



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2018 – 11:21 PM EST

PDB ID : 6EOS
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

<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

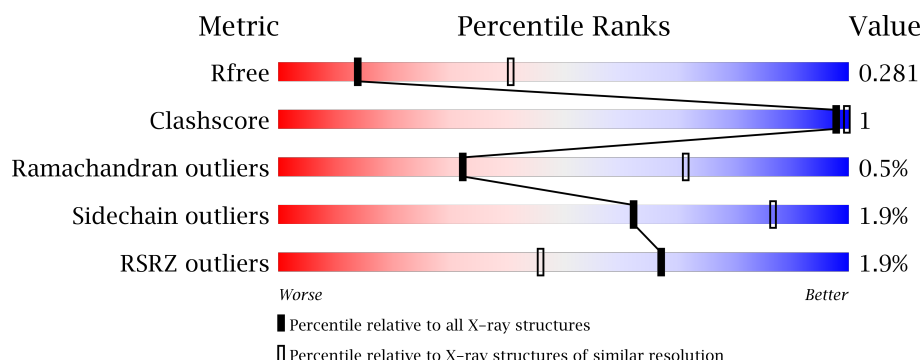
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	<div> <div> <div>0.1%</div> <div>87%</div> <div>9%</div> </div> <div> <div>6%</div> <div>83%</div> <div>7%</div> <div>10%</div> </div> </div>
1	B	898	<div> <div>0.1%</div> <div>88%</div> <div>8%</div> </div> <div> <div>6%</div> <div>83%</div> <div>7%</div> <div>10%</div> </div>
1	C	898	<div> <div>0.1%</div> <div>87%</div> <div>9%</div> </div> <div> <div>6%</div> <div>83%</div> <div>7%</div> <div>10%</div> </div>
1	D	898	<div> <div>0.1%</div> <div>89%</div> <div>8%</div> </div> <div> <div>6%</div> <div>83%</div> <div>7%</div> <div>10%</div> </div>
1	E	898	<div> <div>0.1%</div> <div>87%</div> <div>9%</div> </div> <div> <div>6%</div> <div>83%</div> <div>7%</div> <div>10%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	898	<div><div></div><div>2%</div><div>86%</div><div>5%</div><div>9%</div></div>

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			

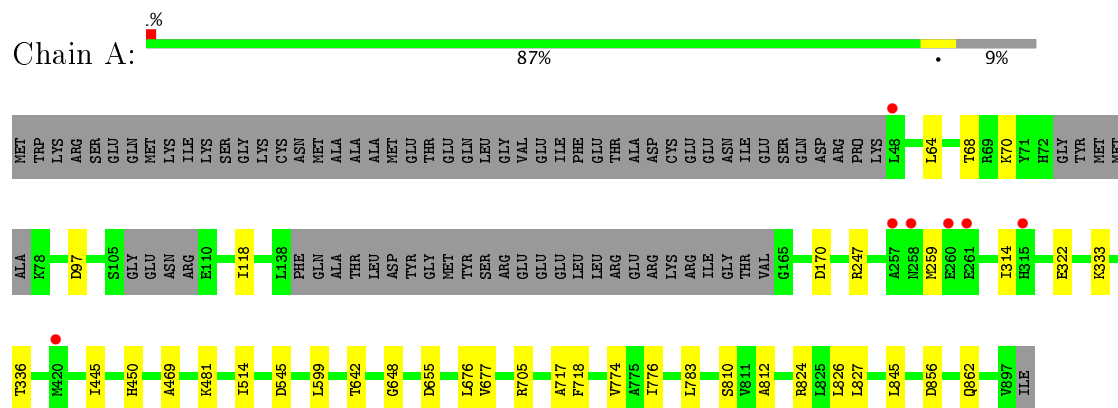
- Molecule 2 is water.

