Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 07:20 AM EDT

PDB ID	:	3KTM
Title	:	Structure of the Heparin-induced E1-Dimer of the Amyloid Precursor Protein (APP)
Authors	:	Dahms, S.O.; Hoefgen, S.; Roeser, D.; Schlott, B.; Guhrs, K.H.; Than, M.E.
Deposited on	:	2009-11-25
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

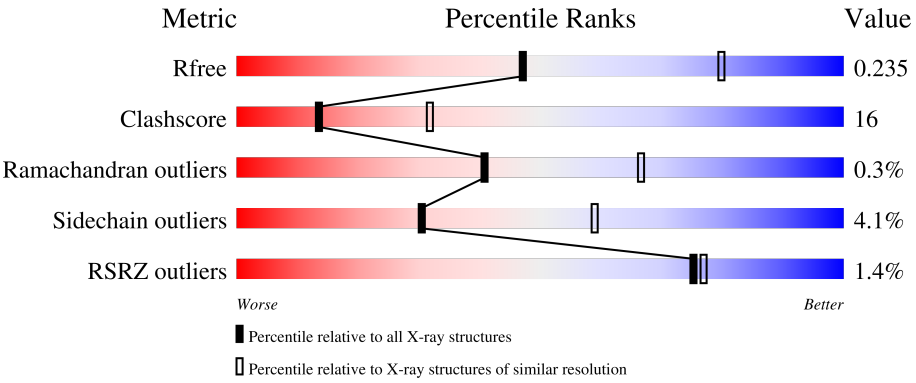
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	191	65% 24% 8%
1	B	191	60% 31% 9%
1	C	191	61% 28% 9%
1	D	191	69% 18% 9%
1	E	191	3% 71% 21% 7%

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Mol	Chain	Length	Quality of chain
1	F	191	61% 28% 8%
1	G	191	57% 32% 9%
1	H	191	62% 28% 8%

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
4	ACT	C	8	-	-	-	X
4	ACT	H	6	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11436 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 Amyloid beta A4 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	32	0	0
			1392	878	245	252	17			
1	B	173	Total	C	N	O	S	27	0	0
			1369	863	241	248	17			
1	C	174	Total	C	N	O	S	20	0	0
			1374	866	242	249	17			
1	D	173	Total	C	N	O	S	26	0	0
			1373	867	241	248	17			
1	E	177	Total	C	N	O	S	35	0	0
			1401	883	247	254	17			
1	F	175	Total	C	N	O	S	37	0	0
			1392	878	245	252	17			
1	G	174	Total	C	N	O	S	50	0	0
			1382	872	242	251	17			
1	H	175	Total	C	N	O	S	38	0	0
			1382	872	243	250	17			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP P05067
A	191	ILE	-	expression tag	UNP P05067
A	192	GLU	-	expression tag	UNP P05067
A	193	GLY	-	expression tag	UNP P05067
A	194	ARG	-	expression tag	UNP P05067
A	195	LYS	-	expression tag	UNP P05067
A	196	LEU	-	expression tag	UNP P05067
A	197	ALA	-	expression tag	UNP P05067
A	198	ALA	-	expression tag	UNP P05067
A	199	ALA	-	expression tag	UNP P05067
A	200	LEU	-	expression tag	UNP P05067
A	201	GLU	-	expression tag	UNP P05067
A	202	HIS	-	expression tag	UNP P05067

