Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:21 AM UTC

PDB ID	:	2BHM / pdb_00002bhm
Title	:	Crystal structure of VirB8 from Brucella suis
Authors	:	Bayliss, R.; Baron, C.; Waksman, G.
Deposited on	:	2005-01-14
Resolution	:	2.40 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:

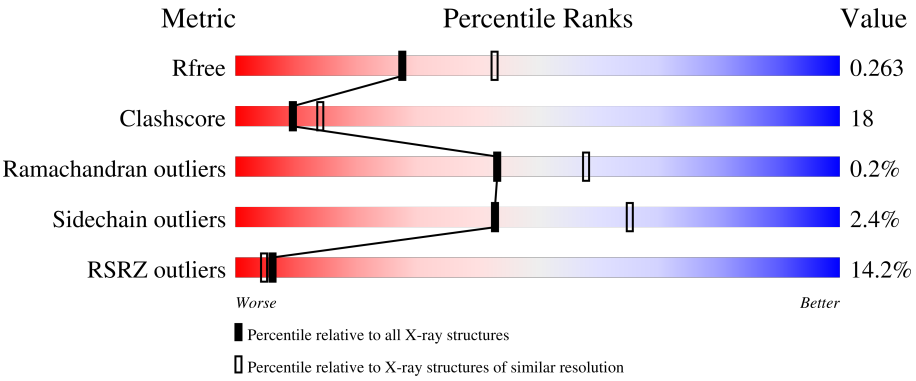
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 <=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	164	10% 56% 24% · 18%
1	B	164	7% 62% 18% · 18%
1	C	164	20% 47% 32% · 18%
1	D	164	7% 51% 27% · 18%
1	E	164	14% 53% 27% · 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5382 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 TYPE IV SECRETION SYSTEM PROTEIN VIRB8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	2	1
			1077	678	179	216	4			
1	B	135	Total	C	N	O	S	0	0	1
			1063	670	176	214	3			
1	C	135	Total	C	N	O	S	0	0	1
			1063	670	176	214	3			
1	D	134	Total	C	N	O	S	0	0	1
			1055	666	175	211	3			
1	E	135	Total	C	N	O	S	0	0	1
			1063	670	176	214	3			

- Molecule 2 is water.

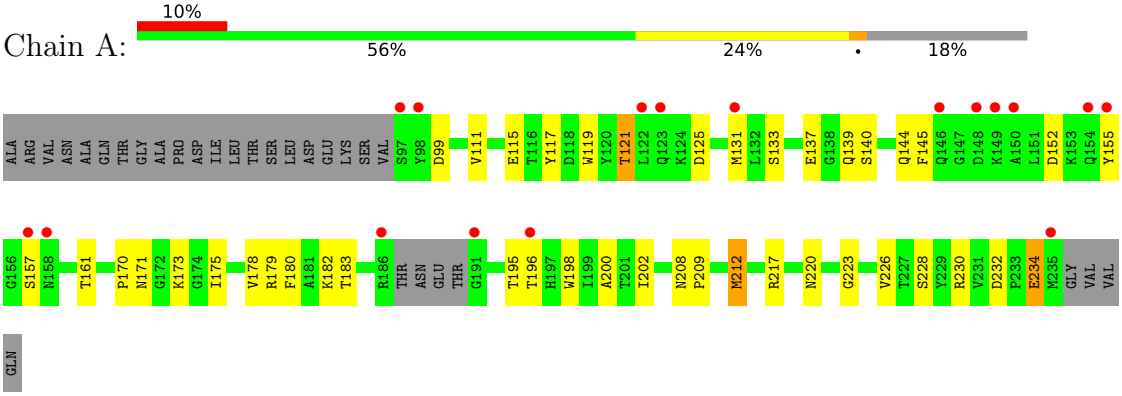
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total	O	0	0
			16	16		
2	B	13	Total	O	0	0
			13	13		
2	C	3	Total	O	0	0
			3	3		
2	D	25	Total	O	0	0
			25	25		
2	E	4	Total	O	0	0
			4	4		

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.

