Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:55 PM GMT

PDB ID	:	4QAB
Title	:	X-RAY STRUCTURE of ACETYLCHOLINE BINDING PROTEIN (ACHBP) IN COMPLEX WITH 4-(MORPHOLIN-4-YL)-6-[4-(TRIFLUOROMETHYL)PHENYL]PYRIMIDIN-2-AMINE
Authors	:	Kaczanowska, K.; Harel, M.; Radic', Z.; Changeux, J.-P.; Finn, M.G.; Taylor, P.
Deposited on	:	2014-05-03
Resolution	:	2.98 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

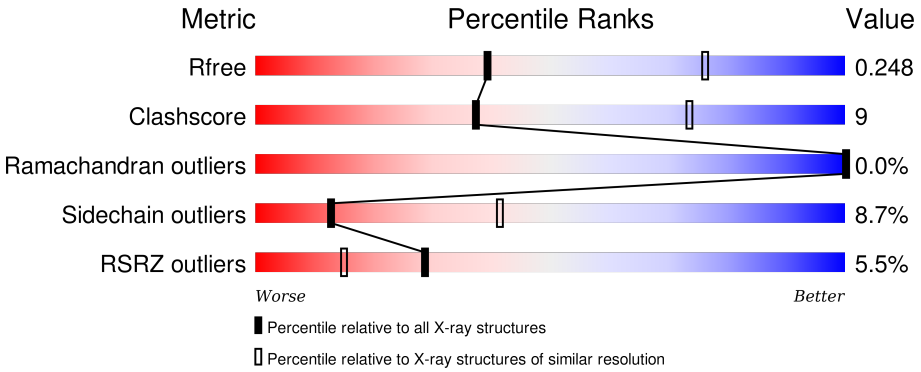
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.98 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}	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	217	5% 76% 18%
1	B	217	3% 74% 17% 6%
1	C	217	6% 76% 17% 5%
1	D	217	6% 71% 24%
1	E	217	6% 77% 17% 5%

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Mol	Chain	Length	Quality of chain
1	F	217	6% 73% 18% 5%
1	G	217	6% 73% 22%
1	H	217	3% 69% 24%
1	I	217	5% 75% 19%
1	J	217	7% 69% 23% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	KK2	I	301	-	-	-	X
3	NAG	B	302	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17236 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	208	Total	C	N	O	S	0	1	0
			1673	1047	284	337	5			
1	B	205	Total	C	N	O	S	0	2	0
			1650	1032	280	333	5			
1	C	207	Total	C	N	O	S	0	1	0
			1665	1043	283	334	5			
1	D	213	Total	C	N	O	S	0	1	0
			1711	1067	290	349	5			
1	E	207	Total	C	N	O	S	0	2	0
			1664	1039	282	338	5			
1	F	208	Total	C	N	O	S	0	4	0
			1689	1057	284	343	5			
1	G	210	Total	C	N	O	S	0	2	0
			1693	1058	286	344	5			
1	H	209	Total	C	N	O	S	0	3	0
			1690	1057	285	343	5			
1	I	209	Total	C	N	O	S	0	4	0
			1694	1060	285	344	5			
1	J	207	Total	C	N	O	S	0	3	0
			1676	1050	283	338	5			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASP	-	EXPRESSION TAG	UNP P58154
A	-6	TYR	-	EXPRESSION TAG	UNP P58154
A	-5	LYS	-	EXPRESSION TAG	UNP P58154
A	-4	ASP	-	EXPRESSION TAG	UNP P58154
A	-3	ASP	-	EXPRESSION TAG	UNP P58154
A	-2	ASP	-	EXPRESSION TAG	UNP P58154
A	-1	ASP	-	EXPRESSION TAG	UNP P58154
A	0	LYS	-	EXPRESSION TAG	UNP P58154
B	-7	ASP	-	EXPRESSION TAG	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	TYR	-	EXPRESSION TAG	UNP P58154
B	-5	LYS	-	EXPRESSION TAG	UNP P58154
B	-4	ASP	-	EXPRESSION TAG	UNP P58154
B	-3	ASP	-	EXPRESSION TAG	UNP P58154
B	-2	ASP	-	EXPRESSION TAG	UNP P58154
B	-1	ASP	-	EXPRESSION TAG	UNP P58154
B	0	LYS	-	EXPRESSION TAG	UNP P58154
C	-7	ASP	-	EXPRESSION TAG	UNP P58154
C	-6	TYR	-	EXPRESSION TAG	UNP P58154
C	-5	LYS	-	EXPRESSION TAG	UNP P58154
C	-4	ASP	-	EXPRESSION TAG	UNP P58154
C	-3	ASP	-	EXPRESSION TAG	UNP P58154
C	-2	ASP	-	EXPRESSION TAG	UNP P58154
C	-1	ASP	-	EXPRESSION TAG	UNP P58154
C	0	LYS	-	EXPRESSION TAG	UNP P58154
D	-7	ASP	-	EXPRESSION TAG	UNP P58154
D	-6	TYR	-	EXPRESSION TAG	UNP P58154
D	-5	LYS	-	EXPRESSION TAG	UNP P58154
D	-4	ASP	-	EXPRESSION TAG	UNP P58154
D	-3	ASP	-	EXPRESSION TAG	UNP P58154
D	-2	ASP	-	EXPRESSION TAG	UNP P58154
D	-1	ASP	-	EXPRESSION TAG	UNP P58154
D	0	LYS	-	EXPRESSION TAG	UNP P58154
E	-7	ASP	-	EXPRESSION TAG	UNP P58154
E	-6	TYR	-	EXPRESSION TAG	UNP P58154
E	-5	LYS	-	EXPRESSION TAG	UNP P58154
E	-4	ASP	-	EXPRESSION TAG	UNP P58154
E	-3	ASP	-	EXPRESSION TAG	UNP P58154
E	-2	ASP	-	EXPRESSION TAG	UNP P58154
E	-1	ASP	-	EXPRESSION TAG	UNP P58154
E	0	LYS	-	EXPRESSION TAG	UNP P58154
F	-7	ASP	-	EXPRESSION TAG	UNP P58154
F	-6	TYR	-	EXPRESSION TAG	UNP P58154
F	-5	LYS	-	EXPRESSION TAG	UNP P58154
F	-4	ASP	-	EXPRESSION TAG	UNP P58154
F	-3	ASP	-	EXPRESSION TAG	UNP P58154
F	-2	ASP	-	EXPRESSION TAG	UNP P58154
F	-1	ASP	-	EXPRESSION TAG	UNP P58154
F	0	LYS	-	EXPRESSION TAG	UNP P58154
G	-7	ASP	-	EXPRESSION TAG	UNP P58154
G	-6	TYR	-	EXPRESSION TAG	UNP P58154
G	-5	LYS	-	EXPRESSION TAG	UNP P58154

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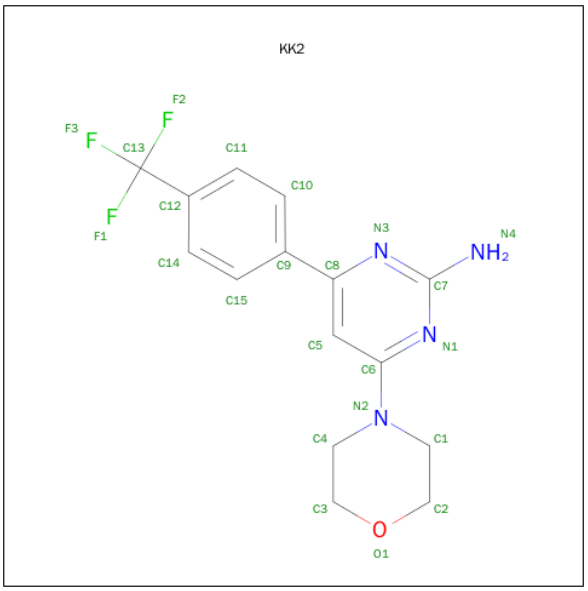
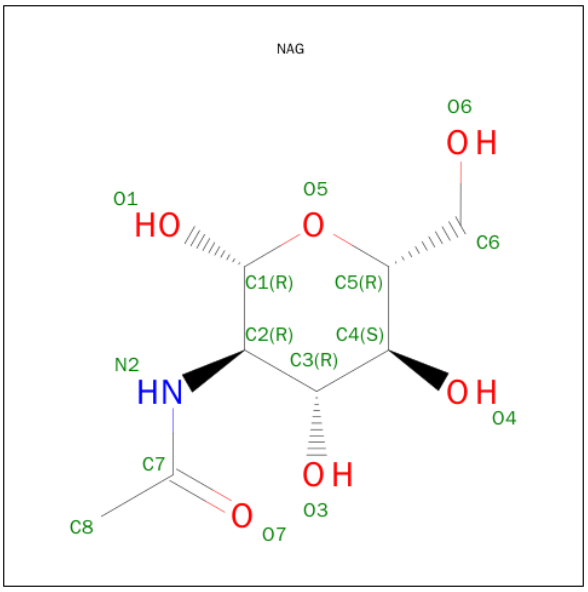
Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	ASP	-	EXPRESSION TAG	UNP P58154
G	-3	ASP	-	EXPRESSION TAG	UNP P58154
G	-2	ASP	-	EXPRESSION TAG	UNP P58154
G	-1	ASP	-	EXPRESSION TAG	UNP P58154
G	0	LYS	-	EXPRESSION TAG	UNP P58154
H	-7	ASP	-	EXPRESSION TAG	UNP P58154
H	-6	TYR	-	EXPRESSION TAG	UNP P58154
H	-5	LYS	-	EXPRESSION TAG	UNP P58154
H	-4	ASP	-	EXPRESSION TAG	UNP P58154
H	-3	ASP	-	EXPRESSION TAG	UNP P58154
H	-2	ASP	-	EXPRESSION TAG	UNP P58154
H	-1	ASP	-	EXPRESSION TAG	UNP P58154
H	0	LYS	-	EXPRESSION TAG	UNP P58154
I	-7	ASP	-	EXPRESSION TAG	UNP P58154
I	-6	TYR	-	EXPRESSION TAG	UNP P58154
I	-5	LYS	-	EXPRESSION TAG	UNP P58154
I	-4	ASP	-	EXPRESSION TAG	UNP P58154
I	-3	ASP	-	EXPRESSION TAG	UNP P58154
I	-2	ASP	-	EXPRESSION TAG	UNP P58154
I	-1	ASP	-	EXPRESSION TAG	UNP P58154
I	0	LYS	-	EXPRESSION TAG	UNP P58154
J	-7	ASP	-	EXPRESSION TAG	UNP P58154
J	-6	TYR	-	EXPRESSION TAG	UNP P58154
J	-5	LYS	-	EXPRESSION TAG	UNP P58154
J	-4	ASP	-	EXPRESSION TAG	UNP P58154
J	-3	ASP	-	EXPRESSION TAG	UNP P58154
J	-2	ASP	-	EXPRESSION TAG	UNP P58154
J	-1	ASP	-	EXPRESSION TAG	UNP P58154
J	0	LYS	-	EXPRESSION TAG	UNP P58154

