



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2023 – 05:48 PM EDT

PDB ID : 2GA0
Title : Variable Small Protein 1 of Borrelia turicatae (VspA or Vsp1)
Authors : Lawson, C.L.; Yung, B.H.; Barbour, A.G.; Zuckert, W.R.
Deposited on : 2006-03-07
Resolution : 2.70 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

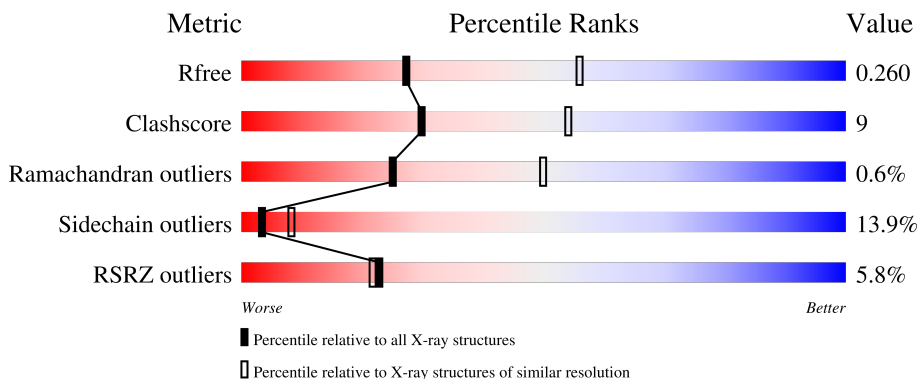
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



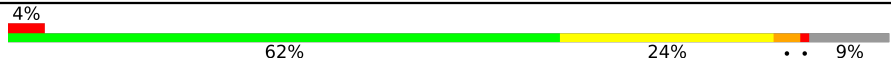


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	181	
1	B	181	
1	C	181	
1	D	181	
1	E	181	

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Mol	Chain	Length	Quality of chain
1	F	181	
1	G	181	
1	H	181	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9606 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 surface protein VspA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
1	A	164	1182	740	196	246	0	0	0
1	B	164	1182	740	196	246	0	0	0
1	C	164	1182	740	196	246	0	0	0
1	D	164	1182	740	196	246	0	0	0
1	E	164	1182	740	196	246	0	0	0
1	F	164	1182	740	196	246	0	0	0
1	G	164	1182	740	196	246	0	0	0
1	H	164	1182	740	196	246	0	0	0

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Ni 2	0	0
2	B	2	Total 2	Ni 2	0	0
2	C	1	Total 1	Ni 1	0	0
2	D	2	Total 2	Ni 2	0	0
2	E	2	Total 2	Ni 2	0	0
2	F	1	Total 1	Ni 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total 2	Ni 2	0	0
2	H	2	Total 2	Ni 2	0	0

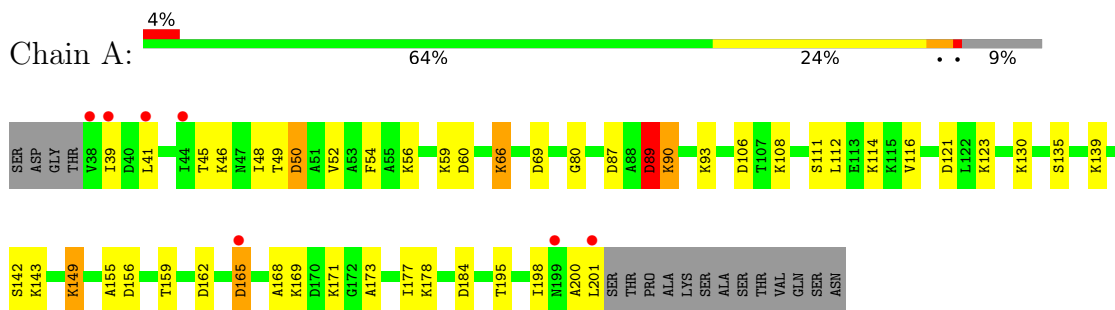
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total 20	O 20	0	0
3	B	16	Total 16	O 16	0	0
3	C	11	Total 11	O 11	0	0
3	D	13	Total 13	O 13	0	0
3	E	16	Total 16	O 16	0	0
3	F	24	Total 24	O 24	0	0
3	G	18	Total 18	O 18	0	0
3	H	18	Total 18	O 18	0	0

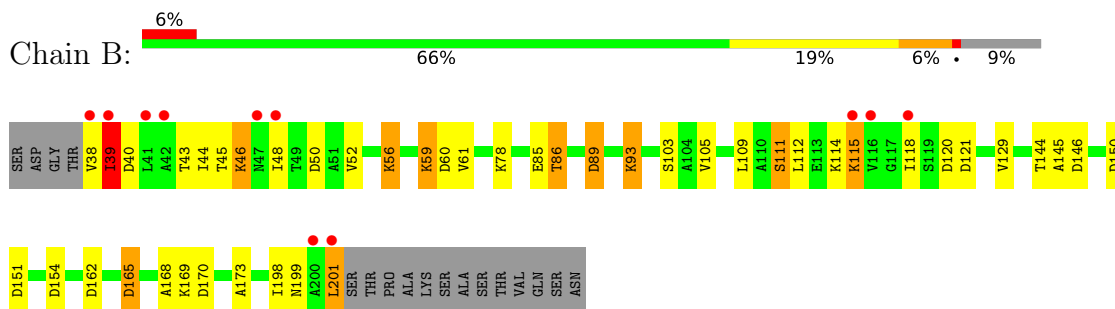
3 Residue-property plots [i](#)

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.