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		

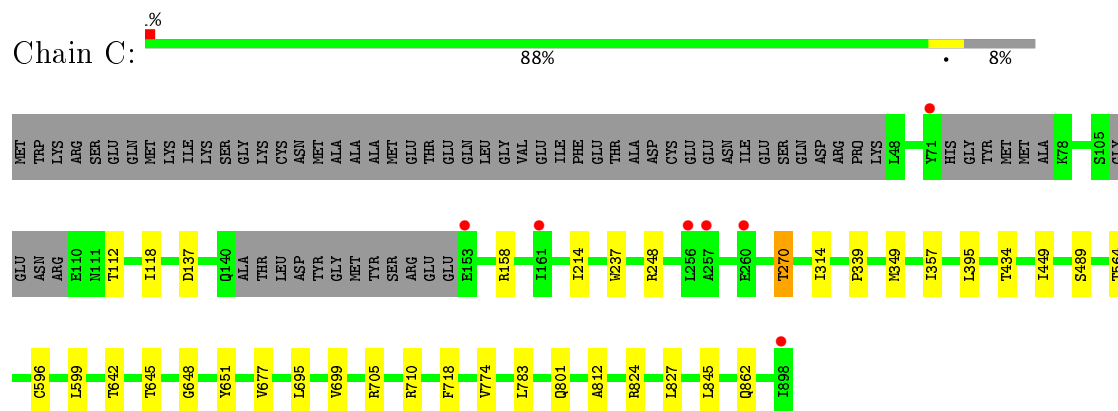
3 Residue-property plots

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.

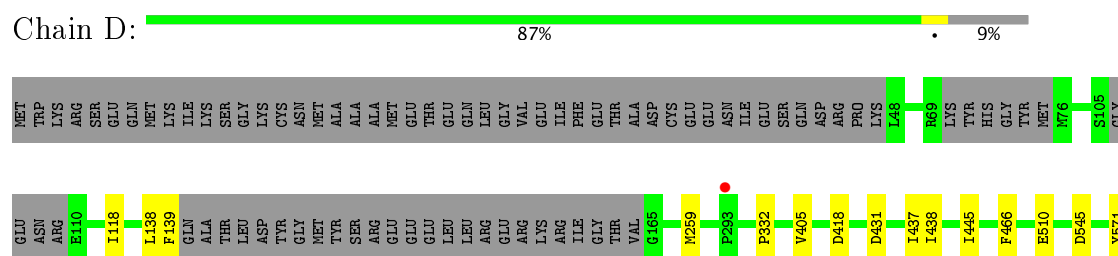
• Molecule 1: Dipeptidyl peptidase 8



• Molecule 1: Dipeptidyl peptidase 8

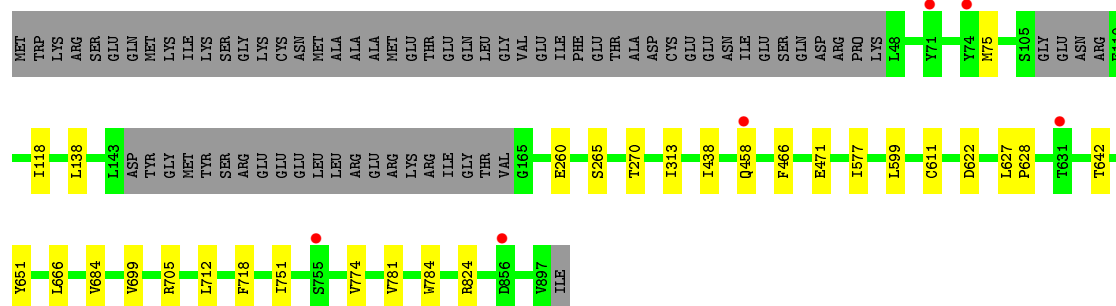
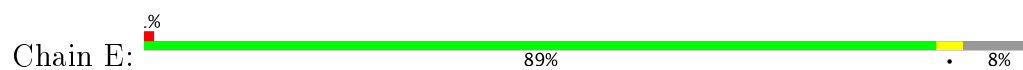


