



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:11 AM GMT

PDB ID : 1PZ8
Title : Modulation of agrin function by alternative splicing and Ca²⁺ binding
Authors : Stetefeld, J.; Alexandrescu, A.T.; Maciejewski, M.W.; Jenny, M.; Rathgeb-Szabo, K.; Schulthess, T.; Landwehr, R.; Frank, S.; Ruegg, M.A.; Kammerer, R.A.
Deposited on : 2003-07-10
Resolution : 2.35 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

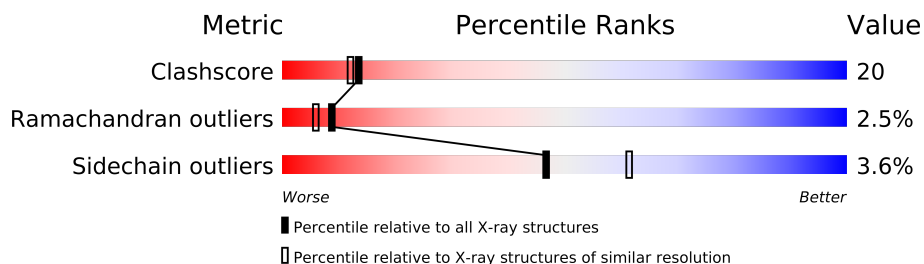
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.35 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))
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	201	
1	B	201	
1	C	201	
1	D	201	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6058 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Agrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	0	0
			1365	863	238	258	6			
1	B	179	Total	C	N	O	S	0	0	0
			1385	874	241	264	6			
1	C	176	Total	C	N	O	S	0	0	0
			1365	863	238	258	6			
1	D	177	Total	C	N	O	S	0	0	0
			1370	866	239	259	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	HIS	PRO	SEE REMARK 999	UNP P31696
A	34	LEU	ASP	SEE REMARK 999	UNP P31696
A	35	SER	ALA	SEE REMARK 999	UNP P31696
A	36	ASN	LEU	SEE REMARK 999	UNP P31696
A	37	GLU	ASP	SEE REMARK 999	UNP P31696
A	38	ILE	TYR	SEE REMARK 999	UNP P31696
A	42	-	PRO	SEE REMARK 999	UNP P31696
A	43	-	SER	SEE REMARK 999	UNP P31696
A	44	-	GLU	SEE REMARK 999	UNP P31696
B	33	HIS	PRO	SEE REMARK 999	UNP P31696
B	34	LEU	ASP	SEE REMARK 999	UNP P31696
B	35	SER	ALA	SEE REMARK 999	UNP P31696
B	36	ASN	LEU	SEE REMARK 999	UNP P31696
B	37	GLU	ASP	SEE REMARK 999	UNP P31696
B	38	ILE	TYR	SEE REMARK 999	UNP P31696
B	42	-	PRO	SEE REMARK 999	UNP P31696
B	43	-	SER	SEE REMARK 999	UNP P31696
B	44	-	GLU	SEE REMARK 999	UNP P31696
C	33	HIS	PRO	SEE REMARK 999	UNP P31696
C	34	LEU	ASP	SEE REMARK 999	UNP P31696
C	35	SER	ALA	SEE REMARK 999	UNP P31696

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Chain	Residue	Modelled	Actual	Comment	Reference
C	36	ASN	LEU	SEE REMARK 999	UNP P31696
C	37	GLU	ASP	SEE REMARK 999	UNP P31696
C	38	ILE	TYR	SEE REMARK 999	UNP P31696
C	42	-	PRO	SEE REMARK 999	UNP P31696
C	43	-	SER	SEE REMARK 999	UNP P31696
C	44	-	GLU	SEE REMARK 999	UNP P31696
D	33	HIS	PRO	SEE REMARK 999	UNP P31696
D	34	LEU	ASP	SEE REMARK 999	UNP P31696
D	35	SER	ALA	SEE REMARK 999	UNP P31696
D	36	ASN	LEU	SEE REMARK 999	UNP P31696
D	37	GLU	ASP	SEE REMARK 999	UNP P31696
D	38	ILE	TYR	SEE REMARK 999	UNP P31696
D	42	-	PRO	SEE REMARK 999	UNP P31696
D	43	-	SER	SEE REMARK 999	UNP P31696
D	44	-	GLU	SEE REMARK 999	UNP P31696

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

- Molecule 3 is water.

