Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:21 PM GMT

PDB ID	:	3WTN
Title	:	Crystal Structure of Lymnaea stagnalis Acetylcholine Binding Protein Complexed with Desnitro-imidacloprid
Authors	:	Okajima, T.; Ihara, M.; Yamashita, A.; Oda, T.; Matsuda, K.
Deposited on	:	2014-04-11
Resolution	:	2.09 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 ⓘ symbol.

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

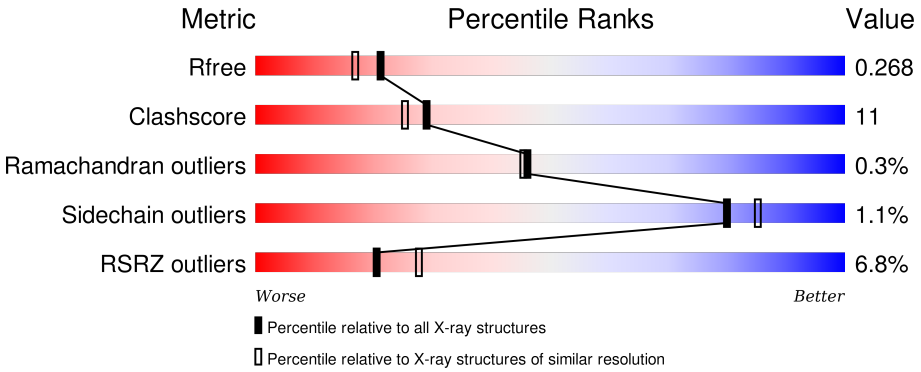
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.09 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	214	5% 76% 21%
1	B	214	4% 84% 13%
1	C	214	2% 82% 14%
1	D	214	7% 77% 19%
1	E	214	4% 74% 22%

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Mol	Chain	Length	Quality of chain
1	F	214	10% 66% 30%
1	G	214	6% 70% 27%
1	H	214	8% 74% 23%
1	I	214	10% 74% 23%
1	J	214	10% 68% 28%

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	N2Y	B	301[A]	-	-	-	X
2	N2Y	B	301[B]	-	-	-	X
2	N2Y	C	301[B]	-	-	X	-
2	N2Y	D	301	-	-	-	X
2	N2Y	E	301[A]	-	-	-	X
2	N2Y	E	301[B]	-	-	-	X
2	N2Y	F	301[A]	-	-	-	X
2	N2Y	F	301[B]	-	-	-	X
2	N2Y	H	301[A]	-	-	-	X
2	N2Y	H	301[B]	-	-	-	X
3	CD	A	302	-	-	-	X
3	CD	C	302	-	-	-	X
4	NA	C	309	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18230 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	2	0
			1669	1040	284	340	5			
1	B	208	Total	C	N	O	S	0	1	0
			1660	1035	284	336	5			
1	C	208	Total	C	N	O	S	0	3	0
			1676	1044	288	339	5			
1	D	208	Total	C	N	O	S	0	1	0
			1663	1037	286	335	5			
1	E	208	Total	C	N	O	S	0	0	0
			1652	1031	282	334	5			
1	F	208	Total	C	N	O	S	0	1	0
			1663	1037	286	335	5			
1	G	208	Total	C	N	O	S	0	1	0
			1660	1035	283	337	5			
1	H	208	Total	C	N	O	S	0	2	0
			1672	1042	287	338	5			
1	I	208	Total	C	N	O	S	0	1	0
			1661	1036	283	337	5			
1	J	208	Total	C	N	O	S	0	0	0
			1652	1031	282	334	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLU	-	EXPRESSION TAG	UNP P58154
A	-2	ALA	-	EXPRESSION TAG	UNP P58154
A	-1	GLU	-	EXPRESSION TAG	UNP P58154
A	0	ALA	-	EXPRESSION TAG	UNP P58154
A	1	ALA	-	EXPRESSION TAG	UNP P58154
A	66	ASP	ASN	SEE REMARK 999	UNP P58154
B	-3	GLU	-	EXPRESSION TAG	UNP P58154
B	-2	ALA	-	EXPRESSION TAG	UNP P58154
B	-1	GLU	-	EXPRESSION TAG	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	EXPRESSION TAG	UNP P58154
B	1	ALA	-	EXPRESSION TAG	UNP P58154
B	66	ASP	ASN	SEE REMARK 999	UNP P58154
C	-3	GLU	-	EXPRESSION TAG	UNP P58154
C	-2	ALA	-	EXPRESSION TAG	UNP P58154
C	-1	GLU	-	EXPRESSION TAG	UNP P58154
C	0	ALA	-	EXPRESSION TAG	UNP P58154
C	1	ALA	-	EXPRESSION TAG	UNP P58154
C	66	ASP	ASN	SEE REMARK 999	UNP P58154
D	-3	GLU	-	EXPRESSION TAG	UNP P58154
D	-2	ALA	-	EXPRESSION TAG	UNP P58154
D	-1	GLU	-	EXPRESSION TAG	UNP P58154
D	0	ALA	-	EXPRESSION TAG	UNP P58154
D	1	ALA	-	EXPRESSION TAG	UNP P58154
D	66	ASP	ASN	SEE REMARK 999	UNP P58154
E	-3	GLU	-	EXPRESSION TAG	UNP P58154
E	-2	ALA	-	EXPRESSION TAG	UNP P58154
E	-1	GLU	-	EXPRESSION TAG	UNP P58154
E	0	ALA	-	EXPRESSION TAG	UNP P58154
E	1	ALA	-	EXPRESSION TAG	UNP P58154
E	66	ASP	ASN	SEE REMARK 999	UNP P58154
F	-3	GLU	-	EXPRESSION TAG	UNP P58154
F	-2	ALA	-	EXPRESSION TAG	UNP P58154
F	-1	GLU	-	EXPRESSION TAG	UNP P58154
F	0	ALA	-	EXPRESSION TAG	UNP P58154
F	1	ALA	-	EXPRESSION TAG	UNP P58154
F	66	ASP	ASN	SEE REMARK 999	UNP P58154
G	-3	GLU	-	EXPRESSION TAG	UNP P58154
G	-2	ALA	-	EXPRESSION TAG	UNP P58154
G	-1	GLU	-	EXPRESSION TAG	UNP P58154
G	0	ALA	-	EXPRESSION TAG	UNP P58154
G	1	ALA	-	EXPRESSION TAG	UNP P58154
G	66	ASP	ASN	SEE REMARK 999	UNP P58154
H	-3	GLU	-	EXPRESSION TAG	UNP P58154
H	-2	ALA	-	EXPRESSION TAG	UNP P58154
H	-1	GLU	-	EXPRESSION TAG	UNP P58154
H	0	ALA	-	EXPRESSION TAG	UNP P58154
H	1	ALA	-	EXPRESSION TAG	UNP P58154
H	66	ASP	ASN	SEE REMARK 999	UNP P58154
I	-3	GLU	-	EXPRESSION TAG	UNP P58154
I	-2	ALA	-	EXPRESSION TAG	UNP P58154
I	-1	GLU	-	EXPRESSION TAG	UNP P58154

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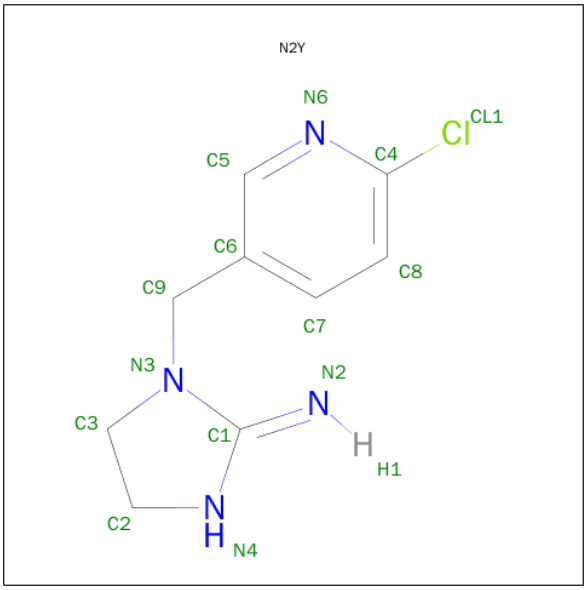
Chain	Residue	Modelled	Actual	Comment	Reference
I	0	ALA	-	EXPRESSION TAG	UNP P58154
I	1	ALA	-	EXPRESSION TAG	UNP P58154
I	66	ASP	ASN	SEE REMARK 999	UNP P58154
J	-3	GLU	-	EXPRESSION TAG	UNP P58154
J	-2	ALA	-	EXPRESSION TAG	UNP P58154
J	-1	GLU	-	EXPRESSION TAG	UNP P58154
J	0	ALA	-	EXPRESSION TAG	UNP P58154
J	1	ALA	-	EXPRESSION TAG	UNP P58154
J	66	ASP	ASN	SEE REMARK 999	UNP P58154

- Molecule 2 is (2Z)-1-[(6-CHLOROPYRIDIN-3-YL)METHYL]IMIDAZOLIDIN-2-IMINE (three-letter code: N2Y) (formula: $C_9H_{11}ClN_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			14	9	1	4		
2	B	1	Total	C	Cl	N	0	1
			28	18	2	8		
2	C	1	Total	C	Cl	N	0	1
			28	18	2	8		
2	D	1	Total	C	Cl	N	0	0
			14	9	1	4		
2	E	1	Total	C	Cl	N	0	1
			28	18	2	8		
2	F	1	Total	C	Cl	N	0	1
			28	18	2	8		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C Cl N 14 9 1 4	0	0
2	H	1	Total C Cl N 28 18 2 8	0	1
2	I	1	Total C Cl N 14 9 1 4	0	0
2	J	1	Total C Cl N 14 9 1 4	0	0

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	5	Total Cd 5 5	0	0
3	J	2	Total Cd 2 2	0	0
3	D	7	Total Cd 7 7	0	0
3	E	6	Total Cd 6 6	0	0
3	H	2	Total Cd 2 2	0	0
3	B	7	Total Cd 7 7	0	0
3	I	6	Total Cd 6 6	0	0
3	C	7	Total Cd 7 7	0	0
3	A	8	Total Cd 8 8	0	0
3	F	4	Total Cd 4 4	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0

- Molecule 5 is water.

