



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:25 AM UTC

PDB ID : 6EOS / pdb_00006eos
Title : DPP8 - Apo, space group 19
Authors : Ross, B.R.; Huber, R.
Deposited on : 2017-10-10
Resolution : 3.10 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:

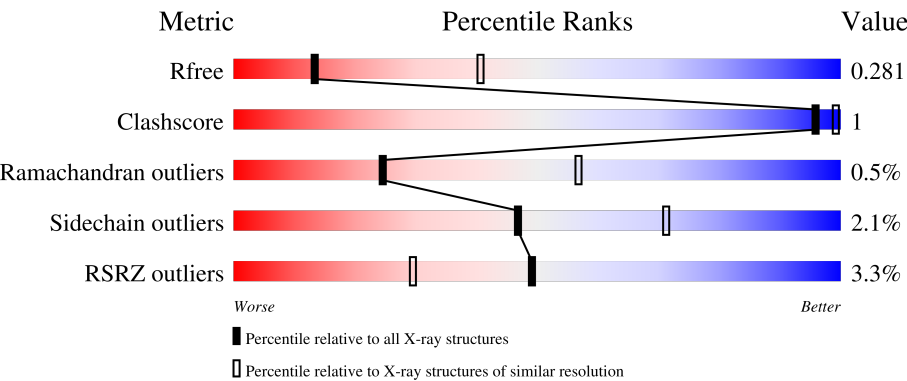
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	% 87%9%
1	B	898	10% 84%7%10%
1	C	898	% 87%5%8%
1	D	898	% 87%9%
1	E	898	2% 87%8%

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Mol	Chain	Length	Quality of chain
1	F	898	3% 85% 6% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 39998 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	815	Total	C	N	O	S	0	0	0
			6620	4257	1107	1230	26			
1	C	829	Total	C	N	O	S	0	0	0
			6740	4334	1130	1250	26			
1	D	815	Total	C	N	O	S	0	0	0
			6613	4253	1104	1229	27			
1	E	825	Total	C	N	O	S	0	0	0
			6697	4308	1118	1243	28			
1	F	815	Total	C	N	O	S	0	0	0
			6620	4257	1107	1230	26			
1	B	811	Total	C	N	O	S	0	0	0
			6583	4233	1100	1224	26			

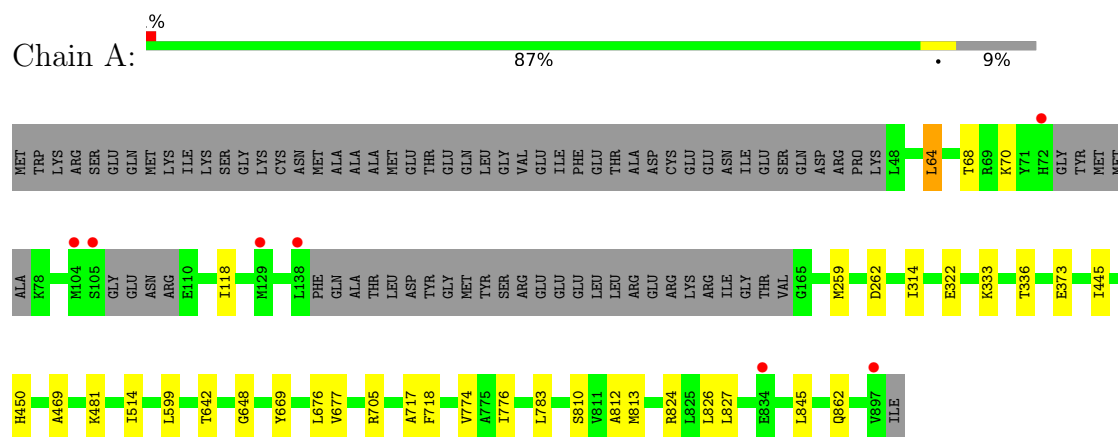
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	32	Total	O	0	0
			32	32		
2	C	23	Total	O	0	0
			23	23		
2	D	21	Total	O	0	0
			21	21		
2	E	21	Total	O	0	0
			21	21		
2	F	20	Total	O	0	0
			20	20		
2	B	8	Total	O	0	0
			8	8		

