2	1.90	0.53
1:B:758:VAL:HB	2:B:902:HOH:O	2.09	0.53
1:A:832:LEU:HD21	1:C:834:ILE:HD12	1.91	0.53
1:B:74:TYR:CE1	1:B:595:MET:HE1	2.43	0.53
1:C:812:HIS:HB3	2:C:901:HOH:O	2.09	0.53
1:D:225:CYS:O	1:D:237:LYS:NZ	2.38	0.52
1:C:58:PHE:CE2	1:C:72:LEU:HD11	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LYS:HB3	1:A:487:ILE:CG2	2.39	0.52
1:D:419:VAL:O	1:D:694:LYS:HE2	2.10	0.51
1:B:809:GLU:OE2	1:B:809:GLU:N	2.42	0.51
1:B:804:HIS:CD2	1:B:816:THR:OG1	2.63	0.51
1:C:210:TRP:NE1	1:C:221:ARG:HD2	2.25	0.51
1:A:834:ILE:HD11	1:C:834:ILE:HD11	1.92	0.51
1:B:74:TYR:CZ	1:B:595:MET:HE1	2.46	0.50
1:D:808:ASP:OD1	1:D:811:VAL:N	2.42	0.50
1:A:272:THR:HG22	1:A:323:GLN:HG2	1.94	0.49
1:B:308:THR:HG21	1:B:767:THR:HB	1.93	0.49
1:C:644:TYR:O	1:C:735:LEU:HD12	2.11	0.49
1:D:626:TYR:HB2	1:D:674:VAL:HB	1.93	0.49
1:B:626:TYR:HB2	1:B:674:VAL:HB	1.94	0.49
1:D:838:GLU:OE2	1:D:844:CYS:HB3	2.13	0.49
1:C:369:LEU:HD23	1:C:375:TRP:O	2.13	0.49
1:D:22:ALA:O	1:D:635:LYS:HA	2.12	0.49
1:C:308:THR:CG2	1:C:767:THR:HB	2.43	0.49
1:C:426:ILE:HD12	1:C:498:ALA:HB2	1.95	0.49
1:C:252:ARG:NH1	1:C:352:ILE:O	2.44	0.48
1:A:804:HIS:HD2	1:A:816:THR:OG1	1.95	0.48
1:C:644:TYR:CE2	1:C:649:VAL:HG21	2.47	0.48
1:A:519:LYS:HB3	1:A:528:TYR:CZ	2.48	0.48
1:A:339:VAL:HG23	1:A:385:LEU:O	2.14	0.47
1:D:243:THR:CG2	1:D:280:VAL:HG11	2.44	0.47
1:B:252:ARG:NE	1:B:254:THR:O	2.46	0.46
1:C:371:ARG:NH1	1:C:768:GLU:OE2	2.46	0.46
1:D:243:THR:HG21	1:D:280:VAL:HG11	1.97	0.46
1:B:798:ASN:HB3	1:B:862:TYR:CG	2.51	0.46
1:A:324:THR:HA	1:A:329:LYS:O	2.16	0.46
1:C:307:ARG:HA	1:C:763:ASP:HA	1.98	0.46
1:B:814:PHE:CE1	1:B:818:PHE:HB2	2.51	0.46
1:C:369:LEU:HG	1:C:376:LEU:HD12	1.97	0.45
1:B:756:VAL:HG11	1:B:759:TRP:CZ3	2.51	0.45
1:A:209:LEU:N	1:A:223:THR:OG1	2.47	0.45
1:C:740:LEU:HD22	1:C:750:ALA:HB3	1.99	0.45
1:D:740:LEU:HD22	1:D:750:ALA:HB3	1.98	0.45
1:A:417:THR:HG21	1:A:420:TRP:C	2.42	0.45
1:A:456:LYS:HB3	1:A:487:ILE:HG23	1.97	0.45
1:C:56:PHE:HA	1:C:73:TYR:O	2.17	0.45
1:C:371:ARG:HB3	1:C:372:PRO:HD3	1.98	0.45
1:A:307:ARG:O	1:A:764:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:849:GLU:O	1:C:853:VAL:HG23	2.17	0.44
