Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 01:48 PM JST

PDB ID	:	5XGL
Title	:	Co-crystal structure of Ac-AChBPP in complex with alpha-conotoxin LvIA
Authors	:	Wang, X.Q.; Xu, M.Y.; Luo, S.L.; Zhu, X.P.
Deposited on	:	2017-04-14
Resolution	:	3.44 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:

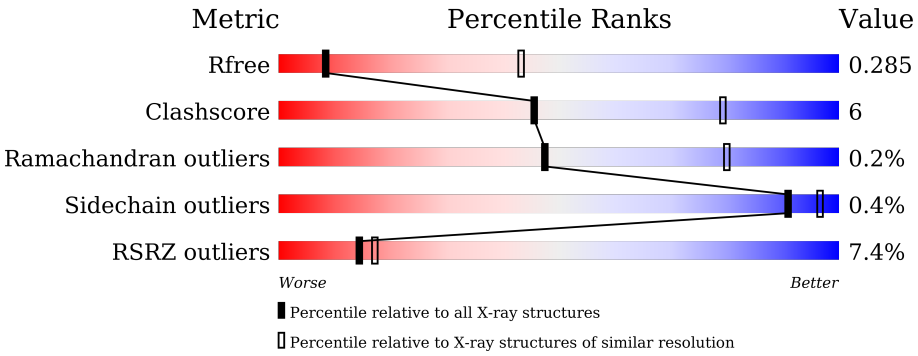
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.44 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	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (3.50-3.38)

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	224	5% 83% 10% 8%
1	B	224	4% 83% 9% 8%
1	D	224	7% 78% 14% 8%
1	G	224	3% 82% 10% 8%
1	I	224	4% 77% 15% 8%
2	C	17	53% 59% 29% 12%

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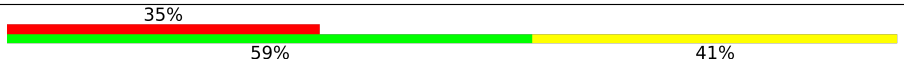
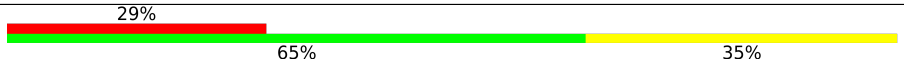
Mol	Chain	Length	Quality of chain
2	E	17	
2	F	17	
2	H	17	
2	J	17	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8835 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 Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1653	1045	271	328	9			
1	B	207	Total	C	N	O	S	0	0	0
			1653	1045	271	328	9			
1	D	207	Total	C	N	O	S	0	0	0
			1653	1045	271	328	9			
1	G	207	Total	C	N	O	S	0	0	0
			1653	1045	271	328	9			
1	I	207	Total	C	N	O	S	0	0	0
			1653	1045	271	328	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	VAL	ALA	conflict	UNP Q8WSF8
A	136	VAL	ALA	conflict	UNP Q8WSF8
A	218	HIS	-	expression tag	UNP Q8WSF8
A	219	HIS	-	expression tag	UNP Q8WSF8
A	220	HIS	-	expression tag	UNP Q8WSF8
A	221	HIS	-	expression tag	UNP Q8WSF8
A	222	HIS	-	expression tag	UNP Q8WSF8
A	223	HIS	-	expression tag	UNP Q8WSF8
B	41	VAL	ALA	conflict	UNP Q8WSF8
B	136	VAL	ALA	conflict	UNP Q8WSF8
B	218	HIS	-	expression tag	UNP Q8WSF8
B	219	HIS	-	expression tag	UNP Q8WSF8
B	220	HIS	-	expression tag	UNP Q8WSF8
B	221	HIS	-	expression tag	UNP Q8WSF8
B	222	HIS	-	expression tag	UNP Q8WSF8
B	223	HIS	-	expression tag	UNP Q8WSF8
D	41	VAL	ALA	conflict	UNP Q8WSF8
D	136	VAL	ALA	conflict	UNP Q8WSF8
D	218	HIS	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	219	HIS	-	expression tag	UNP Q8WSF8
D	220	HIS	-	expression tag	UNP Q8WSF8
D	221	HIS	-	expression tag	UNP Q8WSF8
D	222	HIS	-	expression tag	UNP Q8WSF8
D	223	HIS	-	expression tag	UNP Q8WSF8
G	41	VAL	ALA	conflict	UNP Q8WSF8
G	136	VAL	ALA	conflict	UNP Q8WSF8
G	218	HIS	-	expression tag	UNP Q8WSF8
G	219	HIS	-	expression tag	UNP Q8WSF8
G	220	HIS	-	expression tag	UNP Q8WSF8
G	221	HIS	-	expression tag	UNP Q8WSF8
G	222	HIS	-	expression tag	UNP Q8WSF8
G	223	HIS	-	expression tag	UNP Q8WSF8
I	41	VAL	ALA	conflict	UNP Q8WSF8
I	136	VAL	ALA	conflict	UNP Q8WSF8
I	218	HIS	-	expression tag	UNP Q8WSF8
I	219	HIS	-	expression tag	UNP Q8WSF8
I	220	HIS	-	expression tag	UNP Q8WSF8
I	221	HIS	-	expression tag	UNP Q8WSF8
I	222	HIS	-	expression tag	UNP Q8WSF8
I	223	HIS	-	expression tag	UNP Q8WSF8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	17	Total	C	N	O	S	0	0	1
			114	66	22	22	4			
2	C	17	Total	C	N	O	S	0	0	1
			114	66	22	22	4			
2	E	17	Total	C	N	O	S	0	0	1
			114	66	22	22	4			
2	H	17	Total	C	N	O	S	0	0	1
			114	66	22	22	4			
2	J	17	Total	C	N	O	S	0	0	1
			114	66	22	22	4			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	417	NH2	-	amidation	UNP L8BU87
C	417	NH2	-	amidation	UNP L8BU87
E	417	NH2	-	amidation	UNP L8BU87

