



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:15 AM GMT

PDB ID : 2IBF
Title : Human vinculin's head domain (Vh1, residues 1-258) in complex with two vinculin binding sites of Shigella flexneri's IpaA (residues 565-587)
Authors : Izard, T.
Deposited on : 2006-09-11
Resolution : 3.20 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>

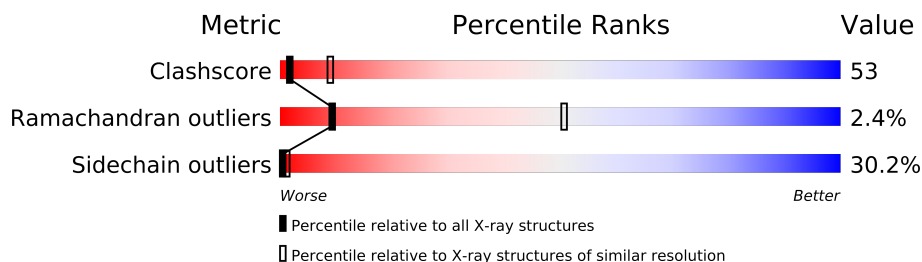
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)

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	266	
2	B	25	
2	D	25	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2359 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 Vinculin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	2020	1272	342	392	14	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	EXPRESSION TAG	UNP P18206
A	-6	GLU	-	EXPRESSION TAG	UNP P18206
A	-5	HIS	-	EXPRESSION TAG	UNP P18206
A	-4	HIS	-	EXPRESSION TAG	UNP P18206
A	-3	HIS	-	EXPRESSION TAG	UNP P18206
A	-2	HIS	-	EXPRESSION TAG	UNP P18206
A	-1	HIS	-	EXPRESSION TAG	UNP P18206
A	0	HIS	-	EXPRESSION TAG	UNP P18206

- Molecule 2 is a protein called Invasin ipaA.

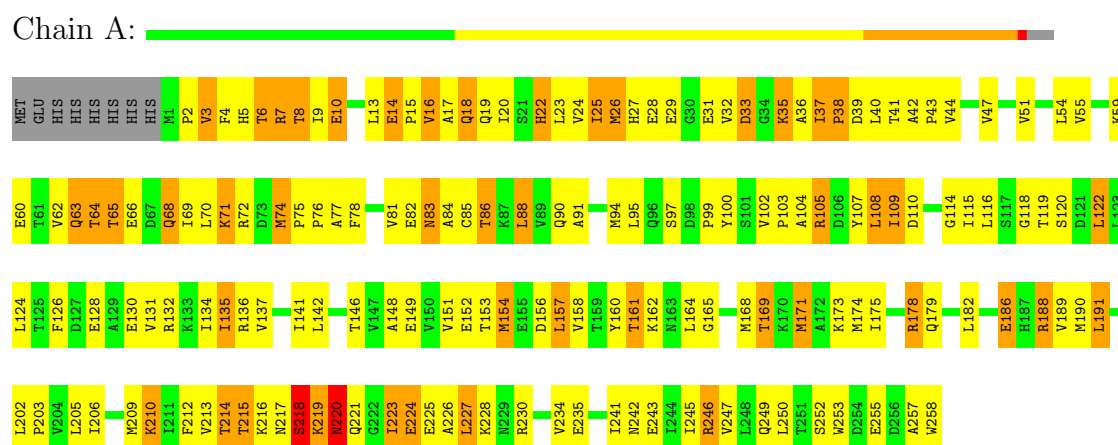
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	25	193	120	32	41	0	0	0
2	D	19	146	93	23	30	0	0	0

3 Residue-property plots

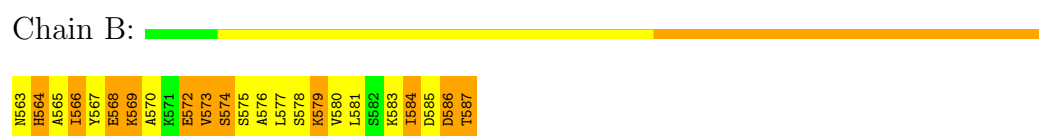
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



• Molecule 2: Invasin ipaA



• Molecule 2: Invasin ipaA



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α , β , γ	154.48Å 154.48Å 154.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.11 – 3.20	Depositor
% Data completeness (in resolution range)	99.0 (109.11-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	BUSTER-TNT 1.3.2	Depositor
R, R_{free}	0.243 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2359	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

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	0.28	0/2047	0.49	0/2773
2	B	0.44	0/194	0.74	1/258 (0.4%)
2	D	0.20	0/146	0.32	0/193
All	All	0.29	0/2387	0.51	1/3224 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	564	HIS	CA-CB-CG	-5.50	104.24	113.60

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	2020	0	2073	227	4
2	B	193	0	197	29	0
2	D	146	0	157	28	0
All	All	2359	0	2427	253	4

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 53.