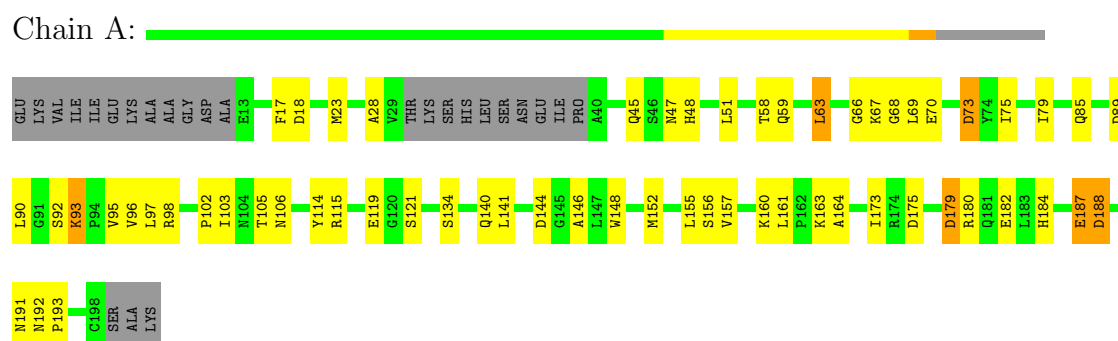
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	155	Total O 155 155	0	0
3	B	150	Total O 150 150	0	0
3	C	143	Total O 143 143	0	0
3	D	121	Total O 121 121	0	0

3 Residue-property plots

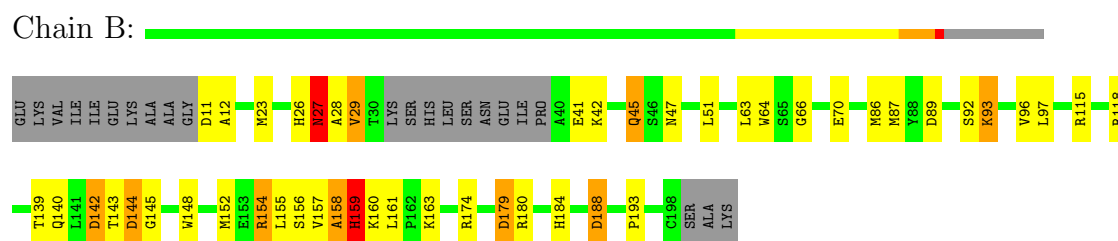
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