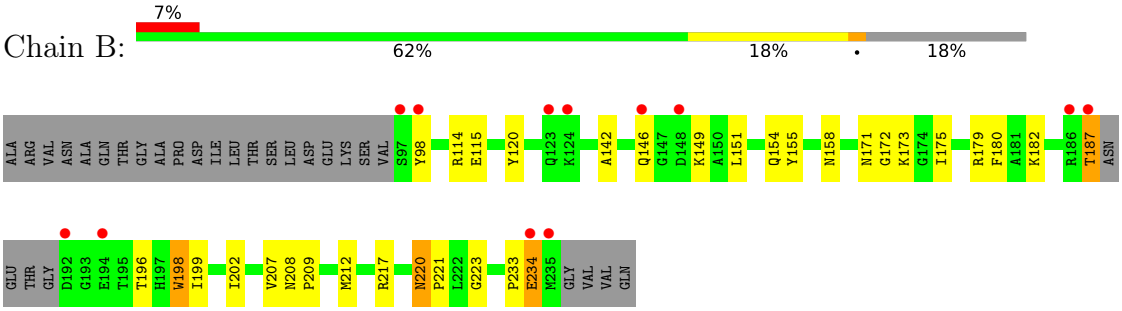
• Molecule 1: TYPE IV SECRETION SYSTEM PROTEIN VIRB8

Chain A:



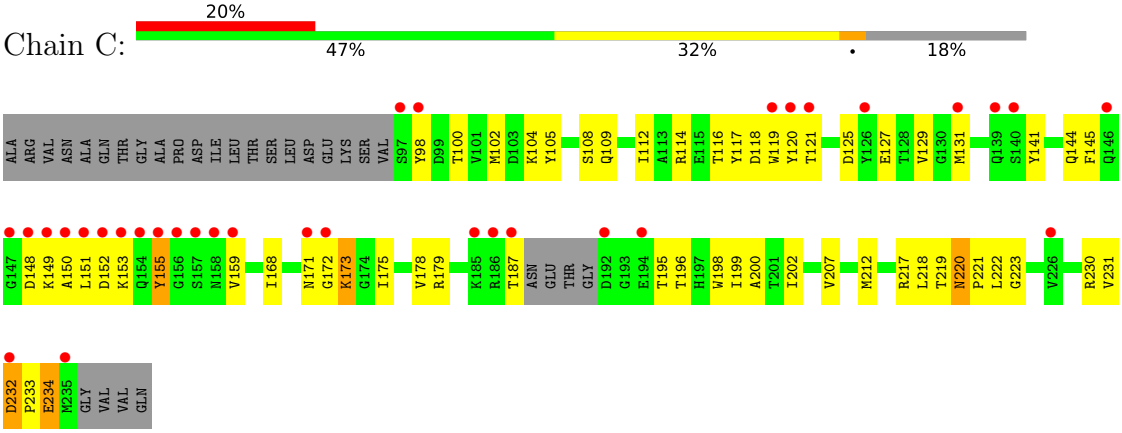
• Molecule 1: TYPE IV SECRETION SYSTEM PROTEIN VIRB8

Chain B:



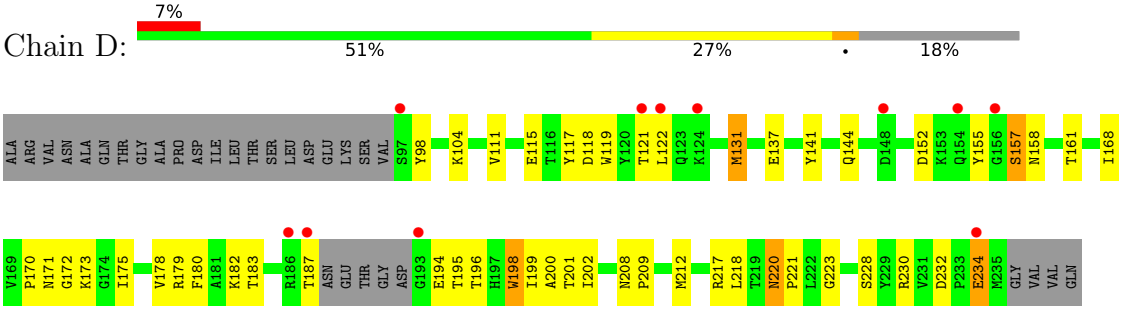
• Molecule 1: TYPE IV SECRETION SYSTEM PROTEIN VIRB8

Chain C:



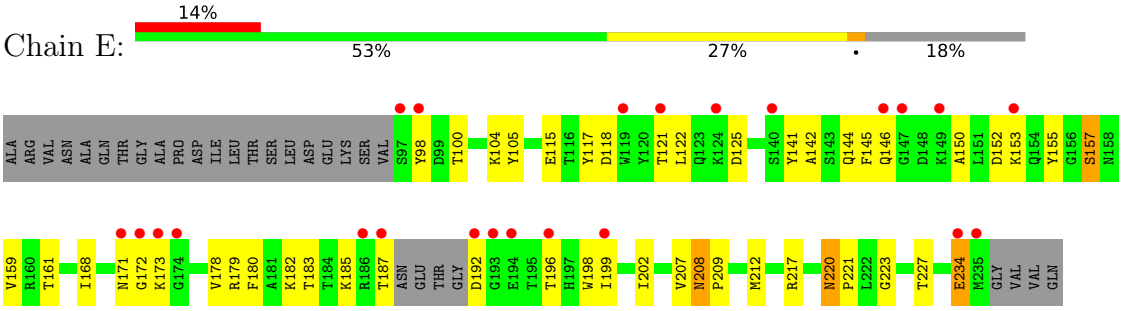
• Molecule 1: TYPE IV SECRETION SYSTEM PROTEIN VIRB8

Chain D:



• Molecule 1: TYPE IV SECRETION SYSTEM PROTEIN VIRB8

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	202.76Å 202.76Å 103.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.60 – 2.40 26.60 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (26.60-2.40) 98.3 (26.60-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.273 0.235 , 0.263	Depositor DCC
R_{free} test set	2083 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	40.0	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5382	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.54	1/1101 (0.1%)	1.07	9/1496 (0.6%)
1	B	0.54	1/1087 (0.1%)	1.07	7/1479 (0.5%)
1	C	0.49	1/1087 (0.1%)	1.03	10/1479 (0.7%)
1	D	0.57	1/1079 (0.1%)	1.14	10/1468 (0.7%)
1	E	0.48	1/1087 (0.1%)	0.98	5/1479 (0.3%)
All	All	0.52	5/5441 (0.1%)	1.06	41/7401 (0.6%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	234	GLU	C-N	-5.80	1.25	1.33
1	A	234	GLU	C-N	-5.76	1.25	1.33
1	C	234	GLU	C-N	-5.32	1.25	1.33
1	D	234	GLU	C-N	-5.07	1.26	1.33
1	E	234	GLU	C-N	-5.07	1.26	1.33

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	220	ASN	CA-C-N	11.44	132.36	119.32
1	D	220	ASN	C-N-CA	11.44	132.36	119.32
1	B	220	ASN	CA-C-N	9.12	129.72	119.32
1	B	220	ASN	C-N-CA	9.12	129.72	119.32
1	B	149	LYS	N-CA-C	-8.71	102.36	113.16
1	E	220	ASN	CA-C-N	8.22	127.78	119.24
1	E	220	ASN	C-N-CA	8.22	127.78	119.24
1	D	155	TYR	N-CA-C	8.18	119.97	111.14
1	C	155	TYR	N-CA-C	7.47	120.88	111.69
1	D	208	ASN	CA-C-N	7.39	127.41	119.28
1	D	208	ASN	C-N-CA	7.39	127.41	119.28
1	C	220	ASN	CA-C-N	7.38	127.74	119.32
1	C	220	ASN	C-N-CA	7.38	127.74	119.32
1	D	158	ASN	N-CA-C	6.96	121.03	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	208	ASN	CA-C-N	6.86	126.83	119.28
1	A	208	ASN	C-N-CA	6.86	126.83	119.28
1	C	202	ILE	N-CA-C	6.76	117.64	108.17
1	B	202	ILE	N-CA-C	6.75	117.56	108.11
1	A	155	TYR	N-CA-C	6.65	118.32	111.14
1	A	170	PRO	N-CA-C	-6.61	101.52	111.57
1	A	202	ILE	N-CA-C	6.28	116.89	108.11
1	C	149	LYS	N-CA-C	-6.16	105.34	112.92
1	D	170	PRO	N-CA-C	-5.90	102.00	111.38
1	D	122	LEU	N-CA-C	5.77	118.06	111.02
1	C	98	TYR	N-CA-C	-5.57	105.21	111.28
1	C	218	LEU	N-CA-C	-5.54	106.50	113.20
1	D	202	ILE	N-CA-C	5.49	116.03	108.12
1	B	198	TRP	N-CA-C	5.44	117.45	109.24
1	A	121	THR	N-CA-C	-5.40	106.56	114.39
1	D	198	TRP	N-CA-C	5.37	116.96	108.96
1	C	114	ARG	N-CA-C	5.35	117.19	111.36
1	E	202	ILE	N-CA-C	5.28	115.56	108.17
1	C	232	ASP	CA-C-N	5.21	126.35	119.84
1	C	232	ASP	C-N-CA	5.21	126.35	119.84
1	A	145	PHE	N-CA-C	-5.15	105.67	112.94
1	E	208	ASN	CA-C-N	5.14	124.94	119.28
1	E	208	ASN	C-N-CA	5.14	124.94	119.28
1	B	114	ARG	N-CA-C	5.12	116.94	111.36
1	A	220	ASN	CA-C-N	5.05	125.33	119.47
1	A	220	ASN	C-N-CA	5.05	125.33	119.47
1	B	120	TYR	N-CA-C	5.04	119.14	113.15

