



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:22 AM UTC

PDB ID : 7TXF / pdb_00007txf
Title : The allosteric binding mode of alphaD-conotoxin VxXXB
Authors : Ho, T.N.T.; Abraham, N.; Lewis, R.J.
Deposited on : 2022-02-09
Resolution : 2.47 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

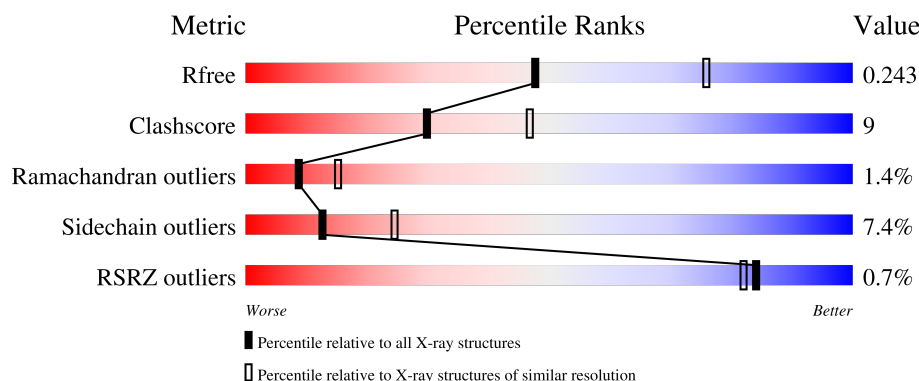
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	205	2% 80% 16% .
1	B	205	75% 24%
1	C	205	75% 18% . .
1	D	205	79% 16% . .
1	E	205	78% 18% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	30	 90% 10%
2	G	30	 63% 23% 10% •
2	H	30	 73% 23% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8771 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 Acetylcholine-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1637	1023	280	329	5			
1	B	205	Total	C	N	O	S	0	0	0
			1637	1023	280	329	5			
1	C	204	Total	C	N	O	S	0	0	0
			1631	1020	279	327	5			
1	D	199	Total	C	N	O	S	0	0	0
			1595	1001	273	316	5			
1	E	200	Total	C	N	O	S	0	0	0
			1599	1003	274	317	5			

- Molecule 2 is a protein called Alpha-conotoxin VxXXB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	30	Total	C	N	O	S	0	0	0
			224	130	48	38	8			
2	G	30	Total	C	N	O	S	0	0	0
			224	130	48	38	8			
2	H	30	Total	C	N	O	S	0	0	0
			224	130	48	38	8			

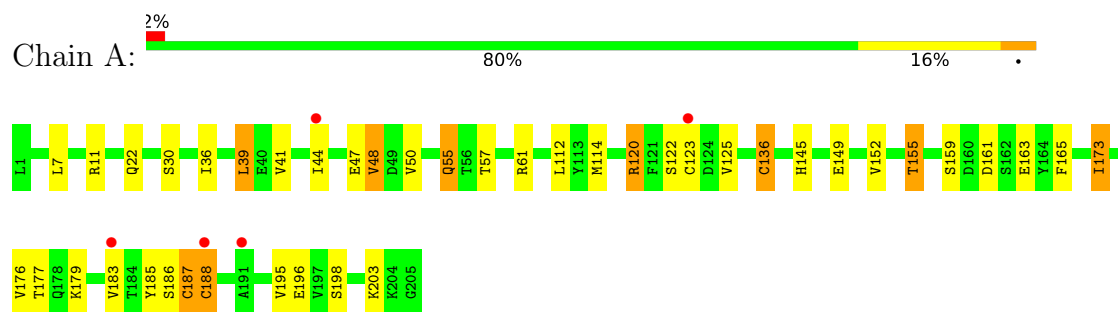
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	8	SER	CYS	conflict	UNP P0C1W6
G	8	SER	CYS	conflict	UNP P0C1W6
H	8	SER	CYS	conflict	UNP P0C1W6

