



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:21 PM EDT

PDB ID : 4P2C / pdb_00004p2c
Title : Complex of Shiga toxin 2e with a neutralizing single-domain antibody
Authors : Lo, A.W.H.; Moonens, K.; De Kerpel, M.; Brys, L.; Pardon, E.; Remaut, H.;
De Greve, H.
Deposited on : 2014-03-03
Resolution : 2.82 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:

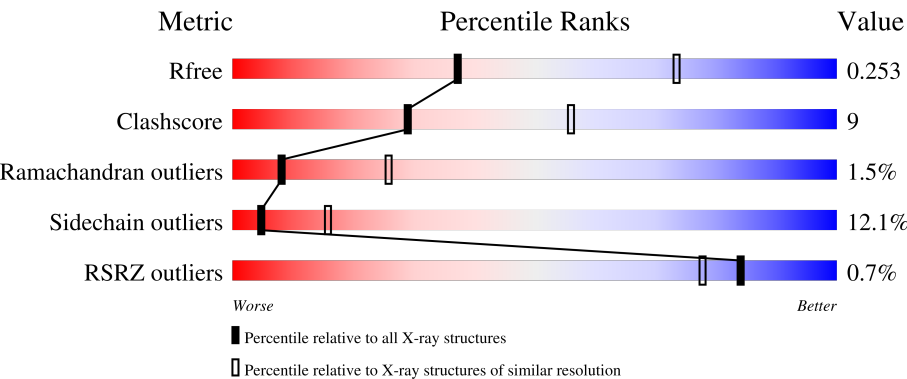
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.82 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	297	2% 60% 27% 7% 6%
2	B	68	74% 25% .
2	C	68	76% 22% .
2	D	68	85% 13% .
2	E	68	78% 21% .

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Mol	Chain	Length	Quality of chain
2	F	68	78% 18%
3	G	128	69% 22% • • 5%
3	H	128	69% 22% • • 6%
3	I	128	% 66% 22% 6% 6%
3	J	128	72% 20% 6% • •
3	K	128	71% 19% • • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9541 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 Shiga toxin 2e, subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2186	1366	390	423	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	SER	TYR	engineered mutation	UNP Q7WUF4
A	167	GLN	GLU	engineered mutation	UNP Q7WUF4
A	274	THR	LYS	variant	UNP Q7WUF4
A	291	SER	PRO	variant	UNP Q7WUF4

- Molecule 2 is a protein called Shiga toxin 2e, subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	68	Total	C	N	O	S	0	0	0
			532	334	91	104	3			
2	C	68	Total	C	N	O	S	0	0	0
			532	334	91	104	3			
2	D	68	Total	C	N	O	S	0	0	0
			532	334	91	104	3			
2	E	68	Total	C	N	O	S	0	0	0
			532	334	91	104	3			
2	F	68	Total	C	N	O	S	0	0	0
			532	334	91	104	3			

- Molecule 3 is a protein called Nanobody 1, Anti-F4+ETEC bacteria VHH variable region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	121	Total	C	N	O	S	0	0	0
			933	579	166	184	4			
3	H	120	Total	C	N	O	S	0	0	0
			924	574	164	182	4			