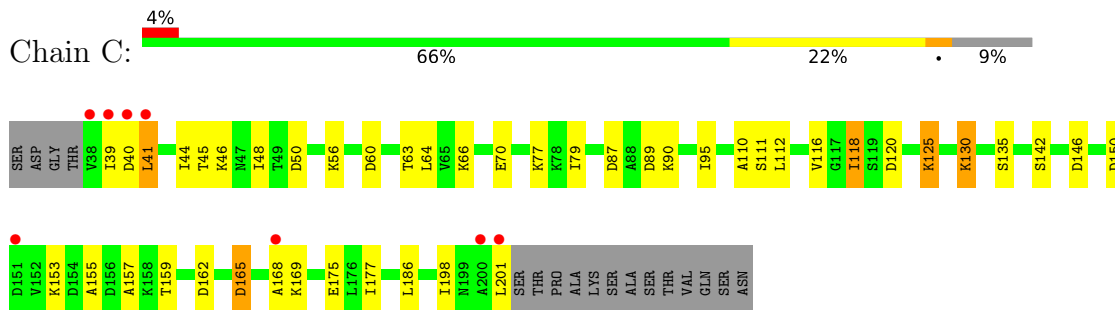
- Molecule 1: surface protein VspA



- Molecule 1: surface protein VspA



- Molecule 1: surface protein VspA

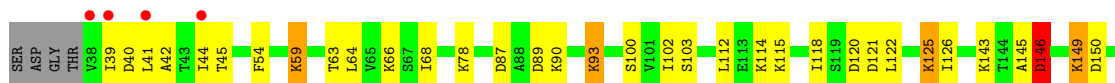


- Molecule 1: surface protein VspA

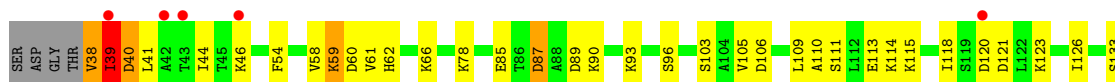




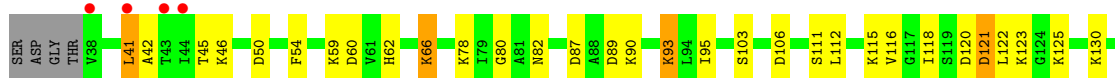
- Molecule 1: surface protein VspA



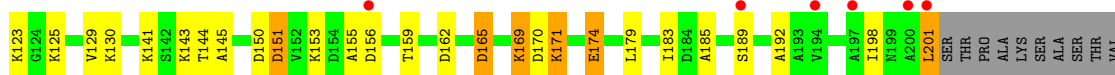
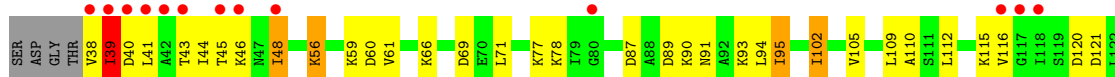
- Molecule 1: surface protein VspA



- Molecule 1: surface protein VspA



- Molecule 1: surface protein VspA



GLN
SER
ASN

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	241.84Å 69.11Å 87.58Å 90.00° 104.95° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 43.54 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-2.70) 98.7 (43.54-2.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.69Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.272 0.216 , 0.260	Depositor DCC
R_{free} test set	1902 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtrriage
Anisotropy	0.428	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9606	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.7245e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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

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	0.77	0/1185	1.04	11/1598 (0.7%)
1	B	0.68	0/1185	1.01	9/1598 (0.6%)
1	C	0.66	0/1185	1.01	10/1598 (0.6%)
1	D	0.66	0/1185	0.97	11/1598 (0.7%)
1	E	0.63	0/1185	0.96	8/1598 (0.5%)
1	F	0.72	0/1185	1.05	13/1598 (0.8%)
1	G	0.70	0/1185	0.97	7/1598 (0.4%)
1	H	0.63	0/1185	1.00	12/1598 (0.8%)
All	All	0.68	0/9480	1.00	81/12784 (0.6%)

There are no bond length outliers.