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	1077	0	1023	38	0
1	B	1063	0	1012	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1063	0	1012	53	0
1	D	1055	0	1008	42	0
1	E	1063	0	1012	39	0
2	A	16	0	0	1	0
2	B	13	0	0	0	0
2	C	3	0	0	0	0
2	D	25	0	0	1	0
2	E	4	0	0	0	0
All	All	5382	0	5067	186	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 18.

All (186) 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:C:150:ALA:HB3	1:C:153:LYS:HG3	1.44	0.99
1:A:196:THR:HG23	1:A:198:TRP:HE1	1.31	0.93
1:A:230:ARG:HG2	1:A:230:ARG:HH11	1.36	0.90
1:C:148:ASP:HA	1:C:153:LYS:HD2	1.53	0.90
1:C:198:TRP:CZ3	1:C:233:PRO:HG3	2.08	0.89
1:A:209:PRO:HA	1:A:212:MET:HE3	1.55	0.87
1:A:179:ARG:NH1	1:A:234:GLU:OE2	2.08	0.87
1:C:131:MET:SD	1:C:219:THR:HG21	2.14	0.86
1:B:209:PRO:HA	1:B:212:MET:HE3	1.60	0.84
1:E:199:ILE:HD11	1:E:234:GLU:HG3	1.61	0.83
1:C:195:THR:HB	1:D:179:ARG:NH1	1.95	0.82
1:D:209:PRO:HA	1:D:212:MET:HE3	1.64	0.79
1:C:141:TYR:O	1:C:144:GLN:HG2	1.83	0.79
1:A:139[A]:GLN:HG3	1:A:140:SER:N	1.99	0.77
1:C:222:LEU:HD21	1:E:98:TYR:HE1	1.49	0.76
1:B:199:ILE:HD11	1:B:234:GLU:HG3	1.66	0.76
1:A:230:ARG:HG2	1:A:230:ARG:NH1	2.00	0.75
1:C:222:LEU:HD21	1:E:98:TYR:CE1	2.21	0.75
1:A:230:ARG:NH1	1:A:232:ASP:OD2	2.22	0.73
1:E:196:THR:HB	1:E:198:TRP:HE1	1.56	0.70
1:A:196:THR:CG2	1:A:198:TRP:HE1	2.03	0.70
1:C:196:THR:HB	1:C:198:TRP:HE1	1.57	0.69
1:C:222:LEU:CD2	1:E:98:TYR:HE1	2.06	0.68
1:A:212:MET:HE1	1:A:223:GLY:HA2	1.75	0.67
1:C:118:ASP:HB3	1:C:121:THR:HB	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ILE:HD11	1:C:234:GLU:CD	2.19	0.67
1:B:196:THR:HB	1:B:198:TRP:HE1	1.60	0.65
1:C:171:ASN:ND2	1:C:175:ILE:HB	2.11	0.65
1:A:171:ASN:ND2	1:A:175:ILE:HB	2.11	0.65
1:C:198:TRP:HZ3	1:C:233:PRO:HG3	1.62	0.65
1:E:171:ASN:HD21	1:E:173:LYS:HB2	1.61	0.65
1:A:139[A]:GLN:NE2	1:D:175:ILE:HD11	2.12	0.64
1:B:212:MET:HE1	1:B:223:GLY:HA2	1.79	0.64
1:D:196:THR:HB	1:D:198:TRP:HE1	1.61	0.64
1:C:171:ASN:HD21	1:C:175:ILE:HB	1.62	0.63
1:A:230:ARG:HH12	1:A:232:ASP:CG	2.07	0.62
1:D:230:ARG:HG2	1:D:230:ARG:HH11	1.65	0.61
1:B:196:THR:HG21	1:B:198:TRP:CZ2	2.34	0.61
1:D:212:MET:HG3	1:D:217:ARG:HG3	1.81	0.61
1:D:179:ARG:NH1	1:D:234:GLU:OE2	2.34	0.61