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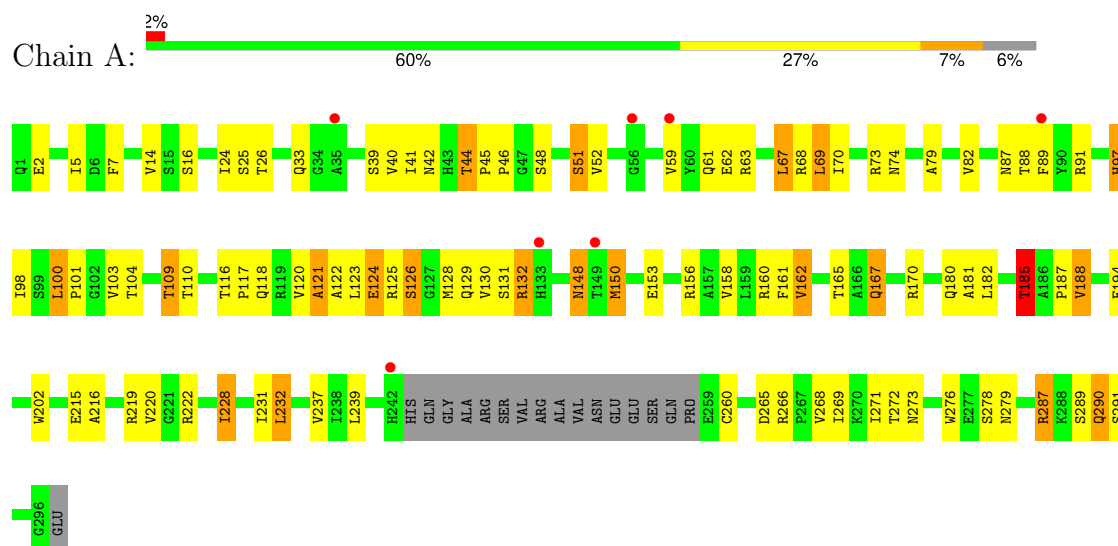
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	120	Total	C	N	O	S	0	0	0
			924	574	164	182	4			
3	J	127	Total	C	N	O	S	0	0	0
			990	613	183	190	4			
3	K	120	Total	C	N	O	S	0	0	0
			924	574	164	182	4			

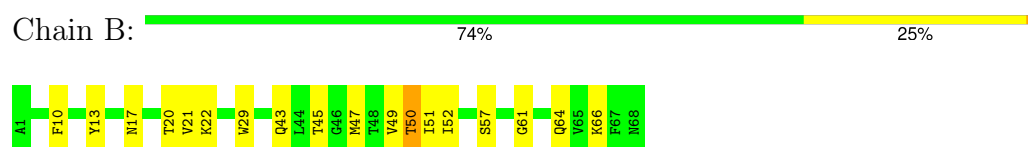
3 Residue-property plots [i](#)

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.

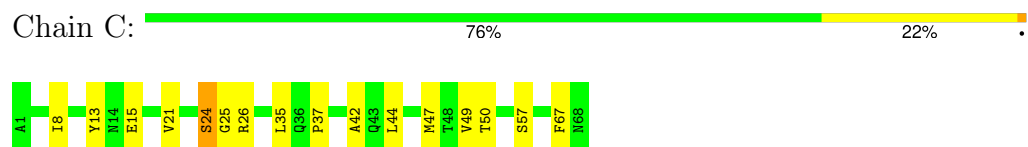
- Molecule 1: Shiga toxin 2e, subunit A



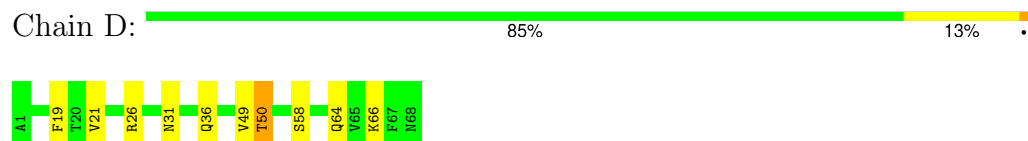
- Molecule 2: Shiga toxin 2e, subunit B



- Molecule 2: Shiga toxin 2e, subunit B



- Molecule 2: Shiga toxin 2e, subunit B



- Molecule 2: Shiga toxin 2e, subunit B

Chain E:  78% 21% .



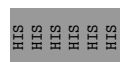
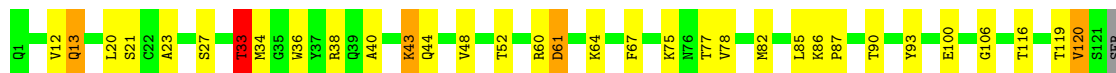
- Molecule 2: Shiga toxin 2e, subunit B

Chain F:  78% 18% .