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	151	ASP	CB-CG-OD2	8.16	125.64	118.30
1	A	50	ASP	CB-CG-OD2	8.14	125.62	118.30
1	A	87	ASP	CB-CG-OD2	8.06	125.56	118.30
1	F	154	ASP	CB-CG-OD2	7.81	125.33	118.30
1	E	87	ASP	CB-CG-OD2	7.80	125.32	118.30
1	A	121	ASP	CB-CG-OD2	7.55	125.09	118.30
1	H	60	ASP	CB-CG-OD2	7.23	124.81	118.30
1	G	121	ASP	CB-CG-OD2	7.22	124.80	118.30
1	C	120	ASP	CB-CG-OD2	7.18	124.76	118.30
1	H	162	ASP	CB-CG-OD2	7.18	124.76	118.30
1	E	120	ASP	CB-CG-OD2	7.17	124.75	118.30
1	B	121	ASP	CB-CG-OD2	7.04	124.64	118.30
1	C	89	ASP	CB-CG-OD2	6.98	124.58	118.30
1	D	40	ASP	CB-CG-OD2	6.97	124.57	118.30
1	B	60	ASP	CB-CG-OD2	6.96	124.57	118.30
1	D	121	ASP	CB-CG-OD2	6.95	124.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	154	ASP	CB-CG-OD2	6.94	124.55	118.30
1	H	156	ASP	CB-CG-OD2	6.84	124.46	118.30
1	C	50	ASP	CB-CG-OD2	6.80	124.42	118.30
1	F	146	ASP	CB-CG-OD2	6.79	124.41	118.30
1	E	89	ASP	CB-CG-OD2	6.78	124.40	118.30
1	A	184	ASP	CB-CG-OD1	6.64	124.28	118.30
1	E	162	ASP	CB-CG-OD2	6.63	124.27	118.30
1	C	146	ASP	CB-CG-OD2	6.62	124.25	118.30
1	B	120	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	60	ASP	CB-CG-OD2	6.50	124.16	118.30
1	F	150	ASP	CB-CG-OD2	6.43	124.08	118.30
1	F	87	ASP	CB-CG-OD2	6.33	124.00	118.30
1	C	87	ASP	CB-CG-OD2	6.32	123.99	118.30
1	F	121	ASP	CB-CG-OD2	6.32	123.99	118.30
1	B	89	ASP	CB-CG-OD2	6.31	123.98	118.30
1	G	60	ASP	CB-CG-OD2	6.21	123.89	118.30
1	H	150	ASP	CB-CG-OD2	6.21	123.89	118.30
1	H	121	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	162	ASP	CB-CG-OD2	6.20	123.88	118.30
1	H	170	ASP	CB-CG-OD2	6.12	123.81	118.30
1	C	165	ASP	CB-CG-OD2	6.09	123.78	118.30
1	F	162	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	60	ASP	CB-CG-OD2	6.05	123.75	118.30
1	D	162	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	170	ASP	CB-CG-OD2	5.99	123.69	118.30
1	G	120	ASP	CB-CG-OD2	5.96	123.67	118.30
1	F	184	ASP	CB-CG-OD1	5.94	123.65	118.30
1	E	40	ASP	CB-CG-OD2	5.83	123.55	118.30
1	E	165	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	165	ASP	CB-CG-OD2	5.78	123.50	118.30
1	G	87	ASP	CB-CG-OD2	5.77	123.49	118.30
1	C	162	ASP	CB-CG-OD2	5.74	123.46	118.30
1	H	69	ASP	CB-CG-OD2	5.74	123.46	118.30
1	H	87	ASP	CB-CG-OD2	5.73	123.45	118.30
1	A	165	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	69	ASP	CB-CG-OD2	5.69	123.42	118.30
1	F	120	ASP	CB-CG-OD2	5.64	123.37	118.30
1	D	150	ASP	CB-CG-OD2	5.63	123.36	118.30
1	B	146	ASP	CB-CG-OD2	5.62	123.36	118.30
1	E	146	ASP	CB-CG-OD2	5.61	123.35	118.30
1	C	150	ASP	CB-CG-OD2	5.61	123.35	118.30
1	G	106	ASP	CB-CG-OD2	5.61	123.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	50	ASP	CB-CG-OD2	5.57	123.32	118.30
1	G	170	ASP	CB-CG-OD2	5.56	123.31	118.30
1	B	162	ASP	CB-CG-OD2	5.55	123.29	118.30
1	F	40	ASP	CB-CG-OD2	5.49	123.24	118.30
1	H	165	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	151	ASP	CB-CG-OD2	5.39	123.15	118.30
1	D	156	ASP	CB-CG-OD2	5.38	123.14	118.30
1	H	120	ASP	CB-CG-OD2	5.35	123.11	118.30
1	H	40	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	154	ASP	CB-CG-OD2	5.33	123.10	118.30
1	H	151	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	40	ASP	CB-CG-OD2	5.32	123.09	118.30
1	F	170	ASP	CB-CG-OD2	5.31	123.08	118.30
1	F	165	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	156	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	89	ASP	CB-CG-OD2	5.24	123.01	118.30
1	G	50	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	106	ASP	CB-CG-OD2	5.17	122.95	118.30
1	E	150	ASP	CB-CG-OD2	5.09	122.88	118.30
1	D	146	ASP	CB-CG-OD2	5.06	122.86	118.30
1	F	156	ASP	CB-CG-OD2	5.04	122.84	118.30
1	D	89	ASP	CB-CG-OD2	5.03	122.83	118.30
1	D	184	ASP	CB-CG-OD2	5.01	122.81	118.30

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	1182	0	1257	37	0
1	B	1182	0	1257	33	0
1	C	1182	0	1257	20	0
1	D	1182	0	1257	31	0
1	E	1182	0	1257	23	0
1	F	1182	0	1257	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1182	0	1257	25	0
1	H	1182	0	1257	28	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	20	0	0	3	0
3	B	16	0	0	4	0
3	C	11	0	0	0	0
3	D	13	0	0	2	0
3	E	16	0	0	2	0
3	F	24	0	0	2	0
3	G	18	0	0	2	0
3	H	18	0	0	4	0
All	All	9606	0	10056	184	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 9.