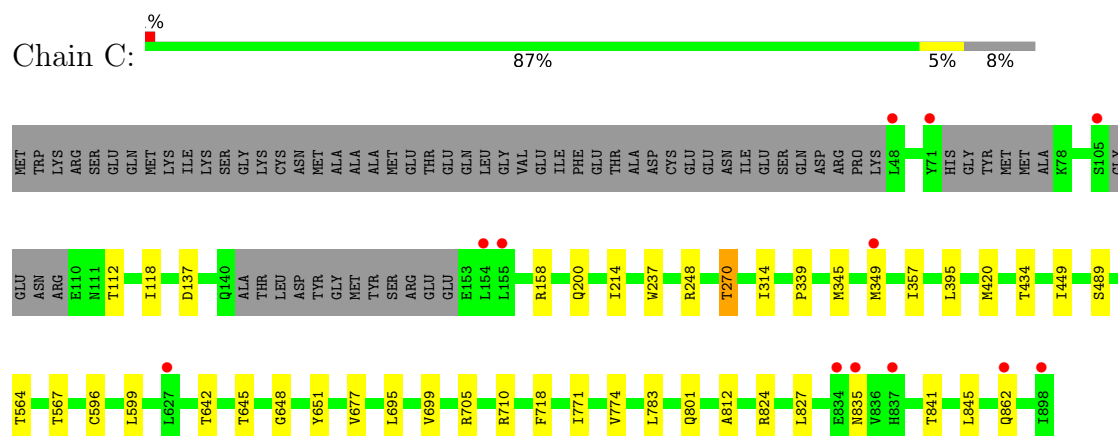
3 Residue-property plots [i](#)

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.

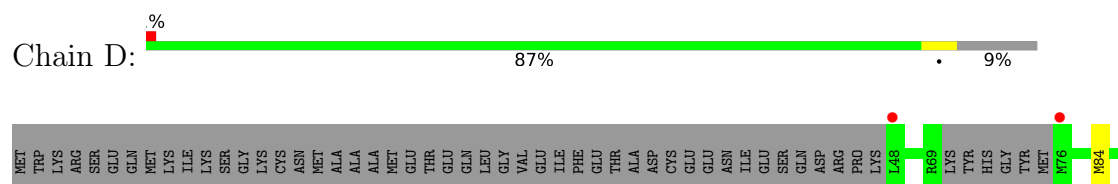
• Molecule 1: Dipeptidyl peptidase 8

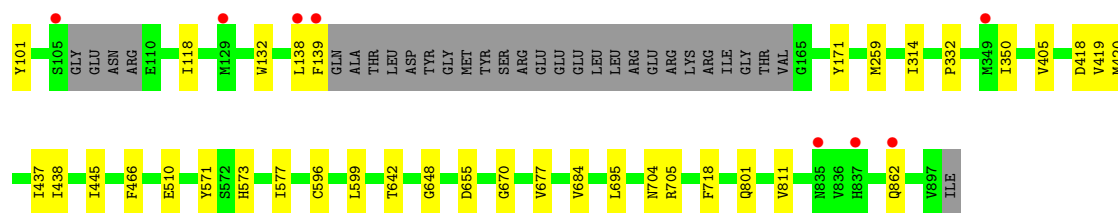


• Molecule 1: Dipeptidyl peptidase 8

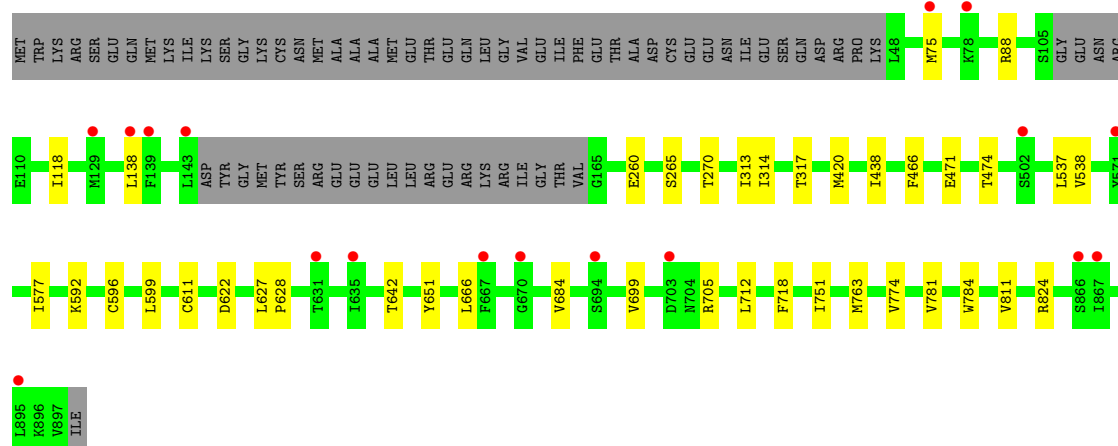
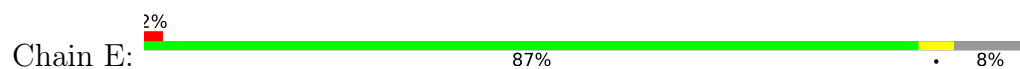