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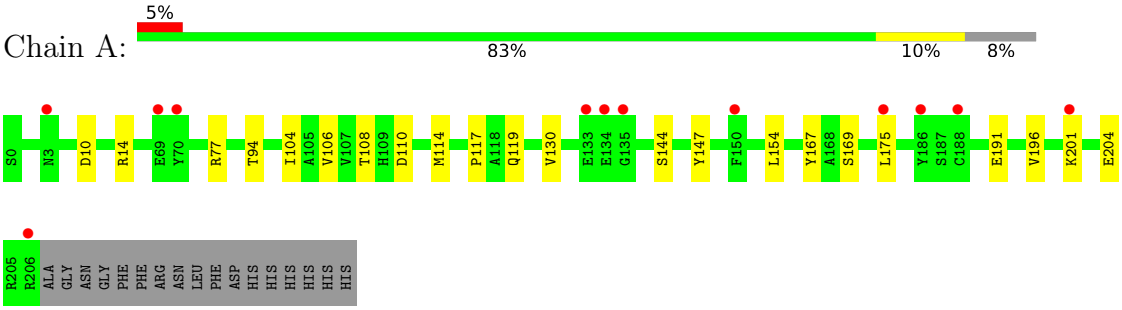
Chain	Residue	Modelled	Actual	Comment	Reference
H	417	NH2	-	amidation	UNP L8BU87
J	417	NH2	-	amidation	UNP L8BU87

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.

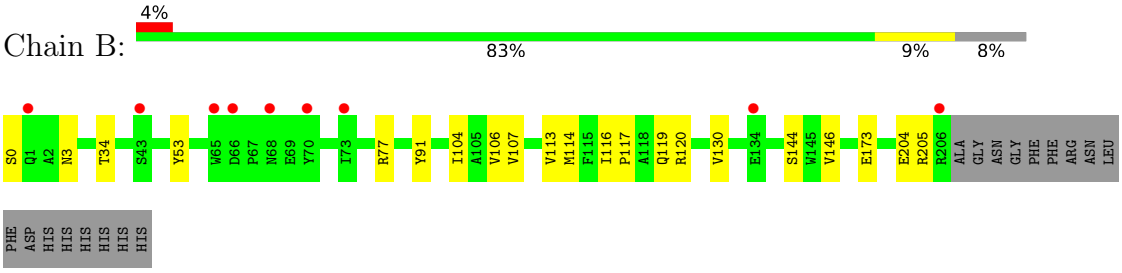
• Molecule 1: Soluble acetylcholine receptor