All (184) 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:165:ASP:HB3	1:A:169:LYS:NZ	1.58	1.18
1:H:112:LEU:HA	3:H:224:HOH:O	1.67	0.94
1:A:165:ASP:HB3	1:A:169:LYS:HZ1	1.29	0.93
1:E:59:LYS:HE3	3:F:238:HOH:O	1.67	0.92
3:E:227:HOH:O	1:F:59:LYS:HG3	1.68	0.91
1:A:143:LYS:HD2	1:A:171:LYS:HG2	1.52	0.89
1:G:42:ALA:O	1:G:45:THR:HG22	1.74	0.86
1:C:56:LYS:HE3	1:D:59:LYS:NZ	1.90	0.86
1:A:165:ASP:HB3	1:A:169:LYS:HZ3	1.39	0.86
1:H:198:ILE:O	1:H:201:LEU:HB2	1.76	0.85
1:G:165:ASP:O	1:G:169:LYS:HE3	1.76	0.85
1:H:112:LEU:HD23	3:H:224:HOH:O	1.74	0.85
1:A:59:LYS:HG3	3:B:228:HOH:O	1.77	0.83
1:B:198:ILE:O	1:B:201:LEU:HB2	1.78	0.83
1:G:198:ILE:O	1:G:201:LEU:HB2	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:ILE:O	1:E:201:LEU:HB2	1.79	0.80
1:A:46:LYS:HE2	1:A:50:ASP:OD1	1.82	0.78
1:F:38:VAL:O	1:F:39:ILE:HG13	1.84	0.78
1:F:165:ASP:OD1	1:F:168:ALA:O	2.02	0.77
1:E:42:ALA:HA	1:E:45:THR:HG22	1.67	0.76
1:A:165:ASP:CB	1:A:169:LYS:NZ	2.47	0.76
1:A:66:LYS:HD2	3:A:217:HOH:O	1.86	0.75
1:C:56:LYS:HE3	1:D:59:LYS:HZ1	1.51	0.75
1:A:149:LYS:HD2	3:A:231:HOH:O	1.88	0.74
1:D:169:LYS:NZ	1:D:169:LYS:HB3	2.04	0.72
1:A:59:LYS:HE2	3:B:228:HOH:O	1.89	0.72
1:D:198:ILE:O	1:D:201:LEU:HB2	1.89	0.72
1:A:165:ASP:O	1:A:169:LYS:HE2	1.91	0.70
1:H:185:ALA:HA	3:H:215:HOH:O	1.91	0.70
1:A:59:LYS:NZ	1:B:56:LYS:HZ2	1.90	0.70
1:A:90:LYS:HE3	1:B:150:ASP:OD1	1.92	0.70
1:G:115:LYS:HD3	1:G:118:ILE:HD11	1.74	0.70
1:D:38:VAL:O	1:D:39:ILE:HG13	1.91	0.69
1:D:199:ASN:HA	3:D:224:HOH:O	1.91	0.68
1:A:165:ASP:CB	1:A:169:LYS:HZ3	2.05	0.68
1:E:54:PHE:CE1	1:E:118:ILE:HD11	2.29	0.68
1:B:86:THR:HG22	3:B:223:HOH:O	1.94	0.67
1:A:59:LYS:NZ	1:B:56:LYS:NZ	2.42	0.66
1:G:80:GLY:HA2	1:H:144:THR:OG1	1.95	0.66
1:F:198:ILE:O	1:F:201:LEU:HB2	1.96	0.65
1:H:192:ALA:HA	3:H:221:HOH:O	1.95	0.64
1:G:66:LYS:HD2	3:G:222:HOH:O	1.95	0.64
1:A:168:ALA:HA	1:C:111:SER:HB2	1.79	0.64
1:F:110:ALA:O	1:F:113:GLU:HG2	1.97	0.64
1:A:165:ASP:O	1:A:169:LYS:CE	2.45	0.64
1:B:38:VAL:C	1:B:39:ILE:HG13	2.17	0.64
1:A:198:ILE:O	1:A:201:LEU:HB2	1.98	0.63
1:H:38:VAL:C	1:H:39:ILE:HG13	2.18	0.63
1:G:201:LEU:HD13	1:H:45:THR:OG1	1.98	0.62
1:A:56:LYS:HZ2	1:B:59:LYS:HZ3	1.48	0.62
1:H:143:LYS:HG3	1:H:171:LYS:HG2	1.80	0.62
1:F:38:VAL:C	1:F:39:ILE:HG13	2.20	0.62
1:D:165:ASP:OD1	1:D:168:ALA:O	2.18	0.61
1:D:70:GLU:OE2	1:D:73:LYS:HE3	2.01	0.60
1:A:59:LYS:HZ3	1:B:56:LYS:HZ2	1.48	0.59
1:D:59:LYS:HE3	3:D:215:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LYS:HZ3	1:B:56:LYS:NZ	2.01	0.58
1:D:66:LYS:HE3	1:D:69:ASP:OD2	2.03	0.58
1:E:201:LEU:HD21	1:F:201:LEU:HD11	1.86	0.57
1:F:115:LYS:HD3	1:F:118:ILE:HD11	1.86	0.57
1:C:110:ALA:HB2	1:C:130:LYS:HE3	1.87	0.56
1:F:61:VAL:HG11	1:F:109:LEU:HD21	1.87	0.56
1:G:93:LYS:HE3	1:H:89:ASP:O	2.05	0.56
1:E:42:ALA:HA	1:E:45:THR:CG2	2.35	0.56
1:H:89:ASP:HB3	1:H:151:ASP:OD2	2.06	0.56