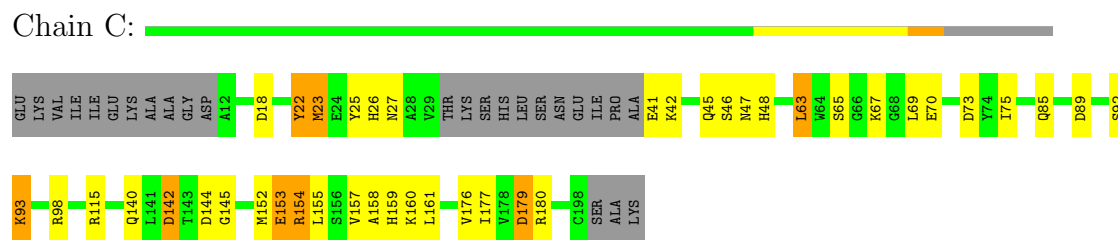
• Molecule 1: Agrin



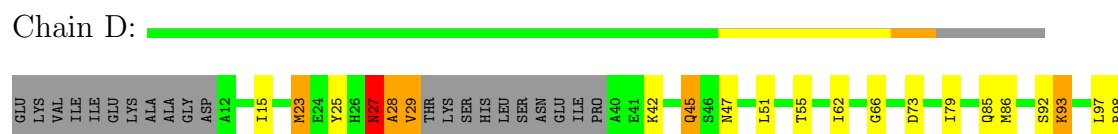
• Molecule 1: Agrin



• Molecule 1: Agrin



• Molecule 1: Agrin



I103	A113	Y114	R115	R118	L141	D142	T143	D144	G145	W148	M152	E153	R154	L155	S156	V157	A158	H159	K160	L161	Y165	S166	D175	V178	D179	R180	Q181	D188	I195	C198	SER	ALA	LYS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.85Å 56.56Å 84.59Å 90.00° 99.75° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.218 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6058	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.65	0/1392	0.83	6/1888 (0.3%)
1	B	0.71	0/1412	0.89	6/1916 (0.3%)
1	C	0.74	0/1392	0.89	6/1888 (0.3%)
1	D	0.78	0/1397	0.97	9/1895 (0.5%)
All	All	0.72	0/5593	0.90	27/7587 (0.4%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	175	ASP	CB-CG-OD2	8.44	125.90	118.30
1	C	144	ASP	CB-CG-OD2	8.01	125.51	118.30
1	B	188	ASP	CB-CG-OD2	7.88	125.40	118.30
1	C	89	ASP	CB-CG-OD2	7.86	125.37	118.30
1	B	89	ASP	CB-CG-OD2	7.52	125.06	118.30
1	D	73	ASP	CB-CG-OD2	7.29	124.87	118.30
1	C	179	ASP	CB-CG-OD2	7.07	124.67	118.30
1	C	73	ASP	CB-CG-OD2	7.00	124.60	118.30
1	A	89	ASP	CB-CG-OD2	6.97	124.57	118.30
1	D	27	ASN	N-CA-C	6.58	128.76	111.00
1	B	11	ASP	CB-CG-OD2	6.14	123.82	118.30
1	A	144	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	18	ASP	CB-CG-OD2	6.05	123.75	118.30
1	D	179	ASP	CB-CG-OD2	6.05	123.75	118.30
1	B	144	ASP	CB-CG-OD2	6.03	123.73	118.30
1	C	18	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	73	ASP	CB-CG-OD2	5.94	123.65	118.30
1	D	144	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	179	ASP	CB-CG-OD2	5.83	123.54	118.30
1	D	27	ASN	CA-C-N	-5.82	104.41	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	ASP	CB-CG-OD2	5.67	123.41	118.30
1	C	142	ASP	CB-CG-OD2	5.47	123.22	118.30
1	D	118	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	188	ASP	CB-CG-OD2	5.36	123.13	118.30
1	D	142	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	188	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	142	ASP	CB-CG-OD2	5.27	123.04	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1365	0	1349	62	0
1	B	1385	0	1365	44	0
1	C	1365	0	1349	57	0
1	D	1370	0	1354	57	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	155	0	0	14	0
3	B	150	0	0	9	0
3	C	143	0	0	13	0
3	D	121	0	0	4	0
All	All	6058	0	5417	220	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (220) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:29:VAL:CG1	1:D:181:GLN:HB3	1.62	1.28