Chain A:



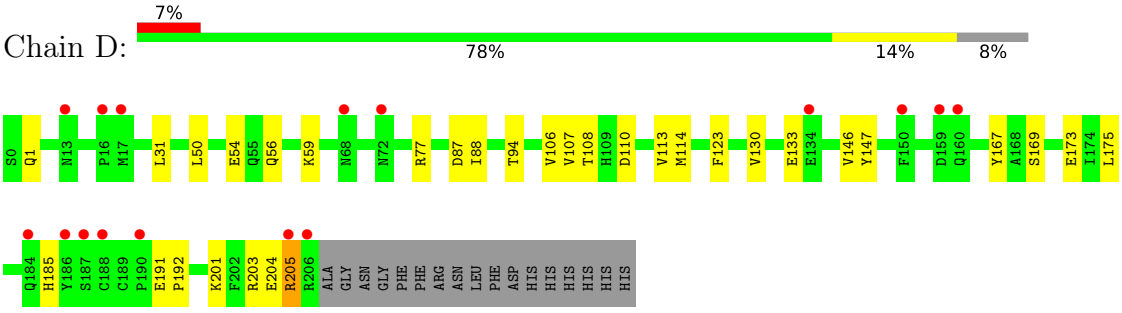
• Molecule 1: Soluble acetylcholine receptor

Chain B:



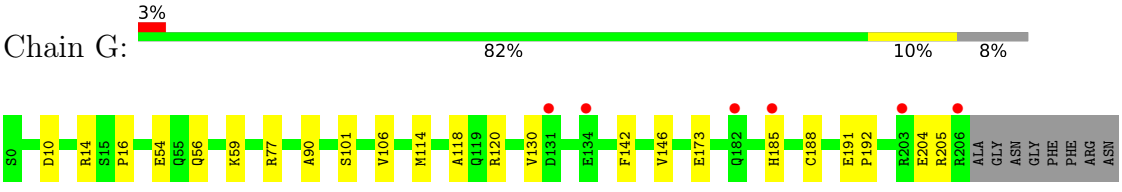
• Molecule 1: Soluble acetylcholine receptor

Chain D:



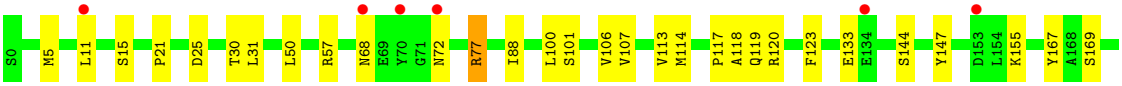
• Molecule 1: Soluble acetylcholine receptor

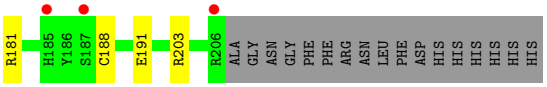
Chain G:



• Molecule 1: Soluble acetylcholine receptor

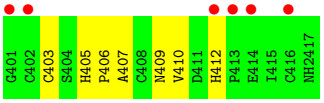
Chain I:





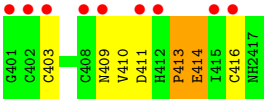
• Molecule 2: Alpha-conotoxin LvIA

Chain F:



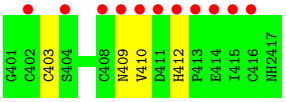
• Molecule 2: Alpha-conotoxin LvIA

Chain C:



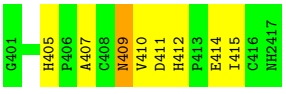
• Molecule 2: Alpha-conotoxin LvIA

Chain E:



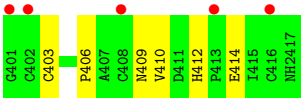
• Molecule 2: Alpha-conotoxin LvIA

Chain H:



• Molecule 2: Alpha-conotoxin LvIA

Chain J:


G401
C402
C403
P406
A407
C408
N409
V410
D411
H412
P413
E414
I415
C416
NH2417

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.39Å 83.99Å 209.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.44 – 3.44 28.44 – 3.44	Depositor EDS
% Data completeness (in resolution range)	97.8 (28.44-3.44) 97.9 (28.44-3.44)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 3.47Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.239 , 0.283 0.240 , 0.285	Depositor DCC
R_{free} test set	908 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	93.7	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.7	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	0.91	EDS
Total number of atoms	8835	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH2