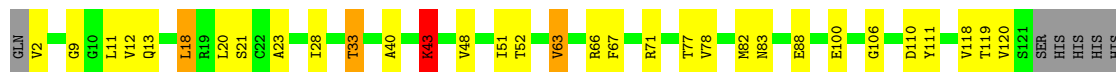
- Molecule 3: Nanobody 1, Anti-F4+ETEC bacteria VHH variable region

Chain G:  69% 22% . . 5%



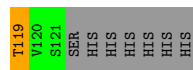
- Molecule 3: Nanobody 1, Anti-F4+ETEC bacteria VHH variable region

Chain H:  69% 22% . . 6%



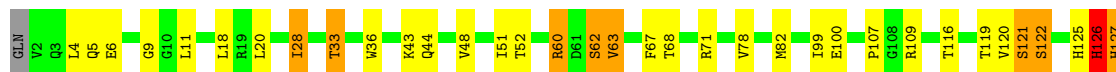
- Molecule 3: Nanobody 1, Anti-F4+ETEC bacteria VHH variable region

Chain I:  % 66% 22% 6% 6%



- Molecule 3: Nanobody 1, Anti-F4+ETEC bacteria VHH variable region

Chain J:  72% 20% 6% ..



H128

- Molecule 3: Nanobody 1, Anti-F4+ETEC bacteria VHH variable region

Chain K:

71%

19%

• • 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	191.84Å 88.19Å 100.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.71 – 2.82 43.71 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.71-2.82) 96.8 (43.71-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1117)	Depositor
R, R_{free}	0.186 , 0.253 0.189 , 0.253	Depositor DCC
R_{free} test set	2120 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 23.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9541	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	0/2225	0.97	7/3025 (0.2%)
2	B	0.68	0/542	0.88	0/732
2	C	0.67	0/542	0.92	0/732
2	D	0.70	0/542	0.95	0/732
2	E	0.62	0/542	0.86	0/732
2	F	0.63	0/542	0.91	0/732
3	G	0.57	1/951 (0.1%)	0.94	1/1286 (0.1%)
3	H	0.54	0/942	0.96	5/1274 (0.4%)
3	I	0.58	0/942	1.00	6/1274 (0.5%)
3	J	0.62	0/1014	0.98	4/1372 (0.3%)
3	K	0.61	0/942	0.97	2/1274 (0.2%)
All	All	0.61	1/9726 (0.0%)	0.95	25/13165 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	33	THR	CA-CB	5.60	1.60	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	121	SER	N-CA-C	9.59	126.47	112.94
3	K	105	TYR	N-CA-C	-8.03	96.08	108.76
3	K	78	VAL	CB-CA-C	-6.99	101.12	110.98
3	H	106	GLY	CA-C-N	6.79	126.75	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	106	GLY	C-N-CA	6.79	126.75	119.28
1	A	61	GLN	N-CA-C	6.73	114.30	108.78
3	I	48	VAL	CB-CA-C	-6.47	106.21	111.71
3	H	43	LYS	N-CA-C	6.23	117.92	110.19
1	A	44	THR	CA-C-N	-5.77	114.44	120.38
1	A	44	THR	C-N-CA	-5.77	114.44	120.38
3	H	28	ILE	N-CA-C	5.61	118.59	113.20
3	I	106	GLY	CA-C-N	5.60	126.84	119.84
3	I	106	GLY	C-N-CA	5.60	126.84	119.84
1	A	61	GLN	CA-C-O	5.58	121.17	117.94
3	J	126	HIS	CA-C-N	5.56	131.72	121.70
3	J	126	HIS	C-N-CA	5.56	131.72	121.70
1	A	231	ILE	N-CA-C	-5.55	104.91	110.30
3	I	40	ALA	CA-C-N	-5.52	114.24	119.76
3	I	40	ALA	C-N-CA	-5.52	114.24	119.76
3	I	105	TYR	N-CA-C	-5.39	101.34	109.85
3	G	120	VAL	N-CA-C	5.36	115.84	108.12
3	H	48	VAL	CB-CA-C	-5.25	107.24	111.71
3	J	107	PRO	N-CA-C	-5.25	107.19	114.27
1	A	97	HIS	N-CA-C	5.12	116.86	111.28
1	A	25	SER	N-CA-C	5.01	116.80	109.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	120	VAL	Peptide
3	J	126	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2186	0	2162	51	0
2	B	532	0	517	9	0
2	C	532	0	517	11	0
2	D	532	0	517	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	532	0	517	8	0
2	F	532	0	517	11	0
3	G	933	0	895	17	0
3	H	924	0	884	14	0
3	I	924	0	884	17	0
3	J	990	0	931	19	0
3	K	924	0	884	13	0
All	All	9541	0	9225	163	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 (163) 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:181:ALA:HA	1:A:187:PRO:HD2	1.52	0.89
2:B:50:THR:HG23	2:B:66:LYS:HB3	1.58	0.82
2:E:50:THR:HG23	2:E:66:LYS:HB3	1.66	0.78
2:F:50:THR:HG23	2:F:66:LYS:HB3	1.64	0.77
3:K:51:ILE:HD13	3:K:71:ARG:HG3	1.69	0.74
3:I:46:GLU:OE2	3:I:60:ARG:NH2	2.21	0.73
3:I:51:ILE:HD13	3:I:71:ARG:HG3	1.71	0.72
3:H:33:THR:HB	3:H:52:THR:HA	1.70	0.72
2:C:24:SER:OG	2:C:25:GLY:N	2.06	0.72
2:D:50:THR:HG23	2:D:66:LYS:HB3	1.71	0.71
3:J:63:VAL:HG13	3:J:67:PHE:HB2	1.73	0.70
3:H:82:MET:HE1	3:H:118:VAL:HG21	1.74	0.69
3:I:90:THR:HG23	3:I:119:THR:HA	1.75	0.69
3:G:33:THR:HB	3:G:52:THR:HA	1.75	0.68
2:E:24:SER:OG	2:E:25:GLY:N	2.25	0.68
3:H:51:ILE:HD13	3:H:71:ARG:HG3	1.77	0.67
3:I:33:THR:HB	3:I:52:THR:HA	1.76	0.67
1:A:123:LEU:HD22	1:A:128:MET:HG3	1.76	0.66
2:D:26:ARG:HH11	2:D:26:ARG:HG3	1.61	0.66