1:H:71:LEU:HB3	1:H:94:LEU:HD11	1.89	0.55
1:H:109:LEU:HD11	1:H:129:VAL:HG12	1.89	0.55
1:A:56:LYS:NZ	1:B:59:LYS:NZ	2.55	0.55
1:E:145:ALA:O	1:E:149:LYS:HG2	2.06	0.55
1:A:56:LYS:NZ	1:B:59:LYS:HZ3	2.05	0.55
1:B:89:ASP:HB3	1:B:151:ASP:OD2	2.07	0.54
1:E:121:ASP:OD2	1:E:125:LYS:NZ	2.41	0.54
1:G:165:ASP:HB3	1:G:169:LYS:NZ	2.22	0.54
1:B:169:LYS:HB3	1:B:173:ALA:HB3	1.90	0.54
1:F:66:LYS:HG3	3:F:237:HOH:O	2.08	0.54
1:A:198:ILE:HG22	1:B:45:THR:HG23	1.89	0.53
1:F:123:LYS:HA	1:F:126:ILE:HD12	1.91	0.53
1:E:173:ALA:O	1:E:177:ILE:HG13	2.08	0.53
1:D:169:LYS:HB3	1:D:169:LYS:HZ1	1.74	0.53
1:G:95:ILE:HD11	1:G:157:ALA:HA	1.91	0.53
1:E:93:LYS:HD3	1:F:89:ASP:O	2.09	0.52
1:D:121:ASP:OD2	1:D:125:LYS:NZ	2.41	0.52
1:B:165:ASP:OD1	1:B:168:ALA:O	2.29	0.51
1:D:62:HIS:HA	1:D:183:ILE:HG12	1.92	0.51
1:C:56:LYS:HE3	1:D:59:LYS:HZ3	1.75	0.51
1:D:38:VAL:C	1:D:39:ILE:HG13	2.31	0.51
1:B:46:LYS:HD2	1:B:50:ASP:OD1	2.10	0.50
1:C:70:GLU:OE2	1:C:70:GLU:HA	2.11	0.50
1:E:187:LEU:O	1:E:191:GLU:HG3	2.12	0.50
1:A:80:GLY:HA2	1:B:144:THR:OG1	2.11	0.50
1:H:169:LYS:HB2	1:H:174:GLU:HG2	1.92	0.50
1:D:80:GLY:HA3	1:D:85:GLU:OE2	2.11	0.50
1:C:198:ILE:O	1:C:201:LEU:HB2	2.12	0.49
1:B:115:LYS:HB3	1:B:118:ILE:HD11	1.94	0.49
1:B:48:ILE:O	1:B:52:VAL:HG23	2.12	0.49
1:C:198:ILE:HG22	1:D:45:THR:HG23	1.93	0.49
1:H:110:ALA:HB2	1:H:130:LYS:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:VAL:HG13	1:B:105:VAL:HG13	1.95	0.49
1:C:56:LYS:CE	1:D:59:LYS:NZ	2.69	0.49
1:D:113:GLU:OE1	1:D:130:LYS:HG2	2.13	0.49
1:E:68:ILE:HG13	1:E:102:ILE:HD11	1.95	0.49
1:E:143:LYS:HG3	1:E:171:LYS:HG2	1.94	0.48
1:H:179:LEU:O	1:H:183:ILE:HG22	2.12	0.48
1:A:90:LYS:CE	1:B:150:ASP:OD1	2.59	0.48
1:A:59:LYS:HZ1	1:B:56:LYS:NZ	2.08	0.48
1:D:71:LEU:HB3	1:D:94:LEU:HD11	1.96	0.48
1:F:62:HIS:HD2	1:F:183:ILE:HG23	1.78	0.47
1:H:61:VAL:HG13	1:H:105:VAL:HG13	1.94	0.47
1:A:89:ASP:O	1:B:93:LYS:HD3	2.14	0.47
1:G:122:LEU:HD21	1:G:189:SER:HB3	1.97	0.47
1:D:169:LYS:NZ	1:D:169:LYS:CB	2.76	0.47
1:C:41:LEU:HD11	1:D:201:LEU:HD22	1.97	0.47
1:C:118:ILE:HD12	1:C:118:ILE:HA	1.54	0.46
1:E:63:THR:OG1	1:F:60:ASP:OD2	2.32	0.46
1:H:155:ALA:O	1:H:159:THR:HG23	2.15	0.46
3:E:230:HOH:O	1:F:66:LYS:HE3	2.15	0.46
1:F:93:LYS:O	1:F:96:SER:HB2	2.15	0.46
1:F:61:VAL:HG13	1:F:105:VAL:HG13	1.97	0.46
1:B:38:VAL:O	1:B:39:ILE:HG13	2.16	0.46
1:B:46:LYS:HB3	1:B:46:LYS:HE3	1.50	0.45
1:D:39:ILE:HG22	1:D:40:ASP:H	1.80	0.45
1:E:146:ASP:N	1:E:146:ASP:OD1	2.50	0.45
1:A:165:ASP:CB	1:A:169:LYS:HZ1	2.15	0.45
1:A:169:LYS:HB3	1:A:173:ALA:HB3	1.99	0.45
1:C:175:GLU:OE1	1:C:175:GLU:N	2.50	0.44
1:E:169:LYS:HB3	1:E:173:ALA:HB3	1.99	0.44
1:G:54:PHE:HE1	1:G:112:LEU:HD22	1.82	0.44
1:G:121:ASP:OD2	1:G:125:LYS:NZ	2.43	0.44
1:C:165:ASP:OD1	1:C:168:ALA:O	2.35	0.44
1:B:40:ASP:O	1:B:44:ILE:HD12	2.17	0.44
1:G:59:LYS:HG3	3:G:218:HOH:O	2.17	0.44
1:B:86:THR:CG2	3:B:223:HOH:O	2.62	0.44