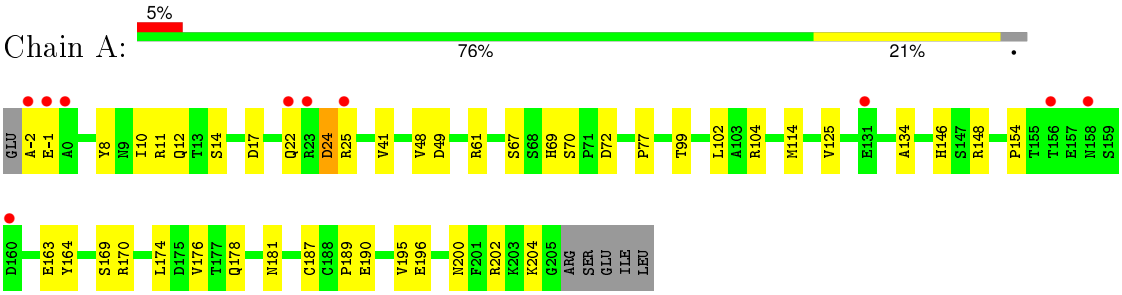
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	154	Total O 154 154	0	0
5	B	199	Total O 199 199	0	0
5	C	181	Total O 181 181	0	0
5	D	133	Total O 133 133	0	0
5	E	136	Total O 136 136	0	0
5	F	90	Total O 90 90	0	0
5	G	125	Total O 125 125	0	0
5	H	130	Total O 130 130	0	0
5	I	88	Total O 88 88	0	0
5	J	100	Total O 100 100	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.

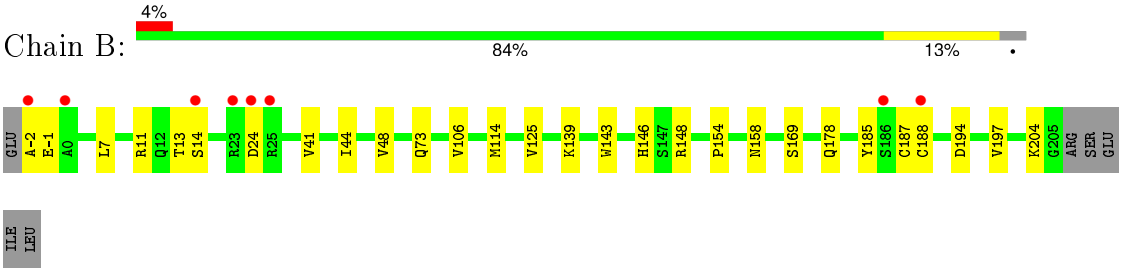
- Molecule 1: Acetylcholine-binding protein

Chain A:



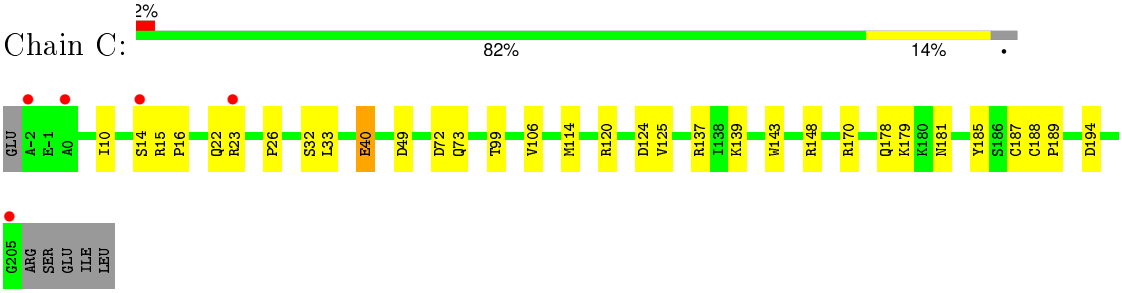
- Molecule 1: Acetylcholine-binding protein

Chain B:



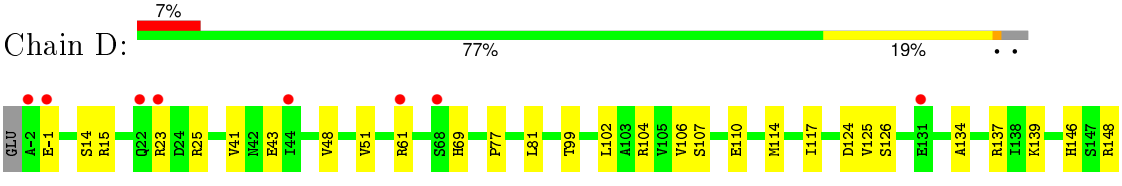
- Molecule 1: Acetylcholine-binding protein

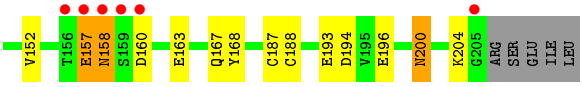
Chain C:



- Molecule 1: Acetylcholine-binding protein

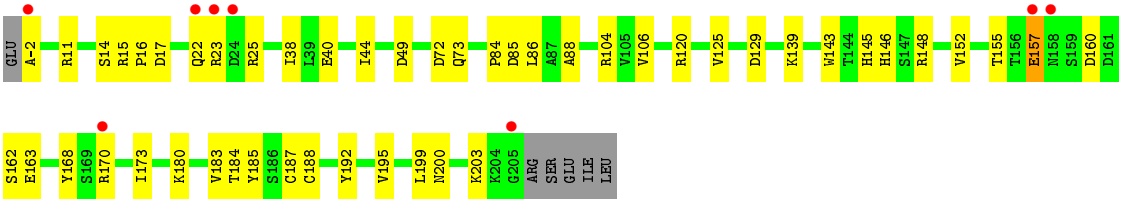
Chain D:





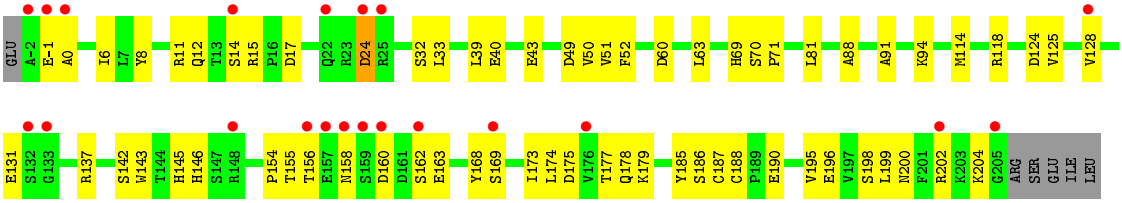
• Molecule 1: Acetylcholine-binding protein

Chain E:



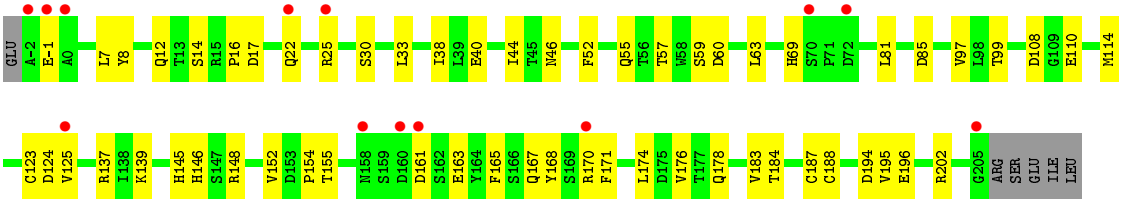
• Molecule 1: Acetylcholine-binding protein

Chain F:



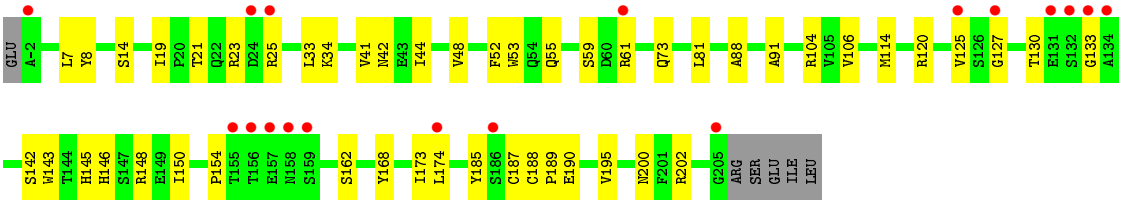
• Molecule 1: Acetylcholine-binding protein

Chain G:



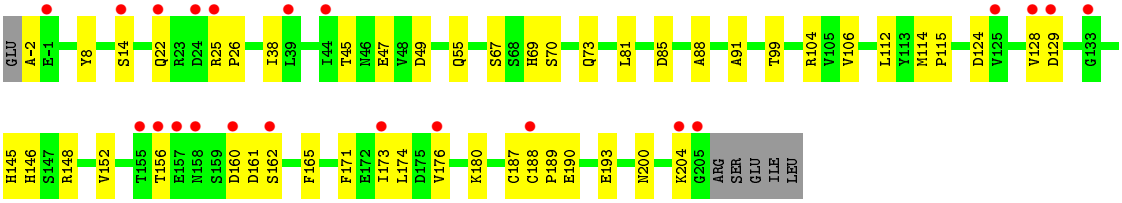
• Molecule 1: Acetylcholine-binding protein

Chain H:

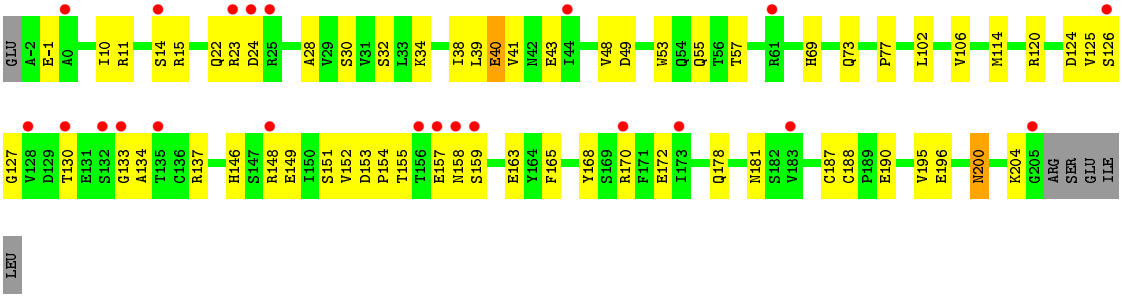


• Molecule 1: Acetylcholine-binding protein

Chain I:



- Molecule 1: Acetylcholine-binding protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.01Å 118.40Å 243.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.84 – 2.09 47.84 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.84-2.09) 98.6 (47.84-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.08Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.213 , 0.262 0.220 , 0.268	Depositor DCC
R_{free} test set	6567 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 66.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 131183 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18230	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% 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: NA, N2Y, CD