All (253) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:255:GLU:OE2	1:A:258:TRP:CD1	1.84	1.28
1:A:4:PHE:CE1	1:A:13:LEU:HB2	1.69	1.25
1:A:255:GLU:OE2	1:A:258:TRP:HD1	0.92	1.20
1:A:255:GLU:O	1:A:255:GLU:CD	1.79	1.20
1:A:23:LEU:HB3	1:A:109:ILE:HD11	1.31	1.09
1:A:179:GLN:HA	1:A:182:LEU:HD12	1.21	1.09
1:A:102:VAL:HG13	1:A:103:PRO:HD3	1.31	1.06
1:A:255:GLU:O	1:A:255:GLU:OE1	1.72	1.06
1:A:37:ILE:HG21	2:B:584:ILE:HG23	1.39	1.03
1:A:217:ASN:O	1:A:219:LYS:N	1.95	1.00
1:A:72:ARG:NH2	1:A:257:ALA:HA	1.75	0.99
1:A:68:GLN:OE1	1:A:68:GLN:HA	1.63	0.98
1:A:6:THR:HG22	1:A:9:ILE:H	1.27	0.97
2:D:568:GLU:HB3	2:D:571:LYS:HD2	1.49	0.94
1:A:157:LEU:HG	2:D:573:VAL:HG21	1.45	0.94
1:A:4:PHE:CE1	1:A:13:LEU:CB	2.51	0.93
1:A:182:LEU:HD11	1:A:191:LEU:HD12	1.53	0.91
1:A:132:ARG:O	1:A:136:ARG:HG3	1.73	0.88
1:A:179:GLN:HA	1:A:182:LEU:CD1	2.03	0.87
1:A:135:ILE:HG23	1:A:245:ILE:HG23	1.56	0.86
1:A:4:PHE:CZ	1:A:13:LEU:HB2	2.10	0.86
1:A:37:ILE:HG21	2:B:584:ILE:CG2	2.06	0.84
2:B:569:LYS:HA	2:B:572:GLU:HG3	1.60	0.84
1:A:23:LEU:CB	1:A:109:ILE:HD11	2.08	0.83
1:A:102:VAL:CG1	1:A:103:PRO:HD3	2.09	0.82
1:A:19:GLN:HB2	2:B:581:LEU:HD23	1.62	0.81
1:A:6:THR:CG2	1:A:9:ILE:H	1.93	0.81
1:A:27:HIS:HA	1:A:32:VAL:HB	1.62	0.79
1:A:42:ALA:HB3	1:A:43:PRO:HD3	1.64	0.79
1:A:23:LEU:HD12	1:A:109:ILE:CD1	2.14	0.78
1:A:165:GLY:HA2	2:D:580:VAL:HG11	1.63	0.78
1:A:23:LEU:HD12	1:A:109:ILE:HD11	1.66	0.77
1:A:20:ILE:HG12	2:B:581:LEU:HD21	1.66	0.77
1:A:24:VAL:O	1:A:28:GLU:HG2	1.84	0.77
1:A:168:MET:HG2	1:A:202:LEU:HD22	1.64	0.77
1:A:241:ILE:O	1:A:245:ILE:HG13	1.86	0.76
1:A:72:ARG:HG3	1:A:72:ARG:HH11	1.51	0.75
1:A:74:MET:N	1:A:75:PRO:HD2	2.02	0.75
1:A:255:GLU:HG2	1:A:258:TRP:HE1	1.51	0.75
1:A:108:LEU:HD11	2:B:584:ILE:HD12	1.67	0.75
1:A:18:GLN:HE21	1:A:18:GLN:HA	1.51	0.75
1:A:26:MET:HB2	1:A:32:VAL:HG23	1.69	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:81:VAL:HG13	1:A:118:GLY:HA3	1.68	0.74
1:A:33:ASP:HA	1:A:105:ARG:HD3	1.68	0.74
1:A:43:PRO:HB2	2:B:580:VAL:HG22	1.70	0.73
1:A:148:ALA:HB2	1:A:160:TYR:CZ	2.24	0.73
1:A:186:GLU:O	1:A:190:MET:HG3	1.88	0.73
1:A:68:GLN:CA	1:A:68:GLN:OE1	2.36	0.73
1:A:6:THR:HG23	1:A:8:THR:H	1.53	0.73
1:A:72:ARG:HH21	1:A:257:ALA:HA	1.54	0.72