• Molecule 1: Dipeptidyl peptidase 8

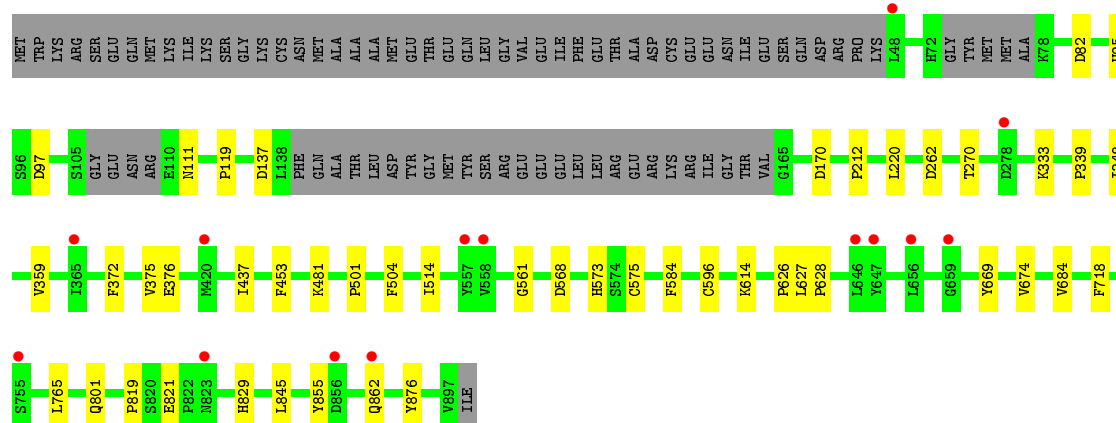
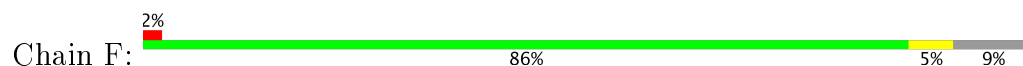




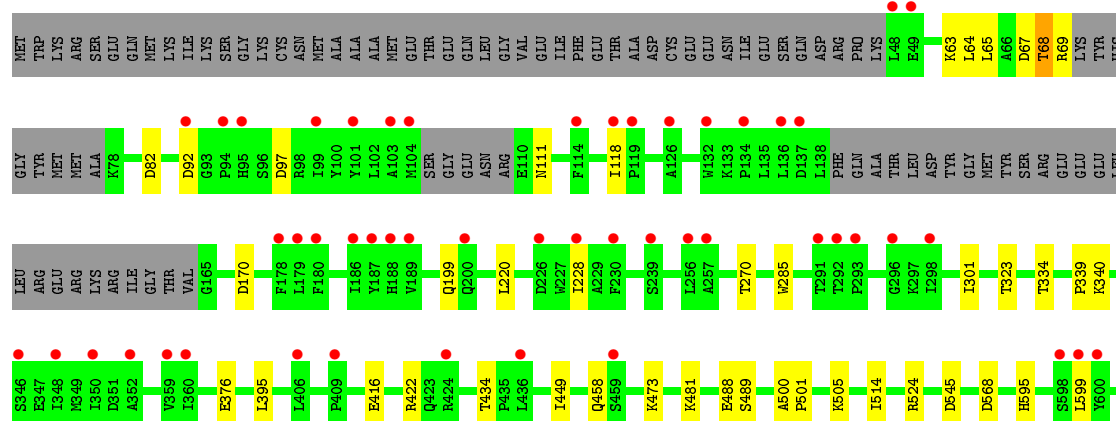
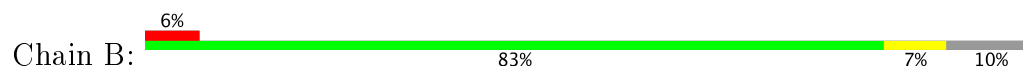
• Molecule 1: Dipeptidyl peptidase 8



• Molecule 1: Dipeptidyl peptidase 8



• Molecule 1: Dipeptidyl peptidase 8





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 44.46 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.40-3.10) 99.9 (44.46-3.10)	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 0.248 , 0.281	Depositor DCC
R_{free} test set	9593 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	83.4	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 59.0	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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	0/6805	0.58	0/9234
1	B	0.39	0/6766	0.57	0/9182
1	C	0.36	0/6925	0.58	0/9393
1	D	0.36	0/6797	0.57	0/9223
1	E	0.36	0/6885	0.59	0/9343
1	F	0.37	0/6805	0.58	0/9234
All	All	0.37	0/40983	0.58	0/55609