• Molecule 1: Dipeptidyl peptidase 8

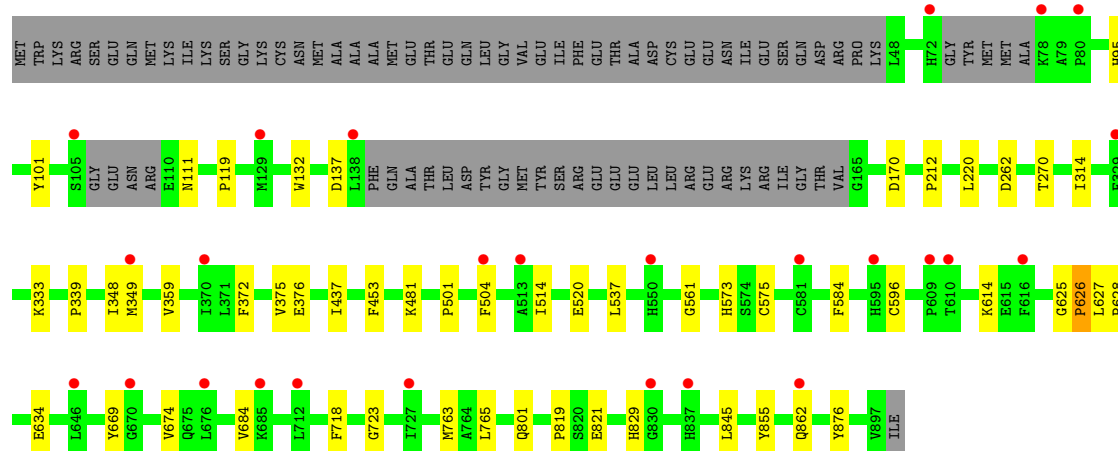
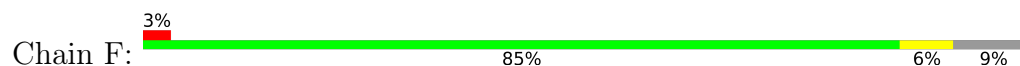




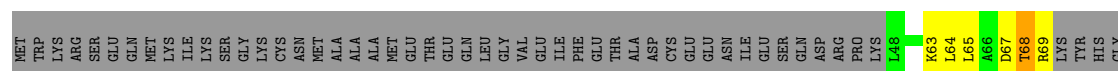
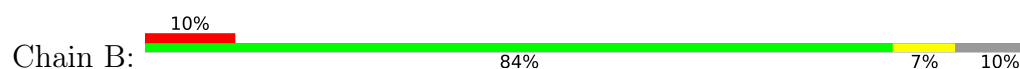
• Molecule 1: Dipeptidyl peptidase 8