1:A:14:GLU:HB3	1:A:15:PRO:HD3	1.72	0.72
2:D:567:TYR:HB2	2:D:569:LYS:HG2	1.71	0.71
1:A:255:GLU:HG2	1:A:258:TRP:NE1	2.05	0.71
1:A:157:LEU:HG	2:D:573:VAL:CG2	2.20	0.71
1:A:72:ARG:HH22	1:A:257:ALA:HA	1.55	0.71
1:A:131:VAL:HG11	1:A:252:SER:OG	1.90	0.71
2:B:565:ALA:O	2:B:568:GLU:N	2.23	0.70
2:B:569:LYS:O	2:B:573:VAL:HG13	1.91	0.70
2:D:568:GLU:HB3	2:D:571:LYS:CD	2.21	0.70
1:A:4:PHE:HE1	1:A:13:LEU:HD12	1.57	0.70
1:A:81:VAL:CG1	1:A:118:GLY:HA3	2.22	0.69
1:A:75:PRO:HA	1:A:78:PHE:CD2	2.29	0.68
1:A:10:GLU:O	1:A:14:GLU:HB2	1.93	0.68
1:A:37:ILE:HD11	1:A:105:ARG:NH1	2.09	0.68
2:D:568:GLU:CB	2:D:571:LYS:HD2	2.23	0.68
1:A:205:LEU:O	1:A:209:MET:HG3	1.94	0.68
1:A:223:ILE:HD12	1:A:226:ALA:HB3	1.75	0.67
1:A:134:ILE:HD12	1:A:178:ARG:HD3	1.76	0.67
1:A:63:GLN:NE2	1:A:63:GLN:HA	2.09	0.66
1:A:4:PHE:HE1	1:A:13:LEU:CD1	2.09	0.66
1:A:179:GLN:CA	1:A:182:LEU:HD12	2.13	0.66
1:A:215:THR:O	1:A:218:SER:O	2.13	0.66
1:A:158:VAL:O	1:A:162:LYS:HG2	1.96	0.66
1:A:44:VAL:HG22	1:A:88:LEU:HD13	1.78	0.65
1:A:77:ALA:HB3	1:A:122:LEU:HD22	1.77	0.65
1:A:18:GLN:NE2	1:A:18:GLN:HA	2.10	0.65
1:A:75:PRO:HG2	1:A:76:PRO:HD3	1.79	0.65
1:A:219:LYS:O	1:A:220:ASN:CB	2.45	0.64
1:A:214:THR:O	1:A:218:SER:N	2.30	0.64
1:A:4:PHE:CE1	1:A:13:LEU:HD12	2.33	0.64
1:A:224:GLU:O	1:A:228:LYS:HG3	1.99	0.63
1:A:47:VAL:O	1:A:51:VAL:HG23	1.98	0.63
1:A:4:PHE:CZ	1:A:13:LEU:CB	2.81	0.63
1:A:169:THR:OG1	2:D:584:ILE:HD12	1.98	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:23:LEU:CD1	1:A:109:ILE:HD11	2.29	0.62
1:A:6:THR:HG22	1:A:9:ILE:N	2.06	0.62
1:A:206:ILE:HG13	2:D:577:LEU:HD13	1.81	0.62
1:A:83:ASN:HA	1:A:86:THR:HG23	1.82	0.62
1:A:245:ILE:O	1:A:249:GLN:HB2	1.99	0.62
1:A:75:PRO:O	1:A:78:PHE:HB2	1.99	0.62
1:A:94:MET:HE2	1:A:104:ALA:HA	1.82	0.62
1:A:23:LEU:HB3	1:A:109:ILE:CD1	2.19	0.61
1:A:206:ILE:HD13	1:A:209:MET:HE2	1.82	0.61
1:A:72:ARG:HG3	1:A:72:ARG:NH1	2.16	0.61
1:A:62:VAL:HG13	1:A:71:LYS:HG3	1.83	0.61
1:A:134:ILE:CD1	1:A:178:ARG:HD3	2.30	0.61
2:D:577:LEU:HG	2:D:581:LEU:HD13	1.82	0.60
1:A:130:GLU:OE1	2:B:564:HIS:HE1	1.85	0.60
1:A:74:MET:HE1	1:A:122:LEU:CD1	2.32	0.60
1:A:60:GLU:O	1:A:64:THR:HG23	2.01	0.60
1:A:94:MET:HE2	1:A:104:ALA:CA	2.31	0.60
1:A:4:PHE:HE1	1:A:13:LEU:CB	2.11	0.60
1:A:20:ILE:O	1:A:24:VAL:HG23	2.03	0.59