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	0.34	0/1705	0.62	0/2327
1	B	0.37	0/1696	0.65	0/2315
1	C	0.36	0/1712	0.64	0/2336
1	D	0.35	0/1699	0.64	0/2319
1	E	0.33	0/1688	0.63	0/2304
1	F	0.31	0/1699	0.60	0/2318
1	G	0.33	0/1696	0.61	0/2315
1	H	0.32	0/1708	0.63	0/2331
1	I	0.31	0/1697	0.60	0/2316
1	J	0.31	0/1688	0.58	0/2304
All	All	0.33	0/16988	0.62	0/23185

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1669	0	1595	43	0
1	B	1660	0	1594	23	0
1	C	1676	0	1612	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1663	0	1602	32	0
1	E	1652	0	1588	34	0
1	F	1663	0	1601	66	0
1	G	1660	0	1591	40	0
1	H	1672	0	1606	46	0
1	I	1661	0	1594	45	0
1	J	1652	0	1588	50	0
2	A	14	0	10	0	0
2	B	28	0	20	2	0
2	C	28	0	20	6	0
2	D	14	0	10	0	0
2	E	28	0	20	4	0
2	F	28	0	20	2	0
2	G	14	0	10	0	0
2	H	28	0	20	4	0
2	I	14	0	10	0	0
2	J	14	0	10	0	0
3	A	8	0	0	0	0
3	B	7	0	0	0	0
3	C	7	0	0	0	0
3	D	7	0	0	0	0
3	E	6	0	0	0	0
3	F	4	0	0	0	0
3	G	5	0	0	0	0
3	H	2	0	0	0	0
3	I	6	0	0	0	0
3	J	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	154	0	0	2	0
5	B	199	0	0	0	0
5	C	181	0	0	3	0
5	D	133	0	0	3	0
5	E	136	0	0	3	0
5	F	90	0	0	3	0
5	G	125	0	0	4	0
5	H	130	0	0	3	0
5	I	88	0	0	2	0
5	J	100	0	0	4	0
All	All	18230	0	16121	378	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 11.