- Molecule 2 is 4-(MORPHOLIN-4-YL)-6-[4-(TRIFLUOROMETHYL)PHENYL]PYRIMIDIN-2-AMINE (three-letter code: KK2) (formula: $C_{15}H_{15}F_3N_4O$).



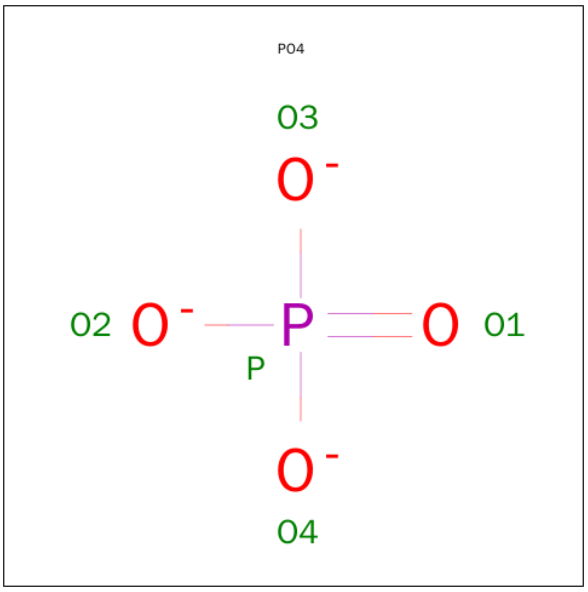
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	B	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	C	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	D	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	E	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	F	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	G	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	H	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	I	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	J	1	Total	C	F	N	O	0	0
			23	15	3	4	1		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	E	1	Total C N O 14 8 1 5	0	0
3	G	1	Total C N O 14 8 1 5	0	0
3	H	1	Total C N O 14 8 1 5	0	0
3	I	1	Total C N O 14 8 1 5	0	0
3	J	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0
4	G	1	Total O P 5 4 1	0	0
4	H	1	Total O P 5 4 1	0	0
4	I	1	Total O P 5 4 1	0	0
4	J	1	Total O P 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	6	Total O 6 6	0	0
5	B	3	Total O 3 3	0	0

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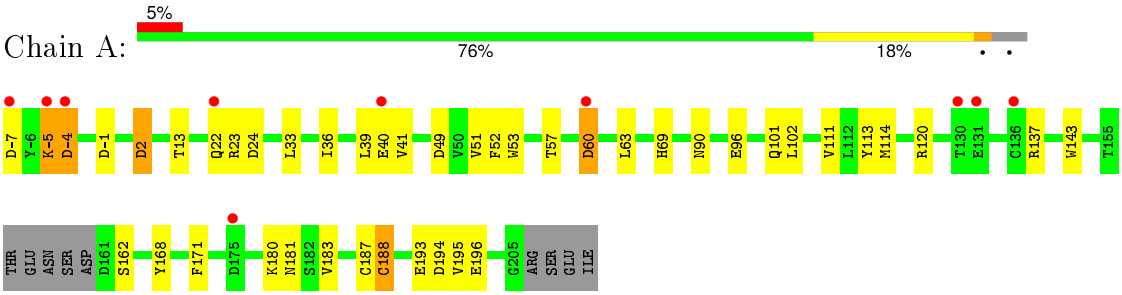
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O 1 1	0	0
5	D	3	Total O 3 3	0	0
5	E	4	Total O 4 4	0	0
5	F	3	Total O 3 3	0	0
5	G	1	Total O 1 1	0	0
5	I	2	Total O 2 2	0	0
5	J	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

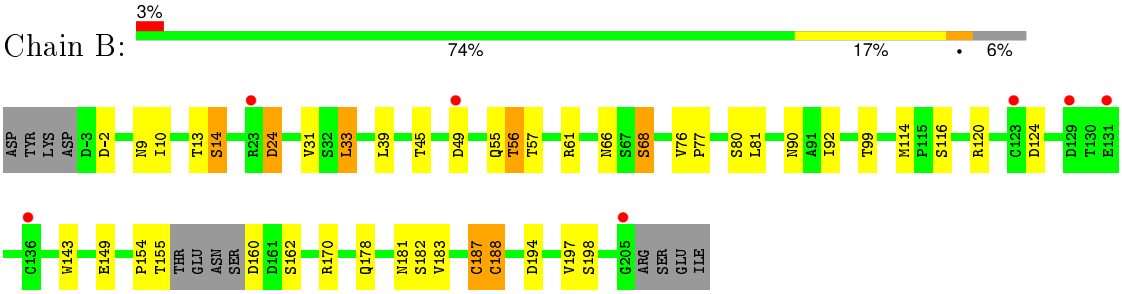
- Molecule 1: Acetylcholine-binding protein

Chain A:



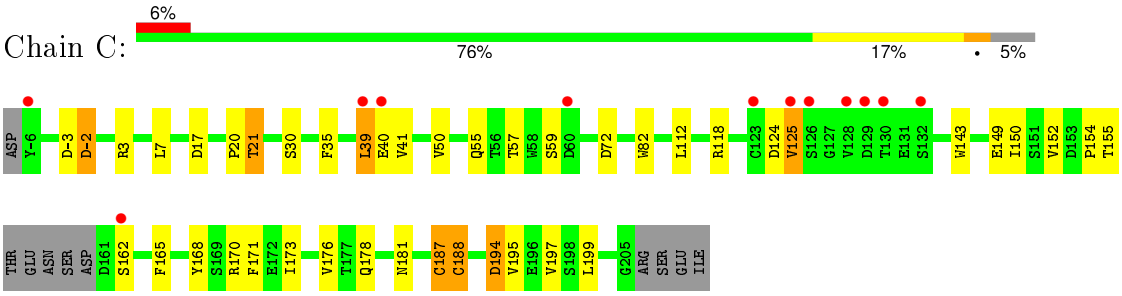
- Molecule 1: Acetylcholine-binding protein

Chain B:



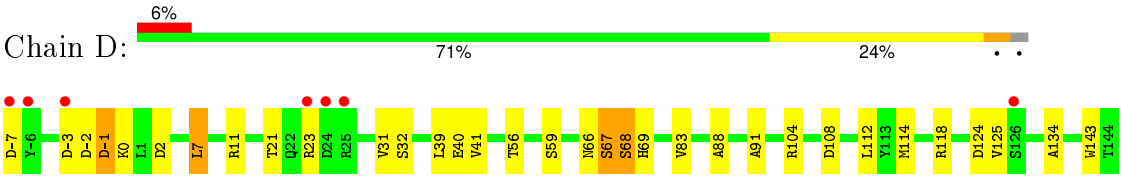
- Molecule 1: Acetylcholine-binding protein

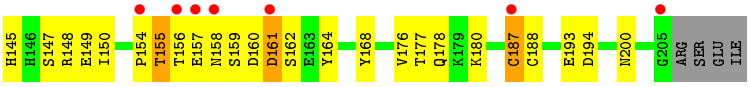
Chain C:



- Molecule 1: Acetylcholine-binding protein

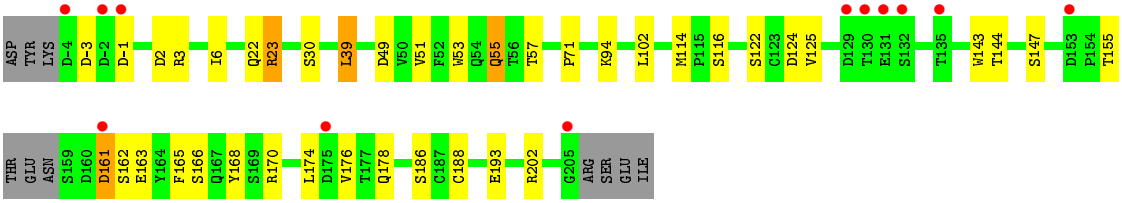
Chain D:





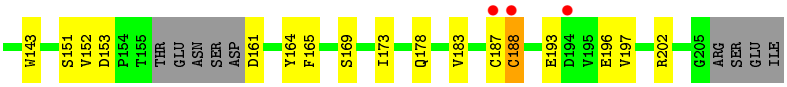
• Molecule 1: Acetylcholine-binding protein