1:A:43:PRO:HB2	2:B:580:VAL:CG2	2.32	0.59
1:A:202:LEU:N	1:A:203:PRO:HD2	2.19	0.58
1:A:84:ALA:HB1	1:A:114:GLY:HA3	1.86	0.58
1:A:75:PRO:CB	1:A:76:PRO:HD3	2.34	0.57
1:A:210:LYS:O	1:A:214:THR:HB	2.03	0.57
1:A:179:GLN:O	1:A:188:ARG:HG3	2.05	0.57
1:A:77:ALA:CB	1:A:122:LEU:HD22	2.34	0.57
1:A:219:LYS:O	1:A:220:ASN:HB3	2.05	0.56
1:A:151:VAL:HG13	1:A:156:ASP:HB3	1.88	0.56
1:A:223:ILE:CD1	1:A:226:ALA:HB3	2.35	0.56
1:A:154:MET:HB3	2:D:569:LYS:HB3	1.88	0.56
1:A:23:LEU:CG	1:A:109:ILE:HD11	2.36	0.56
1:A:154:MET:HG3	2:D:569:LYS:HB3	1.87	0.56
1:A:85:CYS:HA	1:A:115:ILE:HD11	1.86	0.56
1:A:215:THR:CG2	1:A:223:ILE:HD13	2.35	0.55
1:A:6:THR:CG2	1:A:9:ILE:HG13	2.37	0.55
1:A:130:GLU:OE1	2:B:564:HIS:CE1	2.59	0.55
1:A:242:ASN:O	1:A:246:ARG:HD3	2.06	0.55
1:A:75:PRO:CG	1:A:76:PRO:HD3	2.36	0.55
1:A:47:VAL:HG12	2:B:576:ALA:HB1	1.88	0.55
1:A:85:CYS:CA	1:A:115:ILE:HD11	2.36	0.55
1:A:165:GLY:HA3	2:D:580:VAL:HG21	1.89	0.55
1:A:255:GLU:CD	1:A:258:TRP:CD1	2.76	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:37:ILE:CG2	2:B:584:ILE:HA	2.38	0.54
1:A:6:THR:HG21	1:A:9:ILE:HG13	1.90	0.54
1:A:206:ILE:HD13	1:A:209:MET:CE	2.37	0.54
1:A:108:LEU:HD11	2:B:584:ILE:CD1	2.36	0.53
1:A:154:MET:CG	2:D:569:LYS:HB3	2.38	0.53
1:A:37:ILE:HD11	1:A:105:ARG:HH12	1.74	0.53
1:A:152:GLU:HB3	1:A:216:LYS:HE3	1.91	0.53
1:A:74:MET:CE	1:A:122:LEU:HD13	2.39	0.53
1:A:55:VAL:O	1:A:59:LYS:HG3	2.08	0.53
1:A:161:THR:HG23	1:A:206:ILE:HD12	1.90	0.53
1:A:161:THR:CG2	1:A:206:ILE:HD12	2.39	0.53
1:A:215:THR:HG21	1:A:223:ILE:HD13	1.90	0.52
1:A:134:ILE:HG12	1:A:174:MET:HE2	1.91	0.52
1:A:14:GLU:HA	1:A:14:GLU:OE1	2.10	0.52
1:A:91:ALA:O	1:A:95:LEU:HD12	2.10	0.52
1:A:148:ALA:HB2	1:A:160:TYR:OH	2.09	0.52
1:A:70:LEU:CD1	1:A:126:PHE:HA	2.39	0.52
2:B:568:GLU:O	2:B:572:GLU:HG2	2.09	0.52
1:A:74:MET:HE3	1:A:126:PHE:HB2	1.90	0.52
1:A:134:ILE:HG12	1:A:174:MET:CE	2.40	0.52
1:A:16:VAL:O	1:A:20:ILE:HG13	2.09	0.52
2:D:571:LYS:HD3	2:D:572:GLU:N	2.25	0.51
1:A:75:PRO:HB2	1:A:76:PRO:HD3	1.92	0.51
1:A:94:MET:HE2	1:A:104:ALA:HB2	1.92	0.51
1:A:40:LEU:O	1:A:44:VAL:HB	2.11	0.51
2:B:575:SER:O	2:B:579:LYS:HG2	2.10	0.51
1:A:214:THR:HG22	1:A:215:THR:N	2.26	0.51
1:A:162:LYS:HD3	2:D:576:ALA:HB1	1.93	0.51