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:29:VAL:HG22	1:D:181:GLN:CG	1.64	1.26
1:D:29:VAL:HG13	1:D:181:GLN:CB	1.79	1.12
1:D:27:ASN:OD1	1:D:145:GLY:HA3	1.58	1.01
1:D:29:VAL:HG22	1:D:181:GLN:HG2	1.00	1.00
1:C:27:ASN:OD1	1:C:145:GLY:HA3	1.65	0.96
1:B:157:VAL:HG13	1:B:161:LEU:HB2	1.45	0.95
1:D:29:VAL:CG2	1:D:181:GLN:HG2	1.96	0.94
1:C:155:LEU:HD22	1:C:157:VAL:HB	1.49	0.94
1:A:47:ASN:HD22	1:A:115:ARG:HE	1.14	0.93
1:A:191:ASN:OD1	3:A:785:HOH:O	1.88	0.91
1:B:158:ALA:C	3:B:770:HOH:O	2.11	0.87
1:D:29:VAL:CG2	1:D:181:GLN:CG	2.52	0.87
1:D:29:VAL:HG13	1:D:181:GLN:HB3	0.87	0.86
1:C:27:ASN:HD21	1:C:145:GLY:CA	1.89	0.85
1:C:157:VAL:HG13	1:C:161:LEU:HB2	1.60	0.82
1:C:159:HIS:CD2	3:C:760:HOH:O	2.31	0.82
1:B:23:MET:HG2	1:B:193:PRO:HG3	1.62	0.81
1:D:66:GLY:O	1:D:148:TRP:HZ3	1.62	0.81
1:C:27:ASN:HD21	1:C:145:GLY:HA2	1.46	0.80
1:C:152:MET:SD	1:C:155:LEU:HG	2.25	0.77
1:C:180:ARG:HG2	3:C:838:HOH:O	1.85	0.77
1:D:45:GLN:HA	1:D:45:GLN:HE21	1.49	0.77
1:C:154:ARG:H	1:C:154:ARG:HD2	1.49	0.76
1:B:152:MET:HG2	1:B:155:LEU:HG	1.68	0.76
1:C:27:ASN:CG	1:C:145:GLY:HA3	2.07	0.75
1:B:45:GLN:HA	1:B:45:GLN:HE21	1.51	0.74
1:A:157:VAL:HG12	1:A:157:VAL:O	1.88	0.74
1:A:45:GLN:HG3	3:A:836:HOH:O	1.86	0.74
1:D:27:ASN:CG	1:D:145:GLY:HA3	2.07	0.73
1:D:29:VAL:CG1	1:D:181:GLN:CB	2.52	0.73
1:D:179:ASP:O	1:D:180:ARG:HB2	1.90	0.71
1:A:47:ASN:ND2	1:A:115:ARG:HH21	1.89	0.71
1:C:27:ASN:ND2	1:C:145:GLY:HA3	2.06	0.70
1:C:48:HIS:HB3	3:C:761:HOH:O	1.90	0.70
1:A:157:VAL:HG11	1:A:161:LEU:HD12	1.72	0.70
1:B:42:LYS:O	1:B:142:ASP:HA	1.92	0.68
1:C:27:ASN:ND2	1:C:145:GLY:CA	2.57	0.68
1:A:59:GLN:HE21	1:A:164:ALA:HB2	1.59	0.67
1:C:160:LYS:HD3	3:C:775:HOH:O	1.93	0.67
1:D:29:VAL:CB	1:D:181:GLN:HB3	2.26	0.66
1:B:154:ARG:HD2	1:B:154:ARG:H	1.61	0.65
1:D:29:VAL:HG11	1:D:178:VAL:O	1.97	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:47:ASN:ND2	1:B:115:ARG:HH21	1.95	0.64
1:D:157:VAL:HG22	1:D:161:LEU:HD12	1.80	0.63
1:B:66:GLY:O	1:B:148:TRP:HZ3	1.82	0.63
1:B:156:SER:CA	3:B:772:HOH:O	2.46	0.63
1:D:47:ASN:HD22	1:D:115:ARG:HE	1.47	0.62
1:A:90:LEU:HA	3:A:732:HOH:O	1.99	0.62
1:D:157:VAL:HG13	1:D:161:LEU:HB2	1.81	0.61
1:A:47:ASN:ND2	1:A:115:ARG:HE	1.93	0.61
1:A:47:ASN:HD22	1:A:115:ARG:NE	1.93	0.61
1:B:159:HIS:N	3:B:770:HOH:O	2.31	0.61
1:A:73:ASP:HB3	3:A:732:HOH:O	2.00	0.61
1:B:156:SER:HA	3:B:772:HOH:O	2.00	0.61
1:A:163:LYS:HE3	3:A:763:HOH:O	2.01	0.61