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	0.27	0/1693	0.48	0/2309
1	B	0.27	0/1693	0.48	0/2309
1	D	0.27	0/1693	0.48	0/2309
1	G	0.27	0/1693	0.47	0/2309
1	I	0.27	0/1693	0.47	0/2309
2	C	0.40	0/116	0.57	0/158
2	E	0.43	0/116	0.55	0/158
2	F	0.35	0/116	0.49	0/158
2	H	0.34	0/116	0.40	0/158
2	J	0.30	0/116	0.43	0/158
All	All	0.28	0/9045	0.48	0/12335

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	G	0	1
1	I	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	188	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	I	188	CYS	Peptide

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	1653	0	1590	21	0
1	B	1653	0	1590	21	0
1	D	1653	0	1590	23	0
1	G	1653	0	1590	17	0
1	I	1653	0	1590	24	0
2	C	114	0	91	11	0
2	E	114	0	92	7	0
2	F	114	0	92	8	0
2	H	114	0	92	6	0
2	J	114	0	92	5	0
All	All	8835	0	8409	111	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 6.

All (111) 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:114:MET:HB3	2:C:410:VAL:HG13	1.38	1.02
1:B:114:MET:HB3	2:E:410:VAL:HG13	1.50	0.94
2:C:413:PRO:HG2	2:C:414:GLU:H	1.33	0.93
1:A:191:GLU:OE2	2:F:412:HIS:NE2	2.13	0.79
1:G:146:VAL:O	1:I:77:ARG:NH1	2.17	0.78
2:H:411:ASP:OD1	1:I:77:ARG:NH2	2.16	0.77
1:A:117:PRO:HG2	1:A:119:GLN:HE21	1.51	0.76
1:G:191:GLU:OE2	2:H:412:HIS:NE2	2.20	0.75
2:F:410:VAL:HG13	1:G:114:MET:HB3	1.70	0.72
1:I:191:GLU:OE2	2:J:412:HIS:NE2	2.24	0.70
1:A:77:ARG:NH2	2:C:411:ASP:OD1	2.26	0.68
2:C:413:PRO:HG2	2:C:414:GLU:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:PRO:HG2	1:B:119:GLN:HE21	1.60	0.66
1:B:106:VAL:HB	2:E:410:VAL:HG12	1.78	0.65
1:B:0:SER:HA	1:B:3:ASN:HD22	1.60	0.65
2:E:403:CYS:HA	2:E:409:ASN:OD1	1.97	0.64
1:I:133:GLU:O	1:I:203:ARG:NH2	2.31	0.64
1:D:31:LEU:HD11	1:D:88:ILE:HG21	1.79	0.63
1:A:106:VAL:HB	2:C:410:VAL:HG12	1.82	0.62
2:H:409:ASN:ND2	1:I:114:MET:SD	2.72	0.61
1:D:114:MET:HB3	2:J:410:VAL:HG13	1.81	0.61
1:D:77:ARG:HG3	1:D:106:VAL:HG22	1.83	0.60
1:D:108:THR:OG1	1:D:110:ASP:OD1	2.15	0.60
1:I:30:THR:HB	1:I:57:ARG:HB3	1.83	0.60
1:A:108:THR:OG1	1:A:110:ASP:OD1	2.18	0.59
2:C:413:PRO:O	2:C:416:CYS:N	2.35	0.59
1:I:31:LEU:HD11	1:I:88:ILE:HG21	1.85	0.59