1:C:520:ASP:OD2	1:C:540:ARG:NE	2.51	0.44
1:D:412:VAL:CG1	1:D:441:PHE:CE1	3.00	0.44
1:C:712:VAL:HG12	1:C:719:ILE:HG13	1.99	0.44
1:A:413:TYR:CE1	1:A:457:VAL:HG21	2.53	0.43
1:B:645:GLY:HA3	1:B:735:LEU:CD1	2.48	0.43
1:D:631:LEU:HD13	1:D:632:GLN:N	2.32	0.43
1:C:237:LYS:HA	1:C:280:VAL:O	2.17	0.43
1:B:368:PHE:CE2	1:B:379:VAL:CG1	3.01	0.43
1:C:411:VAL:HG23	1:C:479:PHE:HB2	1.99	0.43
1:D:237:LYS:NZ	1:D:237:LYS:HB2	2.34	0.43
1:D:379:VAL:HG12	1:D:411:VAL:HG22	2.01	0.43
1:D:456:LYS:HB3	1:D:487:ILE:HG23	2.00	0.43
1:B:201:PHE:CD1	1:B:214:ILE:HG23	2.53	0.43
1:A:319:LEU:O	1:A:336:LYS:N	2.52	0.43
1:C:58:PHE:HZ	1:C:560:VAL:HG23	1.83	0.43
1:A:712:VAL:HG12	1:A:719:ILE:CD1	2.46	0.43
1:C:511:LYS:HA	1:C:532:TYR:CE2	2.54	0.43
1:C:804:HIS:HD2	1:C:816:THR:OG1	2.02	0.43
1:A:371:ARG:HB3	1:A:372:PRO:HD3	2.00	0.42
1:A:250:PHE:O	1:A:251:ASP:C	2.61	0.42
1:A:644:TYR:O	1:A:735:LEU:HD12	2.20	0.42
1:D:324:THR:HA	1:D:329:LYS:O	2.18	0.42
1:B:712:VAL:HG12	1:B:719:ILE:HG13	2.02	0.42
1:C:506:VAL:HG22	1:C:513:VAL:HG23	2.00	0.42
1:D:258:TRP:CH2	1:D:275:ILE:HD11	2.54	0.42
1:D:225:CYS:O	1:D:237:LYS:HB2	2.20	0.42
1:A:71:ARG:NE	1:A:90:GLU:OE1	2.52	0.41
1:B:308:THR:CG2	1:B:767:THR:HB	2.51	0.41
1:D:757:THR:HA	1:D:786:VAL:HG22	2.03	0.41
1:B:506:VAL:HG22	1:B:513:VAL:HG23	2.03	0.41
1:C:626:TYR:HB2	1:C:674:VAL:HB	2.02	0.41
1:D:417:THR:HG21	1:D:420:TRP:C	2.46	0.41
1:A:305:TYR:CZ	1:A:763:ASP:HB3	2.56	0.41
1:A:804:HIS:CD2	1:A:816:THR:OG1	2.73	0.41
1:B:773:VAL:HG22	1:B:774:PRO:HD2	2.03	0.41
1:C:252:ARG:NE	1:C:254:THR:O	2.52	0.41
1:C:519:LYS:HB3	1:C:528:TYR:CZ	2.55	0.41
1:D:308:THR:HG21	1:D:781:TYR:HH	1.85	0.41
1:D:308:THR:HG23	1:D:768:GLU:HG3	2.02	0.41
1:A:680:ARG:HG3	1:A:704:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:TYR:CZ	1:B:763:ASP:HB3	2.56	0.41
1:A:497:LEU:HD11	1:A:525:HIS:ND1	2.36	0.41
1:A:757:THR:HA	1:A:786:VAL:HG22	2.03	0.41
1:B:225:CYS:SG	1:B:239:ALA:HB2	2.61	0.41
1:C:804:HIS:CD2	1:C:816:THR:OG1	2.74	0.41
1:A:701:GLU:O	1:A:705:GLN:HG2	2.20	0.40
1:B:751:ILE:HD13	1:B:855:LEU:HD12	2.03	0.40
1:D:751:ILE:CG2	1:D:803:LEU:HD11	2.51	0.40
1:D:611:PHE:CZ	1:D:623:GLY:HA3	2.56	0.40