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Chain	Residue	Modelled	Actual	Comment	Reference
A	203	HIS	-	expression tag	UNP P05067
A	204	HIS	-	expression tag	UNP P05067
A	205	HIS	-	expression tag	UNP P05067
A	206	HIS	-	expression tag	UNP P05067
A	207	HIS	-	expression tag	UNP P05067
B	17	MET	-	initiating methionine	UNP P05067
B	191	ILE	-	expression tag	UNP P05067
B	192	GLU	-	expression tag	UNP P05067
B	193	GLY	-	expression tag	UNP P05067
B	194	ARG	-	expression tag	UNP P05067
B	195	LYS	-	expression tag	UNP P05067
B	196	LEU	-	expression tag	UNP P05067
B	197	ALA	-	expression tag	UNP P05067
B	198	ALA	-	expression tag	UNP P05067
B	199	ALA	-	expression tag	UNP P05067
B	200	LEU	-	expression tag	UNP P05067
B	201	GLU	-	expression tag	UNP P05067
B	202	HIS	-	expression tag	UNP P05067
B	203	HIS	-	expression tag	UNP P05067
B	204	HIS	-	expression tag	UNP P05067
B	205	HIS	-	expression tag	UNP P05067
B	206	HIS	-	expression tag	UNP P05067
B	207	HIS	-	expression tag	UNP P05067
C	17	MET	-	initiating methionine	UNP P05067
C	191	ILE	-	expression tag	UNP P05067
C	192	GLU	-	expression tag	UNP P05067
C	193	GLY	-	expression tag	UNP P05067
C	194	ARG	-	expression tag	UNP P05067
C	195	LYS	-	expression tag	UNP P05067
C	196	LEU	-	expression tag	UNP P05067
C	197	ALA	-	expression tag	UNP P05067
C	198	ALA	-	expression tag	UNP P05067
C	199	ALA	-	expression tag	UNP P05067
C	200	LEU	-	expression tag	UNP P05067
C	201	GLU	-	expression tag	UNP P05067
C	202	HIS	-	expression tag	UNP P05067
C	203	HIS	-	expression tag	UNP P05067
C	204	HIS	-	expression tag	UNP P05067
C	205	HIS	-	expression tag	UNP P05067
C	206	HIS	-	expression tag	UNP P05067
C	207	HIS	-	expression tag	UNP P05067
D	17	MET	-	initiating methionine	UNP P05067

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Chain	Residue	Modelled	Actual	Comment	Reference
D	191	ILE	-	expression tag	UNP P05067
D	192	GLU	-	expression tag	UNP P05067
D	193	GLY	-	expression tag	UNP P05067
D	194	ARG	-	expression tag	UNP P05067
D	195	LYS	-	expression tag	UNP P05067
D	196	LEU	-	expression tag	UNP P05067
D	197	ALA	-	expression tag	UNP P05067
D	198	ALA	-	expression tag	UNP P05067
D	199	ALA	-	expression tag	UNP P05067
D	200	LEU	-	expression tag	UNP P05067
D	201	GLU	-	expression tag	UNP P05067
D	202	HIS	-	expression tag	UNP P05067
D	203	HIS	-	expression tag	UNP P05067
D	204	HIS	-	expression tag	UNP P05067
D	205	HIS	-	expression tag	UNP P05067
D	206	HIS	-	expression tag	UNP P05067
D	207	HIS	-	expression tag	UNP P05067
E	17	MET	-	initiating methionine	UNP P05067
E	191	ILE	-	expression tag	UNP P05067
E	192	GLU	-	expression tag	UNP P05067
E	193	GLY	-	expression tag	UNP P05067
E	194	ARG	-	expression tag	UNP P05067
E	195	LYS	-	expression tag	UNP P05067
E	196	LEU	-	expression tag	UNP P05067
E	197	ALA	-	expression tag	UNP P05067
E	198	ALA	-	expression tag	UNP P05067
E	199	ALA	-	expression tag	UNP P05067
E	200	LEU	-	expression tag	UNP P05067
E	201	GLU	-	expression tag	UNP P05067
E	202	HIS	-	expression tag	UNP P05067
E	203	HIS	-	expression tag	UNP P05067
E	204	HIS	-	expression tag	UNP P05067
E	205	HIS	-	expression tag	UNP P05067
E	206	HIS	-	expression tag	UNP P05067
E	207	HIS	-	expression tag	UNP P05067
F	17	MET	-	initiating methionine	UNP P05067
F	191	ILE	-	expression tag	UNP P05067
F	192	GLU	-	expression tag	UNP P05067
F	193	GLY	-	expression tag	UNP P05067
F	194	ARG	-	expression tag	UNP P05067
F	195	LYS	-	expression tag	UNP P05067
F	196	LEU	-	expression tag	UNP P05067