1:B:77:ARG:HD3	1:B:106:VAL:HG22	1.84	0.59
1:D:77:ARG:CG	1:D:106:VAL:HG22	2.33	0.58
1:A:117:PRO:HG2	1:A:119:GLN:NE2	2.18	0.58
1:D:130:VAL:HG22	1:D:204:GLU:HG3	1.84	0.58
1:B:173:GLU:HB2	1:B:205:ARG:HG3	1.85	0.58
1:D:191:GLU:OE2	2:E:412:HIS:NE2	2.32	0.58
2:C:413:PRO:CG	2:C:414:GLU:H	2.11	0.57
2:J:403:CYS:O	2:J:409:ASN:ND2	2.37	0.57
1:D:133:GLU:O	1:D:203:ARG:NH2	2.35	0.57
1:G:54:GLU:OE2	1:G:56:GLN:NE2	2.36	0.56
2:F:405:HIS:CE1	2:F:407:ALA:HB3	2.42	0.55
1:B:114:MET:CB	2:E:410:VAL:HG13	2.33	0.54
1:D:107:VAL:HG22	1:D:113:VAL:HG22	1.91	0.53
1:G:10:ASP:O	1:G:14:ARG:HB2	2.09	0.53
1:B:107:VAL:HG22	1:B:113:VAL:HG22	1.91	0.53
2:J:406:PRO:O	2:J:410:VAL:HG23	2.09	0.53
1:D:167:TYR:CZ	1:D:169:SER:HB2	2.44	0.52
1:G:173:GLU:HB2	1:G:205:ARG:HD3	1.91	0.52
1:A:77:ARG:CG	1:A:106:VAL:HG22	2.39	0.52
1:I:107:VAL:HG22	1:I:113:VAL:HG22	1.91	0.52
1:D:175:LEU:HD12	1:D:201:LYS:HG2	1.92	0.51
1:G:77:ARG:CG	1:G:106:VAL:HG22	2.41	0.51
2:H:414:GLU:HG2	2:H:415:ILE:HG13	1.92	0.51
1:A:106:VAL:HB	2:C:410:VAL:CG1	2.41	0.51
1:D:185:HIS:NE2	1:D:192:PRO:HB3	2.26	0.51
1:B:130:VAL:HG22	1:B:204:GLU:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASP:O	1:A:14:ARG:HB2	2.11	0.50
2:F:405:HIS:HE1	2:F:407:ALA:HB3	1.76	0.50
2:F:410:VAL:HG11	1:G:106:VAL:HB	1.93	0.50
1:G:77:ARG:HG2	1:G:106:VAL:HG22	1.92	0.50
2:C:413:PRO:CG	2:C:414:GLU:N	2.69	0.49
1:B:116:ILE:HD13	2:E:409:ASN:HD22	1.77	0.49
1:A:114:MET:CB	2:C:410:VAL:HG13	2.27	0.48
1:A:77:ARG:HG3	1:A:106:VAL:HG22	1.95	0.48
1:B:106:VAL:HB	2:E:410:VAL:CG1	2.43	0.48
1:G:16:PRO:HG2	1:I:5:MET:SD	2.53	0.48
1:I:167:TYR:CZ	1:I:169:SER:HB2	2.48	0.48
2:C:403:CYS:HA	2:C:409:ASN:OD1	2.14	0.47
2:F:410:VAL:CG1	1:G:106:VAL:HB	2.45	0.47
1:B:77:ARG:HG3	1:D:147:TYR:CE1	2.49	0.47
1:A:154:LEU:HD13	1:A:196:VAL:HG23	1.97	0.47
1:B:120:ARG:HD2	1:D:94:THR:O	2.15	0.47
1:D:185:HIS:CE1	1:D:192:PRO:HB3	2.50	0.47
1:I:101:SER:HB3	1:I:118:ALA:HB3	1.97	0.47
1:A:167:TYR:CZ	1:A:169:SER:HB2	2.50	0.46
1:I:50:LEU:HG	1:I:123:PHE:HE1	1.80	0.46
1:I:117:PRO:HG2	1:I:119:GLN:HE21	1.80	0.46
1:D:173:GLU:HB2	1:D:205:ARG:HD2	1.97	0.46
1:A:175:LEU:HD12	1:A:201:LYS:HG2	1.97	0.46