1:C:64:LEU:HD23	1:C:64:LEU:HA	1.69	0.44
1:G:198:ILE:HG22	1:H:45:THR:HG23	1.99	0.44
1:C:125:LYS:HB3	1:C:186:LEU:HD13	2.00	0.44
1:G:143:LYS:HD2	1:G:171:LYS:HG2	1.99	0.44
1:B:56:LYS:HE3	1:B:56:LYS:HB3	1.40	0.43
1:C:112:LEU:HD23	1:C:112:LEU:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:LYS:HD2	1:H:77:LYS:O	2.18	0.43
1:A:66:LYS:HE2	3:A:234:HOH:O	2.18	0.43
1:B:111:SER:O	1:B:114:LYS:HB2	2.19	0.43
1:C:155:ALA:O	1:C:159:THR:HG23	2.19	0.43
1:D:40:ASP:OD1	1:D:40:ASP:C	2.57	0.43
1:H:125:LYS:HE2	1:H:189:SER:OG	2.18	0.43
1:E:115:LYS:HB3	1:E:118:ILE:HD12	2.01	0.43
1:G:59:LYS:HE2	1:H:56:LYS:HE3	2.00	0.43
1:F:54:PHE:O	1:F:58:VAL:HG23	2.19	0.42
1:D:60:ASP:OD1	1:D:108:LYS:HD3	2.19	0.42
1:A:48:ILE:O	1:A:52:VAL:HG23	2.19	0.42
1:G:139:LYS:NZ	1:G:175:GLU:OE2	2.52	0.42
1:A:54:PHE:HE1	1:A:112:LEU:HD22	1.85	0.42
1:D:149:LYS:HG3	1:D:152:VAL:HG22	2.02	0.42
1:E:122:LEU:O	1:E:126:ILE:HG13	2.20	0.42
1:F:40:ASP:O	1:F:44:ILE:HD12	2.19	0.42
1:H:183:ILE:O	1:H:183:ILE:HG13	2.18	0.42
1:C:63:THR:HB	1:D:63:THR:HG21	2.01	0.42
1:E:64:LEU:HD23	1:E:64:LEU:HA	1.81	0.42
1:B:59:LYS:HA	1:B:59:LYS:HD2	1.77	0.42
1:F:111:SER:O	1:F:114:LYS:HB2	2.18	0.42
1:H:91:ASN:O	1:H:95:ILE:HG12	2.20	0.42
1:E:42:ALA:CA	1:E:45:THR:HG22	2.44	0.41
1:H:144:THR:HG23	1:H:145:ALA:N	2.35	0.41
1:B:109:LEU:CD1	1:B:129:VAL:HG12	2.51	0.41
1:E:54:PHE:CE2	1:E:122:LEU:HD13	2.54	0.41
1:E:100:SER:O	1:E:103:SER:HB2	2.20	0.41
1:A:173:ALA:O	1:A:177:ILE:HG13	2.20	0.41
1:G:198:ILE:O	1:G:201:LEU:CB	2.61	0.41
1:H:102:ILE:HD12	1:H:102:ILE:HA	1.93	0.41
1:G:174:GLU:HA	1:G:177:ILE:HD12	2.03	0.41
1:D:61:VAL:HG13	1:D:105:VAL:HG13	2.03	0.41
1:D:127:THR:HG22	1:D:131:ASN:ND2	2.36	0.41
1:E:93:LYS:NZ	1:F:87:ASP:O	2.33	0.41
1:G:82:ASN:C	1:H:141:LYS:HD3	2.41	0.41
1:A:200:ALA:O	1:A:201:LEU:C	2.60	0.41
1:A:59:LYS:HZ1	1:B:56:LYS:HZ1	1.68	0.40
1:B:144:THR:HG23	1:B:145:ALA:N	2.36	0.40
1:C:56:LYS:CE	1:D:59:LYS:HZ3	2.31	0.40
1:D:38:VAL:O	1:D:38:VAL:HG23	2.22	0.40
1:F:103:SER:O	1:F:106:ASP:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:ASP:HB3	1:G:151:ASP:OD2	2.21	0.40
1:A:155:ALA:O	1:A:159:THR:HG23	2.21	0.40
1:G:62:HIS:HD2	1:G:183:ILE:HG23	1.87	0.40
1:C:95:ILE:HD11	1:C:157:ALA:HA	2.03	0.40
1:G:198:ILE:HG12	1:H:48:ILE:HD11	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	162/181 (90%)	154 (95%)	6 (4%)	2 (1%)	13	32
1	B	162/181 (90%)	152 (94%)	9 (6%)	1 (1%)	25	50
1	C	162/181 (90%)	155 (96%)	7 (4%)	0	100	100
1	D	162/181 (90%)	155 (96%)	6 (4%)	1 (1%)	25	50
1	E	162/181 (90%)	155 (96%)	6 (4%)	1 (1%)	25	50
1	F	162/181 (90%)	154 (95%)	7 (4%)	1 (1%)	25	50
1	G	162/181 (90%)	155 (96%)	6 (4%)	1 (1%)	25	50
1	H	162/181 (90%)	155 (96%)	6 (4%)	1 (1%)	25	50
All	All	1296/1448 (90%)	1235 (95%)	53 (4%)	8 (1%)	25	50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	ILE
1	D	39	ILE
1	E	41	LEU
1	F	39	ILE
1	H	39	ILE