1:A:33:ASP:HA	1:A:105:ARG:CD	2.40	0.51
1:A:37:ILE:HG21	2:B:584:ILE:HA	1.92	0.51
2:B:563:ASN:C	2:B:565:ALA:H	2.14	0.51
1:A:151:VAL:HG13	1:A:156:ASP:CB	2.41	0.51
1:A:7:ARG:HH11	1:A:7:ARG:CG	2.24	0.51
1:A:3:VAL:HG22	1:A:3:VAL:O	2.11	0.50
1:A:65:THR:CG2	1:A:71:LYS:HD2	2.42	0.50
2:D:568:GLU:HB3	2:D:571:LYS:NZ	2.26	0.50
1:A:152:GLU:C	1:A:213:VAL:HG23	2.32	0.50
2:D:570:ALA:O	2:D:574:SER:OG	2.30	0.50
1:A:37:ILE:CB	1:A:38:PRO:HD2	2.42	0.50
1:A:102:VAL:N	1:A:103:PRO:CD	2.75	0.50
2:D:567:TYR:CD1	2:D:567:TYR:N	2.79	0.49
1:A:13:LEU:HD21	1:A:119:THR:CG2	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:32:VAL:CG1	1:A:105:ARG:HG2	2.42	0.49
1:A:217:ASN:O	1:A:218:SER:C	2.43	0.49
1:A:90:GLN:O	1:A:94:MET:HG3	2.12	0.49
1:A:157:LEU:CG	2:D:573:VAL:HG21	2.30	0.49
1:A:14:GLU:HB3	1:A:15:PRO:CD	2.42	0.49
1:A:33:ASP:OD1	1:A:102:VAL:HG23	2.13	0.49
1:A:94:MET:HE2	1:A:104:ALA:CB	2.43	0.49
1:A:54:LEU:HD13	2:B:570:ALA:HA	1.95	0.48
1:A:160:TYR:CE2	1:A:209:MET:HE1	2.49	0.48
1:A:174:MET:O	1:A:178:ARG:HB2	2.13	0.48
1:A:212:PHE:CE1	1:A:227:LEU:HD22	2.48	0.48
1:A:35:LYS:HD2	2:B:587:THR:OXT	2.14	0.48
1:A:6:THR:HG23	1:A:8:THR:N	2.27	0.48
1:A:7:ARG:HG2	1:A:7:ARG:NH1	2.29	0.48
1:A:26:MET:CB	1:A:32:VAL:HG23	2.43	0.48
2:B:563:ASN:HD22	2:B:563:ASN:HA	1.34	0.47
2:D:577:LEU:HD11	2:D:581:LEU:HD11	1.97	0.47
1:A:13:LEU:HD21	1:A:119:THR:HG21	1.97	0.47
1:A:171:MET:O	1:A:175:ILE:HG12	2.15	0.47
1:A:255:GLU:HG2	1:A:258:TRP:CD1	2.49	0.46
1:A:214:THR:CG2	1:A:215:THR:N	2.78	0.46
1:A:109:ILE:HG22	1:A:110:ASP:N	2.31	0.46
1:A:69:ILE:HD12	1:A:69:ILE:H	1.81	0.46
1:A:22:HIS:HD2	1:A:26:MET:CE	2.29	0.46
1:A:215:THR:HG22	1:A:223:ILE:CD1	2.45	0.46
1:A:165:GLY:CA	2:D:580:VAL:HG11	2.40	0.46
1:A:182:LEU:CD1	1:A:191:LEU:HD12	2.36	0.45
1:A:74:MET:HE1	1:A:122:LEU:HD13	1.95	0.45
2:B:579:LYS:H	2:B:579:LYS:HG2	1.61	0.45
1:A:84:ALA:CB	1:A:114:GLY:HA3	2.45	0.45
1:A:227:LEU:CD1	1:A:230:ARG:NH2	2.79	0.45
1:A:74:MET:N	1:A:75:PRO:CD	2.78	0.45
1:A:169:THR:O	1:A:173:LYS:HG3	2.17	0.45
1:A:95:LEU:CD2	1:A:105:ARG:NH2	2.80	0.45
1:A:210:LYS:NZ	2:D:570:ALA:HB1	2.31	0.45
1:A:6:THR:O	1:A:10:GLU:HB2	2.17	0.45
1:A:39:ASP:OD1	1:A:41:THR:HB	2.17	0.45
1:A:44:VAL:HG22	1:A:88:LEU:CD1	2.45	0.44
1:A:13:LEU:O	1:A:17:ALA:HB2	2.16	0.44