1:A:308:THR:HG22	1:A:774:PRO:HD3	2.04	0.40
1:B:751:ILE:HG21	1:B:855:LEU:HD12	2.04	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	743/869 (86%)	692 (93%)	50 (7%)	1 (0%)	48	80
1	B	742/869 (85%)	700 (94%)	42 (6%)	0	100	100
1	C	742/869 (85%)	697 (94%)	44 (6%)	1 (0%)	48	80
1	D	741/869 (85%)	691 (93%)	49 (7%)	1 (0%)	48	80
All	All	2968/3476 (85%)	2780 (94%)	185 (6%)	3 (0%)	48	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	294	ALA
1	C	462	LYS
1	A	67	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	680/759 (90%)	664 (98%)	16 (2%)	43	73
1	B	678/759 (89%)	655 (97%)	23 (3%)	32	66
1	C	678/759 (89%)	658 (97%)	20 (3%)	37	70
1	D	678/759 (89%)	658 (97%)	20 (3%)	37	70
All	All	2714/3036 (89%)	2635 (97%)	79 (3%)	37	70

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	SER
1	A	150	LEU
1	A	176	LYS
1	A	185	SER
1	A	238	SER
1	A	279	GLU
1	A	288	ILE
1	A	314	LYS
1	A	343	SER
1	A	369	LEU
1	A	379	VAL
1	A	390	THR
1	A	393	GLU
1	A	447	CYS
1	A	469	SER
1	A	480	LYS
1	B	102	LEU
1	B	226	HIS
1	B	265	GLU
1	B	283	SER
1	B	287	VAL
1	B	292	SER
1	B	343	SER
1	B	351	TYR

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Mol	Chain	Res	Type
1	B	376	LEU
1	B	378	LEU
1	B	401	ARG
1	B	412	VAL
1	B	447	CYS
1	B	456	LYS
1	B	463	SER
1	B	480	LYS
1	B	481	CYS
1	B	487	ILE
1	B	502	SER
1	B	627	LYS
1	B	677	ILE
1	B	767	THR
1	B	810	ASN
1	C	156	SER
1	C	221	ARG
1	C	226	HIS
1	C	288	ILE
1	C	292	SER
1	C	314	LYS
1	C	336	LYS
1	C	343	SER
1	C	379	VAL
1	C	447	CYS
1	C	456	LYS
1	C	566	VAL
1	C	627	LYS
1	C	677	ILE
1	C	684	GLN
1	C	688	ARG
1	C	748	LYS
1	C	758	VAL
1	C	767	THR
1	C	796	GLU
1	D	36	SER
1	D	173	SER
1	D	209	LEU
1	D	233	LEU
1	D	237	LYS
1	D	271	LYS
1	D	288	ILE

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Mol	Chain	Res	Type
1	D	371	ARG
1	D	390	THR
1	D	391	GLU
1	D	394	GLU
1	D	447	CYS
1	D	470	GLU
1	D	487	ILE
1	D	631	LEU
1	D	683	CYS
1	D	714	GLU
1	D	782	GLU
1	D	804	HIS
1	D	865	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	A	206	ASN
1	A	327	GLN
1	A	334	GLN
1	A	340	GLN
1	A	554	GLN
1	A	555	ASN
1	A	648	GLN
1	A	804	HIS
1	A	815	HIS
1	A	833	GLN
1	B	25	GLN
1	B	54	HIS