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Mol	Chain	Res	Type
1	A	41	LEU
1	A	89	ASP
1	G	41	LEU

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	126/140 (90%)	108 (86%)	18 (14%)	3 8
1	B	126/140 (90%)	111 (88%)	15 (12%)	5 12
1	C	126/140 (90%)	107 (85%)	19 (15%)	3 7
1	D	126/140 (90%)	109 (86%)	17 (14%)	4 9
1	E	126/140 (90%)	110 (87%)	16 (13%)	4 10
1	F	126/140 (90%)	113 (90%)	13 (10%)	7 16
1	G	126/140 (90%)	107 (85%)	19 (15%)	3 7
1	H	126/140 (90%)	103 (82%)	23 (18%)	1 4
All	All	1008/1120 (90%)	868 (86%)	140 (14%)	3 8

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ILE
1	A	45	THR
1	A	49	THR
1	A	66	LYS
1	A	90	LYS
1	A	93	LYS
1	A	108	LYS
1	A	111	SER
1	A	114	LYS
1	A	116	VAL
1	A	123	LYS
1	A	130	LYS

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Mol	Chain	Res	Type
1	A	135	SER
1	A	139	LYS
1	A	142	SER
1	A	149	LYS
1	A	178	LYS
1	A	195	THR
1	B	39	ILE
1	B	43	THR
1	B	46	LYS
1	B	56	LYS
1	B	59	LYS
1	B	78	LYS
1	B	85	GLU
1	B	86	THR
1	B	93	LYS
1	B	103	SER
1	B	111	SER
1	B	112	LEU
1	B	115	LYS
1	B	199	ASN
1	B	201	LEU
1	C	39	ILE
1	C	41	LEU
1	C	44	ILE
1	C	45	THR
1	C	46	LYS
1	C	48	ILE
1	C	66	LYS
1	C	77	LYS
1	C	79	ILE
1	C	90	LYS
1	C	116	VAL
1	C	118	ILE
1	C	125	LYS
1	C	130	LYS
1	C	135	SER
1	C	142	SER
1	C	153	LYS
1	C	169	LYS
1	C	177	ILE
1	D	39	ILE
1	D	41	LEU

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Mol	Chain	Res	Type
1	D	56	LYS
1	D	59	LYS
1	D	60	ASP
1	D	66	LYS
1	D	78	LYS
1	D	93	LYS
1	D	112	LEU
1	D	115	LYS
1	D	116	VAL
1	D	123	LYS
1	D	142	SER
1	D	146	ASP
1	D	169	LYS
1	D	174	GLU
1	D	201	LEU
1	E	39	ILE
1	E	44	ILE
1	E	59	LYS
1	E	66	LYS
1	E	78	LYS
1	E	90	LYS
1	E	93	LYS
1	E	112	LEU
1	E	114	LYS
1	E	125	LYS
1	E	146	ASP
1	E	149	LYS
1	E	153	LYS
1	E	166	THR
1	E	169	LYS
1	E	201	LEU
1	F	38	VAL
1	F	39	ILE
1	F	41	LEU
1	F	46	LYS
1	F	59	LYS
1	F	78	LYS
1	F	85	GLU
1	F	90	LYS
1	F	133	SER
1	F	135	SER
1	F	150	ASP

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Mol	Chain	Res	Type
1	F	153	LYS
1	F	174	GLU
1	G	41	LEU
1	G	46	LYS
1	G	66	LYS
1	G	78	LYS
1	G	90	LYS
1	G	93	LYS
1	G	103	SER
1	G	111	SER
1	G	116	VAL
1	G	123	LYS
1	G	130	LYS
1	G	134	THR
1	G	135	SER
1	G	142	SER
1	G	169	LYS
1	G	170	ASP
1	G	189	SER
1	G	191	GLU
1	G	195	THR
1	H	39	ILE
1	H	41	LEU
1	H	43	THR
1	H	44	ILE
1	H	46	LYS
1	H	48	ILE
1	H	56	LYS
1	H	59	LYS
1	H	66	LYS
1	H	78	LYS
1	H	90	LYS
1	H	93	LYS
1	H	95	ILE
1	H	102	ILE
1	H	115	LYS
1	H	116	VAL
1	H	123	LYS
1	H	153	LYS
1	H	165	ASP
1	H	169	LYS
1	H	171	LYS

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Mol	Chain	Res	Type
1	H	174	GLU
1	H	201	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	47	ASN
1	D	131	ASN
1	E	47	ASN
1	G	47	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 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.