3:I:31:LEU:HG	3:I:103:THR:HG21	1.76	0.66
3:J:9:GLY:HA2	3:J:18:LEU:HD13	1.76	0.65
1:A:24:ILE:O	1:A:42:ASN:ND2	2.29	0.65
3:K:23:ALA:HA	3:K:77:THR:HG22	1.76	0.65
3:J:126:HIS:HA	3:J:127:HIS:HB3	1.78	0.65
3:H:63:VAL:HG13	3:H:67:PHE:HB2	1.78	0.64
1:A:82:VAL:HG12	1:A:89:PHE:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:61:ASP:N	3:I:61:ASP:OD1	2.22	0.63
3:G:23:ALA:HA	3:G:77:THR:HG22	1.81	0.63
3:H:23:ALA:HA	3:H:77:THR:HG22	1.81	0.63
1:A:109:THR:HG23	1:A:110:THR:HG23	1.81	0.62
3:G:87:PRO:HA	3:G:120:VAL:HG23	1.80	0.62
1:A:185:THR:O	1:A:187:PRO:HD3	1.99	0.62
3:I:33:THR:HG22	3:I:100:GLU:HG2	1.81	0.61
2:D:31:ASN:O	3:I:103:THR:HG23	2.01	0.60
1:A:44:THR:HG21	1:A:73:ARG:HB3	1.84	0.60
3:G:85:LEU:HB3	3:G:120:VAL:HG11	1.85	0.59
3:J:11:LEU:HD13	3:J:119:THR:HB	1.84	0.59
3:G:61:ASP:HA	3:G:64:LYS:HD2	1.85	0.57
3:K:33:THR:HG23	3:K:100:GLU:HG2	1.87	0.57
3:I:106:GLY:O	3:I:108:GLY:N	2.38	0.57
3:G:20:LEU:HG	3:G:82:MET:HE2	1.87	0.56
1:A:269:ILE:HG13	1:A:278:SER:HB3	1.87	0.56
3:J:51:ILE:HD13	3:J:71:ARG:HG3	1.86	0.56
3:H:9:GLY:HA2	3:H:18:LEU:HD13	1.87	0.56
3:K:33:THR:HG22	3:K:52:THR:HA	1.87	0.55
1:A:87:ASN:HD21	1:A:103:VAL:HA	1.71	0.55
2:E:45:THR:HG21	2:F:44:LEU:HD11	1.89	0.55
1:A:7:PHE:O	1:A:132:ARG:NH2	2.40	0.55
3:K:99:ILE:HG13	3:K:109:ARG:HA	1.87	0.55
1:A:109:THR:HG22	1:A:148:ASN:O	2.06	0.54
2:C:47:MET:HE2	2:C:67:PHE:HB3	1.88	0.54
2:D:64:GLN:HB2	2:E:15:GLU:HG3	1.89	0.54
1:A:118:GLN:HG2	1:A:124:GLU:HA	1.88	0.54
3:J:20:LEU:HG	3:J:82:MET:HE2	1.90	0.54
3:I:20:LEU:HG	3:I:82:MET:HE2	1.89	0.54
1:A:202:TRP:CZ3	1:A:239:LEU:HD13	2.43	0.53
3:J:28:ILE:HG12	3:J:99:ILE:HD11	1.91	0.53
2:F:52:ILE:HB	2:F:64:GLN:HG2	1.89	0.53
3:G:13:GLN:H	3:G:13:GLN:CD	2.18	0.52
3:J:126:HIS:HA	3:J:127:HIS:CB	2.39	0.52
1:A:122:ALA:HB3	1:A:156:ARG:NH2	2.24	0.52
3:J:33:THR:HG22	3:J:100:GLU:HG2	1.92	0.52
2:E:42:ALA:HA	2:E:47:MET:HE3	1.90	0.52
1:A:153:GLU:HA	1:A:156:ARG:HD2	1.90	0.52
1:A:272:THR:HG22	1:A:273:ASN:H	1.74	0.52
1:A:87:ASN:ND2	1:A:103:VAL:HA	2.25	0.51
3:J:18:LEU:HB2	3:J:82:MET:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:103:THR:O	3:K:109:ARG:NH2	2.44	0.50
1:A:121:ALA:HB1	1:A:156:ARG:HG3	1.93	0.50
2:E:52:ILE:HD12	2:E:64:GLN:HG2	1.93	0.50
3:J:122:SER:HB2	3:J:125:HIS:CD2	2.46	0.50
3:H:40:ALA:HB3	3:H:43:LYS:HE3	1.93	0.49
1:A:272:THR:HG22	1:A:273:ASN:N	2.28	0.49
3:J:33:THR:HB	3:J:52:THR:HA	1.94	0.49
1:A:68:ARG:HB2	1:A:82:VAL:HG22	1.95	0.49
3:K:60:ARG:HG3	3:K:63:VAL:HB	1.94	0.49
3:H:20:LEU:HG	3:H:82:MET:HE2	1.95	0.49
2:B:10:PHE:CE2	2:B:22:LYS:HD2	2.48	0.49
2:B:64:GLN:HB2	2:C:15:GLU:HG3	1.95	0.49
3:G:40:ALA:HB3	3:G:43:LYS:HE3	1.94	0.49
3:H:33:THR:HG22	3:H:100:GLU:OE2	2.12	0.49
3:J:33:THR:HG22	3:J:100:GLU:OE2	2.13	0.48
1:A:88:THR:HG22	1:A:104:THR:HB	1.95	0.48
1:A:130:VAL:HG22	1:A:160:ARG:HG2	1.96	0.48
1:A:219:ARG:HG2	1:A:276:TRP:CH2	2.49	0.48
1:A:287:ARG:HD3	2:C:37:PRO:HB2	1.96	0.48
3:G:34:MET:HE2	3:G:78:VAL:HG21	1.96	0.48
1:A:69:LEU:HD21	1:A:161:PHE:HB3	1.96	0.48
1:A:125:ARG:O	1:A:126:SER:HB3	2.12	0.48
3:G:38:ARG:HB3	3:G:93:TYR:CE1	2.49	0.48
2:C:26:ARG:HG3	2:C:26:ARG:HH11	1.79	0.47
3:G:75:LYS:O	3:G:77:THR:HG23	2.14	0.47
3:H:33:THR:HG22	3:H:100:GLU:HG2	1.97	0.47
1:A:269:ILE:HG22	1:A:271:ILE:HG13	1.96	0.47
3:G:33:THR:HG22	3:G:100:GLU:CG	2.45	0.47
3:I:61:ASP:HA	3:I:64:LYS:HG3	1.95	0.47
1:A:44:THR:HG21	1:A:73:ARG:HD3	1.95	0.47
3:H:12:VAL:HG23	3:H:120:VAL:HG22	1.97	0.47
3:H:66:ARG:HB3	3:H:83:ASN:O	2.15	0.47