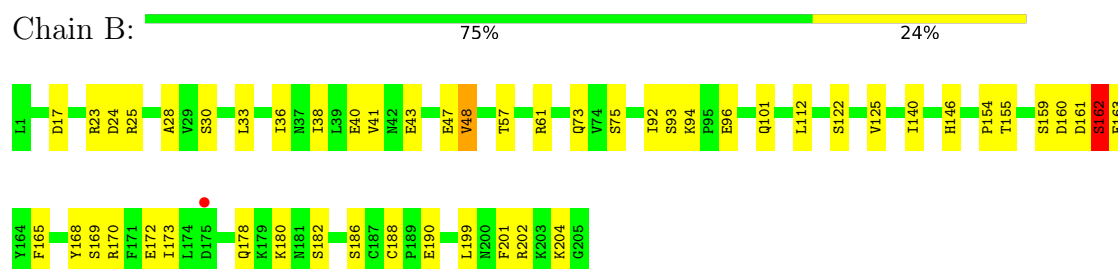
3 Residue-property plots [i](#)

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.

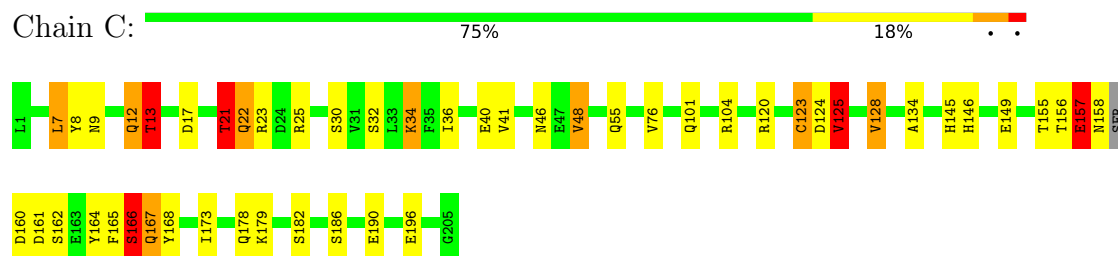
• Molecule 1: Acetylcholine-binding protein



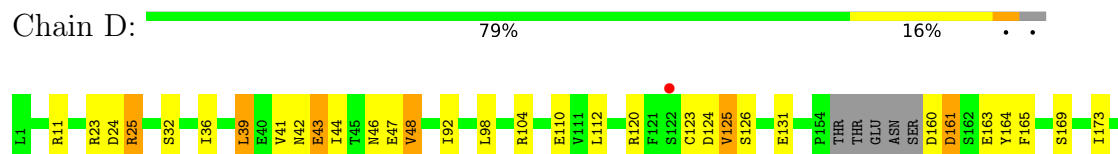
• Molecule 1: Acetylcholine-binding protein

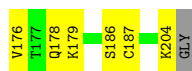


• Molecule 1: Acetylcholine-binding protein



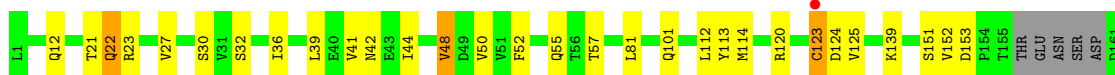
• Molecule 1: Acetylcholine-binding protein





- Molecule 1: Acetylcholine-binding protein

Chain E: 78% 18% ..



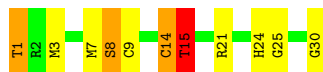
- Molecule 2: Alpha-conotoxin VxXXB

Chain F: 90% 10%



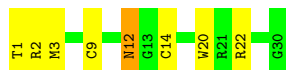
- Molecule 2: Alpha-conotoxin VxXXB

Chain G: 63% 23% 10% .



- Molecule 2: Alpha-conotoxin VxXXB

Chain H: 73% 23% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.91Å 119.57Å 150.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.36 – 2.47 46.36 – 2.47	Depositor EDS
% Data completeness (in resolution range)	94.0 (46.36-2.47) 75.8 (46.36-2.47)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.198 , 0.246 (Not available) , 0.243	Depositor DCC
R_{free} test set	1876 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8771	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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 [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	0.93	1/1673 (0.1%)	1.07	2/2282 (0.1%)
1	B	1.05	4/1673 (0.2%)	1.13	5/2282 (0.2%)
1	C	0.94	1/1666 (0.1%)	1.09	5/2271 (0.2%)
1	D	0.91	1/1630 (0.1%)	1.03	0/2223
1	E	1.09	2/1634 (0.1%)	1.10	0/2227
2	F	0.93	0/230	1.20	0/306
2	G	0.89	0/230	1.19	1/306 (0.3%)
2	H	0.82	0/230	1.05	0/306
All	All	0.98	9/8966 (0.1%)	1.09	13/12203 (0.1%)