All (378) 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:17[A]:ASP:HB2	1:B:11:ARG:HH21	1.12	1.09
1:A:17[B]:ASP:HB2	1:B:11:ARG:HH21	1.13	1.03
1:E:40:GLU:HB2	1:E:49:ASP:HB2	1.48	0.94
1:E:152:VAL:HG12	1:E:195:VAL:HG23	1.56	0.87
1:A:17[B]:ASP:HB2	1:B:11:ARG:NH2	1.95	0.79
1:A:189:PRO:HG2	1:A:190[A]:GLU:OE1	1.83	0.78
1:J:127:GLY:O	1:J:130:THR:HG22	1.85	0.77
1:F:11:ARG:HH12	1:J:15:ARG:HH21	1.33	0.77
1:A:17[A]:ASP:HB2	1:B:11:ARG:NH2	1.95	0.75
1:H:59:SER:HB2	1:H:61:ARG:HH12	1.52	0.73
1:F:11:ARG:NH1	1:J:15:ARG:HH21	1.86	0.73
1:F:168:TYR:CE1	1:J:124:ASP:HB2	2.25	0.71
1:H:23:ARG:HD3	1:H:25:ARG:HH22	1.56	0.71
1:J:15:ARG:HG3	5:J:495:HOH:O	1.91	0.71
1:D:110:GLU:HG3	5:D:528:HOH:O	1.91	0.70
1:F:156:THR:HG22	1:F:158:ASN:ND2	2.07	0.69
1:G:14:SER:HA	5:G:495:HOH:O	1.92	0.69
1:F:173:ILE:HD12	1:F:199:LEU:HD11	1.75	0.68
1:J:130:THR:HG23	1:J:133:GLY:H	1.57	0.68
1:H:187:CYS:SG	1:H:188:CYS:N	2.67	0.68
1:A:187:CYS:SG	1:B:114:MET:HE1	2.34	0.68
1:H:41:VAL:HG13	1:H:48:VAL:HG12	1.74	0.67
1:I:146:HIS:HB3	1:I:190:GLU:HG3	1.76	0.67
1:H:59:SER:HB2	1:H:61:ARG:NH1	2.09	0.67
1:F:40:GLU:HG2	1:F:49:ASP:CB	2.23	0.67
1:A:22:GLN:OE1	1:A:61:ARG:HD3	1.94	0.67
1:C:14[B]:SER:C	1:C:16:PRO:HD3	2.15	0.67
1:D:41:VAL:HG22	1:D:48:VAL:HG23	1.74	0.67
1:I:152:VAL:HG22	1:I:193:GLU:HB2	1.77	0.67
1:A:148:ARG:HH21	1:A:190[A]:GLU:CG	2.08	0.66
1:F:187:CYS:SG	1:F:188:CYS:N	2.69	0.66
1:D:23:ARG:HD2	1:D:25:ARG:HH12	1.61	0.65
1:E:170:ARG:HH21	1:E:203:LYS:NZ	1.95	0.65
1:I:45:THR:HG22	1:J:170:ARG:NE	2.12	0.65
1:A:181:ASN:ND2	1:A:196:GLU:HG3	2.13	0.64
1:A:41:VAL:HG22	1:A:48:VAL:HG23	1.78	0.64
1:C:179:LYS:HE3	1:C:181:ASN:OD1	1.98	0.64
1:G:170:ARG:HD3	5:G:457:HOH:O	1.98	0.64
1:G:174:LEU:HD11	1:G:202:ARG:HG2	1.80	0.64
1:C:14[A]:SER:C	1:C:16:PRO:HD3	2.18	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:SER:OG	1:F:173:ILE:HB	1.99	0.63
1:F:70:SER:HB2	1:F:71:PRO:HD2	1.80	0.63
1:H:55:GLN:HG3	1:H:114:MET:HE2	1.80	0.63
1:I:187:CYS:SG	1:I:188:CYS:N	2.72	0.62
1:H:127:GLY:HA2	1:H:130:THR:HG23	1.79	0.62
1:G:146:HIS:HD2	1:G:148:ARG:H	1.46	0.62
1:B:187:CYS:SG	1:B:188:CYS:N	2.73	0.62
1:G:55:GLN:HB2	1:G:114:MET:HE3	1.81	0.62
1:E:40:GLU:HB2	1:E:49:ASP:CB	2.26	0.61
1:A:154:PRO:HG3	1:A:195:VAL:HG13	1.83	0.61
1:G:176:VAL:HG12	1:G:178:GLN:HE21	1.66	0.61
1:F:11:ARG:HD2	5:F:457:HOH:O	2.00	0.61
1:A:-2:ALA:HB3	1:F:24:ASP:OD1	2.01	0.61
1:F:11:ARG:HH12	1:J:15:ARG:NH2	1.99	0.61
1:F:14:SER:HB3	5:F:469:HOH:O	1.99	0.60
1:F:40:GLU:HG2	1:F:49:ASP:HB2	1.83	0.60
1:F:40:GLU:HG2	1:F:49:ASP:HB3	1.84	0.59
1:E:14:SER:C	1:E:16:PRO:HD3	2.22	0.59
2:H:301[B]:N2Y:C5	1:I:114:MET:HB3	2.32	0.59
1:B:146:HIS:HD2	1:B:148:ARG:H	1.50	0.59
1:I:22:GLN:HB3	1:I:25:ARG:HB3	1.83	0.59
1:A:-1:GLU:HB3	1:A:69:HIS:O	2.03	0.59
1:A:148:ARG:HH21	1:A:190[A]:GLU:HG3	1.67	0.59
1:H:14:SER:HB3	5:H:491:HOH:O	2.02	0.58
1:A:22:GLN:O	1:A:24:ASP:N	2.35	0.58
1:I:146:HIS:ND1	1:I:190:GLU:HG3	2.18	0.58
1:E:187:CYS:SG	1:E:188:CYS:N	2.76	0.58
1:D:14:SER:HG	1:D:81:LEU:HA	1.69	0.57
1:C:23:ARG:HH21	1:I:69:HIS:CG	2.22	0.57
1:E:155:THR:HG22	1:E:157:GLU:H	1.69	0.57
1:F:156:THR:HG22	1:F:158:ASN:HD21	1.67	0.57
1:F:188:CYS:HB3	1:F:190:GLU:OE2	2.04	0.57
1:H:73:GLN:HG2	1:H:106:VAL:HA	1.86	0.57
1:H:41:VAL:HG12	1:H:125:VAL:HG11	1.86	0.57
1:F:6:ILE:HD12	1:F:71:PRO:HG2	1.85	0.57
1:F:33:LEU:HD22	1:F:52:PHE:CD2	2.39	0.57
1:F:6:ILE:CD1	1:F:71:PRO:HG2	2.34	0.57
1:C:14[B]:SER:O	1:C:16:PRO:HD3	2.03	0.57
1:G:55:GLN:HB2	1:G:114:MET:CE	2.34	0.57
1:I:148:ARG:HG2	1:I:148:ARG:HH11	1.70	0.57
1:F:50:VAL:HG12	1:F:51:VAL:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:14:SER:HB3	5:J:479:HOH:O	2.04	0.56
1:I:73:GLN:HB3	1:I:106:VAL:HA	1.87	0.56
1:E:162:SER:OG	1:E:173:ILE:HB	2.06	0.56
1:J:159:SER:HB2	1:J:163:GLU:OE2	2.05	0.56
1:B:41:VAL:HG22	1:B:48:VAL:HG12	1.88	0.56
1:A:181:ASN:HD22	1:A:196:GLU:HG3	1.71	0.56
1:H:146:HIS:CD2	1:H:190[B]:GLU:HG2	2.40	0.56
1:G:22:GLN:HG2	1:G:25:ARG:NH1	2.21	0.56
1:B:139:LYS:HE3	1:B:194:ASP:OD2	2.06	0.56
1:F:124:ASP:HB2	1:G:168:TYR:CE1	2.41	0.56
1:A:163:GLU:HG2	1:A:164:TYR:CZ	2.41	0.56
1:A:176:VAL:HG12	1:A:178:GLN:NE2	2.21	0.56
1:D:125:VAL:O	1:D:125:VAL:HG12	2.06	0.56
1:I:171:PHE:O	1:I:204:LYS:HD2	2.05	0.56
1:C:125:VAL:O	1:C:125:VAL:HG12	2.05	0.55
1:I:146:HIS:CB	1:I:190:GLU:HG3	2.36	0.55
1:J:125:VAL:HG12	1:J:125:VAL:O	2.06	0.55
1:J:43:GLU:OE2	1:J:126:SER:HA	2.07	0.55
1:A:146:HIS:CE1	1:A:148:ARG:HB2	2.40	0.55
1:I:45:THR:HA	1:J:170:ARG:HD3	1.88	0.55
1:F:190:GLU:CD	1:F:190:GLU:H	2.11	0.55
1:I:55:GLN:HG3	1:I:114:MET:HE2	1.89	0.55
1:H:162:SER:OG	1:H:173:ILE:HB	2.07	0.55
1:A:148:ARG:HH21	1:A:190[A]:GLU:HG2	1.72	0.54
1:A:174:LEU:HD21	1:A:202:ARG:NE	2.22	0.54
1:B:185:TYR:CG	2:B:301[B]:N2Y:H3	2.42	0.54
1:I:124:ASP:HB2	1:J:168:TYR:CE1	2.42	0.54
1:B:73:GLN:HG2	1:B:106:VAL:HG22	1.88	0.54
1:B:41:VAL:HG13	1:B:125:VAL:HG11	1.90	0.54
1:H:189:PRO:HG2	1:H:190[B]:GLU:OE2	2.07	0.54
1:J:181:ASN:OD1	1:J:196:GLU:HG3	2.07	0.54
1:C:23:ARG:HD2	1:I:-2:ALA:O	2.08	0.54
1:A:148:ARG:NH2	1:A:190[A]:GLU:HG3	2.23	0.54
1:C:23:ARG:NH2	1:I:69:HIS:ND1	2.54	0.54
1:G:22:GLN:HG2	1:G:25:ARG:HH11	1.72	0.54
1:C:33:LEU:H	1:C:178:GLN:HE22	1.55	0.54
1:E:73:GLN:HG3	1:E:104:ARG:CZ	2.39	0.53
1:E:160:ASP:O	1:E:163:GLU:HB2	2.07	0.53
1:C:124:ASP:HB2	1:D:168:TYR:CE1	2.42	0.53
1:I:146:HIS:CG	1:I:190:GLU:HG3	2.43	0.53
1:I:162:SER:HB3	1:I:173:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:88:ALA:HB3	1:H:91:ALA:HB2	1.90	0.53
1:J:10:ILE:O	1:J:14:SER:HB2	2.09	0.53
1:H:154:PRO:HG3	1:H:195:VAL:HG13	1.89	0.53
1:E:73:GLN:HG3	1:E:104:ARG:NH2	2.24	0.53
1:D:-1:GLU:HB3	1:D:69:HIS:O	2.07	0.53
1:H:73:GLN:HG2	1:H:106:VAL:HG22	1.90	0.53
1:J:55:GLN:HB2	1:J:114:MET:HE2	1.91	0.52
1:F:32:SER:HA	1:F:178:GLN:HE22	1.75	0.52
1:A:11:ARG:NH1	1:E:17:ASP:OD1	2.42	0.52
1:C:143:TRP:CE2	1:D:99:THR:HG21	2.44	0.52
1:C:14[A]:SER:O	1:C:16:PRO:HD3	2.09	0.52
1:C:120:ARG:HH11	1:C:120:ARG:HG3	1.74	0.52
1:H:33:LEU:HD22	1:H:52:PHE:CD2	2.44	0.52
1:I:161:ASP:OD1	1:I:176:VAL:HB	2.10	0.51
1:D:124:ASP:HB2	1:E:168:TYR:CE1	2.45	0.51
1:J:187:CYS:SG	1:J:188:CYS:N	2.82	0.51
1:B:169:SER:O	1:B:204:LYS:HE2	2.10	0.51
1:G:139:LYS:HE2	1:G:196:GLU:OE2	2.10	0.51
1:I:14:SER:HB3	5:I:472:HOH:O	2.09	0.51
1:H:185:TYR:CG	2:H:301[B]:N2Y:H3	2.45	0.51
1:H:143:TRP:CE2	1:I:99:THR:HG21	2.45	0.51
1:F:39:LEU:HD12	1:F:118:ARG:CZ	2.41	0.51
1:J:28:ALA:HA	1:J:151:SER:OG	2.10	0.51
1:H:19:ILE:HG12	1:H:21:THR:HG23	1.93	0.51
1:G:46:ASN:HB3	1:G:123:CYS:O	2.11	0.51
1:F:137[B]:ARG:HD2	1:F:196:GLU:OE2	2.10	0.51
1:D:23:ARG:HD2	1:D:25:ARG:HH22	1.75	0.51
1:G:124:ASP:HB2	1:H:168:TYR:CE1	2.46	0.51
1:J:146:HIS:HE1	1:J:148:ARG:HB2	1.76	0.51
1:I:190:GLU:CD	1:I:190:GLU:H	2.14	0.50
1:B:125:VAL:HG12	1:B:125:VAL:O	2.10	0.50
1:I:128:VAL:HG13	1:I:129:ASP:N	2.26	0.50
1:D:43:GLU:OE2	1:D:126:SER:HA	2.11	0.50
1:H:120:ARG:HG3	1:H:120:ARG:HH11	1.76	0.50
1:C:187:CYS:SG	1:D:114:MET:HE1	2.51	0.50
1:H:133:GLY:HA3	1:H:202:ARG:HB3	1.92	0.50
1:F:160:ASP:HB3	1:F:163:GLU:HB2	1.93	0.50
1:J:146:HIS:CE1	1:J:148:ARG:HB2	2.47	0.50
1:E:185:TYR:CG	2:E:301[A]:N2Y:H3	2.46	0.50
1:H:146:HIS:CD2	1:H:190[A]:GLU:HG2	2.46	0.49
1:J:22:GLN:O	1:J:24:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:GLN:NE2	1:A:61:ARG:NH1	2.60	0.49
1:C:10:ILE:O	1:C:14[B]:SER:HB3	2.12	0.49
1:G:17[B]:ASP:O	1:H:7:LEU:HD13	2.12	0.49
1:I:180:LYS:NZ	1:I:193:GLU:OE1	2.45	0.49
1:I:112:LEU:HD11	1:I:114:MET:HE2	1.93	0.49
1:D:134:ALA:O	1:D:200:ASN:HA	2.13	0.49
1:B:44:ILE:HG22	1:C:170:ARG:HD3	1.95	0.49
1:I:146:HIS:HB3	1:I:190:GLU:CG	2.41	0.49
1:B:13:THR:O	1:B:14:SER:HB3	2.13	0.49
1:E:85:ASP:OD1	1:E:145:HIS:HD2	1.96	0.49
1:G:85:ASP:OD1	1:G:145:HIS:HD2	1.96	0.49
1:E:73:GLN:HE21	1:E:106:VAL:HG22	1.78	0.49
1:F:174:LEU:HD21	1:F:202:ARG:HD3	1.94	0.49
1:D:15[A]:ARG:NH1	1:H:8:TYR:CD2	2.81	0.48
1:J:-1:GLU:OE1	1:J:69:HIS:HB3	2.13	0.48
1:A:10:ILE:O	1:A:14:SER:HB2	2.13	0.48
1:I:67:SER:HA	1:I:70:SER:OG	2.14	0.48
1:H:61:ARG:HD2	5:H:519:HOH:O	2.12	0.48
1:E:73:GLN:NE2	1:E:106:VAL:HG22	2.29	0.48
1:J:-1:GLU:HB3	1:J:69:HIS:O	2.14	0.48
1:F:146:HIS:CD2	1:F:190:GLU:HG3	2.49	0.48
1:F:14:SER:HG	1:F:81:LEU:HA	1.79	0.48
1:F:39:LEU:HD12	1:F:118:ARG:NE	2.28	0.48
1:B:154:PRO:HB3	1:B:178:GLN:HE21	1.79	0.48
1:F:0:ALA:HB2	1:F:69:HIS:HB2	1.95	0.48
1:F:125:VAL:HG12	1:F:125:VAL:O	2.12	0.48
1:D:137:ARG:HD3	5:D:458:HOH:O	2.14	0.48
1:G:33:LEU:HD22	1:G:52:PHE:CD2	2.48	0.48
1:H:41:VAL:HG12	1:H:125:VAL:CG1	2.44	0.48
1:A:176:VAL:HG12	1:A:178:GLN:HE22	1.78	0.48
1:J:172:GLU:OE2	1:J:204:LYS:HA	2.13	0.48
1:H:125:VAL:HG12	1:H:125:VAL:O	2.12	0.48