1:A:79:ALA:HB2	1:A:98:ILE:HD11	1.97	0.46
3:H:9:GLY:HA2	3:H:18:LEU:CD1	2.45	0.46
3:J:67:PHE:CE1	3:J:82:MET:HB3	2.50	0.46
3:J:33:THR:CG2	3:J:100:GLU:HG2	2.46	0.46
3:I:14:ALA:C	3:I:16:GLY:H	2.22	0.46
1:A:131:SER:HB3	1:A:188:VAL:HG22	1.97	0.45
1:A:228:ILE:O	1:A:228:ILE:HG13	2.15	0.45
1:A:41:ILE:HG21	1:A:74:ASN:HA	1.98	0.45
2:F:10:PHE:CE2	2:F:22:LYS:HD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:GLU:HB3	1:A:68:ARG:HH22	1.82	0.45
1:A:97:HIS:CD2	1:A:98:ILE:HG23	2.52	0.45
1:A:33:GLN:HB2	1:A:232:LEU:HD23	1.99	0.44
2:B:45:THR:HG21	2:C:44:LEU:HD22	1.99	0.44
3:I:34:MET:HB3	3:I:78:VAL:HG21	1.99	0.44
3:I:63:VAL:HG13	3:I:67:PHE:HB2	1.99	0.44
2:C:8:ILE:HD11	2:C:49:VAL:HG21	1.99	0.44
3:J:126:HIS:CA	3:J:127:HIS:HB3	2.47	0.44
1:A:51:SER:O	1:A:68:ARG:NH2	2.51	0.44
3:H:2:VAL:HG11	3:H:111:TYR:CD1	2.52	0.44
1:A:5:ILE:HD12	1:A:165:THR:HG22	1.99	0.44
3:G:67:PHE:CD1	3:G:82:MET:HA	2.53	0.44
2:B:64:GLN:HA	2:C:13:TYR:O	2.18	0.43
3:K:90:THR:HG1	3:K:120:VAL:H	1.66	0.43
2:E:32:ARG:HD2	2:F:17:ASN:OD1	2.18	0.43
2:C:35:LEU:HD23	2:C:35:LEU:HA	1.85	0.43
3:K:108:GLY:O	3:K:109:ARG:HB2	2.18	0.43
3:J:121:SER:O	3:J:125:HIS:CD2	2.72	0.43
2:B:17:ASN:OD1	2:F:32:ARG:HD2	2.19	0.43
1:A:100:LEU:HA	1:A:101:PRO:HD3	1.80	0.42
2:F:10:PHE:C	2:F:10:PHE:CD1	2.97	0.42
3:G:12:VAL:HG13	3:G:120:VAL:HG12	2.01	0.42
1:A:116:THR:HB	1:A:117:PRO:HD3	2.02	0.42
2:B:13:TYR:O	2:F:64:GLN:HA	2.19	0.42
3:G:38:ARG:HB3	3:G:93:TYR:CD1	2.54	0.42
3:K:9:GLY:HA2	3:K:18:LEU:HD13	2.01	0.42
2:C:42:ALA:HB1	2:C:47:MET:HB3	2.02	0.42
2:E:64:GLN:HB2	2:F:15:GLU:HG3	2.02	0.42
1:A:287:ARG:HD3	2:C:37:PRO:CB	2.50	0.41
3:G:33:THR:HG22	3:G:100:GLU:HG2	2.01	0.41
3:J:60:ARG:HD3	3:J:62:SER:OG	2.19	0.41
1:A:116:THR:O	1:A:120:VAL:HG22	2.20	0.41
1:A:132:ARG:NH1	1:A:182:LEU:O	2.44	0.41
2:F:7:LYS:HB2	2:F:7:LYS:HE3	1.94	0.41
3:K:3:GLN:C	3:K:4:LEU:HD12	2.45	0.41
1:A:51:SER:HB3	1:A:70:ILE:CD1	2.51	0.41
1:A:44:THR:HG22	1:A:74:ASN:OD1	2.21	0.41
1:A:162:VAL:O	1:A:167:GLN:HB2	2.21	0.41
2:F:44:LEU:HD23	2:F:44:LEU:HA	1.82	0.41
1:A:5:ILE:HA	1:A:16:SER:HB3	2.03	0.41
3:I:33:THR:HG22	3:I:100:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:36:TRP:O	3:J:48:VAL:HB	2.21	0.41
3:K:9:GLY:HA2	3:K:18:LEU:CD1	2.50	0.41
1:A:129:GLN:O	1:A:160:ARG:NH1	2.54	0.41
1:A:266:ARG:CZ	1:A:269:ILE:HG12	2.51	0.41
1:A:278:SER:O	1:A:278:SER:OG	2.31	0.41
2:B:29:TRP:O	2:B:61:GLY:HA2	2.20	0.41
3:I:48:VAL:HA	3:I:60:ARG:HG2	2.03	0.41
1:A:170:ARG:HA	1:A:237:VAL:HG22	2.03	0.40
1:A:289:SER:O	1:A:290:GLN:CB	2.69	0.40
2:D:19:PHE:HB2	2:D:36:GLN:HG2	2.04	0.40
3:K:22:CYS:HB3	3:K:78:VAL:HG23	2.03	0.40
3:I:60:ARG:HG3	3:I:63:VAL:HB	2.02	0.40
2:B:52:ILE:HB	2:B:64:GLN:HG2	2.03	0.40
3:G:36:TRP:O	3:G:48:VAL:HB	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	276/297 (93%)	232 (84%)	32 (12%)	12 (4%)	2	6
2	B	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
2	C	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
2	D	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
2	E	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
2	F	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
3	G	119/128 (93%)	114 (96%)	4 (3%)	1 (1%)	16	41
3	H	118/128 (92%)	111 (94%)	7 (6%)	0	100	100
3	I	118/128 (92%)	113 (96%)	4 (3%)	1 (1%)	16	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	125/128 (98%)	116 (93%)	7 (6%)	2 (2%)	7	24
3	K	118/128 (92%)	110 (93%)	6 (5%)	2 (2%)	7	23
All	All	1204/1277 (94%)	1116 (93%)	70 (6%)	18 (2%)	8	26