Chain E:



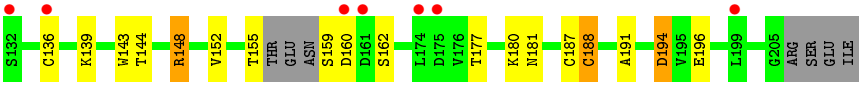
• Molecule 1: Acetylcholine-binding protein

Chain F:



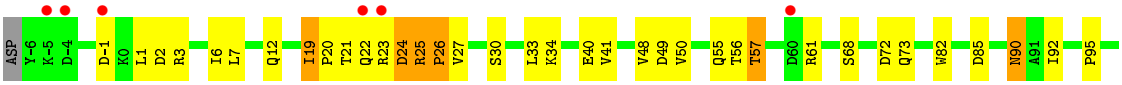
• Molecule 1: Acetylcholine-binding protein

Chain G:



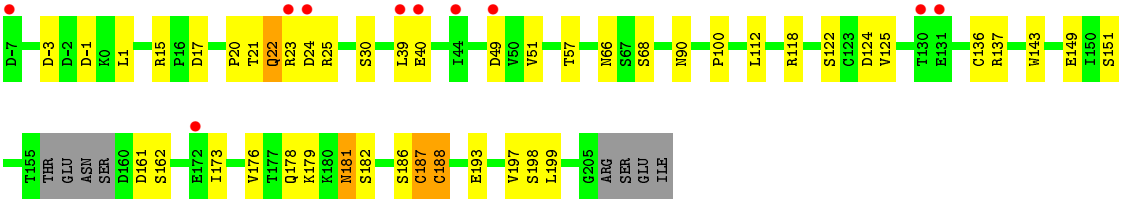
• Molecule 1: Acetylcholine-binding protein

Chain H:



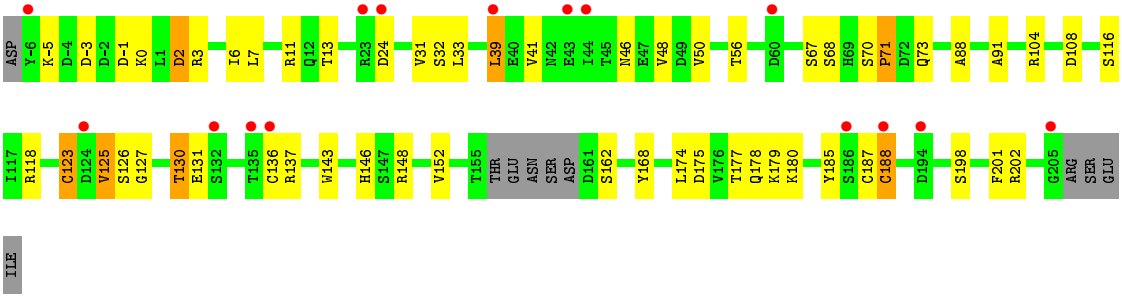
• Molecule 1: Acetylcholine-binding protein

Chain I:



- Molecule 1: Acetylcholine-binding protein

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.64Å 134.01Å 147.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 2.98 49.52 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.52-2.98) 97.4 (49.52-2.98)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	9.32 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.150 , 0.233 0.179 , 0.248	Depositor DCC
R_{free} test set	2000 reflections (4.28%)	DCC
Wilson B-factor (Å^2)	51.5	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 49488 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17236	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4, NAG, KK2

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	0.51	0/1712	0.60	0/2333
1	B	0.46	0/1691	0.60	0/2305
1	C	0.41	0/1704	0.58	0/2322
1	D	0.46	0/1751	0.58	0/2388
1	E	0.45	0/1705	0.59	0/2324
1	F	0.50	0/1737	0.59	0/2367
1	G	0.46	0/1735	0.59	0/2364
1	H	0.58	2/1735 (0.1%)	0.69	3/2364 (0.1%)
1	I	0.44	0/1746	0.59	0/2379
1	J	0.47	1/1721 (0.1%)	0.61	0/2345
All	All	0.48	3/17237 (0.0%)	0.60	3/23491 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	26	PRO	N-CD	5.11	1.55	1.47
1	J	71	PRO	N-CD	5.06	1.54	1.47
1	H	154	PRO	N-CD	5.04	1.54	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	153	ASP	C-N-CD	5.87	140.72	128.40
1	H	25	ARG	C-N-CD	5.72	140.42	128.40
1	H	19	ILE	C-N-CD	5.62	140.20	128.40