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
1	B	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	SER	CA-C	8.86	1.63	1.52
1	B	75	SER	C-O	-6.00	1.16	1.24
1	E	151	SER	CA-C	5.89	1.59	1.52
1	C	166	SER	CA-C	5.68	1.60	1.52
1	E	12	GLN	C-O	-5.68	1.17	1.24
1	B	28	ALA	C-O	-5.32	1.17	1.24
1	A	39	LEU	CA-C	-5.17	1.47	1.53
1	D	39	LEU	CA-C	-5.11	1.47	1.53
1	B	154	PRO	C-O	-5.10	1.18	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	SER	N-CA-C	9.90	123.67	108.42
1	C	21	THR	N-CA-C	8.72	125.75	111.37
1	C	125	VAL	N-CA-C	7.40	124.74	109.34
1	A	136	CYS	CA-CB-SG	-7.06	98.17	114.40
1	B	170	ARG	CB-CG-CD	-6.41	96.57	111.30
1	C	166	SER	N-CA-C	6.36	124.35	110.80
2	G	8	SER	N-CA-C	6.10	120.56	113.18
1	C	12	GLN	N-CA-C	-5.71	102.44	110.50
1	A	187	CYS	CA-CB-SG	5.59	127.25	114.40
1	B	96	GLU	CA-CB-CG	5.39	124.89	114.10
1	B	61	ARG	CB-CG-CD	5.11	123.05	111.30
1	C	104	ARG	CG-CD-NE	-5.07	100.85	112.00
1	B	161	ASP	N-CA-C	-5.03	104.89	111.02