1:C:152:MET:CE	1:C:155:LEU:HD21	2.30	0.61
1:A:59:GLN:NE2	1:A:164:ALA:HB2	2.16	0.60
1:B:152:MET:HG2	1:B:155:LEU:CG	2.30	0.60
1:A:58:THR:O	1:A:79:ILE:HG22	2.02	0.60
1:C:27:ASN:HD21	1:C:145:GLY:HA3	1.64	0.60
1:B:12:ALA:HB1	1:B:174:ARG:HD2	1.83	0.59
1:D:29:VAL:HG22	1:D:181:GLN:HG3	1.75	0.59
1:C:140:GLN:NE2	3:C:755:HOH:O	2.36	0.59
1:B:140:GLN:HG2	3:B:710:HOH:O	2.03	0.59
1:B:64:TRP:HB3	1:B:152:MET:HE1	1.85	0.58
1:D:86:MET:CE	1:D:97:LEU:HD22	2.33	0.58
1:A:45:GLN:CD	1:A:140:GLN:HG2	2.24	0.57
1:C:155:LEU:CD1	3:C:768:HOH:O	2.52	0.57
1:B:42:LYS:N	1:B:143:THR:O	2.38	0.57
1:C:47:ASN:ND2	1:C:115:ARG:HH21	2.03	0.56
1:C:22:TYR:N	1:C:22:TYR:CD1	2.73	0.56
1:C:47:ASN:HD22	1:C:115:ARG:HE	1.54	0.56
1:C:155:LEU:HD12	3:C:768:HOH:O	2.06	0.55
1:A:114:TYR:CE1	1:A:121:SER:HB3	2.41	0.55
1:A:157:VAL:HG11	1:A:161:LEU:CD1	2.37	0.55
1:A:92:SER:O	1:A:93:LYS:HB2	2.07	0.55
1:D:29:VAL:HG11	1:D:181:GLN:N	2.22	0.55
1:C:70:GLU:HA	3:C:840:HOH:O	2.06	0.54
1:D:51:LEU:HD23	1:D:51:LEU:N	2.23	0.54
1:D:86:MET:HE3	1:D:97:LEU:HD22	1.90	0.54
1:A:67:LYS:HG2	1:A:69:LEU:HG	1.90	0.53
1:B:157:VAL:HG12	3:B:779:HOH:O	2.09	0.53
1:B:27:ASN:OD1	1:B:145:GLY:HA2	2.08	0.53
1:D:152:MET:HE2	1:D:155:LEU:HA	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:141:LEU:HG	3:A:732:HOH:O	2.08	0.53
1:A:160:LYS:NZ	3:A:823:HOH:O	2.41	0.52
1:C:179:ASP:O	1:C:180:ARG:HB2	2.09	0.52
1:A:70:GLU:HA	3:A:823:HOH:O	2.08	0.52
1:A:59:GLN:HA	1:A:79:ILE:O	2.10	0.52
1:A:184:HIS:O	1:A:188:ASP:HB2	2.10	0.52
1:D:156:SER:OG	1:D:160:LYS:HE2	2.09	0.52
1:D:160:LYS:HE2	3:D:756:HOH:O	2.09	0.52
1:B:157:VAL:CG1	1:B:161:LEU:HB2	2.30	0.52
1:B:70:GLU:HA	3:B:786:HOH:O	2.09	0.51
1:D:157:VAL:HG11	1:D:165:TYR:C	2.31	0.51
1:D:156:SER:O	1:D:157:VAL:C	2.48	0.51
1:C:67:LYS:HE2	1:C:69:LEU:HD11	1.93	0.51
1:A:45:GLN:OE1	1:A:140:GLN:HG2	2.11	0.51
1:A:155:LEU:O	1:A:157:VAL:N	2.43	0.51
1:A:146:ALA:HB1	1:A:148:TRP:CZ3	2.46	0.51
1:A:148:TRP:CG	1:A:152:MET:HG3	2.46	0.51
1:C:152:MET:SD	1:C:155:LEU:CD2	2.99	0.50
1:A:155:LEU:HD21	3:A:842:HOH:O	2.10	0.50
1:A:75:ILE:HG22	1:A:141:LEU:HD11	1.92	0.50
1:C:63:LEU:HD23	1:C:63:LEU:C	2.31	0.50
1:C:157:VAL:CG1	1:C:161:LEU:HB2	2.38	0.50
1:D:157:VAL:CG1	1:D:165:TYR:HB2	2.41	0.50
1:B:179:ASP:O	1:B:180:ARG:HB2	2.11	0.50
1:C:46:SER:HB2	1:C:115:ARG:O	2.12	0.50
1:A:85:GLN:NE2	1:A:98:ARG:HH21	2.10	0.50
1:C:92:SER:O	1:C:93:LYS:HB2	2.12	0.50
1:D:27:ASN:ND2	3:D:800:HOH:O	2.30	0.49
1:B:92:SER:O	1:B:93:LYS:CB	2.60	0.49