1:J:146:HIS:CE1	1:J:149:GLU:HG3	2.49	0.48
1:A:14:SER:HB3	5:A:516:HOH:O	2.13	0.48
1:E:-2:ALA:N	5:E:521:HOH:O	2.46	0.48
1:A:125:VAL:O	1:A:125:VAL:HG12	2.13	0.48
1:A:190[A]:GLU:N	1:A:190[A]:GLU:OE1	2.47	0.48
1:E:170:ARG:HH21	1:E:203:LYS:HZ3	1.62	0.48
1:C:22:GLN:O	1:C:23:ARG:HB2	2.14	0.48
1:F:179:LYS:HZ1	1:F:196:GLU:CD	2.17	0.48
1:F:50:VAL:CG1	1:F:51:VAL:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:VAL:O	1:E:125:VAL:HG12	2.14	0.47
1:D:187:CYS:SG	1:D:188:CYS:N	2.87	0.47
1:J:41:VAL:HG22	1:J:48:VAL:HG23	1.97	0.47
1:A:148:ARG:NH2	1:A:190[A]:GLU:CG	2.76	0.47
1:H:174:LEU:HB2	1:H:200:ASN:ND2	2.28	0.47
1:B:178:GLN:HG2	1:B:197:VAL:HG22	1.95	0.47
1:C:72:ASP:HB3	5:C:544:HOH:O	2.15	0.47
1:H:148:ARG:NH1	1:H:190[A]:GLU:HG3	2.29	0.47
1:A:174:LEU:HB2	1:A:200:ASN:ND2	2.28	0.47
1:E:22:GLN:O	1:E:23:ARG:HB2	2.15	0.47
1:I:22:GLN:O	1:I:25:ARG:N	2.46	0.47
1:H:42:ASN:OD1	1:H:44:ILE:HB	2.14	0.47
1:G:-1:GLU:HB3	1:G:69:HIS:O	2.15	0.47
1:F:146:HIS:CG	1:F:190:GLU:HG3	2.49	0.47
1:J:157:GLU:C	1:J:159:SER:H	2.18	0.47
1:F:154:PRO:HB3	1:F:178:GLN:OE1	2.14	0.47
1:F:174:LEU:O	1:F:175:ASP:HB2	2.15	0.47
1:I:156:THR:O	1:I:156:THR:HG22	2.15	0.47
1:F:174:LEU:HD11	1:F:202:ARG:HD3	1.98	0.46
1:C:10:ILE:O	1:C:14[A]:SER:HB3	2.15	0.46
1:C:178:GLN:NE2	5:C:497:HOH:O	2.48	0.46
1:G:38:ILE:HG13	1:G:165:PHE:CE1	2.51	0.46
1:A:22:GLN:HG3	1:A:25:ARG:NH2	2.30	0.46
1:I:88:ALA:HB3	1:I:91:ALA:HB2	1.97	0.46
1:F:11:ARG:HH12	1:J:15:ARG:HE	1.61	0.46
1:B:143:TRP:CE2	1:C:99:THR:HG21	2.51	0.46
1:F:177:THR:OG1	1:F:198:SER:HB2	2.16	0.46
2:C:301[B]:N2Y:C5	1:D:114:MET:HB3	2.46	0.46
1:C:188:CYS:HB3	1:C:189:PRO:HD2	1.96	0.46
1:H:174:LEU:HD11	1:H:202:ARG:HD3	1.96	0.46
1:A:114:MET:HB3	2:E:301[A]:N2Y:C5	2.46	0.46
1:D:139:LYS:HE3	1:D:194:ASP:OD2	2.16	0.46
1:J:154:PRO:HG3	1:J:195:VAL:HG13	1.97	0.46
1:H:143:TRP:CZ2	1:I:99:THR:HG21	2.51	0.46
1:C:32:SER:HA	1:C:178:GLN:HE22	1.80	0.45
1:G:125:VAL:O	1:G:125:VAL:HG12	2.16	0.45
1:C:15:ARG:NH2	1:I:8:TYR:CD2	2.84	0.45
1:C:137:ARG:HH11	1:C:137:ARG:HG3	1.81	0.45
1:E:84:PRO:HB2	1:E:86:LEU:HG	1.99	0.45
1:H:185:TYR:CD1	1:H:185:TYR:N	2.84	0.45
1:C:185:TYR:N	1:C:185:TYR:CD1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:HB2	2:E:301[A]:N2Y:CL1	2.53	0.45
1:J:32:SER:OG	1:J:155:THR:HB	2.16	0.45
1:F:146:HIS:HB3	1:F:190:GLU:HG3	1.98	0.45
1:A:99:THR:HG21	1:E:143:TRP:CE2	2.51	0.45
1:J:130:THR:HG23	1:J:133:GLY:N	2.29	0.45
1:C:185:TYR:CG	2:C:301[B]:N2Y:H3	2.52	0.45
1:J:137:ARG:CB	1:J:137:ARG:HH11	2.30	0.45
1:J:30:SER:HB2	1:J:57:THR:OG1	2.17	0.45
1:E:146:HIS:HD2	1:E:148:ARG:H	1.65	0.45
1:F:43:GLU:OE1	1:F:128:VAL:HG12	2.17	0.45
1:I:85:ASP:OD1	1:I:145:HIS:HD2	2.00	0.45
1:F:137[A]:ARG:HD2	1:F:196:GLU:OE2	2.16	0.45
1:D:152:VAL:HG23	1:D:152:VAL:O	2.16	0.45
1:D:167:GLN:O	1:D:204:LYS:NZ	2.50	0.45
1:I:47:GLU:OE2	1:J:39:LEU:HD22	2.17	0.45
1:G:154:PRO:HG3	1:G:195:VAL:HG13	1.99	0.45
1:J:11:ARG:NH2	5:J:491:HOH:O	2.50	0.45
1:G:55:GLN:CB	1:G:114:MET:HE3	2.47	0.44
1:E:160:ASP:HB2	1:E:163:GLU:HB2	1.98	0.44
1:J:55:GLN:HB2	1:J:114:MET:CE	2.47	0.44
1:B:7:LEU:O	1:B:11:ARG:HG3	2.17	0.44
1:A:170:ARG:HD3	1:E:44:ILE:O	2.16	0.44
1:E:72:ASP:HB2	5:E:511:HOH:O	2.18	0.44
1:J:34:LYS:HB2	1:J:53:TRP:HB2	1.99	0.44
1:J:73:GLN:HG2	1:J:106:VAL:HA	1.99	0.44
1:A:134:ALA:O	1:A:200:ASN:HA	2.18	0.44
1:A:8:TYR:O	1:A:12:GLN:HG2	2.18	0.44
1:D:23:ARG:HD2	1:D:25:ARG:NH1	2.30	0.44
1:F:131:GLU:HG3	1:F:202:ARG:NH1	2.32	0.44
1:H:34:LYS:HB2	1:H:53:TRP:HB2	1.99	0.44
2:H:301[B]:N2Y:CL1	1:I:104:ARG:HB2	2.55	0.44
1:E:72:ASP:HB3	5:E:467:HOH:O	2.17	0.44
1:G:8:TYR:CE2	1:G:12:GLN:HG3	2.52	0.44
1:C:120:ARG:NH1	1:C:120:ARG:HG3	2.33	0.44
1:G:30:SER:HB3	1:G:155:THR:HG22	2.00	0.44
1:G:170:ARG:HG3	1:G:171:PHE:CE1	2.53	0.44
1:D:77:PRO:HA	1:D:102:LEU:HD23	2.00	0.44
1:B:-2:ALA:HA	1:F:-1:GLU:HG3	2.00	0.43
1:H:120:ARG:NH1	1:H:120:ARG:HG3	2.33	0.43
1:I:146:HIS:HE1	5:J:409:HOH:O	2.02	0.43
1:C:139:LYS:HE3	1:C:194:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:187:CYS:SG	1:G:188:CYS:N	2.91	0.43
1:G:152:VAL:HG21	1:G:194:ASP:HA	2.01	0.43
1:G:44:ILE:HG13	5:G:471:HOH:O	2.18	0.43
1:H:104:ARG:HG2	5:H:496:HOH:O	2.19	0.43
1:C:187:CYS:SG	2:C:301[B]:N2Y:H4	2.59	0.43
1:E:192:TYR:CZ	2:E:301[B]:N2Y:H9	2.54	0.43
1:J:38:ILE:HG13	1:J:165:PHE:HE1	1.83	0.43
1:A:169:SER:O	1:A:204:LYS:HE2	2.19	0.43
1:F:185:TYR:CG	2:F:301[B]:N2Y:H3	2.54	0.43
1:G:60:ASP:HB3	1:G:63:LEU:HD12	2.00	0.43
1:I:25:ARG:HA	1:I:26:PRO:HD3	1.89	0.43
1:B:41:VAL:HG13	1:B:125:VAL:CG1	2.48	0.43
1:C:143:TRP:CZ2	1:D:99:THR:HG21	2.53	0.43
2:C:301[B]:N2Y:CL1	1:D:104:ARG:HB2	2.56	0.43
1:F:169:SER:O	1:F:204:LYS:HE2	2.19	0.43
1:F:154:PRO:HG3	1:F:195:VAL:HG13	2.01	0.42
1:G:14:SER:OG	1:G:16:PRO:HD3	2.19	0.42
1:H:185:TYR:HB2	2:H:301[B]:N2Y:H3	2.02	0.42
1:F:88:ALA:HB3	1:F:91:ALA:HB2	2.01	0.42
1:H:14:SER:HG	1:H:81:LEU:HA	1.84	0.42
1:E:152:VAL:CG1	1:E:195:VAL:HG23	2.38	0.42
1:I:161:ASP:HB3	1:I:176:VAL:HG23	2.01	0.42
1:D:160:ASP:OD2	1:D:163:GLU:HB2	2.19	0.42
1:H:55:GLN:HG3	1:H:114:MET:CE	2.49	0.42
1:J:134:ALA:O	1:J:200:ASN:HA	2.18	0.42
1:E:88:ALA:HA	1:E:139:LYS:O	2.19	0.42
1:H:142:SER:OG	1:H:145:HIS:HB2	2.19	0.42
1:F:114:MET:HE2	1:F:114:MET:HB2	1.73	0.42
1:F:0:ALA:CB	1:F:69:HIS:HB2	2.49	0.42
1:G:22:GLN:HB3	1:G:25:ARG:HB2	2.00	0.42
1:F:32:SER:OG	1:F:155:THR:HB	2.19	0.42
1:C:185:TYR:HB2	2:C:301[B]:N2Y:H3	2.00	0.42
1:C:40:GLU:H	1:C:49:ASP:HB3	1.83	0.42
1:G:108:ASP:OD2	1:G:110:GLU:HG2	2.20	0.42
1:B:-1:GLU:OE2	1:B:-1:GLU:HA	2.20	0.42
1:E:38:ILE:HD11	1:E:199:LEU:HD21	2.02	0.42
1:C:187:CYS:C	1:C:188:CYS:SG	2.97	0.42
1:J:38:ILE:HG13	1:J:165:PHE:CE1	2.54	0.42
1:A:67:SER:HA	1:A:70:SER:OG	2.20	0.42
1:F:0:ALA:HB3	1:F:69:HIS:O	2.20	0.42
1:A:77:PRO:HA	1:A:102:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:120:ARG:HG3	1:J:120:ARG:HH11	1.85	0.41
1:A:72:ASP:HB3	5:A:483:HOH:O	2.20	0.41
1:J:40:GLU:O	1:J:48:VAL:HA	2.20	0.41
1:G:59:SER:HB2	5:G:415:HOH:O	2.19	0.41
1:I:174:LEU:HB2	1:I:200:ASN:ND2	2.34	0.41
1:F:187:CYS:SG	2:F:301[B]:N2Y:H4	2.60	0.41
1:G:161:ASP:OD1	1:G:176:VAL:HB	2.20	0.41
1:I:14:SER:HG	1:I:81:LEU:HA	1.84	0.41
1:G:137:ARG:NH1	1:H:168:TYR:OH	2.52	0.41
1:J:154:PRO:HG3	1:J:195:VAL:CG1	2.50	0.41
1:F:60:ASP:HB3	1:F:63:LEU:HD12	2.02	0.41
1:I:115:PRO:HA	5:I:470:HOH:O	2.20	0.41
1:F:186:SER:HG	1:G:163:GLU:CD	2.23	0.41
1:H:41:VAL:CG1	1:H:125:VAL:HG13	2.50	0.41
1:H:146:HIS:CG	1:H:190[A]:GLU:HG2	2.55	0.41
1:A:174:LEU:HD11	1:A:202:ARG:HD3	2.01	0.41
2:B:301[A]:N2Y:H11	1:C:114:MET:CE	2.51	0.41
1:C:143:TRP:NE1	2:C:301[B]:N2Y:H5	2.35	0.41
1:C:187:CYS:SG	1:C:188:CYS:N	2.93	0.41
1:J:146:HIS:CD2	1:J:190:GLU:HG3	2.56	0.41
1:F:174:LEU:HD21	1:F:202:ARG:CD	2.50	0.41
1:D:137:ARG:NE	1:D:196:GLU:OE1	2.52	0.41
1:J:154:PRO:HB3	1:J:178:GLN:OE1	2.21	0.41
1:D:51:VAL:HA	1:D:117:ILE:O	2.20	0.41
1:D:14:SER:HB3	5:D:512:HOH:O	2.20	0.41
1:C:26:PRO:HB3	1:C:148[A]:ARG:C	2.40	0.41
1:I:38:ILE:HG13	1:I:165:PHE:CE1	2.56	0.41
1:F:8:TYR:O	1:F:12:GLN:HG2	2.21	0.41
1:F:143:TRP:CE2	1:G:99:THR:HG21	2.56	0.41
1:D:152:VAL:HG22	1:D:193:GLU:HB2	2.03	0.41
1:G:183:VAL:HG12	1:G:184:THR:N	2.36	0.41
1:F:179:LYS:HG2	5:F:440:HOH:O	2.19	0.41
1:H:145:HIS:HB2	1:H:150:ILE:HD12	2.02	0.41
1:E:180:LYS:C	1:E:180:LYS:HD3	2.42	0.41
1:F:94:LYS:NZ	1:F:94:LYS:HB3	2.36	0.41
1:J:153:ASP:HA	1:J:154:PRO:HD3	1.93	0.41
1:G:30:SER:HB2	1:G:57:THR:OG1	2.21	0.41
1:D:157:GLU:O	1:D:158:ASN:HB3	2.20	0.41
1:F:17:ASP:O	1:G:7:LEU:HD13	2.21	0.41
1:E:183:VAL:HG12	1:E:184:THR:N	2.36	0.41
1:J:77:PRO:HA	1:J:102:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ARG:HD3	5:C:470:HOH:O	2.20	0.40
1:C:73:GLN:HG2	1:C:106:VAL:HA	2.04	0.40
1:I:188:CYS:HB3	1:I:189:PRO:HD2	2.03	0.40
1:J:152:VAL:HG22	1:J:195:VAL:CG2	2.51	0.40
1:F:94:LYS:HE2	1:G:97:VAL:O	2.21	0.40
1:D:146:HIS:HD2	1:D:148:ARG:H	1.68	0.40
1:F:14:SER:O	1:F:15:ARG:HB2	2.21	0.40
1:I:161:ASP:HB3	1:I:176:VAL:CG2	2.51	0.40
1:D:106:VAL:HG12	1:D:107:SER:N	2.36	0.40
1:F:142:SER:OG	1:F:145:HIS:HB2	2.21	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	208/214 (97%)	205 (99%)	2 (1%)	1 (0%)	34 30
1	B	207/214 (97%)	198 (96%)	9 (4%)	0	100 100
1	C	209/214 (98%)	202 (97%)	7 (3%)	0	100 100
1	D	207/214 (97%)	198 (96%)	7 (3%)	2 (1%)	19 13
1	E	206/214 (96%)	201 (98%)	5 (2%)	0	100 100
1	F	207/214 (97%)	197 (95%)	10 (5%)	0	100 100
1	G	207/214 (97%)	198 (96%)	9 (4%)	0	100 100
1	H	208/214 (97%)	198 (95%)	10 (5%)	0	100 100
1	I	207/214 (97%)	198 (96%)	8 (4%)	1 (0%)	34 30
1	J	206/214 (96%)	196 (95%)	7 (3%)	3 (2%)	13 7
All	All	2072/2140 (97%)	1991 (96%)	74 (4%)	7 (0%)	46 45