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6620	0	6439	12	0
1	B	6583	0	6405	17	0
1	C	6740	0	6576	14	0
1	D	6613	0	6433	7	0
1	E	6697	0	6515	13	0
1	F	6620	0	6439	11	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	21	0	0	0	0
2	F	20	0	0	0	0
All	All	39998	0	38807	74	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 (74) 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: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:B:64:LEU:O	1:B:68:THR:HG23	2.14	0.48
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:A:774:VAL:HG12	1:A:824:ARG:HA	1.95	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
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: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:HD3	1:B:688:ARG:HA	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:E:577:ILE:N	1:E:577:ILE:HD12	2.34	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: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
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:B:67:ASP:O	1:B:69:ARG:N	2.53	0.41
1:B:651:TYR:HB2	1:B:699:VAL:HB	2.02	0.41
1:F:437:ILE:HD12	1:F:504:PHE:HB2	2.03	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:B:285:TRP:CH2	1:B:301:ILE:HD11	2.56	0.41
1:B:65:LEU:HD21	1:B:881:LEU:HD11	2.03	0.41
1:C:349:MET:HB3	1:C:357:ILE:HD12	2.03	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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%)	28	67
1	B	803/898 (89%)	728 (91%)	70 (9%)	5 (1%)	28	67
1	C	821/898 (91%)	777 (95%)	42 (5%)	2 (0%)	51	84
1	D	807/898 (90%)	754 (93%)	47 (6%)	6 (1%)	25	64
1	E	819/898 (91%)	765 (93%)	54 (7%)	0	100	100
1	F	807/898 (90%)	750 (93%)	49 (6%)	8 (1%)	18	57
All	All	4864/5388 (90%)	4541 (93%)	297 (6%)	26 (0%)	32	71

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	714 (99%)	10 (1%)	71	90
1	B	720/795 (91%)	694 (96%)	26 (4%)	40	75
1	C	737/795 (93%)	727 (99%)	10 (1%)	71	90
1	D	723/795 (91%)	712 (98%)	11 (2%)	70	89
1	E	731/795 (92%)	724 (99%)	7 (1%)	80	92
1	F	724/795 (91%)	707 (98%)	17 (2%)	56	83
All	All	4359/4770 (91%)	4278 (98%)	81 (2%)	62	87