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	VAL
1	A	279	ASN
1	A	290	GLN
3	I	107	PRO
3	J	122	SER
1	A	45	PRO
1	A	67	LEU
1	A	126	SER
1	A	185	THR
3	J	127	HIS
3	K	108	GLY
1	A	121	ALA
1	A	216	ALA
1	A	188	VAL
1	A	150	MET
3	G	106	GLY
3	K	9	GLY
1	A	46	PRO

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	245/260 (94%)	211 (86%)	34 (14%)	3	11
2	B	59/59 (100%)	51 (86%)	8 (14%)	3	12
2	C	59/59 (100%)	55 (93%)	4 (7%)	14	40
2	D	59/59 (100%)	55 (93%)	4 (7%)	14	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	59/59 (100%)	54 (92%)	5 (8%)	10	30
2	F	59/59 (100%)	52 (88%)	7 (12%)	5	16
3	G	98/105 (93%)	86 (88%)	12 (12%)	5	15
3	H	97/105 (92%)	86 (89%)	11 (11%)	5	18
3	I	97/105 (92%)	82 (84%)	15 (16%)	2	9
3	J	104/105 (99%)	89 (86%)	15 (14%)	3	10
3	K	97/105 (92%)	87 (90%)	10 (10%)	7	22
All	All	1033/1080 (96%)	908 (88%)	125 (12%)	5	16

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	26	THR
1	A	39	SER
1	A	40	VAL
1	A	48	SER
1	A	51	SER
1	A	52	VAL
1	A	62	GLU
1	A	63	ARG
1	A	67	LEU
1	A	69	LEU
1	A	91	ARG
1	A	100	LEU
1	A	109	THR
1	A	124	GLU
1	A	132	ARG
1	A	148	ASN
1	A	150	MET
1	A	158	VAL
1	A	162	VAL
1	A	167	GLN
1	A	180	GLN
1	A	185	THR
1	A	194	GLU
1	A	215	GLU
1	A	220	VAL
1	A	222	ARG
1	A	228	ILE