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	D	158	ASN
1	J	23	ARG
1	D	157	GLU
1	J	158	ASN
1	I	160	ASP
1	J	40	GLU

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	193/197 (98%)	192 (100%)	1 (0%)	92 95
1	B	192/197 (98%)	189 (98%)	3 (2%)	70 76
1	C	194/197 (98%)	193 (100%)	1 (0%)	92 95
1	D	192/197 (98%)	190 (99%)	2 (1%)	82 87
1	E	191/197 (97%)	184 (96%)	7 (4%)	41 41
1	F	192/197 (98%)	190 (99%)	2 (1%)	82 87
1	G	192/197 (98%)	189 (98%)	3 (2%)	70 76
1	H	193/197 (98%)	193 (100%)	0	100 100
1	I	192/197 (98%)	191 (100%)	1 (0%)	92 95
1	J	191/197 (97%)	189 (99%)	2 (1%)	82 87
All	All	1922/1970 (98%)	1900 (99%)	22 (1%)	80 85

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	B	24	ASP
1	B	158[A]	ASN
1	B	158[B]	ASN
1	C	40	GLU

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Mol	Chain	Res	Type
1	D	61	ARG
1	D	200	ASN
1	E	11	ARG
1	E	15	ARG
1	E	25	ARG
1	E	120	ARG
1	E	129	ASP
1	E	157	GLU
1	E	200	ASN
1	F	24	ASP
1	F	200	ASN
1	G	40	GLU
1	G	81	LEU
1	G	167	GLN
1	I	49	ASP
1	J	49	ASP
1	J	200	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	200	ASN
1	B	22	GLN
1	B	101	GLN
1	B	146	HIS
1	B	178	GLN
1	C	22	GLN
1	C	146	HIS
1	C	178	GLN
1	D	146	HIS
1	D	200	ASN
1	E	12	GLN
1	E	146	HIS
1	E	178	GLN
1	E	200	ASN
1	F	158	ASN
1	F	200	ASN
1	G	12	GLN
1	G	146	HIS
1	G	178	GLN
1	G	200	ASN

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Mol	Chain	Res	Type
1	H	178	GLN
1	H	200	ASN
1	I	145	HIS
1	I	146	HIS
1	I	200	ASN
1	J	12	GLN
1	J	158	ASN
1	J	200	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 71 ligands modelled in this entry, 56 are monoatomic - leaving 15 for Mogul analysis.

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	N2Y	A	301	-	14,15,15	1.92	4 (28%)	17,20,20	1.73	4 (23%)
2	N2Y	B	301[A]	-	14,15,15	1.90	4 (28%)	17,20,20	1.85	5 (29%)
2	N2Y	B	301[B]	-	14,15,15	1.78	5 (35%)	17,20,20	1.83	5 (29%)
2	N2Y	C	301[A]	-	14,15,15	1.96	4 (28%)	17,20,20	1.75	5 (29%)
2	N2Y	C	301[B]	-	14,15,15	1.85	5 (35%)	17,20,20	1.77	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	N2Y	D	301	-	14,15,15	1.96	4 (28%)	17,20,20	1.87	5 (29%)
2	N2Y	E	301[A]	-	14,15,15	1.98	6 (42%)	17,20,20	1.86	5 (29%)
2	N2Y	E	301[B]	-	14,15,15	2.02	5 (35%)	17,20,20	1.94	5 (29%)
2	N2Y	F	301[A]	-	14,15,15	2.04	4 (28%)	17,20,20	1.82	5 (29%)
2	N2Y	F	301[B]	-	14,15,15	1.91	5 (35%)	17,20,20	1.75	5 (29%)
2	N2Y	G	301	-	14,15,15	2.01	4 (28%)	17,20,20	1.67	3 (17%)
2	N2Y	H	301[A]	-	14,15,15	2.06	4 (28%)	17,20,20	1.86	5 (29%)
2	N2Y	H	301[B]	-	14,15,15	1.88	5 (35%)	17,20,20	1.73	5 (29%)
2	N2Y	I	301	-	14,15,15	2.06	4 (28%)	17,20,20	1.75	4 (23%)
2	N2Y	J	301	-	14,15,15	1.96	4 (28%)	17,20,20	1.83	5 (29%)

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	N2Y	A	301	-	-	0/4/14/14	0/2/2/2
2	N2Y	B	301[A]	-	-	0/4/14/14	0/2/2/2
2	N2Y	B	301[B]	-	-	0/4/14/14	0/2/2/2
2	N2Y	C	301[A]	-	-	0/4/14/14	0/2/2/2
2	N2Y	C	301[B]	-	-	0/4/14/14	0/2/2/2
2	N2Y	D	301	-	-	0/4/14/14	0/2/2/2
2	N2Y	E	301[A]	-	-	0/4/14/14	0/2/2/2
2	N2Y	E	301[B]	-	-	0/4/14/14	0/2/2/2
2	N2Y	F	301[A]	-	-	0/4/14/14	0/2/2/2
2	N2Y	F	301[B]	-	-	0/4/14/14	0/2/2/2
2	N2Y	G	301	-	-	0/4/14/14	0/2/2/2
2	N2Y	H	301[A]	-	-	0/4/14/14	0/2/2/2
2	N2Y	H	301[B]	-	-	0/4/14/14	0/2/2/2
2	N2Y	I	301	-	-	0/4/14/14	0/2/2/2
2	N2Y	J	301	-	-	0/4/14/14	0/2/2/2