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	162	SER	Peptide
1	B	24	ASP	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	1637	0	1581	24	0
1	B	1637	0	1583	24	0
1	C	1631	0	1575	42	0
1	D	1595	0	1546	31	0
1	E	1599	0	1552	26	0
2	F	224	0	202	4	0
2	G	224	0	202	6	0
2	H	224	0	202	9	0
All	All	8771	0	8443	147	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 (147) 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:E:152:VAL:HG12	1:E:195:VAL:HG23	1.46	0.96
1:C:55:GLN:HG2	2:H:20:TRP:CD1	2.05	0.91
1:C:9:ASN:O	1:C:12:GLN:O	1.91	0.89
1:D:124:ASP:O	1:D:125:VAL:HG12	1.74	0.85
2:G:7:MET:HE1	2:G:25:GLY:HA2	1.57	0.84
1:E:55:GLN:HG3	1:E:114:MET:HE2	1.59	0.83
1:A:44:ILE:O	1:E:170:ARG:HD3	1.82	0.78
1:D:23:ARG:HD2	1:D:24:ASP:N	1.97	0.78
1:C:168:TYR:HB3	1:D:46:ASN:HD22	1.51	0.75
1:A:22:GLN:HE22	1:A:61:ARG:NH1	1.89	0.71
1:B:162:SER:HB3	1:B:165:PHE:H	1.56	0.71
1:D:165:PHE:CE1	1:D:173:ILE:HD11	2.27	0.70
1:E:32:SER:HA	1:E:178:GLN:HE22	1.57	0.70
1:E:101:GLN:OE1	1:E:113:TYR:OH	2.08	0.69
1:C:55:GLN:CG	2:H:20:TRP:CD1	2.74	0.69
1:E:152:VAL:CG1	1:E:195:VAL:HG23	2.23	0.68
1:D:160:ASP:OD1	1:D:163:GLU:HB2	1.94	0.68
1:C:165:PHE:CG	1:C:173:ILE:HD13	2.29	0.68
1:C:34:LYS:HE2	1:C:55:GLN:CD	2.19	0.67
1:D:32:SER:HA	1:D:178:GLN:HE22	1.60	0.67
1:D:41:VAL:HG12	1:D:48:VAL:HG23	1.76	0.67
1:A:41:VAL:HG22	1:A:48:VAL:HG23	1.78	0.66
1:E:125:VAL:HG12	1:E:125:VAL:O	1.95	0.66
2:H:1:THR:HG21	2:H:12:ASN:HA	1.77	0.65
1:D:23:ARG:CZ	1:D:25:ARG:HB3	2.27	0.64
1:B:38:ILE:HD11	1:B:199:LEU:HD21	1.80	0.63
1:A:165:PHE:CE1	1:A:173:ILE:HD11	2.34	0.63
1:B:41:VAL:HG22	1:B:48:VAL:HG23	1.81	0.62
1:E:41:VAL:HG22	1:E:48:VAL:HG23	1.80	0.62
1:C:55:GLN:HG2	2:H:20:TRP:CG	2.33	0.62
1:C:41:VAL:HG22	1:C:48:VAL:HG23	1.81	0.62
1:E:42:ASN:OD1	1:E:44:ILE:CG1	2.49	0.61
2:G:1:THR:OG1	2:G:8:SER:O	2.19	0.61
1:C:22:GLN:O	1:C:23:ARG:HG2	2.01	0.60
1:D:42:ASN:OD1	1:D:44:ILE:CG1	2.49	0.60
1:B:160:ASP:OD1	1:B:162:SER:HA	2.03	0.59
1:E:123:CYS:O	1:E:125:VAL:HG23	2.01	0.59
1:C:155:THR:O	1:C:157:GLU:N	2.36	0.59
1:B:146:HIS:CG	1:B:190:GLU:HG3	2.38	0.58
1:A:177:THR:HG23	1:A:198:SER:HB2	1.85	0.58
1:B:162:SER:CB	1:B:165:PHE:H	2.17	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:ASN:OD1	1:D:44:ILE:HG13	2.04	0.57
1:E:42:ASN:OD1	1:E:44:ILE:HG12	2.05	0.57
1:C:146:HIS:CG	1:C:190:GLU:HG3	2.40	0.56
1:B:172:GLU:OE2	1:B:202:ARG:NH1	2.38	0.56
1:B:17:ASP:OD2	1:D:11:ARG:NH2	2.31	0.56