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Chain	Residue	Modelled	Actual	Comment	Reference
F	197	ALA	-	expression tag	UNP P05067
F	198	ALA	-	expression tag	UNP P05067
F	199	ALA	-	expression tag	UNP P05067
F	200	LEU	-	expression tag	UNP P05067
F	201	GLU	-	expression tag	UNP P05067
F	202	HIS	-	expression tag	UNP P05067
F	203	HIS	-	expression tag	UNP P05067
F	204	HIS	-	expression tag	UNP P05067
F	205	HIS	-	expression tag	UNP P05067
F	206	HIS	-	expression tag	UNP P05067
F	207	HIS	-	expression tag	UNP P05067
G	17	MET	-	initiating methionine	UNP P05067
G	191	ILE	-	expression tag	UNP P05067
G	192	GLU	-	expression tag	UNP P05067
G	193	GLY	-	expression tag	UNP P05067
G	194	ARG	-	expression tag	UNP P05067
G	195	LYS	-	expression tag	UNP P05067
G	196	LEU	-	expression tag	UNP P05067
G	197	ALA	-	expression tag	UNP P05067
G	198	ALA	-	expression tag	UNP P05067
G	199	ALA	-	expression tag	UNP P05067
G	200	LEU	-	expression tag	UNP P05067
G	201	GLU	-	expression tag	UNP P05067
G	202	HIS	-	expression tag	UNP P05067
G	203	HIS	-	expression tag	UNP P05067
G	204	HIS	-	expression tag	UNP P05067
G	205	HIS	-	expression tag	UNP P05067
G	206	HIS	-	expression tag	UNP P05067
G	207	HIS	-	expression tag	UNP P05067
H	17	MET	-	initiating methionine	UNP P05067
H	191	ILE	-	expression tag	UNP P05067
H	192	GLU	-	expression tag	UNP P05067
H	193	GLY	-	expression tag	UNP P05067
H	194	ARG	-	expression tag	UNP P05067
H	195	LYS	-	expression tag	UNP P05067
H	196	LEU	-	expression tag	UNP P05067
H	197	ALA	-	expression tag	UNP P05067
H	198	ALA	-	expression tag	UNP P05067
H	199	ALA	-	expression tag	UNP P05067
H	200	LEU	-	expression tag	UNP P05067
H	201	GLU	-	expression tag	UNP P05067
H	202	HIS	-	expression tag	UNP P05067