1	B	340	GLN
1	B	422	ASN
1	B	500	HIS
1	B	555	ASN
1	B	705	GLN
1	B	742	HIS
1	B	804	HIS
1	B	857	HIS
1	C	161	HIS
1	C	206	ASN
1	C	424	HIS
1	C	705	GLN

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Mol	Chain	Res	Type
1	C	804	HIS
1	C	810	ASN
1	C	837	ASN
1	C	860	GLN
1	D	157	ASN
1	D	334	GLN
1	D	424	HIS
1	D	588	GLN
1	D	742	HIS

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 [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	767/869 (88%)	0.66	53 (6%)	23	12	29, 52, 83, 103	0
1	B	766/869 (88%)	0.57	44 (5%)	29	15	30, 53, 83, 125	0
1	C	766/869 (88%)	0.74	55 (7%)	21	11	28, 52, 83, 122	0
1	D	765/869 (88%)	0.58	44 (5%)	29	15	29, 53, 84, 112	0
All	All	3064/3476 (88%)	0.64	196 (6%)	25	13	28, 52, 84, 125	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	PRO	6.7
1	A	386	PHE	6.5
1	C	386	PHE	5.4
1	B	233	LEU	4.9
1	B	266	GLY	4.8
1	A	437	ASP	4.7
1	D	248	GLU	4.7
1	D	469	SER	4.6
1	C	399	SER	4.5
1	B	302	SER	4.3
1	C	462	LYS	4.2
1	C	474	PRO	4.1
1	B	20	PRO	4.0
1	C	395	GLN	4.0
1	C	270	LEU	3.9
1	D	391	GLU	3.8
1	C	840	HIS	3.8
1	B	77	MET	3.8
1	A	463	SER	3.7
1	A	474	PRO	3.7
1	D	289	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	22	ALA	3.5
1	D	865	HIS	3.5
1	C	78	PRO	3.5
1	B	52	ALA	3.4
1	A	248	GLU	3.4
1	A	109	LEU	3.4
1	D	397	LEU	3.4
1	A	598	ALA	3.3
1	C	77	MET	3.3
1	A	181	LYS	3.2
1	B	270	LEU	3.2
1	D	841	SER	3.2
1	D	282	GLU	3.2
1	A	717	GLY	3.2
1	D	392	ASN	3.2
1	B	478	GLU	3.1
1	A	840	HIS	3.1
1	D	52	ALA	3.1
1	B	765	GLY	3.1
1	C	233	LEU	3.1
1	C	864	HIS	3.1
1	A	395	GLN	3.1
1	B	384	ALA	3.1
1	B	598	ALA	3.1
1	C	646	GLY	3.1
1	A	20	PRO	3.1
1	A	646	GLY	3.1
1	C	436	GLU	3.1
1	A	78	PRO	3.1
1	B	810	ASN	3.0
1	B	265	GLU	3.0
1	C	791	GLU	3.0
1	B	370	ASP	3.0
1	C	178	LEU	3.0
1	B	840	HIS	3.0
1	C	269	GLY	3.0
1	D	233	LEU	3.0
1	C	314	LYS	3.0
1	B	500	HIS	3.0
1	A	508	GLU	2.9
1	C	383	PRO	2.9
1	A	185	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	267	SER	2.9
1	C	460	VAL	2.9
1	B	474	PRO	2.9
1	B	791	GLU	2.9
1	C	486	GLU	2.9
1	D	394	GLU	2.9
1	B	427	PHE	2.9
1	B	369	LEU	2.9
1	B	425	ASP	2.8
1	C	810	ASN	2.8
1	C	645	GLY	2.8
1	C	463	SER	2.8
1	A	648	GLN	2.8
1	C	83	GLU	2.8