1:C:160:ASP:OD1	1:C:162:SER:HB3	2.05	0.56
1:E:153:ASP:OD1	1:E:180:LYS:NZ	2.38	0.56
1:A:55:GLN:HG3	2:F:20:TRP:CH2	2.41	0.55
1:B:33:LEU:HD21	1:B:140:ILE:CD1	2.34	0.55
1:C:146:HIS:CD2	1:C:190:GLU:HG3	2.41	0.55
1:D:163:GLU:OE1	1:D:164:TYR:CE2	2.59	0.55
1:B:57:THR:HG22	1:B:112:LEU:HD23	1.88	0.55
1:E:30:SER:OG	1:E:57:THR:HG22	2.07	0.55
1:A:55:GLN:NE2	1:A:155:THR:HG21	2.22	0.54
1:C:125:VAL:HA	1:C:134:ALA:HB1	1.90	0.54
1:D:110:GLU:OE1	2:G:21:ARG:NH2	2.41	0.54
1:A:30:SER:OG	1:A:57:THR:HG22	2.07	0.54
1:D:43:GLU:HA	1:D:125:VAL:HG11	1.90	0.54
1:A:55:GLN:HE22	1:A:155:THR:HG21	1.71	0.53
1:D:23:ARG:CD	1:D:24:ASP:N	2.70	0.53
1:A:55:GLN:OE1	2:F:20:TRP:CZ3	2.61	0.53
1:B:160:ASP:CG	1:B:162:SER:HA	2.33	0.53
1:C:145:HIS:HD2	1:C:149:GLU:OE1	1.90	0.53
1:E:42:ASN:OD1	1:E:44:ILE:HG13	2.09	0.53
1:B:146:HIS:CD2	1:B:190:GLU:HG3	2.43	0.53
1:A:47:GLU:OE1	1:A:120:ARG:HD2	2.09	0.53
1:D:92:ILE:HD11	1:D:120:ARG:HG2	1.91	0.53
1:C:165:PHE:CE1	1:C:173:ILE:HD11	2.44	0.52
1:C:34:LYS:CE	1:C:55:GLN:CD	2.81	0.52
1:A:177:THR:CG2	1:A:198:SER:HB2	2.40	0.52
1:A:152:VAL:HG12	1:A:195:VAL:HG23	1.92	0.51
1:C:23:ARG:HH11	1:C:25:ARG:HD3	1.73	0.51
1:E:169:SER:O	1:E:204:LYS:CE	2.59	0.51
1:C:46:ASN:OD1	1:C:125:VAL:HG22	2.11	0.50
1:D:42:ASN:OD1	1:D:44:ILE:HG12	2.10	0.50
1:D:163:GLU:OE1	1:D:164:TYR:CZ	2.64	0.50
2:G:14:CYS:O	2:G:15:THR:CB	2.59	0.50
1:D:47:GLU:HB3	1:D:120:ARG:HH11	1.77	0.50
1:E:22:GLN:O	1:E:23:ARG:HG2	2.11	0.50
1:A:11:ARG:NH2	1:C:17:ASP:OD2	2.41	0.49
1:A:30:SER:OG	1:A:57:THR:CG2	2.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:O	1:E:170:ARG:CD	2.54	0.49
1:C:7:LEU:CD1	1:C:76:VAL:HG22	2.43	0.49
1:D:165:PHE:CD1	1:D:173:ILE:HD11	2.48	0.48
1:C:165:PHE:CD1	1:C:173:ILE:HD13	2.47	0.48
1:D:23:ARG:HG2	1:D:24:ASP:H	1.79	0.48
1:A:145:HIS:HD2	1:A:149:GLU:OE1	1.97	0.48
1:C:166:SER:O	1:C:167:GLN:HG2	2.14	0.48
1:A:161:ASP:HB3	1:A:176:VAL:HG23	1.96	0.47
1:C:166:SER:O	1:C:167:GLN:CB	2.62	0.47
1:B:169:SER:O	1:B:204:LYS:CE	2.62	0.47
1:D:23:ARG:CG	1:D:24:ASP:H	2.27	0.47
1:C:168:TYR:HB3	1:D:46:ASN:ND2	2.27	0.47
1:B:57:THR:CG2	1:B:112:LEU:HD23	2.44	0.47
1:B:30:SER:HB3	1:B:155:THR:HG22	1.96	0.47
1:C:34:LYS:HG2	1:C:164:TYR:CE1	2.50	0.47
1:E:30:SER:OG	1:E:57:THR:CG2	2.63	0.47
2:H:1:THR:HG21	2:H:12:ASN:HD22	1.79	0.47
1:A:112:LEU:HD13	1:A:112:LEU:C	2.38	0.47
1:C:8:TYR:CE1	1:C:12:GLN:NE2	2.83	0.47
2:H:2:ARG:HG3	2:H:14:CYS:O	2.16	0.46
1:C:46:ASN:OD1	1:C:124:ASP:O	2.33	0.46