1:A:2:PRO:C	1:A:4:PHE:H	2.20	0.44
1:A:164:LEU:O	1:A:168:MET:HB2	2.18	0.44
1:A:37:ILE:HB	1:A:38:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:568:GLU:HB3	2:D:571:LYS:HZ3	1.82	0.44
2:B:565:ALA:O	2:B:566:ILE:C	2.53	0.44
1:A:78:PHE:CD1	1:A:122:LEU:HD21	2.52	0.44
1:A:146:THR:O	1:A:149:GLU:HG3	2.18	0.44
1:A:158:VAL:HG13	1:A:162:LYS:HZ2	1.83	0.43
2:D:573:VAL:CG1	2:D:574:SER:N	2.80	0.43
1:A:210:LYS:HA	1:A:213:VAL:HG12	2.01	0.43
1:A:243:GLU:O	1:A:247:VAL:HG23	2.18	0.43
2:D:578:SER:O	2:D:582:SER:OG	2.37	0.43
1:A:23:LEU:HD12	1:A:109:ILE:HD13	1.96	0.43
1:A:91:ALA:HB2	1:A:107:TYR:HB2	2.01	0.43
1:A:153:THR:C	1:A:213:VAL:HG21	2.39	0.43
1:A:137:VAL:O	1:A:141:ILE:HG12	2.18	0.42
1:A:27:HIS:CA	1:A:32:VAL:HB	2.40	0.42
1:A:72:ARG:NH2	1:A:257:ALA:CA	2.65	0.42
1:A:74:MET:H	1:A:75:PRO:HD2	1.77	0.42
1:A:128:GLU:HG2	1:A:252:SER:HB2	2.01	0.42
1:A:168:MET:CG	1:A:202:LEU:HD22	2.43	0.42
1:A:169:THR:HG23	1:A:173:LYS:HE3	2.00	0.42
1:A:25:ILE:O	1:A:29:GLU:HG2	2.20	0.42
1:A:36:ALA:HB2	1:A:100:TYR:CZ	2.53	0.42
1:A:37:ILE:HD12	2:B:584:ILE:CG2	2.50	0.42
1:A:72:ARG:CG	1:A:72:ARG:NH1	2.80	0.42
1:A:109:ILE:HD12	1:A:109:ILE:HA	1.80	0.42
1:A:65:THR:HG21	1:A:70:LEU:HD23	2.02	0.42
1:A:7:ARG:CG	1:A:7:ARG:NH1	2.81	0.41
2:B:570:ALA:O	2:B:574:SER:HB3	2.20	0.41
1:A:14:GLU:CB	1:A:15:PRO:HD3	2.46	0.41
1:A:154:MET:CB	2:D:569:LYS:HB3	2.49	0.41
1:A:42:ALA:N	1:A:43:PRO:CD	2.83	0.41
2:B:587:THR:OXT	2:B:587:THR:HG22	2.20	0.41
1:A:227:LEU:HA	1:A:227:LEU:HD13	1.85	0.41
1:A:95:LEU:HD21	1:A:105:ARG:NH2	2.36	0.41
2:B:565:ALA:C	2:B:567:TYR:N	2.72	0.41
1:A:29:GLU:H	1:A:29:GLU:HG2	1.63	0.41
1:A:175:ILE:HG23	1:A:191:LEU:HD22	2.03	0.41
1:A:131:VAL:O	1:A:135:ILE:HG13	2.20	0.41
1:A:28:GLU:HA	1:A:28:GLU:OE1	2.21	0.41
1:A:108:LEU:CD1	2:B:584:ILE:HD12	2.46	0.40
1:A:77:ALA:CB	1:A:122:LEU:CD2	2.99	0.40
2:D:567:TYR:HB2	2:D:569:LYS:CG	2.46	0.40
1:A:202:LEU:O	1:A:206:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:99:PRO:O	1:A:105:ARG:NH2	2.53	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:219:LYS:CB	1:A:219:LYS:CB[18_454]	1.68	0.52
1:A:219:LYS:CG	1:A:219:LYS:CD[18_454]	1.77	0.43
1:A:219:LYS:CG	1:A:219:LYS:CG[18_454]	2.10	0.10
1:A:219:LYS:CD	1:A:219:LYS:CD[18_454]	2.19	0.01