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	1673	0	1610	28	0
1	B	1650	0	1590	25	0
1	C	1665	0	1606	28	0
1	D	1711	0	1639	55	0
1	E	1664	0	1599	25	0
1	F	1689	0	1625	33	0
1	G	1693	0	1625	33	0
1	H	1690	0	1625	36	0
1	I	1694	0	1630	36	0
1	J	1676	0	1618	43	0
2	A	23	0	15	2	0
2	B	23	0	15	1	0
2	C	23	0	15	3	0
2	D	23	0	15	1	0
2	E	23	0	15	1	0
2	F	23	0	15	1	0
2	G	23	0	15	2	0
2	H	23	0	15	1	0
2	I	23	0	15	2	0
2	J	23	0	15	2	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
3	E	14	0	13	0	0
3	G	14	0	13	0	0
3	H	14	0	13	2	0
3	I	14	0	13	1	0
3	J	14	0	13	0	0
4	A	5	0	0	0	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
4	E	10	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	1	0
4	I	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	5	0	0	1	0
5	A	6	0	0	0	0
5	B	3	0	0	0	0
5	C	1	0	0	0	0
5	D	3	0	0	0	0
5	E	4	0	0	0	0
5	F	3	0	0	0	0
5	G	1	0	0	0	0
5	I	2	0	0	0	0
5	J	2	0	0	0	0
All	All	17236	0	16434	312	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 (312) 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:D:156:THR:CG2	1:D:178:GLN:HB2	1.43	1.47
1:D:156:THR:HG21	1:D:178:GLN:CB	1.59	1.31
1:J:123:CYS:SG	1:J:136:CYS:HB3	1.85	1.17
1:D:156:THR:HB	1:D:157:GLU:CG	1.76	1.16
1:F:21:THR:HG21	1:G:-2:ASP:HB3	1.14	1.12
1:C:162:SER:HB2	1:C:165:PHE:HB2	1.31	1.12
1:D:156:THR:CB	1:D:157:GLU:HG2	1.80	1.10
1:D:32:SER:HB2	1:D:155:THR:HG21	1.40	1.04
1:E:22:GLN:C	1:E:23:ARG:HG2	1.81	0.98
1:D:156:THR:HB	1:D:157:GLU:HG2	0.98	0.98
1:D:156:THR:CG2	1:D:178:GLN:CB	2.28	0.95
1:D:156:THR:HG23	1:D:178:GLN:NE2	1.83	0.93
1:H:26:PRO:HG3	1:H:148:ARG:O	1.67	0.93
1:F:21:THR:CG2	1:G:-2:ASP:HB3	2.00	0.87
1:J:123:CYS:SG	1:J:136:CYS:CB	2.62	0.87
1:F:21:THR:HG21	1:G:-2:ASP:CB	2.05	0.85
1:B:92:ILE:HD12	1:C:39:LEU:HD11	1.59	0.83
1:H:24:ASP:O	1:H:25:ARG:HG3	1.79	0.82
1:A:60:ASP:OD1	1:A:63:LEU:HD12	1.78	0.82
1:D:156:THR:HG23	1:D:178:GLN:HE21	1.44	0.80
1:A:39:LEU:HD11	1:A:51:VAL:HG23	1.63	0.79
1:D:32:SER:HB2	1:D:155:THR:CG2	2.14	0.78
1:C:162:SER:HB2	1:C:165:PHE:CB	2.12	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ASP:HB2	1:D:176:VAL:CG2	2.14	0.77
1:D:156:THR:CG2	1:D:178:GLN:NE2	2.48	0.76
1:A:187:CYS:SG	1:A:188:CYS:N	2.58	0.76
1:I:187:CYS:SG	1:I:188:CYS:N	2.58	0.76
1:I:39:LEU:CD2	1:I:51:VAL:HG23	2.17	0.75
1:J:39:LEU:HD13	1:J:118:ARG:HE	1.51	0.75
1:A:40:GLU:H	1:A:49:ASP:HB3	1.53	0.74
1:H:34:LYS:HD2	1:H:164:TYR:HE1	1.53	0.73
1:J:136:CYS:SG	1:J:201:PHE:HE1	2.12	0.73
1:G:55:GLN:HA	1:G:114:MET:HG2	1.71	0.72
1:A:40:GLU:HB2	1:A:49:ASP:HB2	1.71	0.72
1:G:41:VAL:HG22	1:G:48:VAL:HG12	1.70	0.72
1:F:164:TYR:HE2	1:J:185:TYR:CD1	2.07	0.72
1:F:55:GLN:HA	1:F:114:MET:HG2	1.72	0.72
1:H:21:THR:HA	1:H:27:VAL:HG22	1.72	0.72
1:J:187:CYS:SG	1:J:188:CYS:N	2.65	0.69
1:E:22:GLN:O	1:E:23:ARG:HG2	1.93	0.69
1:J:39:LEU:HD22	1:J:118:ARG:NH2	2.08	0.69
1:D:161:ASP:HB2	1:D:176:VAL:HG21	1.75	0.69
1:F:30:SER:HB2	1:F:57:THR:HG23	1.76	0.68
1:A:23:ARG:O	1:A:24:ASP:HB2	1.94	0.68
1:I:39:LEU:O	1:I:40:GLU:HG3	1.95	0.67
1:I:39:LEU:HB2	1:I:49[A]:ASP:HB3	1.76	0.67
1:D:39:LEU:C	1:D:40:GLU:HG3	2.15	0.67
1:D:143:TRP:CE2	2:D:301:KK2:H15	2.30	0.67
1:H:143:TRP:CE2	2:H:301:KK2:H15	2.31	0.66
1:D:161:ASP:CB	1:D:176:VAL:CG2	2.74	0.66
1:E:55:GLN:HG3	1:E:114:MET:HG2	1.78	0.65
1:B:45:THR:HA	1:C:170:ARG:HD2	1.79	0.65
1:I:39:LEU:HD21	1:I:51:VAL:HG23	1.77	0.65
1:D:155:THR:HG23	1:D:155:THR:O	1.97	0.64
1:H:30:SER:HB2	1:H:57:THR:HG23	1.79	0.64
1:B:187:CYS:SG	1:B:188:CYS:N	2.71	0.63
1:G:187:CYS:SG	1:G:188:CYS:N	2.71	0.63
1:C:41:VAL:HG21	1:C:171:PHE:CZ	2.33	0.63
1:J:32:SER:O	1:J:33:LEU:HD23	1.99	0.63
1:G:19:ILE:HD12	1:G:21:THR:HG23	1.80	0.63
1:F:57:THR:HB	1:F:112:LEU:HD23	1.80	0.63
1:J:3:ARG:NH1	4:J:303:PO4:O2	2.32	0.62
3:H:302:NAG:O7	3:H:302:NAG:O3	2.11	0.62
1:D:161:ASP:CB	1:D:176:VAL:HG23	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:SER:HB2	1:D:160:ASP:HB2	1.81	0.62
1:D:161:ASP:HB2	1:D:176:VAL:HG23	1.79	0.62
1:G:-1:ASP:HB2	1:G:2:ASP:HB2	1.82	0.61
1:I:30:SER:HB2	1:I:57:THR:HG23	1.82	0.61
1:I:39:LEU:HD23	1:I:51:VAL:HG23	1.82	0.60
1:B:55:GLN:HA	1:B:114:MET:HG2	1.83	0.60
1:J:41:VAL:HG13	1:J:125:VAL:HG11	1.83	0.60
1:G:-1:ASP:OD2	1:G:-1:ASP:N	2.34	0.60
1:E:22:GLN:HB3	1:E:23:ARG:NE	2.16	0.60
1:B:9:ASN:HD22	1:I:1:LEU:HD21	1.66	0.60
1:A:-1:ASP:HB3	1:A:2:ASP:HB2	1.84	0.60
1:H:85:ASP:HB2	1:I:100:PRO:HG2	1.83	0.60
1:C:162:SER:HB3	1:C:173:ILE:HD12	1.83	0.60
1:I:143:TRP:CE2	2:I:301:KK2:H15	2.36	0.60
1:A:24:ASP:HA	1:B:-2:ASP:HB3	1.85	0.59
1:E:174:LEU:HD11	1:E:202:ARG:HG2	1.84	0.59
1:D:156:THR:CG2	1:D:178:GLN:CG	2.80	0.59
1:J:39:LEU:HD22	1:J:118:ARG:HH21	1.68	0.59
1:B:143:TRP:CE2	2:B:301:KK2:H15	2.37	0.58
1:F:49:ASP:OD1	1:F:120:ARG:HG2	2.03	0.58
1:B:24:ASP:HA	1:C:-2:ASP:HB2	1.86	0.58
1:E:30:SER:HB3	1:E:57:THR:HG23	1.85	0.58
1:F:139:LYS:HG3	1:F:196:GLU:HG3	1.85	0.58
1:D:158:ASN:HA	1:D:159:SER:C	2.24	0.58
1:G:118:ARG:HE	1:G:120:ARG:HH12	1.50	0.58
1:H:34:LYS:HD2	1:H:164:TYR:CE1	2.38	0.58
1:I:137:ARG:NH1	1:I:198:SER:OG	2.37	0.57
1:D:31:VAL:O	1:D:155:THR:HB	2.05	0.57
1:H:49[B]:ASP:OD1	1:H:120:ARG:NE	2.35	0.57
1:D:-1:ASP:OD2	1:D:-1:ASP:N	2.37	0.57
1:C:143:TRP:CE2	2:C:301:KK2:H15	2.39	0.57
1:B:49[B]:ASP:CG	1:B:120:ARG:HG2	2.25	0.57
1:C:41:VAL:HG13	1:C:125:VAL:HG11	1.86	0.57
1:F:187:CYS:SG	1:F:188:CYS:N	2.77	0.57
1:J:136:CYS:SG	1:J:201:PHE:CE1	2.95	0.57
1:F:46:ASN:HB3	1:F:123:CYS:O	2.05	0.57
1:G:127:GLY:HA2	1:G:130:THR:HG23	1.87	0.57
1:E:39:LEU:HD21	1:E:51:VAL:HG23	1.87	0.57
1:J:137:ARG:HH12	1:J:179:LYS:NZ	2.03	0.57
1:I:39:LEU:HD21	1:I:51:VAL:CG2	2.35	0.56
1:D:154:PRO:HD3	1:D:180:LYS:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:17:ASP:OD2	1:J:11:ARG:NH2	2.38	0.56
1:J:39:LEU:HD13	1:J:118:ARG:NE	2.20	0.56
1:H:21:THR:HA	1:H:27:VAL:CG2	2.35	0.56
1:E:55:GLN:HA	1:E:114:MET:HG2	1.88	0.56
1:I:39:LEU:CD1	1:I:118:ARG:NH1	2.69	0.56
1:D:156:THR:HG21	1:D:178:GLN:HB2	0.62	0.56
1:J:185:TYR:OH	2:J:301:KK2:H1	2.06	0.56
1:F:47:GLU:HB3	1:F:120:ARG:HH21	1.71	0.56
1:B:178:GLN:HG2	1:B:197:VAL:HG22	1.88	0.55
1:C:20:PRO:HA	1:D:0:LYS:HD2	1.88	0.55
1:I:20:PRO:HA	1:J:0:LYS:HE3	1.89	0.55
1:H:-1:ASP:HB3	1:H:2:ASP:HB2	1.88	0.55
1:F:40:GLU:HB2	1:F:49:ASP:HB2	1.89	0.55
1:C:187:CYS:SG	1:C:188:CYS:N	2.80	0.55
1:F:41:VAL:HG13	1:F:125:VAL:HG11	1.89	0.54
1:H:26:PRO:HG3	1:H:148:ARG:C	2.28	0.54
1:J:123:CYS:HG	1:J:136:CYS:CB	2.20	0.54
1:I:23:ARG:HB3	1:I:25:ARG:HH21	1.72	0.54
2:C:301:KK2:H6	1:D:164:TYR:CD1	2.42	0.54
1:F:37:ASN:OD1	1:F:169:SER:HB2	2.07	0.54
1:D:155:THR:CG2	1:D:155:THR:O	2.54	0.54
1:F:24:ASP:HA	1:G:-2:ASP:HB2	1.90	0.54
1:J:146:HIS:CE1	1:J:148:ARG:HG3	2.43	0.54
1:D:156:THR:CG2	1:D:178:GLN:CD	2.76	0.54
1:G:148:ARG:HH22	1:G:191:ALA:H	1.54	0.54
1:D:41:VAL:CG1	1:D:125:VAL:HG11	2.37	0.54
1:J:88:ALA:HB3	1:J:91:ALA:HB2	1.90	0.53
1:H:55:GLN:HA	1:H:114:MET:HG2	1.88	0.53
3:H:302:NAG:HO3	3:H:302:NAG:C7	2.15	0.53
1:J:41:VAL:HG22	1:J:48:VAL:HG23	1.91	0.52
1:H:48:VAL:HG21	1:H:123:CYS:SG	2.49	0.52
1:J:131:GLU:O	1:J:202:ARG:NH1	2.42	0.52
1:H:41:VAL:HG22	1:H:48:VAL:HG12	1.90	0.52
1:B:31:VAL:HG22	1:B:56:THR:HG23	1.90	0.52
1:E:143:TRP:CE2	2:E:301:KK2:H15	2.44	0.52
1:C:17:ASP:OD2	1:D:11:ARG:NH2	2.43	0.52
1:I:149:GLU:OE2	1:J:3:ARG:NH2	2.43	0.52
1:G:60:ASP:O	1:G:109:GLY:HA3	2.08	0.52
1:D:124:ASP:HB2	1:E:168:TYR:CE1	2.44	0.52
1:J:137:ARG:HH12	1:J:179:LYS:HZ1	1.57	0.52
1:H:40:GLU:OE1	1:H:120:ARG:NH2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:-1:ASP:HB3	1:J:2:ASP:HB2	1.91	0.51
1:I:22:GLN:CG	1:I:23:ARG:HD2	2.40	0.51
1:B:124:ASP:HB2	1:C:168:TYR:CE1	2.46	0.51
1:H:19:ILE:HG22	1:H:82:TRP:CZ2	2.46	0.51
1:I:23:ARG:CB	1:I:25:ARG:HH21	2.23	0.51
1:H:123:CYS:O	1:H:125:VAL:HG23	2.10	0.51
1:F:21:THR:CG2	1:G:-2:ASP:O	2.59	0.51
1:I:39:LEU:HD12	1:I:118:ARG:NH1	2.25	0.51
1:A:102:LEU:HB2	1:E:144:THR:HG21	1.92	0.51
1:C:154:PRO:HD3	1:C:195:VAL:HG22	1.92	0.51