1	D	301	ASP	2.8
1	D	672	TYR	2.8
1	D	727	HIS	2.8
1	B	787	ALA	2.8
1	D	598	ALA	2.8
1	A	289	HIS	2.7
1	B	484	LYS	2.7
1	D	787	ALA	2.7
1	C	101	LEU	2.7
1	C	345	LEU	2.7
1	A	179	GLU	2.7
1	D	296	GLU	2.7
1	A	101	LEU	2.7
1	B	170	PHE	2.7
1	A	484	LYS	2.7
1	D	720	ASP	2.7
1	A	864	HIS	2.7
1	D	78	PRO	2.7
1	D	395	GLN	2.7
1	B	300	THR	2.7
1	D	694	LYS	2.6
1	B	356	GLY	2.6
1	A	693	LEU	2.6
1	C	172	VAL	2.6
1	D	500	HIS	2.6
1	D	386	PHE	2.6
1	C	264	TRP	2.6
1	A	234	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	839	ARG	2.6
1	C	303	TYR	2.6
1	B	301	ASP	2.6
1	B	864	HIS	2.5
1	A	460	VAL	2.5
1	A	498	ALA	2.5
1	D	20	PRO	2.5
1	D	678	ASP	2.5
1	A	303	TYR	2.5
1	C	53	PRO	2.5
1	C	360	ASP	2.5
1	A	56	PHE	2.5
1	A	170	PHE	2.5
1	D	62	THR	2.5
1	C	647	PRO	2.5
1	C	396	ARG	2.5
1	B	171	MET	2.5
1	B	253	PHE	2.5
1	D	810	ASN	2.5
1	D	691	GLY	2.5
1	C	598	ALA	2.4
1	A	568	THR	2.4
1	A	159	LEU	2.4
1	C	468	TRP	2.4
1	C	159	LEU	2.4
1	C	321	GLU	2.4
1	A	187	PRO	2.4
1	C	21	ALA	2.3
1	C	377	GLN	2.3
1	B	424	HIS	2.3
1	C	648	GLN	2.3
1	C	811	VAL	2.3
1	B	660	LYS	2.3
1	C	344	SER	2.3
1	B	443	ARG	2.3
1	A	178	LEU	2.3
1	B	437	ASP	2.3
1	A	265	GLU	2.3
1	A	314	LYS	2.3
1	C	183	GLN	2.3
1	D	842	ILE	2.2
1	B	371	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	393	GLU	2.2
1	A	425	ASP	2.2
1	A	266	GLY	2.2
1	D	638	PRO	2.2
1	B	811	VAL	2.2
1	B	841	SER	2.2
1	C	594	SER	2.2
1	D	297	GLU	2.2
1	C	717	GLY	2.2
1	C	467	ASP	2.2
1	A	105	TRP	2.2
1	D	468	TRP	2.2
1	A	412	VAL	2.1
1	D	677	ILE	2.1
1	C	86	LEU	2.1
1	A	809	GLU	2.1
1	B	501	GLY	2.1
1	C	177	PRO	2.1
1	A	175	MET	2.1
1	C	343	SER	2.1
1	D	399	SER	2.1
1	D	795	ASN	2.1
1	A	176	LYS	2.1
1	A	288	ILE	2.1
1	C	466	TYR	2.1
1	A	444	ALA	2.1
1	B	349	VAL	2.1
1	D	760	MET	2.1
1	D	692	ALA	2.1
1	A	377	GLN	2.1
1	A	200	PHE	2.1
1	B	480	LYS	2.0
1	A	551	SER	2.0
1	B	807	LEU	2.0
1	D	298	ARG	2.0
1	D	534	ALA	2.0
1	D	681	GLY	2.0
1	B	279	GLU	2.0
1	B	84	ASN	2.0
1	C	175	MET	2.0
1	D	817	ASN	2.0
1	B	22	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	251	ASP	2.0
1	A	183	GLN	2.0
1	C	431	PRO	2.0
1	D	334	GLN	2.0
1	C	485	GLU	2.0
1	D	101	LEU	2.0
1	A	426	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.