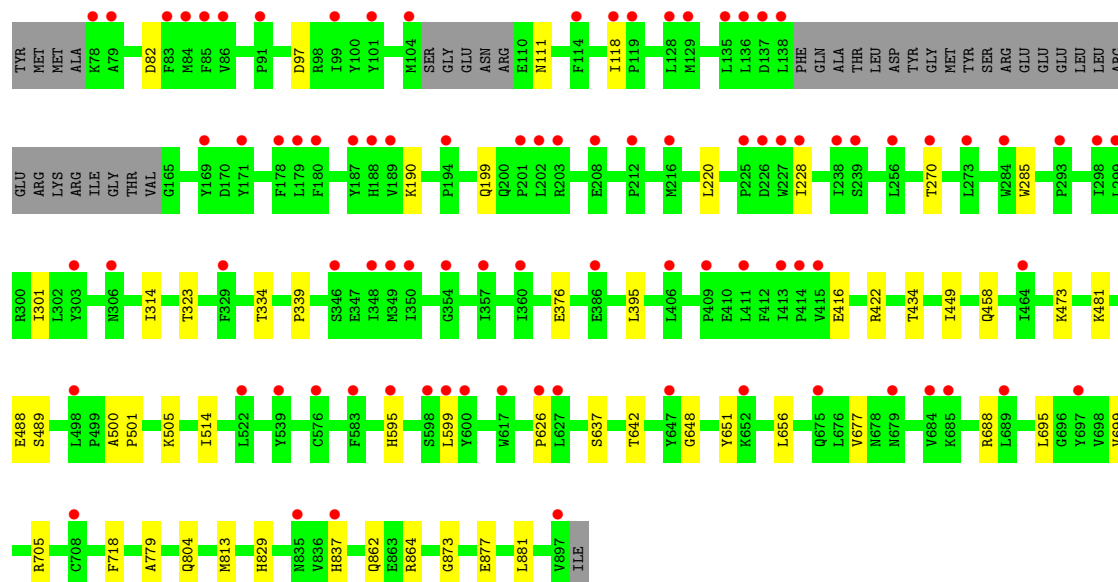


• Molecule 1: Dipeptidyl peptidase 8



• Molecule 1: Dipeptidyl peptidase 8





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	148.12Å 266.78Å 268.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.40 – 3.10 44.40 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.40-3.10) 99.9 (44.40-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.247 , 0.283 0.247 , 0.281	Depositor DCC
R_{free} test set	9593 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	83.4	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	39998	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.28% 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	0.50	1/6805 (0.0%)	0.75	1/9234 (0.0%)
1	B	0.57	0/6766	0.76	0/9182
1	C	0.50	0/6925	0.75	0/9393
1	D	0.51	0/6797	0.74	0/9223
1	E	0.52	0/6885	0.76	0/9343
1	F	0.54	0/6805	0.77	0/9234
All	All	0.53	1/40983 (0.0%)	0.76	1/55609 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	262	ASP	CA-C	5.89	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	669	TYR	N-CA-C	-5.29	105.04	112.12

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	6620	0	6439	12	0
1	B	6583	0	6405	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6740	0	6576	15	0
1	D	6613	0	6433	10	0
1	E	6697	0	6515	15	0
1	F	6620	0	6439	15	0
2	A	32	0	0	0	0
2	B	8	0	0	0	0
2	C	23	0	0	0	0
2	D	21	0	0	0	0
2	E	21	0	0	0	0
2	F	20	0	0	0	0
All	All	39998	0	38807	84	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 1.