1:F:164:TYR:HE2	1:J:185:TYR:HD1	1.55	0.50
1:H:90:ASN:HD21	1:H:138:ILE:HA	1.75	0.50
1:E:22:GLN:HB3	1:E:23:ARG:CZ	2.42	0.50
1:I:39:LEU:HB2	1:I:49[B]:ASP:HB2	1.92	0.50
1:J:152:VAL:O	1:J:180:LYS:NZ	2.42	0.50
1:I:161:ASP:OD2	1:I:176:VAL:HG21	2.11	0.50
1:B:181:ASN:HB3	1:B:194:ASP:OD1	2.12	0.50
1:H:41:VAL:HG13	1:H:125:VAL:HG11	1.93	0.50
1:F:143:TRP:CE2	2:F:301:KK2:H15	2.47	0.50
1:G:36:ILE:HD11	1:G:53:TRP:HB2	1.94	0.50
1:C:41:VAL:CG2	1:C:171:PHE:CZ	2.94	0.49
1:H:3:ARG:NH2	4:H:303:PO4:O1	2.27	0.49
1:E:162:SER:HA	1:E:165:PHE:HB3	1.94	0.49
1:A:39:LEU:HD11	1:A:51:VAL:CG2	2.38	0.49
1:D:187:CYS:SG	1:D:188:CYS:N	2.86	0.49
1:D:39:LEU:O	1:D:40:GLU:HG3	2.13	0.49
1:H:48:VAL:CG2	1:H:123:CYS:SG	3.00	0.49
1:D:88:ALA:HB3	1:D:91:ALA:HB2	1.94	0.49
1:J:143:TRP:CE2	2:J:301:KK2:H15	2.48	0.49
1:I:66:ASN:ND2	3:I:302:NAG:H61	2.27	0.49
1:I:178:GLN:HG2	1:I:197:VAL:HG13	1.93	0.49
1:G:144:THR:HG21	1:H:102:LEU:HB2	1.95	0.48
1:G:41:VAL:HG13	1:G:125:VAL:HG11	1.95	0.48
1:H:187:CYS:SG	1:H:188:CYS:N	2.86	0.48
1:D:39:LEU:HD12	1:D:118:ARG:HE	1.78	0.48
1:G:19:ILE:HG22	1:G:82:TRP:CZ2	2.49	0.48
1:A:41:VAL:HG21	1:A:171:PHE:CZ	2.48	0.48
1:I:124:ASP:HB2	1:J:168:TYR:CE1	2.49	0.48
1:D:66:ASN:OD1	1:D:68:SER:OG	2.32	0.48
1:A:33:LEU:HD22	1:A:52:PHE:CD1	2.48	0.48
1:J:108:ASP:N	1:J:108:ASP:OD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194[B]:ASP:OD1	1:A:195:VAL:N	2.46	0.47
1:H:22:GLN:O	1:H:23:ARG:C	2.51	0.47
1:J:33:LEU:H	1:J:178:GLN:HE22	1.63	0.47
1:G:139:LYS:HG2	1:G:196:GLU:HG3	1.95	0.47
1:G:118:ARG:HE	1:G:120:ARG:NH1	2.13	0.47
1:G:143:TRP:CZ2	1:H:99:THR:HG21	2.50	0.47
1:H:112:LEU:HD23	1:H:114:MET:HE3	1.96	0.47
1:D:68:SER:O	1:D:69:HIS:ND1	2.47	0.47
1:J:137:ARG:NH1	1:J:179:LYS:NZ	2.62	0.47
1:C:21:THR:HG21	1:D:-2:ASP:O	2.15	0.47
2:G:301:KK2:H6	1:H:164:TYR:CD2	2.50	0.47
1:F:-1:ASP:HB3	1:F:2:ASP:HB2	1.97	0.47
1:E:147:SER:HB3	1:E:193:GLU:HG3	1.97	0.47
1:A:60:ASP:OD1	1:A:63:LEU:CD1	2.58	0.46
1:A:39:LEU:CD1	1:A:51:VAL:HG23	2.40	0.46
1:E:39:LEU:HD23	1:E:49[A]:ASP:OD1	2.15	0.46
1:I:22:GLN:HG2	1:I:23:ARG:HD2	1.98	0.46
1:A:137:ARG:HD3	1:A:196:GLU:OE2	2.16	0.46
1:J:67:SER:HA	1:J:70:SER:HB2	1.98	0.46
1:D:156:THR:HG22	1:D:178:GLN:CD	2.35	0.46
1:E:161:ASP:O	1:E:162:SER:HB2	2.15	0.46
1:F:165:PHE:CD1	1:F:173:ILE:HD11	2.51	0.46
1:I:173:ILE:HG12	1:I:199:LEU:HD11	1.98	0.46
1:E:6:ILE:HD12	1:E:71:PRO:HG2	1.98	0.46
1:H:22:GLN:HE22	1:H:61:ARG:HH11	1.62	0.45
1:D:161:ASP:CB	1:D:176:VAL:HG21	2.42	0.45
1:D:149:GLU:OE2	1:E:3:ARG:NH2	2.49	0.45
1:A:53:TRP:HE1	1:A:114:MET:HB3	1.82	0.45
1:G:60:ASP:O	1:G:109:GLY:CA	2.64	0.45
1:D:162:SER:OG	1:D:162:SER:O	2.33	0.45
1:I:57:THR:HB	1:I:112:LEU:HD23	1.98	0.45
1:F:48:VAL:HG12	1:F:123:CYS:SG	2.56	0.45
1:F:41:VAL:CG1	1:F:125:VAL:HG11	2.46	0.45
1:A:22:GLN:O	1:A:23:ARG:HB2	2.16	0.45
1:A:101:GLN:HG2	1:A:113:TYR:OH	2.17	0.45
1:J:127:GLY:HA2	1:J:130:THR:HG23	1.99	0.45
1:H:95:PRO:HG3	1:H:119:GLN:NE2	2.31	0.45
1:A:143:TRP:CE2	2:A:301:KK2:H12	2.52	0.45
1:F:40:GLU:O	1:F:41:VAL:HG23	2.17	0.45
1:D:158:ASN:HB3	1:D:160:ASP:HA	1.98	0.44
1:C:124:ASP:HB2	1:D:168:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1:LEU:HA	1:I:1:LEU:HD12	1.69	0.44
1:B:10:ILE:O	1:B:14:SER:HB3	2.17	0.44
1:F:151:SER:HA	1:F:193[B]:GLU:OE1	2.17	0.44
1:B:49[B]:ASP:OD2	1:B:120:ARG:HG2	2.17	0.44
1:A:180:LYS:HE3	1:A:193:GLU:OE1	2.17	0.44
1:I:39:LEU:CB	1:I:49[A]:ASP:HB3	2.45	0.44
1:A:96:GLU:HG3	1:E:94:LYS:HD2	1.99	0.44
1:D:159:SER:HA	1:D:160:ASP:HA	1.49	0.44
1:B:80:SER:O	1:B:81:LEU:HD23	2.18	0.44
1:A:168:TYR:CE1	1:E:124:ASP:HB2	2.53	0.44
1:B:9:ASN:ND2	1:I:1:LEU:HD21	2.33	0.44
1:C:30:SER:HB3	1:C:155:THR:HG22	1.99	0.44
1:D:-7:ASP:N	1:D:67:SER:O	2.50	0.43
1:G:152:VAL:O	1:G:180:LYS:HE3	2.17	0.43
1:G:181:ASN:HB3	1:G:194[A]:ASP:OD2	2.18	0.43
1:A:-4:ASP:OD1	1:A:69:HIS:O	2.35	0.43
1:C:152:VAL:HG23	1:C:152:VAL:O	2.16	0.43
1:A:-7:ASP:OD1	1:A:-5:LYS:HB2	2.18	0.43
1:D:134:ALA:O	1:D:200:ASN:ND2	2.39	0.43
1:G:60:ASP:O	1:G:109:GLY:O	2.37	0.43
1:A:60:ASP:OD2	1:A:111:VAL:HG23	2.18	0.43
1:E:53:TRP:CZ2	1:E:114:MET:HE3	2.54	0.43
1:E:161:ASP:OD2	1:E:176:VAL:HG23	2.18	0.43
1:C:181:ASN:HB2	1:C:194:ASP:OD1	2.18	0.43
1:G:143:TRP:CE2	2:G:301:KK2:H15	2.53	0.43
1:F:39:LEU:HD12	1:F:49:ASP:HB3	2.00	0.43
1:D:145:HIS:HB2	1:D:150:ILE:HD12	2.01	0.43
1:F:42:ASN:OD1	1:F:44:ILE:HB	2.19	0.43
1:C:176:VAL:HG22	1:C:199:LEU:HD13	2.01	0.43
1:C:35:PHE:CZ	1:C:199:LEU:HD22	2.53	0.43
1:B:39:LEU:O	1:B:170:ARG:NH1	2.52	0.43
1:E:22:GLN:O	1:E:23:ARG:CG	2.65	0.43
1:H:2:ASP:O	1:H:6:ILE:HG13	2.19	0.42
1:J:174:LEU:HD21	1:J:202:ARG:HG2	2.00	0.42
2:A:301:KK2:H1	2:A:301:KK2:H9	1.85	0.42
1:H:73:GLN:NE2	1:H:104:ARG:HH21	2.17	0.42
1:J:46:ASN:OD1	1:J:125:VAL:HG23	2.19	0.42
1:J:73:GLN:HG3	1:J:104:ARG:HH21	1.84	0.42
1:D:7:LEU:HD22	1:D:11:ARG:HE	1.83	0.42
1:J:-5:LYS:HE2	1:J:-5:LYS:HB3	1.78	0.42
1:D:157:GLU:OE2	1:D:177:THR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:GLN:HG2	1:F:197:VAL:HG22	2.01	0.42
1:I:22:GLN:HG3	1:I:23:ARG:HD2	2.00	0.42
1:F:152:VAL:HG22	1:F:193[A]:GLU:CG	2.50	0.42
1:G:159:SER:HA	1:G:160:ASP:HA	1.74	0.42
1:C:3:ARG:NH2	4:C:303:PO4:O3	2.37	0.42
1:F:40:GLU:C	1:F:41:VAL:HG23	2.40	0.42
1:I:151:SER:HB2	1:I:193:GLU:OE1	2.20	0.42
1:I:39:LEU:HD11	1:I:118:ARG:NH1	2.35	0.41
1:B:90:ASN:OD1	1:B:90:ASN:N	2.53	0.41
1:B:99:THR:HG23	1:B:116:SER:HB3	2.02	0.41
1:D:156:THR:HB	1:D:157:GLU:CA	2.49	0.41
1:F:22:GLN:NE2	1:F:61:ARG:HD3	2.34	0.41
1:J:7:LEU:HD12	1:J:7:LEU:HA	1.86	0.41
1:B:76:VAL:HG12	1:B:77:PRO:O	2.20	0.41
1:C:82:TRP:HZ2	1:C:150:ILE:HD11	1.85	0.41
1:B:92:ILE:HD12	1:C:39:LEU:CD1	2.40	0.41
1:B:33:LEU:HG	1:B:197:VAL:HG21	2.03	0.41
1:J:2:ASP:HB3	1:J:71:PRO:HD3	2.02	0.41
1:G:48:VAL:HG22	1:G:123:CYS:SG	2.60	0.41
1:G:1:LEU:HD12	1:G:1:LEU:HA	1.87	0.41
1:C:178:GLN:HG2	1:C:197:VAL:HG22	2.03	0.41
1:G:143:TRP:CE2	1:H:99:THR:HG21	2.56	0.41
2:C:301:KK2:F3	1:D:104:ARG:HG3	2.11	0.41
1:A:33:LEU:HD22	1:A:52:PHE:HD1	1.86	0.41
1:G:-4:ASP:O	1:G:71:PRO:HA	2.21	0.41
1:A:36:ILE:HB	1:A:51:VAL:O	2.21	0.41
1:C:-2:ASP:N	1:C:-2:ASP:OD1	2.53	0.41
1:H:33:LEU:H	1:H:178:GLN:HE22	1.69	0.41
1:E:102:LEU:HA	1:E:102:LEU:HD23	1.87	0.41
1:B:92:ILE:O	1:C:118:ARG:HD2	2.20	0.40
2:I:301:KK2:F3	1:J:104:ARG:HG2	2.11	0.40
1:F:48:VAL:CG1	1:F:123:CYS:SG	3.09	0.40
1:B:66:ASN:OD1	1:B:68:SER:OG	2.39	0.40
1:D:147:SER:HB3	1:D:193:GLU:HG3	2.04	0.40
1:H:127:GLY:HA2	1:H:130:THR:HG23	2.03	0.40
1:J:6:ILE:HD11	1:J:71:PRO:HD2	2.03	0.40
1:H:1:LEU:HA	1:H:1:LEU:HD12	1.81	0.40
1:G:7:LEU:CD1	1:G:76:VAL:HG22	2.51	0.40
1:J:146:HIS:HE1	1:J:148:ARG:HG3	1.87	0.40
1:I:90:ASN:N	1:I:90:ASN:OD1	2.54	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	205/217 (94%)	196 (96%)	9 (4%)	0	100	100
1	B	203/217 (94%)	196 (97%)	6 (3%)	1 (0%)	34	75
1	C	204/217 (94%)	198 (97%)	6 (3%)	0	100	100
1	D	212/217 (98%)	208 (98%)	4 (2%)	0	100	100
1	E	205/217 (94%)	204 (100%)	1 (0%)	0	100	100
1	F	208/217 (96%)	199 (96%)	9 (4%)	0	100	100
1	G	208/217 (96%)	204 (98%)	4 (2%)	0	100	100
1	H	208/217 (96%)	205 (99%)	3 (1%)	0	100	100
1	I	209/217 (96%)	208 (100%)	1 (0%)	0	100	100
1	J	206/217 (95%)	203 (98%)	3 (2%)	0	100	100
All	All	2068/2170 (95%)	2021 (98%)	46 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	154	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	195/203 (96%)	183 (94%)	12 (6%)	23	59
1	B	193/203 (95%)	176 (91%)	17 (9%)	12	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	194/203 (96%)	176 (91%)	18 (9%)	11 38
1	D	200/203 (98%)	181 (90%)	19 (10%)	11 36
1	E	195/203 (96%)	178 (91%)	17 (9%)	13 41
1	F	198/203 (98%)	177 (89%)	21 (11%)	8 30
1	G	198/203 (98%)	181 (91%)	17 (9%)	13 42
1	H	198/203 (98%)	183 (92%)	15 (8%)	16 49
1	I	199/203 (98%)	182 (92%)	17 (8%)	13 43
1	J	196/203 (97%)	177 (90%)	19 (10%)	10 35
All	All	1966/2030 (97%)	1794 (91%)	172 (9%)	13 41