1:B:115:GLU:HB3	1:B:182:LYS:HE3	1.83	0.61
1:D:117:TYR:OH	1:D:152:ASP:HA	2.01	0.60
1:A:111:VAL:HG21	1:A:178:VAL:HG11	1.82	0.60
1:A:230:ARG:NH2	1:D:144:GLN:OE1	2.34	0.60
1:B:158:ASN:HA	1:B:187:THR:HB	1.84	0.59
1:C:199:ILE:HD11	1:C:234:GLU:OE2	2.02	0.59
1:D:199:ILE:HD11	1:D:234:GLU:OE2	2.02	0.59
1:E:142:ALA:O	1:E:146:GLN:HG3	2.02	0.59
1:C:155:TYR:HD2	1:C:159:VAL:HG21	1.68	0.59
1:C:155:TYR:HD2	1:C:159:VAL:CG2	2.15	0.59
1:E:196:THR:HB	1:E:198:TRP:NE1	2.17	0.59
1:D:171:ASN:OD1	1:D:171:ASN:C	2.47	0.58
1:D:230:ARG:NH1	1:D:232:ASP:OD1	2.36	0.58
1:C:212:MET:HE1	1:C:223:GLY:HA2	1.84	0.58
1:E:196:THR:HG21	1:E:198:TRP:CZ2	2.39	0.57
1:A:131[A]:MET:HE2	2:A:2015:HOH:O	2.05	0.57
1:B:212:MET:HG3	1:B:217:ARG:HG3	1.88	0.56
1:A:121:THR:HG22	1:A:125:ASP:OD2	2.05	0.56
1:C:121:THR:HG22	1:C:125:ASP:OD2	2.06	0.56
1:C:155:TYR:HD2	1:C:159:VAL:CB	2.19	0.56
1:E:141:TYR:O	1:E:144:GLN:HG2	2.06	0.56
1:C:155:TYR:HD2	1:C:159:VAL:HB	1.72	0.55
1:C:121:THR:HG22	1:C:125:ASP:CG	2.32	0.55
1:D:137:GLU:OE2	1:D:228:SER:HA	2.07	0.54
1:D:230:ARG:HH11	1:D:230:ARG:CG	2.20	0.54
1:C:155:TYR:CD2	1:C:159:VAL:HB	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ASN:ND2	1:B:175:ILE:HB	2.23	0.53
1:E:185:LYS:HE2	1:E:192:ASP:HA	1.89	0.53
1:E:212:MET:HG3	1:E:217:ARG:HG3	1.89	0.53
1:C:195:THR:HB	1:D:179:ARG:HH12	1.74	0.53
1:D:200:ALA:HA	1:D:230:ARG:O	2.08	0.53
1:E:121:THR:HG22	1:E:125:ASP:CG	2.34	0.53
1:A:139[A]:GLN:HE22	1:D:175:ILE:HD11	1.73	0.53
1:E:179:ARG:NH1	1:E:234:GLU:OE2	2.41	0.52
1:B:179:ARG:HD3	1:B:234:GLU:OE2	2.09	0.52
1:E:100:THR:HG22	1:E:104:LYS:HE3	1.91	0.52
1:C:148:ASP:HA	1:C:153:LYS:CD	2.35	0.52
1:A:230:ARG:NH1	1:A:230:ARG:CG	2.69	0.51
1:C:117:TYR:OH	1:C:152:ASP:HA	2.09	0.51
1:E:122:LEU:HD11	1:E:145:PHE:CE2	2.45	0.51
1:A:161:THR:HA	1:A:183:THR:O	2.09	0.51
1:D:118:ASP:HB3	1:D:121:THR:HB	1.93	0.51
1:B:209:PRO:O	1:B:212:MET:HG2	2.10	0.51
1:D:171:ASN:OD1	1:D:172:GLY:N	2.43	0.51
1:E:157:SER:O	1:E:187:THR:OG1	2.28	0.51
1:D:212:MET:HE1	1:D:223:GLY:HA2	1.93	0.50
1:A:230:ARG:NH1	1:A:232:ASP:CG	2.68	0.50
1:D:209:PRO:O	1:D:212:MET:HG2	2.11	0.50
1:A:144:GLN:CD	1:D:230:ARG:NH2	2.70	0.50
1:C:118:ASP:O	1:C:119:TRP:C	2.55	0.50
1:A:200:ALA:HA	1:A:230:ARG:O	2.11	0.49