All (84) 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:64:LEU:O	1:A:68:THR:HG23	1.93	0.67
1:F:101:TYR:HH	1:F:132:TRP:CD1	2.14	0.65
1:D:101:TYR:HH	1:D:132:TRP:CD1	2.18	0.62
1:A:333:LYS:HG2	1:A:336:THR:HG23	1.90	0.53
1:E:666:LEU:HD23	1:E:751:ILE:HD12	1.91	0.52
1:E:774:VAL:HG12	1:E:824:ARG:HA	1.90	0.52
1:C:651:TYR:HB2	1:C:699:VAL:HB	1.92	0.52
1:B:434:THR:HG21	1:B:489:SER:HB2	1.92	0.52
1:B:500:ALA:HB1	1:B:501:PRO:HD2	1.93	0.51
1:A:642:THR:HG21	1:A:705:ARG:NH1	2.25	0.51
1:A:783:LEU:HD13	1:A:812:ALA:HB3	1.93	0.50
1:F:348:ILE:HG23	1:F:359:VAL:HG22	1.94	0.49
1:D:648:GLY:HA2	1:D:677:VAL:HG21	1.93	0.49
1:C:270:THR:HG21	1:C:339:PRO:HG2	1.95	0.48
1:C:774:VAL:HG12	1:C:824:ARG:HA	1.95	0.48
1:B:64:LEU:O	1:B:68:THR:HG23	2.14	0.48
1:A:774:VAL:HG12	1:A:824:ARG:HA	1.95	0.48
1:D:84:MET:HE1	1:D:171:TYR:CG	2.48	0.48
1:E:781:VAL:HG11	1:E:784:TRP:CZ3	2.49	0.47
1:B:648:GLY:HA2	1:B:677:VAL:HG21	1.95	0.47
1:C:648:GLY:HA2	1:C:677:VAL:HG21	1.95	0.47
1:B:395:LEU:HD21	1:B:449:ILE:HD11	1.97	0.47
1:A:450:HIS:CE1	1:A:469:ALA:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ILE:HD12	1:C:599:LEU:HD22	1.97	0.46
1:F:669:TYR:CE2	1:F:674:VAL:HG21	2.50	0.46
1:C:395:LEU:HD21	1:C:449:ILE:HD11	1.97	0.46
1:E:763:MET:HE2	1:E:811:VAL:HG13	1.98	0.45
1:F:627:LEU:HD12	1:F:628:PRO:HD2	1.98	0.45
1:D:642:THR:HG21	1:D:705:ARG:NH1	2.32	0.45
1:B:688:ARG:HA	1:B:688:ARG:HD3	1.84	0.45
1:B:873:GLY:O	1:B:877:GLU:HG3	2.16	0.45
1:A:481:LYS:HB2	1:A:514:ILE:HD11	1.98	0.45
1:E:642:THR:HG21	1:E:705:ARG:NH1	2.31	0.45
1:C:434:THR:HG21	1:C:489:SER:CB	2.47	0.45
1:C:645:THR:O	1:C:710:ARG:NH1	2.47	0.44
1:B:118:ILE:HD12	1:B:599:LEU:CD2	2.48	0.44
1:D:118:ILE:HD12	1:D:599:LEU:CD2	2.47	0.44
1:E:118:ILE:HD12	1:E:599:LEU:HD22	2.00	0.44
1:F:101:TYR:HH	1:F:132:TRP:CG	2.35	0.44
1:B:481:LYS:HB2	1:B:514:ILE:HD11	1.99	0.44
1:E:651:TYR:HB2	1:E:699:VAL:HB	2.01	0.43
1:F:95:HIS:HA	1:F:119:PRO:HA	2.01	0.43
1:E:577:ILE:HD12	1:E:577:ILE:N	2.34	0.43
1:B:220:LEU:HD23	1:B:228:ILE:HG22	2.00	0.43
1:B:270:THR:HG21	1:B:339:PRO:HG2	2.01	0.43
1:B:642:THR:HG21	1:B:705:ARG:NH1	2.33	0.43
1:A:648:GLY:HA2	1:A:677:VAL:HG21	2.01	0.43
1:C:642:THR:HG21	1:C:705:ARG:NH1	2.34	0.43
1:E:118:ILE:HD12	1:E:599:LEU:CD2	2.48	0.42
1:C:237:TRP:CZ2	1:C:248:ARG:HD2	2.55	0.42
1:C:270:THR:HG21	1:C:339:PRO:CG	2.49	0.42
1:F:723:GLY:HA3	1:F:763:MET:HE3	2.00	0.42
1:B:779:ALA:HA	1:B:829:HIS:CD2	2.55	0.42
1:E:75:MET:HG2	1:E:684:VAL:HG22	2.00	0.42
1:D:405:VAL:HG22	1:D:437:ILE:HG12	2.01	0.42
1:D:670:GLY:HA3	1:D:704:ASN:HD21	1.85	0.42
1:A:118:ILE:HD12	1:A:599:LEU:CD2	2.50	0.42
1:A:776:ILE:HG23	1:A:826:LEU:HD23	2.00	0.42
1:E:627:LEU:HD12	1:E:628:PRO:HD2	2.00	0.42
1:F:573:HIS:HB3	1:F:575:CYS:SG	2.60	0.42
1:F:845:LEU:HD22	1:F:855:TYR:CZ	2.55	0.42
1:E:260:GLU:HG3	1:E:313:ILE:HD13	2.02	0.42
1:C:783:LEU:HD13	1:C:812:ALA:HB3	2.01	0.41
1:F:481:LYS:HB2	1:F:514:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:VAL:HG13	1:D:420:MET:HE3	2.02	0.41
1:E:438:ILE:HD12	1:E:466:PHE:CE2	2.55	0.41
1:A:783:LEU:HD12	1:A:810:SER:HB3	2.02	0.41
1:D:438:ILE:HD12	1:D:466:PHE:CE2	2.56	0.41
1:F:625:GLY:O	1:F:626:PRO:C	2.64	0.41
1:B:67:ASP:O	1:B:69:ARG:N	2.53	0.41
1:F:437:ILE:HD12	1:F:504:PHE:HB2	2.03	0.41
1:B:651:TYR:HB2	1:B:699:VAL:HB	2.02	0.41
1:F:270:THR:HG21	1:F:339:PRO:CG	2.51	0.41
1:E:471:GLU:HB3	1:E:712:LEU:HD22	2.03	0.41
1:A:827:LEU:HD12	1:A:845:LEU:HD21	2.03	0.41
1:C:349:MET:HB3	1:C:357:ILE:HD12	2.03	0.41
1:B:65:LEU:HD21	1:B:881:LEU:HD11	2.03	0.41
1:B:285:TRP:CH2	1:B:301:ILE:HD11	2.56	0.41
1:C:827:LEU:HD12	1:C:845:LEU:HD21	2.04	0.40
1:D:571:TYR:HB2	1:D:573:HIS:CE1	2.57	0.40
1:C:420:MET:HA	1:C:420:MET:HE2	2.04	0.40
1:F:372:PHE:HB3	1:F:375:VAL:HG21	2.02	0.40
1:F:765:LEU:HD11	1:F:819:PRO:HG2	2.03	0.40
1:E:420:MET:HE2	1:E:420:MET:HA	2.04	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	807/898 (90%)	767 (95%)	35 (4%)	5 (1%)	21	52
1	B	803/898 (89%)	728 (91%)	70 (9%)	5 (1%)	21	52
1	C	821/898 (91%)	777 (95%)	42 (5%)	2 (0%)	43	73
1	D	807/898 (90%)	754 (93%)	47 (6%)	6 (1%)	18	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	819/898 (91%)	765 (93%)	54 (7%)	0	100	100
1	F	807/898 (90%)	750 (93%)	49 (6%)	8 (1%)	12	41
All	All	4864/5388 (90%)	4541 (93%)	297 (6%)	26 (0%)	24	57