1:C:157:VAL:O	1:C:157:VAL:CG1	2.60	0.49
1:D:29:VAL:CG1	1:D:181:GLN:N	2.76	0.49
1:D:152:MET:HG2	1:D:154:ARG:O	2.13	0.49
1:A:85:GLN:HE21	1:A:98:ARG:HH21	1.60	0.49
1:A:95:VAL:HB	1:A:134:SER:HA	1.95	0.48
1:C:152:MET:HE1	1:C:155:LEU:HD21	1.95	0.48
1:B:157:VAL:HG13	1:B:161:LEU:HD12	1.96	0.48
1:D:23:MET:HB3	1:D:25:TYR:CE1	2.49	0.48
1:D:92:SER:O	1:D:93:LYS:HB2	2.13	0.48
1:C:27:ASN:OD1	1:C:145:GLY:CA	2.50	0.48
1:C:179:ASP:O	1:C:180:ARG:CB	2.61	0.48
1:C:85:GLN:HE21	1:C:98:ARG:HH21	1.60	0.48
1:C:152:MET:SD	1:C:155:LEU:CG	2.99	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:48:HIS:CD2	3:C:724:HOH:O	2.66	0.48
1:C:27:ASN:HB2	3:C:846:HOH:O	2.14	0.48
1:B:27:ASN:HB2	1:B:145:GLY:CA	2.44	0.47
1:A:63:LEU:C	1:A:63:LEU:HD23	2.35	0.47
1:C:176:VAL:O	1:C:177:ILE:HD13	2.15	0.47
1:A:157:VAL:HG11	1:A:161:LEU:CG	2.45	0.47
1:B:27:ASN:HB2	1:B:145:GLY:HA3	1.96	0.47
1:A:66:GLY:O	1:A:148:TRP:HZ3	1.98	0.47
1:D:27:ASN:O	1:D:28:ALA:O	2.32	0.47
1:A:157:VAL:HG13	1:A:160:LYS:HB3	1.95	0.47
1:A:184:HIS:HB2	1:A:187:GLU:OE1	2.15	0.47
1:B:92:SER:O	1:B:93:LYS:HB2	2.13	0.47
1:C:23:MET:HG2	1:C:25:TYR:OH	2.14	0.47
1:D:159:HIS:N	1:D:159:HIS:ND1	2.57	0.47
1:D:180:ARG:HG3	3:D:780:HOH:O	2.14	0.47
1:C:65:SER:HB3	1:C:75:ILE:HG23	1.97	0.47
1:A:96:VAL:C	1:A:97:LEU:HD12	2.35	0.47
1:B:152:MET:HG2	1:B:155:LEU:CD1	2.45	0.46
1:D:155:LEU:CD2	1:D:158:ALA:H	2.28	0.46
1:D:92:SER:O	1:D:93:LYS:CB	2.63	0.46
1:D:42:LYS:NZ	1:D:42:LYS:HB3	2.31	0.46
1:C:42:LYS:HB3	1:C:42:LYS:NZ	2.30	0.46
1:D:85:GLN:HE21	1:D:98:ARG:HH21	1.62	0.46
1:A:51:LEU:HD23	1:A:51:LEU:N	2.31	0.46
1:A:157:VAL:CG1	1:A:157:VAL:O	2.61	0.46
1:A:105:THR:O	1:A:106:ASN:HB3	2.16	0.46
1:A:92:SER:O	1:A:93:LYS:CB	2.62	0.46
1:B:157:VAL:CG1	1:B:161:LEU:HD12	2.46	0.45
1:C:152:MET:HE3	1:C:155:LEU:HD11	1.97	0.45
1:B:87:MET:HE3	1:B:96:VAL:HG22	1.98	0.45
1:C:41:GLU:OE1	1:C:142:ASP:HB3	2.16	0.45
1:A:102:PRO:HD2	3:A:820:HOH:O	2.17	0.45
1:D:29:VAL:HG11	1:D:181:GLN:H	1.82	0.45
1:C:26:HIS:CG	1:C:27:ASN:N	2.85	0.45
1:C:154:ARG:H	1:C:154:ARG:CD	2.19	0.44
1:B:157:VAL:HG13	1:B:161:LEU:CB	2.33	0.44
1:D:179:ASP:CG	3:D:753:HOH:O	2.56	0.44
1:D:156:SER:OG	1:D:160:LYS:CE	2.66	0.44
1:D:155:LEU:HD21	1:D:166:SER:OG	2.18	0.44
1:B:160:LYS:NZ	3:B:736:HOH:O	2.29	0.44
1:D:27:ASN:ND2	1:D:145:GLY:CA	2.80	0.44
1:D:157:VAL:HG11	1:D:165:TYR:HB2	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:157:VAL:HG11	1:D:165:TYR:CB	2.48	0.44