No monomer is involved in short contacts.

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	164/181 (90%)	-0.06	7 (4%) 35 33	15, 19, 21, 22	0
1	B	164/181 (90%)	0.09	11 (6%) 17 16	17, 19, 21, 22	0
1	C	164/181 (90%)	0.09	8 (4%) 29 28	17, 19, 21, 22	0
1	D	164/181 (90%)	0.05	7 (4%) 35 33	16, 19, 21, 23	0
1	E	164/181 (90%)	0.17	9 (5%) 25 24	17, 19, 21, 23	0
1	F	164/181 (90%)	0.08	8 (4%) 29 28	16, 19, 21, 22	0
1	G	164/181 (90%)	0.01	7 (4%) 35 33	16, 19, 21, 22	0
1	H	164/181 (90%)	0.65	19 (11%) 4 3	16, 19, 21, 22	0
All	All	1312/1448 (90%)	0.13	76 (5%) 23 22	15, 19, 21, 23	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	201	LEU	8.6
1	B	39	ILE	7.9
1	C	201	LEU	7.2
1	E	41	LEU	5.7
1	F	43	THR	5.6
1	F	201	LEU	5.5
1	A	201	LEU	5.3
1	A	38	VAL	4.9
1	E	201	LEU	4.9
1	H	42	ALA	4.8
1	H	116	VAL	4.8
1	H	117	GLY	4.7
1	B	41	LEU	4.5
1	H	39	ILE	4.5
1	C	38	VAL	4.5
1	G	165	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	H	200	ALA	4.4
1	B	116	VAL	4.1
1	H	41	LEU	4.0
1	C	39	ILE	3.8
1	B	201	LEU	3.7
1	A	165	ASP	3.7
1	E	44	ILE	3.7
1	D	39	ILE	3.6
1	H	118	ILE	3.5
1	G	44	ILE	3.4
1	A	39	ILE	3.4
1	F	200	ALA	3.3
1	D	38	VAL	3.3
1	A	199	ASN	3.3
1	C	168	ALA	3.3
1	E	38	VAL	3.2
1	D	43	THR	3.2
1	F	42	ALA	3.1
1	H	45	THR	3.1
1	F	46	LYS	3.0
1	F	168	ALA	2.9
1	G	41	LEU	2.9
1	F	120	ASP	2.9
1	C	41	LEU	2.9
1	H	38	VAL	2.8
1	G	38	VAL	2.8
1	H	189	SER	2.8
1	B	118	ILE	2.7
1	H	48	ILE	2.6
1	A	41	LEU	2.6
1	H	197	ALA	2.6
1	E	165	ASP	2.6
1	D	201	LEU	2.5
1	G	199	ASN	2.5
1	E	168	ALA	2.5
1	D	199	ASN	2.4
1	C	151	ASP	2.4
1	B	38	VAL	2.4
1	B	42	ALA	2.4
1	G	201	LEU	2.4
1	E	199	ASN	2.3
1	H	46	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	40	ASP	2.3
1	H	43	THR	2.3
1	B	48	ILE	2.3
1	H	80	GLY	2.3
1	G	43	THR	2.3
1	D	44	ILE	2.3
1	F	39	ILE	2.3
1	B	200	ALA	2.2
1	C	200	ALA	2.2
1	E	39	ILE	2.2
1	A	44	ILE	2.1
1	H	156	ASP	2.1
1	B	115	LYS	2.1
1	C	40	ASP	2.1
1	H	194	VAL	2.1
1	B	47	ASN	2.1
1	D	41	LEU	2.0
1	E	153	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NI	H	13	1/1	0.71	0.07	80,80,80,80	0
2	NI	H	10	1/1	0.81	0.09	49,49,49,49	0
2	NI	E	5	1/1	0.84	0.09	48,48,48,48	0
2	NI	B	4	1/1	0.86	0.06	65,65,65,65	0
2	NI	D	1	1/1	0.88	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NI	A	14	1/1	0.89	0.06	61,61,61,61	0
2	NI	E	12	1/1	0.89	0.12	74,74,74,74	0
2	NI	C	3	1/1	0.91	0.11	43,43,43,43	0
2	NI	D	8	1/1	0.94	0.07	67,67,67,67	0
2	NI	G	11	1/1	0.94	0.06	67,67,67,67	0
2	NI	A	7	1/1	0.95	0.14	41,41,41,41	0
2	NI	F	6	1/1	0.98	0.18	43,43,43,43	0
2	NI	G	9	1/1	0.99	0.16	47,47,47,47	0
2	NI	B	2	1/1	0.99	0.14	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.