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	THR
1	C	158	ARG
1	F	561	GLY
1	A	70	LYS
1	D	138	LEU
1	D	418	ASP
1	D	684	VAL
1	F	137	ASP
1	F	262	ASP
1	B	111	ASN
1	B	864	ARG
1	A	322	GLU
1	A	717	ALA
1	D	259	MET
1	F	453	PHE
1	F	626	PRO
1	B	458	GLN
1	B	626	PRO
1	A	259	MET
1	D	445	ILE
1	F	212	PRO
1	A	445	ILE
1	F	501	PRO
1	D	332	PRO
1	F	684	VAL
1	C	214	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	724/795 (91%)	717 (99%)	7 (1%)	68	79
1	B	720/795 (91%)	697 (97%)	23 (3%)	34	64
1	C	737/795 (93%)	721 (98%)	16 (2%)	45	71
1	D	723/795 (91%)	711 (98%)	12 (2%)	53	74
1	E	731/795 (92%)	717 (98%)	14 (2%)	50	73
1	F	724/795 (91%)	705 (97%)	19 (3%)	40	68
All	All	4359/4770 (91%)	4268 (98%)	91 (2%)	47	71

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LEU
1	A	314	ILE
1	A	373	GLU
1	A	676	LEU
1	A	718	PHE
1	A	813	MET
1	A	862	GLN
1	C	112	THR
1	C	137	ASP
1	C	200	GLN
1	C	270	THR
1	C	314	ILE
1	C	345	MET
1	C	564	THR
1	C	567	THR
1	C	596	CYS
1	C	695	LEU
1	C	718	PHE
1	C	771	ILE
1	C	801	GLN
1	C	835	ASN
1	C	841	THR
1	C	862	GLN
1	D	139	PHE
1	D	314	ILE
1	D	350	ILE
1	D	510	GLU
1	D	577	ILE
1	D	596	CYS
1	D	655	ASP

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Mol	Chain	Res	Type
1	D	695	LEU
1	D	718	PHE
1	D	801	GLN
1	D	811	VAL
1	D	862	GLN
1	E	88	ARG
1	E	138	LEU
1	E	265	SER
1	E	270	THR
1	E	314	ILE
1	E	317	THR
1	E	474	THR
1	E	537	LEU
1	E	538	VAL
1	E	592	LYS
1	E	596	CYS
1	E	611	CYS
1	E	622	ASP
1	E	718	PHE
1	F	111	ASN
1	F	170	ASP
1	F	220	LEU
1	F	314	ILE
1	F	333	LYS
1	F	349	MET
1	F	376	GLU
1	F	520	GLU
1	F	537	LEU
1	F	584	PHE
1	F	596	CYS
1	F	614	LYS
1	F	634	GLU
1	F	718	PHE
1	F	801	GLN
1	F	821	GLU
1	F	829	HIS
1	F	862	GLN
1	F	876	TYR
1	B	63	LYS
1	B	82	ASP
1	B	97	ASP
1	B	190	LYS