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Mol	Chain	Res	Type
1	A	232	LEU
1	A	260	CYS
1	A	265	ASP
1	A	268	VAL
1	A	287	ARG
1	A	291	SER
2	B	20	THR
2	B	21	VAL
2	B	43	GLN
2	B	47	MET
2	B	49	VAL
2	B	50	THR
2	B	51	ILE
2	B	57	SER
2	C	21	VAL
2	C	24	SER
2	C	50	THR
2	C	57	SER
2	D	21	VAL
2	D	49	VAL
2	D	50	THR
2	D	58	SER
2	E	21	VAL
2	E	49	VAL
2	E	50	THR
2	E	51	ILE
2	E	55	THR
2	F	7	LYS
2	F	21	VAL
2	F	44	LEU
2	F	49	VAL
2	F	50	THR
2	F	57	SER
2	F	65	VAL
3	G	13	GLN
3	G	21	SER
3	G	27	SER
3	G	33	THR
3	G	43	LYS
3	G	44	GLN
3	G	60	ARG
3	G	61	ASP

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Mol	Chain	Res	Type
3	G	86	LYS
3	G	90	THR
3	G	116	THR
3	G	119	THR
3	H	11	LEU
3	H	13	GLN
3	H	18	LEU
3	H	21	SER
3	H	33	THR
3	H	43	LYS
3	H	63	VAL
3	H	78	VAL
3	H	88	GLU
3	H	110	ASP
3	H	119	THR
3	I	5	GLN
3	I	6	GLU
3	I	11	LEU
3	I	12	VAL
3	I	19	ARG
3	I	28	ILE
3	I	33	THR
3	I	60	ARG
3	I	61	ASP
3	I	62	SER
3	I	63	VAL
3	I	77	THR
3	I	103	THR
3	I	110	ASP
3	I	119	THR
3	J	4	LEU
3	J	5	GLN
3	J	6	GLU
3	J	28	ILE
3	J	33	THR
3	J	43	LYS
3	J	44	GLN
3	J	60	ARG
3	J	62	SER
3	J	63	VAL
3	J	68	THR
3	J	78	VAL

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Mol	Chain	Res	Type
3	J	109	ARG
3	J	116	THR
3	J	126	HIS
3	K	11	LEU
3	K	32	SER
3	K	45	ARG
3	K	58	ASN
3	K	63	VAL
3	K	68	THR
3	K	78	VAL
3	K	82	MET
3	K	90	THR
3	K	119	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	1	GLN
1	A	18	ASN
1	A	83	ASN
1	A	87	ASN
1	A	201	ASN
1	A	227	ASN
2	C	14	ASN
3	G	117	GLN
3	J	125	HIS
3	K	39	GLN

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 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, 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	280/297 (94%)	0.14	7 (2%) 58 48	8, 50, 76, 91	0
2	B	68/68 (100%)	-0.76	0 100 100	9, 18, 29, 34	0
2	C	68/68 (100%)	-0.79	0 100 100	7, 16, 30, 36	0
2	D	68/68 (100%)	-0.80	0 100 100	6, 13, 26, 29	0
2	E	68/68 (100%)	-0.82	0 100 100	7, 13, 27, 36	0
2	F	68/68 (100%)	-0.82	0 100 100	8, 18, 30, 38	0
3	G	121/128 (94%)	-0.21	0 100 100	13, 35, 66, 75	0
3	H	120/128 (93%)	-0.50	0 100 100	10, 31, 46, 58	0
3	I	120/128 (93%)	-0.43	1 (0%) 82 75	10, 29, 53, 65	0
3	J	127/128 (99%)	-0.66	0 100 100	9, 19, 35, 59	0
3	K	120/128 (93%)	-0.43	0 100 100	10, 26, 47, 68	0
All	All	1228/1277 (96%)	-0.41	8 (0%) 84 78	6, 25, 66, 91	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	ALA	3.1
1	A	149	THR	3.0
1	A	59	VAL	2.6
1	A	242	HIS	2.5
1	A	133	HIS	2.3
1	A	56	GLY	2.2
3	I	107	PRO	2.2
1	A	89	PHE	2.1

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.