1:B:47:ASN:HD21	1:B:115:ARG:HH21	1.63	0.44
1:B:70:GLU:HG3	3:B:727:HOH:O	2.17	0.44
1:B:41:GLU:OE1	1:B:144:ASP:HB3	2.18	0.44
1:B:51:LEU:HD23	1:B:51:LEU:N	2.33	0.44
1:B:26:HIS:CG	1:B:27:ASN:N	2.86	0.44
1:B:163:LYS:HD3	1:B:163:LYS:HA	1.87	0.44
1:C:27:ASN:ND2	3:C:835:HOH:O	2.50	0.44
1:B:86:MET:HE3	1:B:97:LEU:HD22	2.00	0.44
1:A:182:GLU:HG2	1:A:184:HIS:CD2	2.53	0.43
1:C:155:LEU:HB3	3:C:843:HOH:O	2.18	0.43
1:B:154:ARG:O	1:B:155:LEU:HG	2.18	0.43
1:B:184:HIS:O	1:B:188:ASP:HB2	2.18	0.43
1:A:45:GLN:HE21	1:A:45:GLN:HA	1.83	0.43
1:A:23:MET:HG2	1:A:193:PRO:HG3	2.01	0.43
1:A:103:ILE:HG13	1:A:103:ILE:O	2.18	0.43
1:A:48:HIS:HE1	3:A:727:HOH:O	2.00	0.43
1:D:29:VAL:CG1	1:D:178:VAL:O	2.66	0.43
1:C:92:SER:O	1:C:93:LYS:CB	2.66	0.43
1:B:157:VAL:C	1:B:159:HIS:H	2.22	0.43
1:A:45:GLN:NE2	1:A:140:GLN:HG2	2.34	0.43
1:D:156:SER:OG	1:D:160:LYS:NZ	2.52	0.43
1:D:62:ILE:HD11	1:D:79:ILE:HG13	2.00	0.42
1:D:103:ILE:HG13	1:D:103:ILE:O	2.19	0.42
1:C:23:MET:HB3	1:C:25:TYR:CE1	2.54	0.42
1:D:15:ILE:HD12	1:D:195:ILE:HG23	2.01	0.42
1:A:17:PHE:CE2	1:A:173:ILE:HD12	2.54	0.42
1:A:157:VAL:CG1	1:A:161:LEU:HB2	2.48	0.42
1:A:157:VAL:HG22	1:A:160:LYS:HE2	2.00	0.42
1:B:118:ARG:HG3	1:B:139:THR:HG22	2.01	0.42
1:A:184:HIS:CB	1:A:187:GLU:OE1	2.67	0.42
1:A:179:ASP:O	1:A:180:ARG:HB2	2.19	0.42
1:A:160:LYS:HD3	3:A:778:HOH:O	2.19	0.42
1:D:86:MET:SD	1:D:113:ALA:HB1	2.60	0.42
1:D:29:VAL:CG2	1:D:181:GLN:CB	2.98	0.41
1:C:26:HIS:ND1	1:C:27:ASN:N	2.68	0.41
1:A:191:ASN:O	1:A:192:ASN:C	2.58	0.41
1:A:68:GLY:HA3	1:A:152:MET:HE3	2.01	0.41
1:C:158:ALA:C	1:C:159:HIS:CD2	2.93	0.41
1:C:158:ALA:C	1:C:159:HIS:HD2	2.23	0.41
1:A:85:GLN:NE2	1:A:98:ARG:NH2	2.69	0.41
1:A:155:LEU:HD11	3:A:842:HOH:O	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:26:HIS:CG	1:B:27:ASN:H	2.39	0.41
1:A:157:VAL:HG12	1:A:161:LEU:HB2	2.03	0.41
1:C:63:LEU:HD23	1:C:63:LEU:O	2.21	0.41
1:C:65:SER:HB3	1:C:75:ILE:CG2	2.50	0.40
1:D:141:LEU:HD23	1:D:141:LEU:C	2.42	0.40
1:D:29:VAL:CG1	1:D:181:GLN:CA	2.99	0.40
1:C:153:GLU:HB3	1:C:154:ARG:HD2	2.03	0.40
1:A:175:ASP:HB2	3:A:786:HOH:O	2.22	0.40
1:C:45:GLN:HB3	3:C:758:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	172/201 (86%)	157 (91%)	12 (7%)	3 (2%)	14	11
1	B	175/201 (87%)	158 (90%)	11 (6%)	6 (3%)	6	3
1	C	172/201 (86%)	160 (93%)	10 (6%)	2 (1%)	19	19
1	D	173/201 (86%)	159 (92%)	8 (5%)	6 (4%)	6	3
All	All	692/804 (86%)	634 (92%)	41 (6%)	17 (2%)	9	6