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Mol	Chain	Res	Type
1	B	199	GLN
1	B	314	ILE
1	B	323	THR
1	B	334	THR
1	B	376	GLU
1	B	416	GLU
1	B	422	ARG
1	B	473	LYS
1	B	488	GLU
1	B	505	LYS
1	B	595	HIS
1	B	637	SER
1	B	656	LEU
1	B	695	LEU
1	B	718	PHE
1	B	804	GLN
1	B	813	MET
1	B	837	HIS
1	B	862	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	72	HIS
1	A	173	GLN
1	A	200	GLN
1	A	274	GLN
1	A	315	HIS
1	A	525	HIS
1	A	530	GLN
1	A	593	ASN
1	A	673	GLN
1	A	709	HIS
1	A	858	GLN
1	C	123	ASN
1	C	181	GLN
1	C	274	GLN
1	C	315	HIS
1	C	450	HIS
1	C	559	ASN
1	C	591	GLN

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Mol	Chain	Res	Type
1	C	724	GLN
1	C	814	GLN
1	C	858	GLN
1	C	882	HIS
1	C	885	GLN
1	D	123	ASN
1	D	200	GLN
1	D	315	HIS
1	D	403	GLN
1	D	579	GLN
1	D	704	ASN
1	D	730	GLN
1	D	814	GLN
1	D	829	HIS
1	D	858	GLN
1	E	95	HIS
1	E	111	ASN
1	E	274	GLN
1	E	315	HIS
1	E	366	GLN
1	E	423	GLN
1	E	454	HIS
1	E	704	ASN
1	E	730	GLN
1	E	801	GLN
1	E	804	GLN
1	E	814	GLN
1	E	862	GLN
1	F	60	GLN
1	F	81	HIS
1	F	95	HIS
1	F	199	GLN
1	F	315	HIS
1	F	550	HIS
1	F	591	GLN
1	F	724	GLN
1	F	730	GLN
1	F	814	GLN
1	F	862	GLN
1	F	885	GLN
1	B	111	ASN
1	B	123	ASN