1:B:168:TYR:CE1	1:E:124:ASP:HB2	2.51	0.46
1:D:187:CYS:SG	2:H:22:ARG:HA	2.56	0.46
1:D:124:ASP:O	1:D:125:VAL:CG1	2.57	0.46
1:C:12:GLN:O	1:C:13:THR:HB	2.15	0.45
1:B:93:SER:C	1:D:98:LEU:HD22	2.40	0.45
1:C:165:PHE:CD1	1:C:173:ILE:CD1	3.00	0.45
1:A:114:MET:SD	2:F:20:TRP:HZ2	2.40	0.45
1:A:165:PHE:CG	1:A:173:ILE:HD13	2.52	0.45
1:C:40:GLU:OE1	1:C:120:ARG:NH1	2.42	0.45
1:A:185:TYR:HB2	1:A:188:CYS:SG	2.57	0.45
2:G:7:MET:CE	2:G:24:HIS:O	2.64	0.44
1:C:158:ASN:ND2	1:C:162:SER:CB	2.80	0.44
1:D:43:GLU:HA	1:D:125:VAL:CG1	2.47	0.44
1:E:125:VAL:O	1:E:125:VAL:CG1	2.63	0.44
1:C:8:TYR:HE1	1:C:12:GLN:NE2	2.16	0.44
1:C:55:GLN:CG	2:H:20:TRP:NE1	2.81	0.44
1:C:123:CYS:O	1:C:125:VAL:HG13	2.18	0.44
1:E:162:SER:O	1:E:162:SER:OG	2.35	0.44
1:D:23:ARG:CG	1:D:24:ASP:N	2.82	0.43
1:D:47:GLU:OE1	1:D:120:ARG:HD3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LYS:HE2	1:C:55:GLN:NE2	2.32	0.43
1:B:38:ILE:HG21	1:B:201:PHE:CE2	2.53	0.43
1:D:161:ASP:OD1	1:D:176:VAL:HG12	2.18	0.43
1:B:47:GLU:HG2	1:B:92:ILE:CD1	2.49	0.43
2:H:2:ARG:HB2	2:H:9:CYS:SG	2.59	0.43
1:C:165:PHE:CE1	1:C:173:ILE:CD1	3.01	0.43
1:E:139:LYS:HG2	1:E:196:GLU:HG2	2.01	0.43
1:B:173:ILE:HG12	1:B:199:LEU:HD11	2.01	0.42
1:E:21:THR:HG22	1:E:27:VAL:HG23	2.00	0.42
1:A:55:GLN:HG3	2:F:20:TRP:CZ2	2.54	0.42
1:C:41:VAL:HG11	1:C:128:VAL:HG11	2.01	0.42
1:E:50:VAL:HG12	1:E:52:PHE:HD2	1.85	0.42
1:E:39:LEU:HD23	1:E:39:LEU:HA	1.90	0.41
1:C:179:LYS:HE3	1:C:196:GLU:OE1	2.21	0.41
1:B:47:GLU:HG2	1:B:92:ILE:HD11	2.03	0.41
1:E:41:VAL:HG21	1:E:201:PHE:HE2	1.84	0.41
1:B:188:CYS:HB3	1:B:190:GLU:OE2	2.21	0.41
1:B:180:LYS:HB3	2:G:30:GLY:C	2.46	0.41
1:B:33:LEU:HD11	1:B:140:ILE:HD11	2.02	0.41
1:C:32:SER:HA	1:C:178:GLN:HE22	1.86	0.41
1:A:39:LEU:HA	1:A:39:LEU:HD23	1.92	0.40
1:C:21:THR:HG23	1:C:22:GLN:N	2.35	0.40
1:C:30:SER:HB3	1:C:155:THR:HG22	2.03	0.40
1:D:169:SER:O	1:D:204:LYS:CE	2.70	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	203/205 (99%)	197 (97%)	5 (2%)	1 (0%)	24 40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	203/205 (99%)	198 (98%)	4 (2%)	1 (0%)	24	40
1	C	200/205 (98%)	187 (94%)	5 (2%)	8 (4%)	2	2
1	D	195/205 (95%)	189 (97%)	4 (2%)	2 (1%)	12	22
1	E	196/205 (96%)	194 (99%)	2 (1%)	0	100	100
2	F	28/30 (93%)	28 (100%)	0	0	100	100
2	G	28/30 (93%)	24 (86%)	1 (4%)	3 (11%)	0	0
2	H	28/30 (93%)	28 (100%)	0	0	100	100
All	All	1081/1115 (97%)	1045 (97%)	21 (2%)	15 (1%)	9	15