1:D:141:TYR:O	1:D:144:GLN:HG2	2.12	0.49
1:E:117:TYR:OH	1:E:152:ASP:HA	2.12	0.49
1:B:207:VAL:O	1:B:208:ASN:C	2.55	0.49
1:E:212:MET:HE1	1:E:223:GLY:HA2	1.95	0.49
1:A:119:TRP:HZ3	1:A:152:ASP:HB2	1.78	0.49
1:C:196:THR:HB	1:C:198:TRP:NE1	2.25	0.49
1:C:200:ALA:HB2	1:C:231:VAL:HG22	1.93	0.49
1:C:102:MET:HG2	1:C:222:LEU:CD1	2.43	0.49
1:C:200:ALA:HA	1:C:230:ARG:O	2.12	0.49
1:A:212:MET:HG3	1:A:217:ARG:HG3	1.94	0.49
1:C:168:ILE:HG12	1:C:178:VAL:HG22	1.95	0.48
1:C:222:LEU:CD2	1:E:98:TYR:CE1	2.88	0.48
1:D:161:THR:HA	1:D:183:THR:O	2.13	0.48
1:A:196:THR:HG23	1:A:198:TRP:NE1	2.14	0.48
1:B:196:THR:HB	1:B:198:TRP:NE1	2.27	0.48
1:E:171:ASN:CG	1:E:172:GLY:N	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:PRO:HA	1:E:212:MET:HE3	1.94	0.48
1:D:196:THR:HG21	1:D:198:TRP:CZ2	2.49	0.48
1:E:121:THR:HG22	1:E:125:ASP:OD2	2.14	0.48
1:B:220:ASN:N	1:B:221:PRO:HD3	2.29	0.47
1:A:171:ASN:OD1	1:A:173:LYS:N	2.37	0.47
1:C:127:GLU:O	1:C:131:MET:HG2	2.15	0.47
1:D:179:ARG:HG3	2:D:2015:HOH:O	2.14	0.47
1:A:209:PRO:HA	1:A:212:MET:CE	2.35	0.47
1:C:145:PHE:HA	1:C:150:ALA:HB1	1.97	0.47
1:D:111:VAL:HG21	1:D:178:VAL:HG11	1.97	0.47
1:D:209:PRO:HA	1:D:212:MET:CE	2.39	0.47
1:D:119:TRP:HZ3	1:D:152:ASP:HB2	1.79	0.47
1:E:220:ASN:N	1:E:221:PRO:HD3	2.31	0.46
1:D:157:SER:O	1:D:187:THR:OG1	2.32	0.46
1:D:161:THR:CG2	1:D:182:LYS:HG2	2.46	0.46
1:E:115:GLU:HB3	1:E:182:LYS:HE3	1.98	0.46
1:B:212:MET:HE1	1:B:223:GLY:CA	2.44	0.46
1:B:198:TRP:CZ3	1:B:233:PRO:HG3	2.50	0.46
1:C:221:PRO:HG2	1:E:105:TYR:CG	2.51	0.46
1:D:201:THR:HB	1:D:230:ARG:HB3	1.99	0.45
1:C:148:ASP:CA	1:C:153:LYS:HD2	2.36	0.45
1:B:142:ALA:O	1:B:146:GLN:HG3	2.16	0.45
1:B:171:ASN:OD1	1:B:173:LYS:N	2.50	0.45
1:C:120:TYR:CD1	1:C:120:TYR:N	2.84	0.45
1:E:100:THR:O	1:E:104:LYS:HG3	2.17	0.45
1:A:121:THR:HG22	1:A:125:ASP:CG	2.41	0.44
1:E:155:TYR:HB3	1:E:159:VAL:HB	1.98	0.44
1:E:168:ILE:HG12	1:E:178:VAL:HG22	1.99	0.44
1:B:151:LEU:HD22	1:B:155:TYR:CE1	2.52	0.44
1:C:196:THR:HG21	1:C:198:TRP:CZ2	2.53	0.44
1:D:115:GLU:HG3	1:D:180:PHE:CZ	2.53	0.44
1:B:115:GLU:HG3	1:B:180:PHE:CE1	2.53	0.44
1:D:182:LYS:O	1:D:195:THR:HA	2.18	0.44
1:C:125:ASP:O	1:C:129:VAL:HG23	2.16	0.44
1:D:98:TYR:CD2	1:D:98:TYR:C	2.95	0.44