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301[B]	N2Y	C9-C6	2.01	1.55	1.51
2	I	301	N2Y	C8-C4	2.02	1.42	1.37
2	E	301[B]	N2Y	C8-C4	2.03	1.42	1.37
2	B	301[A]	N2Y	C8-C4	2.09	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301[B]	N2Y	C7-C6	2.10	1.43	1.38
2	E	301[A]	N2Y	C7-C8	2.13	1.42	1.38
2	F	301[A]	N2Y	C8-C4	2.17	1.42	1.37
2	C	301[B]	N2Y	C7-C6	2.17	1.43	1.38
2	B	301[B]	N2Y	C5-C6	2.17	1.42	1.38
2	D	301	N2Y	C9-C6	2.17	1.55	1.51
2	F	301[B]	N2Y	C7-C6	2.20	1.43	1.38
2	G	301	N2Y	C8-C4	2.22	1.42	1.37
2	H	301[B]	N2Y	C7-C6	2.23	1.43	1.38
2	C	301[A]	N2Y	C8-C4	2.23	1.42	1.37
2	A	301	N2Y	C8-C4	2.24	1.42	1.37
2	H	301[A]	N2Y	C8-C4	2.26	1.42	1.37
2	F	301[B]	N2Y	C8-C4	2.26	1.42	1.37
2	J	301	N2Y	C8-C4	2.26	1.42	1.37
2	C	301[B]	N2Y	C5-C6	2.26	1.42	1.38
2	H	301[B]	N2Y	C8-C4	2.28	1.42	1.37
2	H	301[B]	N2Y	C5-C6	2.33	1.42	1.38
2	E	301[A]	N2Y	C7-C6	2.34	1.43	1.38
2	C	301[B]	N2Y	C8-C4	2.39	1.43	1.37
2	E	301[A]	N2Y	C8-C4	2.42	1.43	1.37
2	B	301[B]	N2Y	C8-C4	2.50	1.43	1.37
2	F	301[B]	N2Y	C5-C6	2.57	1.42	1.38
2	E	301[A]	N2Y	C5-C6	2.60	1.42	1.38
2	B	301[B]	N2Y	C1-N3	2.99	1.42	1.35
2	B	301[A]	N2Y	C5-C6	3.00	1.43	1.38
2	J	301	N2Y	C5-C6	3.01	1.43	1.38
2	F	301[A]	N2Y	C5-C6	3.09	1.43	1.38
2	G	301	N2Y	C1-N3	3.09	1.42	1.35
2	D	301	N2Y	C5-C6	3.09	1.43	1.38
2	H	301[B]	N2Y	C1-N3	3.23	1.42	1.35
2	A	301	N2Y	C1-N3	3.23	1.42	1.35
2	H	301[A]	N2Y	C5-C6	3.26	1.43	1.38
2	E	301[B]	N2Y	C5-C6	3.28	1.43	1.38
2	C	301[A]	N2Y	C5-C6	3.29	1.43	1.38
2	B	301[A]	N2Y	C1-N3	3.30	1.42	1.35
2	J	301	N2Y	C1-N3	3.36	1.43	1.35
2	C	301[A]	N2Y	C1-N3	3.36	1.43	1.35
2	C	301[B]	N2Y	C1-N3	3.37	1.43	1.35
2	F	301[B]	N2Y	C1-N3	3.39	1.43	1.35
2	I	301	N2Y	C1-N3	3.40	1.43	1.35
2	A	301	N2Y	C5-C6	3.42	1.44	1.38
2	H	301[A]	N2Y	C1-N3	3.44	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301[A]	N2Y	C1-N4	3.46	1.40	1.35
2	E	301[A]	N2Y	C1-N3	3.49	1.43	1.35
2	E	301[B]	N2Y	C1-N3	3.52	1.43	1.35
2	F	301[A]	N2Y	C1-N3	3.53	1.43	1.35
2	G	301	N2Y	C5-C6	3.57	1.44	1.38
2	A	301	N2Y	C1-N4	3.58	1.40	1.35
2	I	301	N2Y	C5-C6	3.60	1.44	1.38
2	D	301	N2Y	C1-N4	3.62	1.40	1.35
2	B	301[B]	N2Y	C1-N4	3.68	1.40	1.35
2	E	301[B]	N2Y	C1-N4	3.71	1.40	1.35
2	D	301	N2Y	C1-N3	3.72	1.43	1.35
2	C	301[B]	N2Y	C1-N4	3.77	1.41	1.35
2	C	301[A]	N2Y	C1-N4	3.81	1.41	1.35
2	E	301[A]	N2Y	C1-N4	3.82	1.41	1.35
2	F	301[B]	N2Y	C1-N4	3.83	1.41	1.35
2	H	301[B]	N2Y	C1-N4	3.90	1.41	1.35
2	H	301[A]	N2Y	C1-N4	3.91	1.41	1.35
2	F	301[A]	N2Y	C1-N4	3.93	1.41	1.35
2	J	301	N2Y	C1-N4	3.98	1.41	1.35
2	I	301	N2Y	C1-N4	4.02	1.41	1.35
2	G	301	N2Y	C1-N4	4.09	1.41	1.35