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	156	THR
1	C	161	ASP
1	D	125	VAL
1	D	161	ASP
2	G	14	CYS
2	G	15	THR
1	A	159	SER
1	C	13	THR
1	C	22	GLN
1	C	125	VAL
1	C	167	GLN
1	B	159	SER
1	C	157	GLU
1	C	166	SER
2	G	9	CYS

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	191/191 (100%)	171 (90%)	20 (10%)	6	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	191/191 (100%)	176 (92%)	15 (8%)	11	22
1	C	190/191 (100%)	177 (93%)	13 (7%)	14	28
1	D	186/191 (97%)	174 (94%)	12 (6%)	15	30
1	E	186/191 (97%)	178 (96%)	8 (4%)	26	48
2	F	25/25 (100%)	23 (92%)	2 (8%)	11	21
2	G	25/25 (100%)	22 (88%)	3 (12%)	5	9
2	H	25/25 (100%)	23 (92%)	2 (8%)	11	21
All	All	1019/1030 (99%)	944 (93%)	75 (7%)	13	24

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	36	ILE
1	A	48	VAL
1	A	50	VAL
1	A	55	GLN
1	A	120	ARG
1	A	122	SER
1	A	123	CYS
1	A	125	VAL
1	A	136	CYS
1	A	155	THR
1	A	163	GLU
1	A	173	ILE
1	A	179	LYS
1	A	183	VAL
1	A	186	SER
1	A	187	CYS
1	A	188	CYS
1	A	196	GLU
1	A	203	LYS
1	B	23	ARG
1	B	25	ARG
1	B	36	ILE
1	B	40	GLU
1	B	43	GLU
1	B	48	VAL
1	B	73	GLN
1	B	94	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	101	GLN
1	B	122	SER
1	B	125	VAL
1	B	163	GLU
1	B	178	GLN
1	B	182	SER
1	B	186	SER
1	C	7	LEU
1	C	13	THR
1	C	21	THR
1	C	34	LYS
1	C	36	ILE
1	C	48	VAL
1	C	101	GLN
1	C	123	CYS
1	C	125	VAL
1	C	128	VAL
1	C	157	GLU
1	C	182	SER
1	C	186	SER
1	D	25	ARG
1	D	36	ILE
1	D	39	LEU
1	D	43	GLU
1	D	48	VAL
1	D	104	ARG
1	D	112	LEU
1	D	123	CYS
1	D	126	SER
1	D	131	GLU
1	D	179	LYS
1	D	186	SER
1	E	22	GLN
1	E	36	ILE
1	E	48	VAL
1	E	81	LEU
1	E	112	LEU
1	E	120	ARG
1	E	123	CYS
1	E	179	LYS
2	F	15	THR
2	F	21	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	1	THR
2	G	3	MET
2	G	15	THR
2	H	3	MET
2	H	12	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	54	GLN
1	A	55	GLN
1	A	101	GLN
1	A	145	HIS
1	A	200	ASN
1	B	69	HIS
1	B	101	GLN
1	B	158	ASN
1	B	178	GLN
1	B	200	ASN
1	C	12	GLN
1	C	54	GLN
1	C	101	GLN
1	C	145	HIS
1	C	158	ASN
1	C	200	ASN
1	D	22	GLN
1	D	46	ASN
1	D	178	GLN
1	D	181	ASN
1	D	200	ASN
1	E	178	GLN
1	E	200	ASN
2	F	24	HIS
2	H	12	ASN
2	H	24	HIS

5.3.3 RNA ⓘ

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 [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	205/205 (100%)	0.08	5 (2%) 59 56	49, 78, 126, 169	0
1	B	205/205 (100%)	-0.01	1 (0%) 87 85	44, 72, 109, 135	0
1	C	204/205 (99%)	-0.01	0 100 100	52, 81, 127, 173	0
1	D	199/205 (97%)	0.00	1 (0%) 87 85	56, 83, 121, 142	0
1	E	200/205 (97%)	-0.16	1 (0%) 87 85	46, 59, 94, 125	0
2	F	30/30 (100%)	0.17	0 100 100	66, 77, 100, 123	0
2	G	30/30 (100%)	0.52	0 100 100	93, 120, 146, 148	0
2	H	30/30 (100%)	0.36	0 100 100	96, 111, 129, 143	0
All	All	1103/1115 (98%)	0.01	8 (0%) 84 82	44, 76, 124, 173	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	VAL	3.7
1	A	191	ALA	3.3
1	E	123	CYS	2.8
1	A	123	CYS	2.6
1	D	122	SER	2.4
1	A	44	ILE	2.1
1	A	188	CYS	2.1
1	B	175	ASP	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.