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	LYS
1	A	-4	ASP
1	A	2	ASP
1	A	13	THR
1	A	57	THR
1	A	60	ASP
1	A	90	ASN
1	A	120	ARG
1	A	162	SER
1	A	181	ASN
1	A	183	VAL
1	A	188	CYS
1	B	13	THR
1	B	14	SER
1	B	24	ASP
1	B	33	LEU
1	B	56	THR
1	B	57	THR
1	B	61	ARG
1	B	68	SER
1	B	149	GLU
1	B	155	THR
1	B	160	ASP
1	B	162	SER
1	B	182	SER
1	B	183	VAL

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Mol	Chain	Res	Type
1	B	187	CYS
1	B	188	CYS
1	B	198	SER
1	C	-3	ASP
1	C	-2	ASP
1	C	7	LEU
1	C	21	THR
1	C	39	LEU
1	C	40	GLU
1	C	50	VAL
1	C	55	GLN
1	C	57	THR
1	C	59	SER
1	C	72[A]	ASP
1	C	72[B]	ASP
1	C	112	LEU
1	C	125	VAL
1	C	149	GLU
1	C	187	CYS
1	C	188	CYS
1	C	194	ASP
1	D	-3	ASP
1	D	-1	ASP
1	D	2	ASP
1	D	7	LEU
1	D	21	THR
1	D	23	ARG
1	D	56	THR
1	D	59	SER
1	D	67	SER
1	D	68	SER
1	D	83	VAL
1	D	108	ASP
1	D	112	LEU
1	D	114	MET
1	D	148	ARG
1	D	155	THR
1	D	161	ASP
1	D	187	CYS
1	D	194	ASP
1	E	-3	ASP
1	E	-1	ASP

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Mol	Chain	Res	Type
1	E	2	ASP
1	E	23	ARG
1	E	39	LEU
1	E	55	GLN
1	E	116	SER
1	E	122	SER
1	E	125	VAL
1	E	155	THR
1	E	161	ASP
1	E	163	GLU
1	E	166	SER
1	E	170	ARG
1	E	178	GLN
1	E	186	SER
1	E	188	CYS
1	F	-3	ASP
1	F	-2	ASP
1	F	-1	ASP
1	F	2	ASP
1	F	12	GLN
1	F	24	ASP
1	F	39	LEU
1	F	40	GLU
1	F	49	ASP
1	F	56	THR
1	F	57	THR
1	F	59	SER
1	F	94	LYS
1	F	116	SER
1	F	125	VAL
1	F	139	LYS
1	F	153	ASP
1	F	161	ASP
1	F	183	VAL
1	F	188	CYS
1	F	202	ARG
1	G	-3	ASP
1	G	-1	ASP
1	G	22	GLN
1	G	30	SER
1	G	50	VAL
1	G	56	THR

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Mol	Chain	Res	Type
1	G	104	ARG
1	G	119	GLN
1	G	128	VAL
1	G	136	CYS
1	G	148	ARG
1	G	155	THR
1	G	162	SER
1	G	177	THR
1	G	188	CYS
1	G	194[A]	ASP
1	G	194[B]	ASP
1	H	7	LEU
1	H	12	GLN
1	H	20	PRO
1	H	24	ASP
1	H	50	VAL
1	H	56	THR
1	H	57	THR
1	H	68	SER
1	H	72	ASP
1	H	90	ASN
1	H	92	ILE
1	H	136	CYS
1	H	161	ASP
1	H	188	CYS
1	H	194	ASP
1	I	-3	ASP
1	I	-1	ASP
1	I	15	ARG
1	I	21	THR
1	I	22	GLN
1	I	24	ASP
1	I	68	SER
1	I	122	SER
1	I	125	VAL
1	I	136	CYS
1	I	162	SER
1	I	179	LYS
1	I	181	ASN
1	I	182	SER
1	I	186	SER
1	I	187	CYS

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Mol	Chain	Res	Type
1	I	188	CYS
1	J	-3	ASP
1	J	2	ASP
1	J	13	THR
1	J	24	ASP
1	J	31	VAL
1	J	39	LEU
1	J	50	VAL
1	J	56	THR
1	J	68	SER
1	J	116	SER
1	J	123	CYS
1	J	125	VAL
1	J	126	SER
1	J	130	THR
1	J	162	SER
1	J	175	ASP
1	J	177	THR
1	J	188	CYS
1	J	198	SER