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301[B]	N2Y	C8-C4-N6	-2.22	120.96	124.71
2	F	301[A]	N2Y	C8-C4-N6	-2.22	120.96	124.71
2	H	301[A]	N2Y	C8-C4-N6	-2.16	121.06	124.71
2	J	301	N2Y	C8-C4-N6	-2.12	121.12	124.71
2	B	301[A]	N2Y	C8-C4-N6	-2.12	121.13	124.71
2	E	301[A]	N2Y	C8-C4-N6	-2.08	121.18	124.71
2	B	301[B]	N2Y	C8-C4-N6	-2.07	121.20	124.71
2	D	301	N2Y	C8-C4-N6	-2.07	121.21	124.71
2	I	301	N2Y	C8-C4-N6	-2.05	121.24	124.71
2	H	301[B]	N2Y	C8-C4-N6	-2.04	121.25	124.71
2	C	301[B]	N2Y	C8-C4-N6	-2.04	121.25	124.71
2	C	301[A]	N2Y	C8-C4-N6	-2.04	121.26	124.71
2	F	301[B]	N2Y	C8-C4-N6	-2.01	121.30	124.71
2	D	301	N2Y	C3-C2-N4	2.08	105.42	102.72
2	B	301[B]	N2Y	C9-N3-C1	2.08	127.90	123.99
2	G	301	N2Y	C9-N3-C1	2.09	127.92	123.99
2	E	301[B]	N2Y	C3-C2-N4	2.13	105.48	102.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301[A]	N2Y	C3-C2-N4	2.16	105.53	102.72
2	F	301[A]	N2Y	C3-C2-N4	2.18	105.54	102.72
2	A	301	N2Y	C9-N3-C1	2.18	128.08	123.99
2	J	301	N2Y	C3-C2-N4	2.18	105.55	102.72
2	H	301[A]	N2Y	C3-C2-N4	2.21	105.59	102.72
2	E	301[A]	N2Y	C3-C2-N4	2.22	105.60	102.72
2	H	301[B]	N2Y	C3-C2-N4	2.22	105.60	102.72
2	F	301[B]	N2Y	C3-C2-N4	2.24	105.63	102.72
2	C	301[A]	N2Y	C3-C2-N4	2.25	105.64	102.72
2	A	301	N2Y	C3-C2-N4	2.26	105.66	102.72
2	I	301	N2Y	C9-N3-C1	2.27	128.25	123.99
2	C	301[A]	N2Y	C9-N3-C1	2.32	128.34	123.99
2	C	301[B]	N2Y	C9-N3-C1	2.34	128.38	123.99
2	H	301[B]	N2Y	C9-N3-C1	2.34	128.39	123.99
2	B	301[A]	N2Y	C9-N3-C1	2.37	128.44	123.99
2	H	301[A]	N2Y	C9-N3-C1	2.37	128.44	123.99
2	E	301[A]	N2Y	C9-N3-C1	2.37	128.45	123.99
2	B	301[B]	N2Y	C3-C2-N4	2.40	105.83	102.72
2	C	301[B]	N2Y	C3-C2-N4	2.41	105.85	102.72
2	J	301	N2Y	C9-N3-C1	2.42	128.53	123.99
2	F	301[A]	N2Y	C9-N3-C1	2.48	128.65	123.99
2	F	301[B]	N2Y	C9-N3-C1	2.53	128.73	123.99
2	E	301[B]	N2Y	C9-N3-C1	2.54	128.76	123.99
2	D	301	N2Y	C9-N3-C1	2.64	128.94	123.99
2	H	301[B]	N2Y	C6-C9-N3	2.70	117.69	113.10
2	F	301[B]	N2Y	C6-C9-N3	2.72	117.73	113.10
2	G	301	N2Y	C6-C9-N3	2.87	117.99	113.10
2	C	301[A]	N2Y	C6-C9-N3	2.96	118.14	113.10
2	A	301	N2Y	C6-C9-N3	3.01	118.22	113.10
2	C	301[B]	N2Y	C6-C9-N3	3.04	118.27	113.10
2	I	301	N2Y	C6-C9-N3	3.09	118.36	113.10
2	F	301[A]	N2Y	C6-C9-N3	3.13	118.43	113.10
2	J	301	N2Y	C6-C9-N3	3.32	118.75	113.10
2	H	301[A]	N2Y	C6-C9-N3	3.51	119.08	113.10
2	D	301	N2Y	C6-C9-N3	3.56	119.16	113.10
2	B	301[A]	N2Y	C6-C9-N3	3.57	119.18	113.10
2	E	301[A]	N2Y	C6-C9-N3	3.59	119.22	113.10
2	B	301[B]	N2Y	C6-C9-N3	3.63	119.27	113.10
2	E	301[B]	N2Y	C6-C9-N3	3.96	119.83	113.10
2	G	301	N2Y	C5-N6-C4	4.01	121.55	116.45
2	A	301	N2Y	C5-N6-C4	4.10	121.67	116.45
2	I	301	N2Y	C5-N6-C4	4.20	121.80	116.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	N2Y	C5-N6-C4	4.30	121.92	116.45
2	C	301[A]	N2Y	C5-N6-C4	4.31	121.94	116.45
2	B	301[B]	N2Y	C5-N6-C4	4.39	122.03	116.45
2	E	301[B]	N2Y	C5-N6-C4	4.41	122.06	116.45
2	B	301[A]	N2Y	C5-N6-C4	4.43	122.08	116.45
2	F	301[B]	N2Y	C5-N6-C4	4.43	122.09	116.45
2	C	301[B]	N2Y	C5-N6-C4	4.44	122.09	116.45
2	J	301	N2Y	C5-N6-C4	4.44	122.09	116.45
2	H	301[B]	N2Y	C5-N6-C4	4.44	122.09	116.45
2	F	301[A]	N2Y	C5-N6-C4	4.45	122.11	116.45
2	H	301[A]	N2Y	C5-N6-C4	4.46	122.12	116.45
2	E	301[A]	N2Y	C5-N6-C4	4.52	122.20	116.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301[A]	N2Y	1	0
2	B	301[B]	N2Y	1	0
2	C	301[B]	N2Y	6	0
2	E	301[A]	N2Y	3	0
2	E	301[B]	N2Y	1	0
2	F	301[B]	N2Y	2	0
2	H	301[B]	N2Y	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	208/214 (97%)	0.14	10 (4%) 34 43	21, 31, 56, 81	0
1	B	208/214 (97%)	0.04	8 (3%) 44 53	17, 25, 48, 60	0
1	C	208/214 (97%)	-0.01	5 (2%) 62 68	19, 27, 47, 59	0
1	D	208/214 (97%)	0.27	14 (6%) 21 28	21, 32, 58, 86	0
1	E	208/214 (97%)	0.31	8 (3%) 44 53	20, 35, 59, 81	0
1	F	208/214 (97%)	0.58	21 (10%) 9 12	26, 41, 67, 89	0
1	G	208/214 (97%)	0.35	13 (6%) 23 31	21, 37, 61, 88	0
1	H	208/214 (97%)	0.41	18 (8%) 13 17	19, 40, 67, 90	1 (0%)
1	I	208/214 (97%)	0.54	22 (10%) 8 11	25, 43, 65, 88	0
1	J	208/214 (97%)	0.60	22 (10%) 8 11	25, 44, 68, 88	0
All	All	2080/2140 (97%)	0.32	141 (6%) 20 28	17, 35, 63, 90	1 (0%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	205	GLY	9.8
1	A	156	THR	8.0
1	I	205	GLY	7.5
1	F	-2	ALA	6.9
1	H	156	THR	6.1
1	I	157	GLU	6.0
1	I	128	VAL	5.5
1	A	23	ARG	5.4
1	E	205	GLY	5.3
1	J	157	GLU	5.3
1	G	205	GLY	5.3
1	G	158	ASN	4.8
1	H	158	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
1	J	44	ILE	4.8
1	E	157	GLU	4.7
1	D	159	SER	4.6
1	B	-2	ALA	4.4
1	E	158	ASN	4.4
1	F	205	GLY	4.4
1	I	156	THR	4.3
1	A	158	ASN	4.3
1	J	23	ARG	4.3
1	D	205	GLY	4.2
1	H	157	GLU	4.0
1	F	159	SER	3.9
1	E	23	ARG	3.9
1	J	156	THR	3.8
1	E	22	GLN	3.8
1	I	162	SER	3.7
1	F	24	ASP	3.7
1	J	24	ASP	3.7
1	I	158	ASN	3.6
1	H	159	SER	3.6
1	F	157	GLU	3.6
1	H	24	ASP	3.6
1	D	160	ASP	3.6
1	G	-1	GLU	3.5
1	J	158	ASN	3.5
1	F	162	SER	3.5
1	A	-1	GLU	3.4
1	F	156	THR	3.4
1	E	24	ASP	3.4
1	H	174	LEU	3.3
1	J	132	SER	3.3
1	A	-2	ALA	3.3
1	I	22	GLN	3.2
1	F	160	ASP	3.2
1	D	157	GLU	3.2
1	F	-1	GLU	3.2
1	C	23	ARG	3.1
1	F	0	ALA	3.1
1	D	44	ILE	3.1
1	I	155	THR	3.1
1	J	170	ARG	3.1
1	D	-2	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	161	ASP	3.1
1	G	25	ARG	3.0
1	I	24	ASP	3.0
1	H	155	THR	3.0
1	H	131	GLU	3.0
1	J	25	ARG	3.0
1	C	-2	ALA	2.9
1	J	159	SER	2.9
1	H	25	ARG	2.9
1	F	158	ASN	2.9
1	B	24	ASP	2.9
1	J	205	GLY	2.9
1	I	173	ILE	2.8
1	G	-2	ALA	2.8
1	B	14	SER	2.8
1	J	14	SER	2.8
1	C	0	ALA	2.7
1	G	70	SER	2.7
1	J	128	VAL	2.6
1	I	125	VAL	2.6
1	C	205	GLY	2.6
1	A	22	GLN	2.6
1	I	160	ASP	2.6
1	G	22	GLN	2.6
1	J	126	SER	2.5
1	C	14[A]	SER	2.5
1	I	39	LEU	2.5
1	G	72	ASP	2.5
1	B	25	ARG	2.5
1	A	131	GLU	2.5
1	G	0	ALA	2.4
1	I	44	ILE	2.4
1	D	131	GLU	2.4
1	F	128	VAL	2.4
1	F	25	ARG	2.4
1	E	170	ARG	2.4
1	H	133	GLY	2.4
1	I	129	ASP	2.3
1	H	186	SER	2.3
1	J	183	VAL	2.3
1	I	176	VAL	2.3
1	H	61	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	204	LYS	2.3
1	I	25	ARG	2.3
1	B	186	SER	2.3
1	D	68	SER	2.3
1	E	-2	ALA	2.3
1	F	14	SER	2.2
1	F	132	SER	2.2
1	F	169	SER	2.2
1	D	158	ASN	2.2
1	G	125	VAL	2.2
1	H	127	GLY	2.2
1	B	0	ALA	2.2
1	H	134	ALA	2.2
1	J	173	ILE	2.2
1	I	-1	GLU	2.2
1	D	61	ARG	2.2
1	F	148	ARG	2.2
1	J	130	THR	2.2
1	J	148	ARG	2.2
1	G	160	ASP	2.2
1	A	0	ALA	2.2
1	A	160	ASP	2.1
1	D	-1	GLU	2.1
1	I	188	CYS	2.1
1	H	-2	ALA	2.1
1	F	133	GLY	2.1
1	H	132	SER	2.1
1	A	25	ARG	2.1
1	B	23	ARG	2.1
1	D	22	GLN	2.1
1	G	170	ARG	2.1
1	I	14	SER	2.1
1	D	23	ARG	2.1
1	F	22	GLN	2.1
1	F	176	VAL	2.1
1	D	156	THR	2.1
1	F	202	ARG	2.1
1	J	0	ALA	2.1
1	J	61	ARG	2.0
1	H	125	VAL	2.0
1	J	135	THR	2.0
1	B	188	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	133	GLY	2.0
1	J	133	GLY	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
4	NA	C	309	1/1	0.92	0.16	4.40	28,28,28,28	0
2	N2Y	H	301[B]	14/14	0.89	0.20	4.36	34,38,49,49	14
2	N2Y	H	301[A]	14/14	0.89	0.20	4.36	16,34,40,40	14
3	CD	C	302	1/1	1.00	0.11	3.41	29,29,29,29	0
3	CD	A	302	1/1	1.00	0.11	3.17	30,30,30,30	0
2	N2Y	F	301[A]	14/14	0.89	0.20	3.01	7,30,37,38	14
2	N2Y	F	301[B]	14/14	0.89	0.20	2.94	34,37,48,48	14
2	N2Y	B	301[B]	14/14	0.91	0.19	2.76	1,19,27,28	14
2	N2Y	B	301[A]	14/14	0.91	0.19	2.76	2,26,40,40	14
2	N2Y	E	301[B]	14/14	0.88	0.20	2.69	6,28,35,35	14
2	N2Y	E	301[A]	14/14	0.88	0.20	2.69	26,33,42,42	14
2	N2Y	D	301	14/14	0.88	0.15	2.10	3,22,30,30	0
2	N2Y	C	301[B]	14/14	0.90	0.18	1.99	28,34,45,45	14
2	N2Y	C	301[A]	14/14	0.90	0.18	1.99	1,23,31,32	14
3	CD	D	302	1/1	1.00	0.12	1.71	32,32,32,32	0
2	N2Y	A	301	14/14	0.89	0.13	1.06	2,22,26,29	0
3	CD	E	302	1/1	1.00	0.12	1.03	26,26,26,26	0
2	N2Y	I	301	14/14	0.88	0.13	0.34	15,34,38,39	0
3	CD	F	303	1/1	0.76	0.16	0.13	98,98,98,98	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CD	B	305	1/1	1.00	0.10	0.06	28,28,28,28	0
2	N2Y	G	301	14/14	0.88	0.12	-0.11	12,31,37,37	0
2	N2Y	J	301	14/14	0.88	0.12	-0.25	19,32,40,40	0
3	CD	I	306	1/1	0.97	0.10	-0.73	70,70,70,70	1
3	CD	B	302	1/1	1.00	0.09	-1.33	34,34,34,34	0
3	CD	F	304	1/1	0.89	0.09	-1.46	58,58,58,58	1
4	NA	B	309	1/1	0.60	0.11	-1.50	52,52,52,52	0
3	CD	I	304	1/1	0.99	0.06	-1.68	38,38,38,38	0
3	CD	G	303	1/1	0.98	0.07	-2.57	51,51,51,51	1
3	CD	D	304	1/1	0.92	0.09	-2.67	75,75,75,75	1
3	CD	G	305	1/1	0.96	0.07	-2.85	75,75,75,75	1
3	CD	D	305	1/1	0.98	0.04	-2.88	44,44,44,44	0
3	CD	E	307	1/1	0.99	0.06	-3.42	55,55,55,55	1
3	CD	D	306	1/1	0.99	0.04	-5.48	52,52,52,52	1
3	CD	C	305	1/1	0.97	0.04	-	65,65,65,65	0
3	CD	I	305	1/1	0.94	0.05	-	66,66,66,66	1
3	CD	A	304	1/1	0.86	0.08	-	83,83,83,83	1
3	CD	C	308	1/1	0.93	0.14	-	78,78,78,78	1
3	CD	B	303	1/1	0.88	0.09	-	83,83,83,83	0
3	CD	D	308	1/1	0.90	0.06	-	89,89,89,89	1
3	CD	C	304	1/1	0.95	0.07	-	60,60,60,60	1
3	CD	B	308	1/1	0.86	0.07	-	50,50,50,50	1
3	CD	E	303	1/1	0.94	0.10	-	69,69,69,69	0
3	CD	G	304	1/1	0.90	0.09	-	75,75,75,75	1
3	CD	F	305	1/1	0.96	0.05	-	76,76,76,76	1
3	CD	G	302	1/1	0.95	0.06	-	79,79,79,79	1
3	CD	E	306	1/1	0.95	0.09	-	66,66,66,66	0
3	CD	A	309	1/1	0.87	0.09	-	46,46,46,46	1
3	CD	C	307	1/1	0.95	0.07	-	85,85,85,85	0
3	CD	E	305	1/1	0.90	0.11	-	76,76,76,76	0
3	CD	B	304	1/1	0.91	0.07	-	92,92,92,92	1
3	CD	A	303	1/1	0.92	0.07	-	74,74,74,74	1
3	CD	F	302	1/1	0.84	0.07	-	94,94,94,94	0
3	CD	C	303	1/1	0.98	0.04	-	51,51,51,51	0
3	CD	E	304	1/1	0.70	0.09	-	83,83,83,83	1
3	CD	A	307	1/1	0.86	0.07	-	92,92,92,92	1
3	CD	A	306	1/1	0.98	0.04	-	68,68,68,68	1
3	CD	C	306	1/1	0.99	0.10	-	33,33,33,33	0
3	CD	H	302	1/1	0.93	0.07	-	66,66,66,66	0
3	CD	J	302	1/1	0.90	0.08	-	75,75,75,75	0
3	CD	G	306	1/1	0.90	0.18	-	48,48,48,48	1
3	CD	B	306	1/1	0.95	0.07	-	84,84,84,84	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CD	H	303	1/1	0.96	0.06	-	76,76,76,76	1
3	CD	J	303	1/1	0.92	0.06	-	79,79,79,79	1
3	CD	I	303	1/1	0.87	0.08	-	91,91,91,91	1
3	CD	D	307	1/1	0.90	0.10	-	89,89,89,89	1
3	CD	B	307	1/1	0.76	0.10	-	47,47,47,47	1
3	CD	A	305	1/1	0.81	0.06	-	91,91,91,91	0
3	CD	I	302	1/1	0.93	0.07	-	87,87,87,87	0
3	CD	D	303	1/1	0.92	0.07	-	84,84,84,84	1
3	CD	A	308	1/1	0.87	0.17	-	55,55,55,55	1
3	CD	I	307	1/1	0.97	0.10	-	46,46,46,46	1

6.5 Other polymers

There are no such residues in this entry.