1:C:108:SER:O	1:C:112:ILE:HG13	2.17	0.43
1:C:151:LEU:O	1:C:155:TYR:HD1	2.01	0.43
1:B:172:GLY:O	1:B:173:LYS:HG3	2.18	0.43
1:E:161:THR:HA	1:E:183:THR:O	2.19	0.43
1:C:155:TYR:CD2	1:C:159:VAL:HG21	2.49	0.43
1:A:115:GLU:HG3	1:A:180:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:LYS:HE2	1:D:168:ILE:O	2.19	0.43
1:E:161:THR:CG2	1:E:182:LYS:HG2	2.48	0.43
1:A:133:SER:HB3	1:A:226:VAL:HB	2.00	0.42
1:D:218:LEU:HD23	1:D:218:LEU:HA	1.79	0.42
1:C:217:ARG:O	1:C:221:PRO:HG3	2.19	0.42
1:B:198:TRP:HZ3	1:B:233:PRO:HG3	1.83	0.42
1:C:116:THR:HG22	1:C:117:TYR:N	2.34	0.42
1:E:122:LEU:HD11	1:E:145:PHE:CZ	2.53	0.42
1:C:100:THR:O	1:C:104:LYS:HG3	2.19	0.42
1:C:179:ARG:NH1	1:C:234:GLU:OE2	2.51	0.42
1:C:220:ASN:N	1:C:221:PRO:HD3	2.35	0.42
1:E:155:TYR:CD2	1:E:155:TYR:N	2.84	0.42
1:B:217:ARG:O	1:B:221:PRO:HG3	2.20	0.42
1:D:230:ARG:NH1	1:D:230:ARG:CG	2.81	0.42
1:A:117:TYR:OH	1:A:152:ASP:HA	2.18	0.42
1:A:171:ASN:OD1	1:A:171:ASN:C	2.61	0.42
1:A:212:MET:HE1	1:A:223:GLY:CA	2.45	0.42
1:C:232:ASP:HA	1:C:233:PRO:HD3	1.84	0.42
1:E:150:ALA:O	1:E:153:LYS:HB2	2.19	0.42
1:B:171:ASN:OD1	1:B:171:ASN:C	2.61	0.42
1:D:220:ASN:N	1:D:221:PRO:HD3	2.34	0.42
1:E:115:GLU:HG3	1:E:180:PHE:CZ	2.55	0.41
1:E:207:VAL:O	1:E:208:ASN:C	2.63	0.41
1:E:199:ILE:HD11	1:E:234:GLU:CG	2.41	0.41
1:A:209:PRO:O	1:A:212:MET:HG2	2.21	0.41
1:C:105:TYR:O	1:C:109:GLN:HG2	2.21	0.41
1:A:171:ASN:HD21	1:A:175:ILE:HB	1.85	0.41
1:D:131:MET:HE2	1:D:131:MET:HB2	1.74	0.41
1:C:171:ASN:C	1:C:173:LYS:H	2.29	0.41
1:E:118:ASP:HB3	1:E:121:THR:HB	2.02	0.41
1:A:182:LYS:O	1:A:195:THR:HA	2.21	0.41
1:D:121:THR:HG22	1:D:121:THR:O	2.20	0.41
1:D:212:MET:HE1	1:D:223:GLY:CA	2.51	0.41
1:E:171:ASN:OD1	1:E:172:GLY:N	2.50	0.41
1:A:137:GLU:OE2	1:A:228:SER:HA	2.20	0.41
1:B:98:TYR:CD2	1:B:98:TYR:C	3.00	0.40
1:C:121:THR:HG22	1:C:121:THR:O	2.22	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	133/164 (81%)	130 (98%)	3 (2%)	0	100 100
1	B	131/164 (80%)	127 (97%)	4 (3%)	0	100 100
1	C	131/164 (80%)	124 (95%)	6 (5%)	1 (1%)	16 25
1	D	130/164 (79%)	126 (97%)	4 (3%)	0	100 100
1	E	131/164 (80%)	127 (97%)	4 (3%)	0	100 100
All	All	656/820 (80%)	634 (97%)	21 (3%)	1 (0%)	43 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	172	GLY