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

Mol	Chain	Res	Type
1	A	55	GLN
1	B	9	ASN
1	D	178	GLN
1	H	22	GLN
1	H	55	GLN
1	I	181	ASN

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

29 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	KK2	A	301	-	25,25,25	1.30	3 (12%)	36,36,36	1.31	4 (11%)
3	NAG	A	302	1	14,14,15	0.59	0	15,19,21	1.22	1 (6%)
4	PO4	A	303	-	4,4,4	0.50	0	6,6,6	0.27	0
2	KK2	B	301	-	25,25,25	1.13	3 (12%)	36,36,36	1.35	6 (16%)
3	NAG	B	302	1	14,14,15	0.51	0	15,19,21	1.83	3 (20%)
2	KK2	C	301	-	25,25,25	1.11	2 (8%)	36,36,36	1.44	5 (13%)
3	NAG	C	302	1	14,14,15	0.41	0	15,19,21	1.90	2 (13%)
4	PO4	C	303	-	4,4,4	0.57	0	6,6,6	0.28	0
2	KK2	D	301	-	25,25,25	1.00	1 (4%)	36,36,36	1.28	4 (11%)
3	NAG	D	302	1	14,14,15	0.45	0	15,19,21	1.19	1 (6%)
4	PO4	D	303	-	4,4,4	0.53	0	6,6,6	0.27	0
2	KK2	E	301	-	25,25,25	1.08	1 (4%)	36,36,36	1.36	4 (11%)
3	NAG	E	302	1	14,14,15	0.50	0	15,19,21	0.56	0
4	PO4	E	303	-	4,4,4	0.46	0	6,6,6	0.28	0
4	PO4	E	304	-	4,4,4	0.43	0	6,6,6	0.28	0
2	KK2	F	301	-	25,25,25	1.43	4 (16%)	36,36,36	1.39	6 (16%)
4	PO4	F	302	-	4,4,4	0.74	0	6,6,6	0.26	0
2	KK2	G	301	-	25,25,25	1.00	0	36,36,36	1.38	6 (16%)
3	NAG	G	302	1	14,14,15	0.36	0	15,19,21	0.76	1 (6%)
4	PO4	G	303	-	4,4,4	0.48	0	6,6,6	0.27	0
2	KK2	H	301	-	25,25,25	1.18	2 (8%)	36,36,36	1.48	7 (19%)
3	NAG	H	302	1	14,14,15	0.28	0	15,19,21	0.53	0
4	PO4	H	303	-	4,4,4	0.58	0	6,6,6	0.28	0
2	KK2	I	301	-	25,25,25	0.97	0	36,36,36	1.65	7 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	I	302	1	14,14,15	0.34	0	15,19,21	0.77	1 (6%)
4	PO4	I	303	-	4,4,4	0.63	0	6,6,6	0.28	0
2	KK2	J	301	-	25,25,25	0.72	0	36,36,36	1.23	4 (11%)
3	NAG	J	302	1	14,14,15	0.27	0	15,19,21	0.53	0
4	PO4	J	303	-	4,4,4	0.58	0	6,6,6	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KK2	A	301	-	-	0/14/22/22	0/3/3/3
3	NAG	A	302	1	-	2/6/23/26	0/1/1/1
4	PO4	A	303	-	-	0/0/0/0	0/0/0/0
2	KK2	B	301	-	-	0/14/22/22	0/3/3/3
3	NAG	B	302	1	-	0/6/23/26	0/1/1/1
2	KK2	C	301	-	-	0/14/22/22	0/3/3/3
3	NAG	C	302	1	-	0/6/23/26	0/1/1/1
4	PO4	C	303	-	-	0/0/0/0	0/0/0/0
2	KK2	D	301	-	-	0/14/22/22	0/3/3/3
3	NAG	D	302	1	-	0/6/23/26	0/1/1/1
4	PO4	D	303	-	-	0/0/0/0	0/0/0/0
2	KK2	E	301	-	-	0/14/22/22	0/3/3/3
3	NAG	E	302	1	-	0/6/23/26	0/1/1/1
4	PO4	E	303	-	-	0/0/0/0	0/0/0/0
4	PO4	E	304	-	-	0/0/0/0	0/0/0/0
2	KK2	F	301	-	-	0/14/22/22	0/3/3/3
4	PO4	F	302	-	-	0/0/0/0	0/0/0/0
2	KK2	G	301	-	-	0/14/22/22	0/3/3/3
3	NAG	G	302	1	-	0/6/23/26	0/1/1/1
4	PO4	G	303	-	-	0/0/0/0	0/0/0/0
2	KK2	H	301	-	-	0/14/22/22	0/3/3/3
3	NAG	H	302	1	-	0/6/23/26	0/1/1/1
4	PO4	H	303	-	-	0/0/0/0	0/0/0/0
2	KK2	I	301	-	-	0/14/22/22	0/3/3/3
3	NAG	I	302	1	-	0/6/23/26	0/1/1/1
4	PO4	I	303	-	-	0/0/0/0	0/0/0/0
2	KK2	J	301	-	-	0/14/22/22	0/3/3/3
3	NAG	J	302	1	-	0/6/23/26	0/1/1/1
4	PO4	J	303	-	-	0/0/0/0	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	KK2	C7-N3	2.06	1.39	1.35
2	B	301	KK2	C6-N1	2.07	1.37	1.34
2	C	301	KK2	C1-N2	2.09	1.49	1.46
2	C	301	KK2	C4-N2	2.12	1.49	1.46
2	H	301	KK2	C7-N4	2.12	1.38	1.34
2	B	301	KK2	C1-N2	2.23	1.50	1.46
2	B	301	KK2	C6-N2	2.27	1.42	1.37
2	F	301	KK2	C7-N4	2.29	1.38	1.34
2	A	301	KK2	C5-C6	2.31	1.43	1.39
2	H	301	KK2	C6-N2	2.35	1.42	1.37
2	D	301	KK2	C7-N1	2.39	1.39	1.35
2	F	301	KK2	C4-N2	2.41	1.50	1.46
2	A	301	KK2	C6-N1	2.43	1.37	1.34
2	F	301	KK2	C6-N2	2.87	1.43	1.37
2	A	301	KK2	C6-N2	3.24	1.44	1.37
2	F	301	KK2	C9-C8	3.63	1.54	1.48

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	KK2	C1-N2-C6	-3.95	110.83	120.22
2	I	301	KK2	C7-N1-C6	-3.79	113.81	116.73
2	B	301	KK2	C1-N2-C6	-3.42	112.10	120.22
2	I	301	KK2	C15-C9-C8	-3.37	115.75	121.24
2	E	301	KK2	C7-N1-C6	-3.19	114.27	116.73
2	H	301	KK2	C7-N1-C6	-3.15	114.31	116.73
2	G	301	KK2	C7-N1-C6	-3.09	114.35	116.73
2	D	301	KK2	C7-N1-C6	-3.07	114.36	116.73
2	A	301	KK2	C9-C8-N3	-3.05	112.07	116.13
2	F	301	KK2	C7-N1-C6	-2.98	114.43	116.73
2	D	301	KK2	C1-N2-C6	-2.93	113.24	120.22
2	G	301	KK2	C15-C9-C8	-2.91	116.49	121.24
2	G	301	KK2	C1-N2-C6	-2.77	113.63	120.22
2	I	301	KK2	C1-N2-C6	-2.73	113.74	120.22
2	F	301	KK2	C1-N2-C6	-2.68	113.84	120.22
2	C	301	KK2	C7-N1-C6	-2.65	114.69	116.73
2	B	301	KK2	C7-N1-C6	-2.40	114.88	116.73
2	J	301	KK2	C1-N2-C6	-2.17	115.06	120.22
2	J	301	KK2	C7-N1-C6	-2.13	115.09	116.73
2	A	301	KK2	C7-N1-C6	-2.13	115.09	116.73
2	H	301	KK2	C15-C9-C8	-2.10	117.82	121.24
2	F	301	KK2	C4-N2-C6	2.04	125.08	120.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	KK2	C10-C9-C8	2.05	124.58	121.24
2	D	301	KK2	C3-C4-N2	2.06	113.63	110.02
3	I	302	NAG	C3-C4-C5	2.08	113.83	110.20
3	G	302	NAG	C3-C4-C5	2.10	113.86	110.20
2	E	301	KK2	C2-C1-N2	2.11	113.73	110.02
2	G	301	KK2	C8-C5-C6	2.14	118.28	116.77
2	H	301	KK2	C5-C8-C9	2.28	124.91	121.89
2	I	301	KK2	C11-C12-C13	2.30	123.44	119.99
2	J	301	KK2	C3-C4-N2	2.31	114.08	110.02
2	H	301	KK2	C3-C4-N2	2.40	114.24	110.02
2	I	301	KK2	C3-C4-N2	2.52	114.46	110.02
2	F	301	KK2	C3-C4-N2	2.56	114.52	110.02
2	G	301	KK2	C3-C4-N2	2.58	114.55	110.02
2	H	301	KK2	C8-C5-C6	2.58	118.59	116.77
2	B	301	KK2	C3-C4-N2	2.62	114.62	110.02
2	F	301	KK2	C10-C9-C8	2.65	125.57	121.24
3	B	302	NAG	C3-C4-C5	2.70	114.90	110.20
2	B	301	KK2	C2-C1-N2	2.72	114.80	110.02
2	C	301	KK2	C8-C5-C6	2.74	118.70	116.77
2	H	301	KK2	C10-C9-C8	2.75	125.73	121.24
3	C	302	NAG	C3-C4-C5	2.93	115.31	110.20
2	H	301	KK2	C4-N2-C6	3.00	127.35	120.22
2	C	301	KK2	C2-C1-N2	3.02	115.33	110.02
2	E	301	KK2	C8-C5-C6	3.08	118.94	116.77
2	A	301	KK2	C5-C8-C9	3.13	126.05	121.89
2	J	301	KK2	C4-N2-C6	3.25	127.95	120.22
2	B	301	KK2	C8-C5-C6	3.29	119.08	116.77
2	G	301	KK2	C10-C9-C8	3.31	126.65	121.24
2	E	301	KK2	C4-N2-C6	3.36	128.21	120.22
2	D	301	KK2	C8-C5-C6	3.37	119.14	116.77
3	B	302	NAG	O5-C5-C6	3.39	114.68	107.35
2	I	301	KK2	C8-C5-C6	3.39	119.16	116.77
3	A	302	NAG	C2-N2-C7	3.54	127.59	123.04
2	F	301	KK2	C8-C5-C6	3.71	119.38	116.77
3	D	302	NAG	C1-O5-C5	3.78	117.04	112.25
2	C	301	KK2	C3-C4-N2	3.80	116.70	110.02
2	A	301	KK2	C4-N2-C6	3.94	129.59	120.22
2	I	301	KK2	C10-C9-C8	4.00	127.77	121.24
3	B	302	NAG	C1-O5-C5	5.11	118.74	112.25
3	C	302	NAG	C1-O5-C5	6.37	120.33	112.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	NAG	C8-C7-N2-C2
3	A	302	NAG	O7-C7-N2-C2