1:A:104:ILE:HG21	1:B:146:VAL:HG21	1.98	0.46
1:B:77:ARG:CD	1:B:106:VAL:HG22	2.45	0.46
1:D:59:LYS:HE3	1:D:110:ASP:O	2.16	0.45
2:F:403:CYS:HA	2:F:409:ASN:OD1	2.16	0.45
1:D:54:GLU:OE2	1:D:56:GLN:NE2	2.50	0.45
1:I:100:LEU:HD11	1:I:120:ARG:HB2	1.99	0.45
1:B:117:PRO:HG2	1:B:119:GLN:NE2	2.31	0.44
1:G:90:ALA:HB2	1:G:142:PHE:CE2	2.53	0.43
1:A:130:VAL:HG22	1:A:204:GLU:HG3	1.99	0.43
1:B:91:TYR:OH	1:B:144:SER:O	2.30	0.43
1:I:11:LEU:O	1:I:15:SER:HB2	2.18	0.43
1:A:104:ILE:HB	1:B:146:VAL:HG11	2.00	0.43
2:H:405:HIS:CE1	2:H:407:ALA:HB3	2.53	0.43
1:I:77:ARG:HG2	1:I:106:VAL:HG22	1.99	0.43
1:I:191:GLU:CD	2:J:412:HIS:HE2	2.18	0.43
1:A:77:ARG:HG2	1:A:106:VAL:HG22	2.00	0.43
1:B:34:THR:HB	1:B:53:TYR:HB2	1.99	0.43
1:D:50:LEU:HG	1:D:123:PHE:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:SER:HB3	1:G:118:ALA:HB3	2.01	0.42
1:D:87:ASP:OD2	1:D:146:VAL:HG22	2.19	0.42
1:B:77:ARG:HG3	1:D:147:TYR:CZ	2.55	0.42
1:I:155:LYS:HA	1:I:181:ARG:HD2	2.01	0.42
1:D:1:GLN:HG2	1:I:25:ASP:OD2	2.19	0.42
2:F:406:PRO:O	2:F:410:VAL:HG23	2.20	0.42
1:I:77:ARG:CG	1:I:106:VAL:HG22	2.50	0.41
1:B:104:ILE:HB	1:D:146:VAL:HG11	2.01	0.41
1:I:68:ASN:ND2	1:I:72:ASN:OD1	2.51	0.41
1:A:144:SER:OG	1:A:147:TYR:HB2	2.21	0.41
1:G:130:VAL:HG22	1:G:204:GLU:HG3	2.02	0.41
1:I:21:PRO:HD2	1:I:147:TYR:CZ	2.56	0.41
1:G:59:LYS:HE2	1:G:59:LYS:HB3	1.70	0.40
2:H:410:VAL:HG11	1:I:106:VAL:CG2	2.51	0.40
1:I:144:SER:OG	1:I:147:TYR:HB2	2.21	0.40
1:A:94:THR:O	1:G:120:ARG:HD2	2.21	0.40
1:G:185:HIS:NE2	1:G:192:PRO:HB3	2.36	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	205/224 (92%)	202 (98%)	3 (2%)	0	100 100
1	B	205/224 (92%)	202 (98%)	3 (2%)	0	100 100
1	D	205/224 (92%)	200 (98%)	5 (2%)	0	100 100
1	G	205/224 (92%)	203 (99%)	2 (1%)	0	100 100
1	I	205/224 (92%)	202 (98%)	3 (2%)	0	100 100
2	C	15/17 (88%)	12 (80%)	1 (7%)	2 (13%)	0 3
2	E	15/17 (88%)	15 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	F	15/17 (88%)	15 (100%)	0	0	100 100
2	H	15/17 (88%)	15 (100%)	0	0	100 100
2	J	15/17 (88%)	15 (100%)	0	0	100 100
All	All	1100/1205 (91%)	1081 (98%)	17 (2%)	2 (0%)	47 80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	414	GLU
2	C	413	PRO