5.3.2 Protein sidechains (i)

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	118/142 (83%)	115 (98%)	3 (2%)	42 64
1	B	117/142 (82%)	115 (98%)	2 (2%)	53 74
1	C	117/142 (82%)	114 (97%)	3 (3%)	40 63
1	D	116/142 (82%)	112 (97%)	4 (3%)	32 54
1	E	117/142 (82%)	115 (98%)	2 (2%)	53 74
All	All	585/710 (82%)	571 (98%)	14 (2%)	43 65

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ASP
1	A	157	SER
1	A	212	MET
1	B	154	GLN
1	B	187	THR
1	C	173	LYS
1	C	187	THR
1	C	207	VAL
1	D	131	MET
1	D	157	SER
1	D	173	LYS
1	D	194	GLU
1	E	157	SER
1	E	227	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	A	225	ASN
1	B	139	GLN
1	B	146	GLN
1	C	146	GLN
1	C	197	HIS
1	C	205	GLN
1	C	225	ASN
1	E	205	GLN
1	E	225	ASN

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

There are no oligosaccharides 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

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, 95^{th} 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	135/164 (82%)	0.30	17 (12%) 8 6	9, 30, 67, 79	2 (1%)
1	B	135/164 (82%)	0.33	12 (8%) 15 12	23, 38, 66, 86	0
1	C	135/164 (82%)	1.38	33 (24%) 2 1	32, 59, 89, 94	0
1	D	134/164 (81%)	0.25	11 (8%) 17 14	20, 33, 65, 81	0
1	E	135/164 (82%)	1.09	23 (17%) 4 3	31, 53, 83, 93	0
All	All	674/820 (82%)	0.67	96 (14%) 6 5	9, 45, 80, 94	2 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	187	THR	5.5
1	C	98	TYR	5.2
1	C	235	MET	5.2
1	E	97	SER	5.2
1	C	187	THR	4.8
1	E	235	MET	4.7
1	C	152	ASP	4.5
1	E	98	TYR	4.4
1	C	139	GLN	4.4
1	C	97	SER	4.3
1	E	187	THR	4.2
1	C	147	GLY	4.2
1	C	155	TYR	4.1
1	A	98	TYR	3.9
1	C	156	GLY	3.9
1	C	149	LYS	3.8
1	B	97	SER	3.8
1	D	154	GLN	3.7
1	C	148	ASP	3.7
1	C	119	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	186	ARG	3.5
1	B	235	MET	3.5
1	C	185	LYS	3.5
1	E	146	GLN	3.5
1	C	146	GLN	3.4
1	D	187	THR	3.4
1	C	131	MET	3.4
1	E	119	TRP	3.3
1	A	186	ARG	3.3
1	C	151	LEU	3.2
1	E	234	GLU	3.2
1	E	147	GLY	3.1
1	E	171	ASN	3.0
1	A	235	MET	3.0
1	E	172	GLY	3.0
1	E	124	LYS	3.0
1	A	155	TYR	2.9
1	B	124	LYS	2.9
1	C	186	ARG	2.9
1	B	192	ASP	2.9
1	D	124	LYS	2.8
1	C	158	ASN	2.8
1	E	173	LYS	2.8
1	D	186	ARG	2.7
1	A	191	GLY	2.7
1	C	140	SER	2.6
1	E	121	THR	2.6
1	E	153	LYS	2.6
1	A	148	ASP	2.6
1	E	186	ARG	2.6
1	B	234	GLU	2.6
1	B	146	GLN	2.5
1	A	131[A]	MET	2.5
1	B	194	GLU	2.5
1	C	232	ASP	2.5
1	D	234	GLU	2.5
1	A	146	GLN	2.5
1	C	154	GLN	2.5
1	C	171	ASN	2.5
1	E	199	ILE	2.5
1	D	193	GLY	2.4
1	C	153	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	159	VAL	2.4
1	B	148	ASP	2.4
1	D	148	ASP	2.4
1	A	157	SER	2.4
1	E	193	GLY	2.4
1	A	123	GLN	2.4
1	D	121	THR	2.3
1	E	192	ASP	2.3
1	E	174	GLY	2.3
1	A	149	LYS	2.3
1	B	98	TYR	2.3
1	A	150	ALA	2.3
1	C	121	THR	2.3
1	C	192	ASP	2.3
1	E	194	GLU	2.3
1	A	154	GLN	2.2
1	C	157	SER	2.2
1	C	120	TYR	2.2
1	E	140	SER	2.2
1	C	226	VAL	2.2
1	D	97	SER	2.2
1	C	194	GLU	2.2
1	A	122	LEU	2.1
1	C	150	ALA	2.1
1	D	156	GLY	2.1
1	A	97	SER	2.1
1	D	122	LEU	2.1
1	E	149	LYS	2.1
1	C	172	GLY	2.0
1	A	196	THR	2.0
1	E	196	THR	2.0
1	C	126	TYR	2.0
1	B	123	GLN	2.0
1	A	158	ASN	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.