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Mol	Chain	Res	Type
1	B	205	ASN
1	B	213	ASN
1	B	258	ASN
1	B	274	GLN
1	B	315	HIS
1	B	450	HIS
1	B	591	GLN
1	B	709	HIS
1	B	804	GLN
1	B	814	GLN
1	B	829	HIS
1	B	882	HIS
1	B	885	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 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	815/898 (90%)	0.13	7 (0%) 81 63	53, 86, 125, 160	0
1	B	811/898 (90%)	0.87	89 (10%) 10 5	69, 123, 159, 189	0
1	C	829/898 (92%)	0.20	12 (1%) 73 53	64, 91, 127, 174	0
1	D	815/898 (90%)	0.15	10 (1%) 76 58	65, 95, 126, 152	0
1	E	825/898 (91%)	0.30	17 (2%) 63 42	66, 94, 135, 185	0
1	F	815/898 (90%)	0.66	26 (3%) 50 30	76, 112, 141, 168	0
All	All	4910/5388 (91%)	0.38	161 (3%) 49 29	53, 98, 141, 189	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	143	LEU	5.7
1	B	189	VAL	5.6
1	B	349	MET	4.6
1	B	179	LEU	4.6
1	A	138	LEU	4.3
1	A	897	VAL	4.0
1	B	187	TYR	3.9
1	C	154	LEU	3.8
1	F	610	THR	3.8
1	B	837	HIS	3.7
1	B	239	SER	3.4
1	E	139	PHE	3.4
1	B	178	PHE	3.4
1	C	71	TYR	3.4
1	D	139	PHE	3.4
1	D	48	LEU	3.3
1	B	129	MET	3.3
1	D	138	LEU	3.3
1	B	897	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	225	PRO	3.2
1	B	83	PHE	3.2
1	E	867	ILE	3.2
1	B	684	VAL	3.1
1	C	837	HIS	3.1
1	E	138	LEU	3.1
1	B	298	ILE	3.1
1	B	360	ILE	3.0
1	B	293	PRO	3.0
1	B	101	TYR	3.0
1	B	299	LEU	3.0
1	C	898	ILE	3.0
1	B	346	SER	2.9
1	B	238	ILE	2.9
1	B	119	PRO	2.9
1	B	85	PHE	2.9
1	B	598	SER	2.8
1	F	670	GLY	2.8
1	F	646	LEU	2.8
1	A	129	MET	2.8
1	B	99	ILE	2.8
1	B	136	LEU	2.8
1	F	138	LEU	2.8
1	D	349	MET	2.8
1	B	203	ARG	2.8
1	E	694	SER	2.8
1	B	201	PRO	2.7
1	B	583	PHE	2.7
1	F	513	ALA	2.7
1	B	188	HIS	2.7
1	B	697	TYR	2.7
1	B	273	LEU	2.7
1	B	91	PRO	2.7
1	C	48	LEU	2.7
1	B	137	ASP	2.7
1	B	306	ASN	2.7
1	F	504	PHE	2.6
1	B	180	PHE	2.6
1	B	216	MET	2.6
1	B	270	THR	2.6
1	B	227	TRP	2.6
1	D	129	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	105	SER	2.6
1	F	349	MET	2.6
1	E	670	GLY	2.6
1	B	652	LYS	2.6
1	D	105	SER	2.6
1	F	581	CYS	2.5
1	B	626	PRO	2.5
1	F	862	GLN	2.5
1	B	226	ASP	2.5
1	B	348	ILE	2.5
1	B	104	MET	2.5
1	C	155	LEU	2.5
1	B	627	LEU	2.5
1	B	138	LEU	2.5
1	B	498	LEU	2.5
1	B	599	LEU	2.5
1	C	834	GLU	2.5
1	A	104	MET	2.5
1	E	75	MET	2.5
1	B	357	ILE	2.4
1	B	256	LEU	2.4
1	E	667	PHE	2.4
1	B	708	CYS	2.4
1	F	685	LYS	2.4
1	E	895	LEU	2.4
1	D	837	HIS	2.4
1	C	627	LEU	2.4
1	B	194	PRO	2.3
1	F	78	LYS	2.3
1	B	284	TRP	2.3
1	B	202	LEU	2.3
1	B	522	LEU	2.3
1	E	129	MET	2.3
1	B	600	TYR	2.3
1	B	647	TYR	2.3
1	B	350	ILE	2.3
1	D	862	GLN	2.3
1	B	78	LYS	2.3
1	B	409	PRO	2.3
1	F	105	SER	2.3
1	B	114	PHE	2.3
1	B	576	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	118	ILE	2.2
1	F	676	LEU	2.2
1	B	617	TRP	2.2
1	B	228	ILE	2.2
1	B	406	LEU	2.2
1	E	571	TYR	2.2
1	B	169	TYR	2.2
1	D	835	ASN	2.2
1	B	679	ASN	2.2
1	E	631	THR	2.2
1	F	550	HIS	2.2
1	B	86	VAL	2.2
1	A	105	SER	2.2
1	B	413	ILE	2.2
1	F	830	GLY	2.2
1	B	539	TYR	2.2
1	B	208	GLU	2.2
1	B	354	GLY	2.2
1	F	616	PHE	2.2
1	F	727	ILE	2.1
1	C	862	GLN	2.1
1	C	349	MET	2.1
1	E	502	SER	2.1
1	F	80	PRO	2.1
1	B	415	VAL	2.1
1	B	595	HIS	2.1
1	B	303	TYR	2.1
1	B	464	ILE	2.1
1	F	712	LEU	2.1
1	B	135	LEU	2.1
1	B	411	LEU	2.1
1	B	689	LEU	2.1
1	B	84	MET	2.1
1	A	834	GLU	2.1
1	F	609	PRO	2.1
1	F	837	HIS	2.1
1	E	78	LYS	2.1
1	B	171	TYR	2.1
1	B	79	ALA	2.1
1	B	212	PRO	2.1
1	B	386	GLU	2.1
1	E	703	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	76	MET	2.1
1	E	866	SER	2.1
1	C	835	ASN	2.1
1	B	835	ASN	2.1
1	F	370	ILE	2.1
1	B	128	LEU	2.1
1	A	72	HIS	2.1
1	F	129	MET	2.1
1	B	675	GLN	2.1
1	F	329	PHE	2.1
1	B	414	PRO	2.1
1	E	635	ILE	2.0
1	F	72	HIS	2.0
1	F	595	HIS	2.0
1	B	329	PHE	2.0
1	B	685	LYS	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.