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	190/204 (93%)	190 (100%)	0	100 100
1	B	190/204 (93%)	190 (100%)	0	100 100
1	D	190/204 (93%)	189 (100%)	1 (0%)	88 95
1	G	190/204 (93%)	190 (100%)	0	100 100
1	I	190/204 (93%)	189 (100%)	1 (0%)	88 95
2	C	14/14 (100%)	14 (100%)	0	100 100
2	E	14/14 (100%)	14 (100%)	0	100 100
2	F	14/14 (100%)	14 (100%)	0	100 100
2	H	14/14 (100%)	13 (93%)	1 (7%)	14 46
2	J	14/14 (100%)	13 (93%)	1 (7%)	14 46
All	All	1020/1090 (94%)	1016 (100%)	4 (0%)	91 96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	205	ARG

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Mol	Chain	Res	Type
2	H	409	ASN
1	I	77	ARG
2	J	414	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1	GLN
1	B	3	ASN
2	C	412	HIS
1	D	3	ASN
2	H	409	ASN
1	I	55	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides 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	207/224 (92%)	0.25	12 (5%) 23 24	58, 85, 128, 144	0
1	B	207/224 (92%)	0.41	9 (4%) 35 34	60, 85, 136, 155	0
1	D	207/224 (92%)	0.41	16 (7%) 13 16	63, 95, 133, 153	0
1	G	207/224 (92%)	0.17	6 (2%) 51 50	62, 89, 113, 144	0
1	I	207/224 (92%)	0.27	9 (4%) 35 34	62, 92, 118, 140	0
2	C	16/17 (94%)	2.09	9 (56%) 0 0	30, 129, 142, 150	0
2	E	16/17 (94%)	2.93	11 (68%) 0 0	110, 149, 162, 165	0
2	F	16/17 (94%)	1.45	6 (37%) 0 0	110, 131, 145, 157	0
2	H	16/17 (94%)	0.21	0 100 100	83, 101, 122, 125	0
2	J	16/17 (94%)	1.35	5 (31%) 0 0	99, 126, 143, 148	0
All	All	1115/1205 (92%)	0.40	83 (7%) 14 17	30, 91, 134, 165	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	66	ASP	7.4
2	E	414	GLU	5.8
2	E	413	PRO	5.5
2	E	411	ASP	5.4
2	E	416	CYS	4.9
1	D	16	PRO	4.5
2	C	401	GLY	4.2
2	C	412	HIS	4.1
2	E	412	HIS	4.1
1	D	17	MET	4.1
1	B	65	TRP	4.0
2	E	408	CYS	3.8
2	J	402	CYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	206	ARG	3.7
1	B	73	ILE	3.6
2	C	402	CYS	3.6
1	B	206	ARG	3.5
1	B	68	ASN	3.5
1	A	134	GLU	3.4
1	I	134	GLU	3.4
1	D	68	ASN	3.3
2	E	415	ILE	3.2
2	C	411	ASP	3.2
1	I	68	ASN	3.2
2	F	414	GLU	3.2
1	I	185	HIS	3.1
1	D	150	PHE	3.1
1	A	133	GLU	3.0
1	I	206	ARG	3.0
2	C	403	CYS	2.9
2	J	401	GLY	2.9
1	A	175	LEU	2.8
2	E	409	ASN	2.8
1	A	135	GLY	2.7
1	G	131	ASP	2.7
1	D	190	PRO	2.7
2	C	408	CYS	2.7
2	F	402	CYS	2.7
2	F	416	CYS	2.6
1	A	201	LYS	2.6
2	J	408	CYS	2.6
1	A	150	PHE	2.6
1	A	186	TYR	2.6
1	I	153	ASP	2.6
2	C	409	ASN	2.6
1	B	70	TYR	2.6
1	G	134	GLU	2.5
1	G	206	ARG	2.5
2	F	401	GLY	2.5
1	D	186	TYR	2.5
1	D	72	ASN	2.5
1	B	134	GLU	2.4
1	I	70	TYR	2.4
1	A	206	ARG	2.4
1	D	13	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	43	SER	2.4
2	E	402	CYS	2.4
1	D	134	GLU	2.3
2	J	413	PRO	2.3
1	A	188	CYS	2.3
1	G	182	GLN	2.3
1	D	188	CYS	2.2
1	I	187	SER	2.2
1	G	203	ARG	2.2
2	E	410	VAL	2.2
1	D	187	SER	2.2
2	C	416	CYS	2.2
1	A	3	ASN	2.2
1	D	159	ASP	2.2
1	I	11	LEU	2.2
2	F	413	PRO	2.1
1	G	185	HIS	2.1
1	A	69	GLU	2.1
1	D	184	GLN	2.1
2	J	416	CYS	2.1
1	B	1	GLN	2.1
2	E	404	SER	2.1
1	D	160	GLN	2.1
2	F	412	HIS	2.1
1	D	205	ARG	2.0
1	A	70	TYR	2.0
1	I	72	ASN	2.0
2	C	415	ILE	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.