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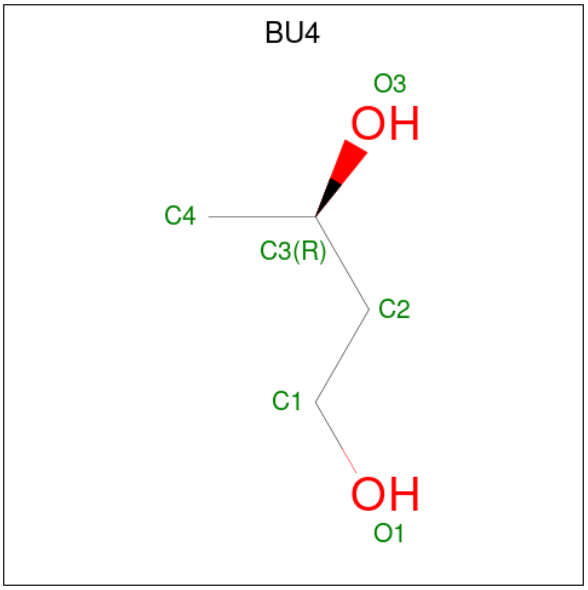
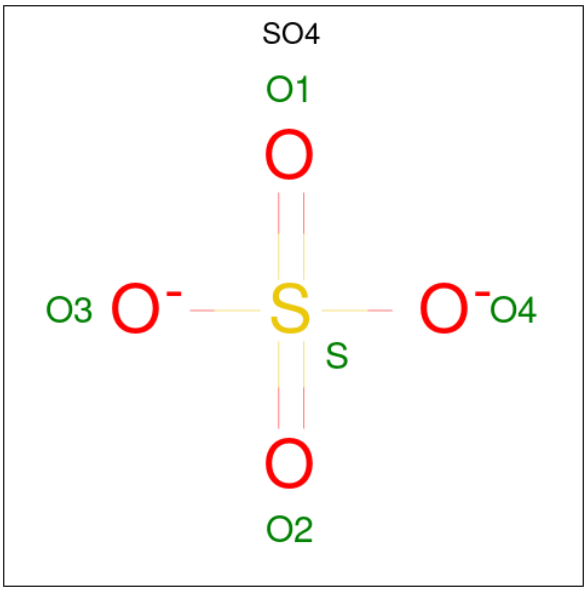
Chain	Residue	Modelled	Actual	Comment	Reference
H	203	HIS	-	expression tag	UNP P05067
H	204	HIS	-	expression tag	UNP P05067
H	205	HIS	-	expression tag	UNP P05067
H	206	HIS	-	expression tag	UNP P05067
H	207	HIS	-	expression tag	UNP P05067

- Molecule 2 is (3R)-butane-1,3-diol (three-letter code: BU4) (formula: $C_4H_{10}O_2$).



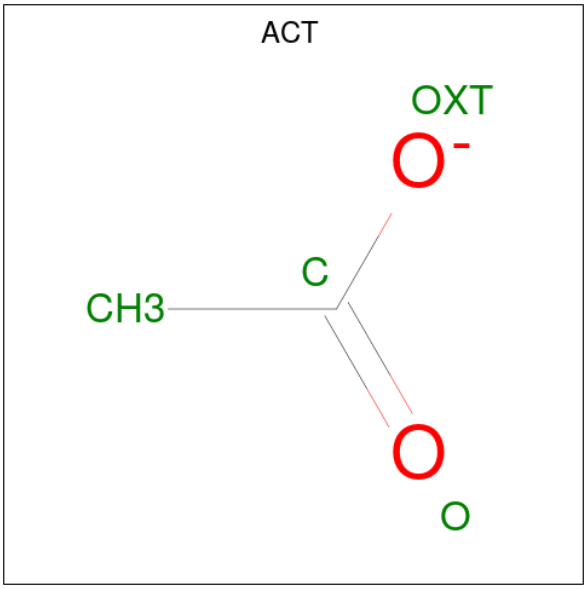
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 4 2	0	0
2	B	1	Total C O 6 4 2	0	0
2	C	1	Total C O 6 4 2	0	0
2	D	1	Total C O 6 4 2	0	0
2	E	1	Total C O 6 4 2	0	0
2	F	1	Total C O 6 4 2	0	0
2	G	1	Total C O 6 4 2	0	0
2	H	1	Total C O 6 4 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