There are no ring outliers.

15 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	KK2	2	0
2	B	301	KK2	1	0
2	C	301	KK2	3	0
4	C	303	PO4	1	0
2	D	301	KK2	1	0
2	E	301	KK2	1	0
2	F	301	KK2	1	0
2	G	301	KK2	2	0
2	H	301	KK2	1	0
3	H	302	NAG	2	0
4	H	303	PO4	1	0
2	I	301	KK2	2	0
3	I	302	NAG	1	0
2	J	301	KK2	2	0
4	J	303	PO4	1	0

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	208/217 (95%)	0.22	10 (4%) 34 19	10, 24, 58, 85	0
1	B	205/217 (94%)	0.14	7 (3%) 49 28	8, 24, 54, 85	0
1	C	207/217 (95%)	0.29	12 (5%) 26 13	9, 27, 56, 76	0
1	D	213/217 (98%)	0.38	14 (6%) 22 10	10, 27, 61, 93	0
1	E	207/217 (95%)	0.27	12 (5%) 26 13	10, 24, 54, 70	0
1	F	208/217 (95%)	0.23	13 (6%) 23 11	9, 25, 55, 93	0
1	G	210/217 (96%)	0.30	14 (6%) 21 10	8, 25, 56, 99	0
1	H	209/217 (96%)	0.14	7 (3%) 50 29	9, 23, 53, 81	0
1	I	209/217 (96%)	0.21	10 (4%) 34 19	6, 23, 59, 80	0
1	J	207/217 (95%)	0.35	15 (7%) 18 9	8, 27, 59, 88	0
All	All	2083/2170 (95%)	0.25	114 (5%) 29 15	6, 25, 58, 99	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-6	TYR	7.6
1	H	22	GLN	6.2
1	D	-7	ASP	4.8
1	J	39	LEU	4.6
1	J	-6	TYR	4.5
1	B	136	CYS	4.3
1	G	160	ASP	4.3
1	A	60	ASP	4.2
1	G	-4	ASP	4.1
1	D	158	ASN	4.1
1	D	157	GLU	4.1
1	D	24	ASP	3.9
1	A	-5	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	I	24	ASP	3.8
1	G	130	THR	3.7
1	C	162	SER	3.7
1	J	136	CYS	3.7
1	D	154	PRO	3.5
1	I	-7	ASP	3.5
1	J	205	GLY	3.5
1	F	-7	ASP	3.5
1	E	-2	ASP	3.5
1	C	130	THR	3.4
1	G	132	SER	3.3
1	C	129	ASP	3.3
1	D	156	THR	3.3
1	G	23	ARG	3.3
1	D	161	ASP	3.2
1	H	23	ARG	3.2
1	G	136	CYS	3.2
1	A	-4	ASP	3.1
1	I	44	ILE	3.1
1	F	60[A]	ASP	3.1
1	C	125	VAL	3.1
1	G	129	ASP	3.0
1	J	186	SER	3.0
1	I	39	LEU	3.0
1	J	132	SER	3.0
1	F	-2	ASP	3.0
1	F	-6	TYR	3.0
1	C	-6	TYR	3.0
1	G	-3	ASP	2.9
1	I	40	GLU	2.9
1	A	130	THR	2.9
1	D	25	ARG	2.9
1	E	-4	ASP	2.9
1	B	123	CYS	2.9
1	C	132	SER	2.8
1	A	-7	ASP	2.8
1	E	131	GLU	2.8
1	J	44	ILE	2.8
1	D	23	ARG	2.8
1	J	60	ASP	2.8
1	H	-5	LYS	2.8
1	C	126	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	187	CYS	2.7
1	I	131	GLU	2.7
1	D	205	GLY	2.6
1	F	194[A]	ASP	2.6
1	I	130	THR	2.6
1	H	60[A]	ASP	2.6
1	E	130	THR	2.6
1	I	23	ARG	2.5
1	I	49[A]	ASP	2.5
1	C	123	CYS	2.5
1	H	-1	ASP	2.5
1	C	40	GLU	2.5
1	E	129	ASP	2.4
1	G	161	ASP	2.4
1	A	136	CYS	2.4
1	E	-1	ASP	2.4
1	E	161	ASP	2.4
1	J	23	ARG	2.4
1	C	128	VAL	2.3
1	F	188	CYS	2.3
1	J	24	ASP	2.3
1	B	131	GLU	2.3
1	F	136	CYS	2.3
1	G	-7	ASP	2.3
1	B	23	ARG	2.3
1	E	153	ASP	2.3
1	J	188	CYS	2.3
1	F	-1	ASP	2.3
1	D	126	SER	2.3
1	J	135	THR	2.2
1	E	175	ASP	2.2
1	E	205	GLY	2.2
1	E	135	THR	2.2
1	C	60	ASP	2.2
1	J	194[A]	ASP	2.2
1	G	174	LEU	2.2
1	B	49[A]	ASP	2.2
1	F	-5	LYS	2.2
1	E	132	SER	2.2
1	B	129	ASP	2.2
1	H	-4	ASP	2.2
1	G	131	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	43	GLU	2.2
1	A	22	GLN	2.2
1	F	39	LEU	2.2
1	H	172[A]	GLU	2.1
1	J	124	ASP	2.1
1	A	40	GLU	2.1
1	I	172[A]	GLU	2.1
1	F	-4	ASP	2.1
1	F	187	CYS	2.1
1	C	39	LEU	2.1
1	A	175	ASP	2.1
1	D	-3	ASP	2.1
1	G	199	LEU	2.1
1	B	205	GLY	2.1
1	G	175	ASP	2.0
1	F	24	ASP	2.0
1	A	131	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	B	302	14/15	0.84	0.28	3.97	38,63,70,72	0
2	KK2	I	301	23/23	0.96	0.22	2.43	14,20,30,32	0
2	KK2	G	301	23/23	0.95	0.19	1.91	10,18,33,43	0
2	KK2	A	301	23/23	0.96	0.23	1.60	13,22,40,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	H	302	14/15	0.71	0.31	1.38	47,60,79,85	0
2	KK2	B	301	23/23	0.94	0.20	1.01	13,20,39,46	0
3	NAG	E	302	14/15	0.73	0.37	0.91	58,70,91,96	0
2	KK2	J	301	23/23	0.96	0.23	0.84	14,27,40,45	0
2	KK2	C	301	23/23	0.96	0.20	0.71	15,26,40,44	0
2	KK2	E	301	23/23	0.97	0.18	0.53	11,14,36,49	0
2	KK2	F	301	23/23	0.96	0.23	0.37	15,25,42,53	0
2	KK2	D	301	23/23	0.96	0.20	0.16	16,22,37,46	0
3	NAG	A	302	14/15	0.87	0.29	0.12	47,72,78,79	0
2	KK2	H	301	23/23	0.96	0.18	0.01	15,24,29,32	0
3	NAG	D	302	14/15	0.70	0.26	-0.14	53,69,91,93	0
4	PO4	J	303	5/5	0.99	0.17	-0.37	10,10,13,17	0
3	NAG	C	302	14/15	0.89	0.24	-0.42	39,58,68,72	0
4	PO4	F	302	5/5	0.99	0.18	-0.80	13,16,19,22	0
4	PO4	G	303	5/5	0.99	0.16	-0.91	10,13,13,14	0
4	PO4	I	303	5/5	0.99	0.15	-0.94	8,9,10,14	0
4	PO4	C	303	5/5	0.99	0.14	-1.12	7,9,10,16	0
4	PO4	E	303	5/5	0.99	0.14	-1.18	10,12,14,15	0
4	PO4	E	304	5/5	0.99	0.13	-1.53	13,15,16,18	0
4	PO4	A	303	5/5	0.99	0.14	-2.01	9,15,15,18	0
4	PO4	H	303	5/5	0.99	0.14	-2.09	10,10,12,23	0
4	PO4	D	303	5/5	0.99	0.13	-2.26	13,14,18,18	0
3	NAG	J	302	14/15	0.76	0.38	-	46,63,82,85	0
3	NAG	I	302	14/15	0.64	0.45	-	47,62,70,74	0
3	NAG	G	302	14/15	0.63	0.51	-	50,66,88,93	0

6.5 Other polymers (i)

There are no such residues in this entry.