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	256/266 (96%)	232 (91%)	18 (7%)	6 (2%)	10	52
2	B	23/25 (92%)	21 (91%)	1 (4%)	1 (4%)	4	30
2	D	17/25 (68%)	17 (100%)	0	0	100	100
All	All	296/316 (94%)	270 (91%)	19 (6%)	7 (2%)	9	51

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	THR
1	A	218	SER
1	A	220	ASN
1	A	3	VAL
1	A	38	PRO
2	B	586	ASP
1	A	253	TRP

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	229/237 (97%)	169 (74%)	60 (26%)	1	2
2	B	22/22 (100%)	8 (36%)	14 (64%)	0	0
2	D	17/22 (77%)	10 (59%)	7 (41%)	0	0
All	All	268/281 (95%)	187 (70%)	81 (30%)	0	1

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

Mol	Chain	Res	Type
1	A	5	HIS
1	A	6	THR
1	A	7	ARG
1	A	8	THR
1	A	10	GLU
1	A	14	GLU
1	A	16	VAL
1	A	18	GLN
1	A	22	HIS
1	A	25	ILE
1	A	26	MET
1	A	31	GLU
1	A	33	ASP
1	A	35	LYS
1	A	37	ILE
1	A	63	GLN
1	A	64	THR
1	A	66	GLU
1	A	68	GLN
1	A	71	LYS
1	A	74	MET
1	A	82	GLU
1	A	83	ASN
1	A	86	THR
1	A	88	LEU
1	A	97	SER
1	A	105	ARG

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Mol	Chain	Res	Type
1	A	108	LEU
1	A	109	ILE
1	A	116	LEU
1	A	120	SER
1	A	122	LEU
1	A	124	LEU
1	A	135	ILE
1	A	142	LEU
1	A	154	MET
1	A	157	LEU
1	A	161	THR
1	A	169	THR
1	A	171	MET
1	A	178	ARG
1	A	186	GLU
1	A	188	ARG
1	A	189	VAL
1	A	191	LEU
1	A	210	LYS
1	A	214	THR
1	A	215	THR
1	A	218	SER
1	A	219	LYS
1	A	220	ASN
1	A	221	GLN
1	A	223	ILE
1	A	224	GLU
1	A	225	GLU
1	A	227	LEU
1	A	234	VAL
1	A	235	GLU
1	A	246	ARG
1	A	250	LEU
2	B	566	ILE
2	B	568	GLU
2	B	569	LYS
2	B	572	GLU
2	B	573	VAL
2	B	574	SER
2	B	577	LEU
2	B	578	SER
2	B	579	LYS

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Mol	Chain	Res	Type
2	B	583	LYS
2	B	584	ILE
2	B	585	ASP
2	B	586	ASP
2	B	587	THR
2	D	567	TYR
2	D	571	LYS
2	D	572	GLU
2	D	573	VAL
2	D	574	SER
2	D	575	SER
2	D	582	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	22	HIS
1	A	27	HIS
1	A	63	GLN
1	A	163	ASN
1	A	193	ASN
1	A	196	ASN
1	A	220	ASN
1	A	229	ASN
2	B	563	ASN
2	B	564	HIS

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 ⓘ

There are no ligands in this entry.

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.