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28	ALA
1	B	29	VAL
1	B	159	HIS
1	D	27	ASN
1	D	28	ALA
1	C	153	GLU
1	D	158	ALA
1	A	156	SER
1	B	27	ASN

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Mol	Chain	Res	Type
1	B	158	ALA
1	A	28	ALA
1	C	93	LYS
1	D	93	LYS
1	D	153	GLU
1	A	93	LYS
1	B	93	LYS
1	D	157	VAL

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	146/166 (88%)	143 (98%)	3 (2%)	66	82
1	B	148/166 (89%)	142 (96%)	6 (4%)	41	54
1	C	146/166 (88%)	142 (97%)	4 (3%)	57	74
1	D	146/166 (88%)	138 (94%)	8 (6%)	30	36
All	All	586/664 (88%)	565 (96%)	21 (4%)	47	61

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LEU
1	A	119	GLU
1	A	187	GLU
1	B	27	ASN
1	B	29	VAL
1	B	45	GLN
1	B	63	LEU
1	B	154	ARG
1	B	159	HIS
1	C	22	TYR
1	C	23	MET
1	C	63	LEU
1	C	154	ARG
1	D	23	MET

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Mol	Chain	Res	Type
1	D	29	VAL
1	D	45	GLN
1	D	55	THR
1	D	143	THR
1	D	155	LEU
1	D	159	HIS
1	D	181	GLN

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

Mol	Chain	Res	Type
1	A	45	GLN
1	A	47	ASN
1	A	59	GLN
1	A	85	GLN
1	A	107	HIS
1	A	117	GLN
1	A	123	GLN
1	A	140	GLN
1	A	184	HIS
1	B	45	GLN
1	B	47	ASN
1	B	59	GLN
1	B	85	GLN
1	B	117	GLN
1	B	123	GLN
1	B	181	GLN
1	C	45	GLN
1	C	47	ASN
1	C	59	GLN
1	C	85	GLN
1	C	117	GLN
1	C	123	GLN
1	C	140	GLN
1	C	159	HIS
1	C	181	GLN
1	D	27	ASN
1	D	45	GLN
1	D	47	ASN
1	D	59	GLN
1	D	85	GLN
1	D	117	GLN

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Mol	Chain	Res	Type
1	D	123	GLN
1	D	140	GLN
1	D	181	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are 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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.