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ASP
1	A	170	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	247	ARG
1	A	314	ILE
1	A	545	ASP
1	A	655	ASP
1	A	676	LEU
1	A	718	PHE
1	A	856	ASP
1	A	862	GLN
1	C	112	THR
1	C	137	ASP
1	C	270	THR
1	C	314	ILE
1	C	564	THR
1	C	596	CYS
1	C	695	LEU
1	C	718	PHE
1	C	801	GLN
1	C	862	GLN
1	D	139	PHE
1	D	431	ASP
1	D	510	GLU
1	D	545	ASP
1	D	577	ILE
1	D	596	CYS
1	D	655	ASP
1	D	695	LEU
1	D	718	PHE
1	D	801	GLN
1	D	862	GLN
1	E	138	LEU
1	E	265	SER
1	E	270	THR
1	E	458	GLN
1	E	611	CYS
1	E	622	ASP
1	E	718	PHE
1	F	82	ASP
1	F	97	ASP
1	F	111	ASN
1	F	170	ASP
1	F	220	LEU
1	F	333	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	376	GLU
1	F	568	ASP
1	F	584	PHE
1	F	596	CYS
1	F	614	LYS
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	92	ASP
1	B	97	ASP
1	B	170	ASP
1	B	199	GLN
1	B	323	THR
1	B	334	THR
1	B	340	LYS
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	524	ARG
1	B	545	ASP
1	B	568	ASP
1	B	595	HIS
1	B	629	ASP
1	B	695	LEU
1	B	718	PHE
1	B	804	GLN
1	B	813	MET
1	B	837	HIS
1	B	862	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	200	GLN
1	A	274	GLN
1	A	573	HIS
1	A	579	GLN
1	A	593	ASN
1	A	704	ASN
1	A	709	HIS
1	A	730	GLN
1	A	858	GLN
1	A	885	GLN
1	C	450	HIS
1	C	591	GLN
1	C	690	ASN
1	C	704	ASN
1	C	730	GLN
1	C	814	GLN
1	C	829	HIS
1	C	882	HIS
1	D	200	GLN
1	D	274	GLN
1	D	591	GLN
1	D	704	ASN
1	D	730	GLN
1	D	814	GLN
1	D	829	HIS
1	D	858	GLN
1	D	885	GLN
1	E	675	GLN
1	F	274	GLN
1	F	458	GLN
1	F	573	HIS
1	F	591	GLN
1	F	730	GLN
1	F	829	HIS
1	F	862	GLN
1	B	213	ASN
1	B	232	HIS
1	B	274	GLN
1	B	591	GLN
1	B	804	GLN
1	B	829	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 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	815/898 (90%)	-0.03	7 (0%) 84 69	57, 86, 125, 160	0
1	B	811/898 (90%)	0.49	56 (6%) 18 7	69, 123, 160, 189	0
1	C	829/898 (92%)	0.04	7 (0%) 86 71	64, 91, 127, 174	0
1	D	815/898 (90%)	-0.03	1 (0%) 95 90	65, 95, 126, 152	0
1	E	825/898 (91%)	0.07	6 (0%) 87 75	66, 94, 135, 185	0
1	F	815/898 (90%)	0.29	14 (1%) 70 49	76, 112, 141, 168	0
All	All	4910/5388 (91%)	0.14	91 (1%) 67 46	57, 98, 141, 189	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	189	VAL	5.8
1	B	187	TYR	5.7
1	B	94	PRO	5.3
1	B	239	SER	4.7
1	E	71	TYR	4.5
1	B	119	PRO	4.4
1	B	180	PHE	4.3
1	B	118	ILE	4.2
1	B	626	PRO	4.0
1	B	178	PHE	3.9
1	B	648	GLY	3.9
1	B	188	HIS	3.8
1	B	352	ALA	3.7
1	B	101	TYR	3.6
1	B	256	LEU	3.4
1	B	126	ALA	3.3
1	C	71	TYR	3.3
1	B	95	HIS	3.3
1	B	598	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	258	ASN	3.1
1	B	137	ASP	3.1
1	B	226	ASP	3.0
1	B	291	THR	3.0
1	B	186	ILE	3.0
1	B	348	ILE	3.0
1	B	99	ILE	3.0
1	B	92	ASP	2.9
1	B	617	TRP	2.9
1	B	658	PRO	2.9
1	E	458	GLN	2.8
1	E	631	THR	2.8
1	A	257	ALA	2.8
1	A	420	MET	2.7
1	B	359	VAL	2.7
1	B	114	PHE	2.7
1	B	132	TRP	2.7
1	B	293	PRO	2.7
1	B	296	GLY	2.7
1	B	104	MET	2.7
1	F	659	GLY	2.6
1	B	406	LEU	2.6
1	C	256	LEU	2.6
1	B	228	ILE	2.6
1	F	856	ASP	2.6
1	A	48	LEU	2.6
1	E	74	TYR	2.6
1	B	350	ILE	2.6
1	F	646	LEU	2.5
1	B	298	ILE	2.5
1	B	230	PHE	2.5
1	B	600	TYR	2.5
1	D	293	PRO	2.5
1	F	558	VAL	2.4
1	B	292	THR	2.4
1	F	755	SER	2.3
1	B	103	ALA	2.3
1	B	360	ILE	2.3
1	F	647	TYR	2.3
1	B	436	LEU	2.3
1	F	656	LEU	2.3
1	B	179	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	856	ASP	2.3
1	F	278	ASP	2.3
1	A	261	GLU	2.2
1	C	260	GLU	2.2
1	C	257	ALA	2.2
1	B	346	SER	2.2
1	B	647	TYR	2.2
1	B	679	ASN	2.2
1	A	315	HIS	2.2
1	C	161	ILE	2.2
1	A	260	GLU	2.2
1	F	557	TYR	2.1
1	B	409	PRO	2.1
1	F	823	ASN	2.1
1	C	898	ILE	2.1
1	B	48	LEU	2.1
1	B	424	ARG	2.1
1	F	48	LEU	2.1
1	E	755	SER	2.1
1	B	200	GLN	2.1
1	F	862	GLN	2.0
1	B	599	LEU	2.0
1	F	420	MET	2.0
1	F	365	ILE	2.0
1	B	49	GLU	2.0
1	B	257	ALA	2.0
1	B	459	SER	2.0
1	B	134	PRO	2.0
1	C	153	GLU	2.0
1	B	136	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.