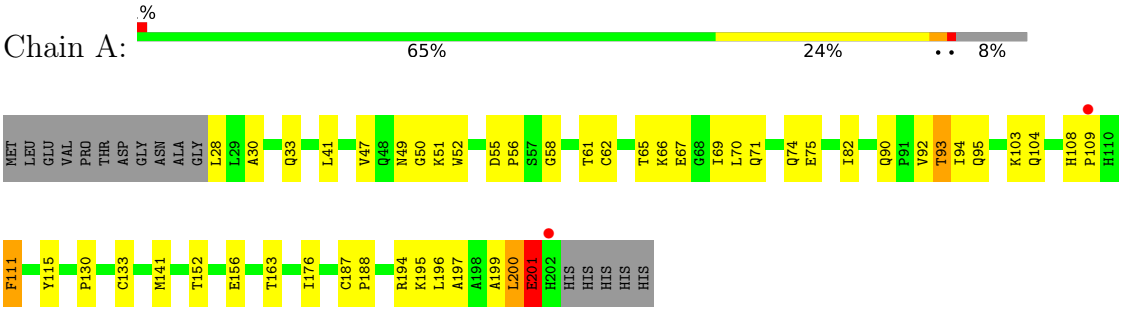
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	41	Total O 41 41	0	0
5	B	36	Total O 36 36	0	0
5	C	47	Total O 47 47	0	0
5	D	53	Total O 53 53	0	0
5	E	29	Total O 29 29	0	0
5	F	36	Total O 36 36	0	0
5	G	9	Total O 9 9	0	0
5	H	31	Total O 31 31	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

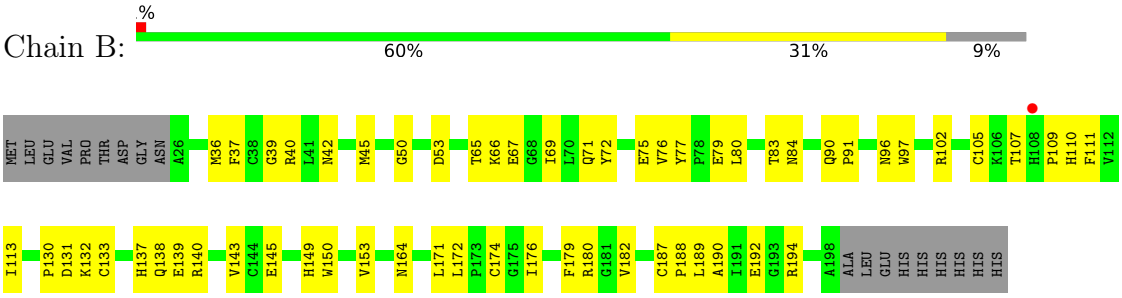
• Molecule 1: Amyloid beta A4 protein

Chain A:



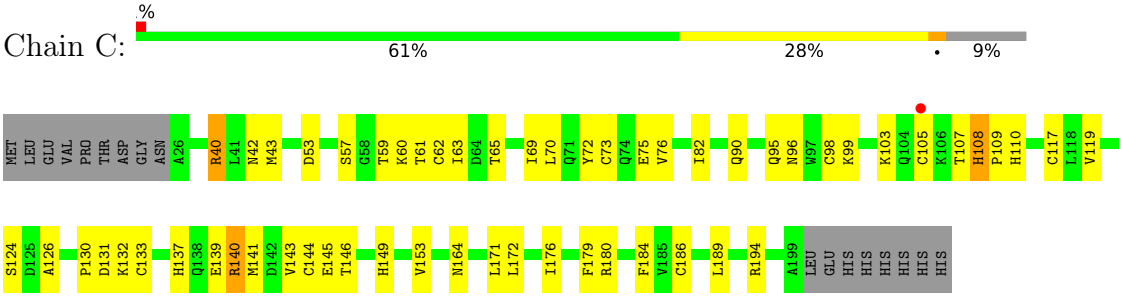
• Molecule 1: Amyloid beta A4 protein

Chain B:



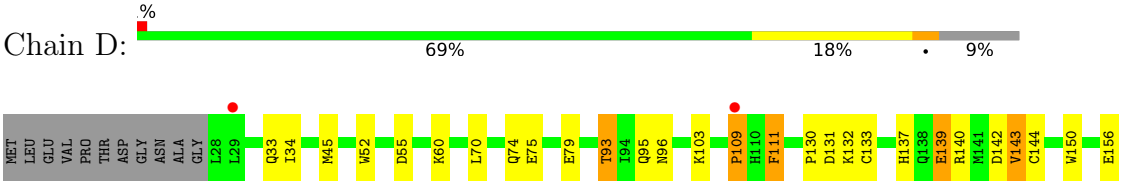
• Molecule 1: Amyloid beta A4 protein

Chain C:



• Molecule 1: Amyloid beta A4 protein

Chain D:

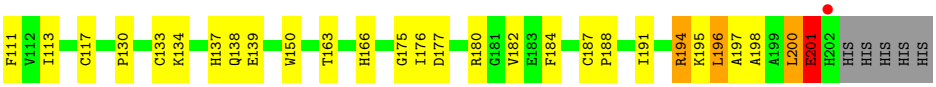


• Molecule 1: Amyloid beta A4 protein

Chain E:

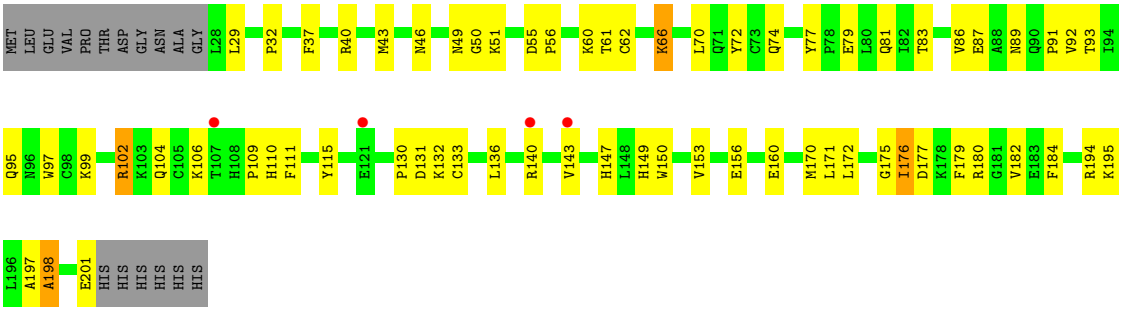
• Molecule 1: Amyloid beta A4 protein

Chain F:



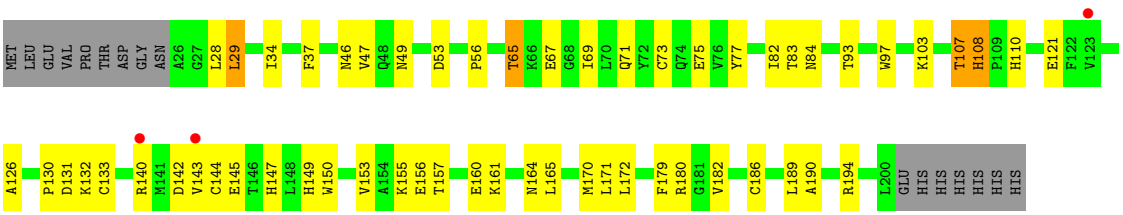
• Molecule 1: Amyloid beta A4 protein

Chain G:



• Molecule 1: Amyloid beta A4 protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	143.99Å 143.99Å 351.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.00 – 2.70 29.38 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.00-2.70) 99.9 (29.38-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.68Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.250 0.201 , 0.235	Depositor DCC
R_{free} test set	3735 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	52.3	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 61.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.009 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.011 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.008 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.010 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.007 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.022 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11436	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, SO4, BU4

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	0.44	0/1425	0.72	1/1929 (0.1%)
1	B	0.41	0/1401	0.68	0/1896
1	C	0.40	0/1406	0.67	0/1903
1	D	0.43	0/1405	0.70	0/1902
1	E	0.39	0/1434	0.67	0/1941
1	F	0.43	0/1425	0.70	0/1929
1	G	0.37	0/1414	0.63	0/1914
1	H	0.41	0/1414	0.67	0/1914
All	All	0.41	0/11324	0.68	1/15328 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	201	GLU	N-CA-C	7.33	130.80	111.00

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	1392	0	1360	41	0
1	B	1369	0	1339	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1374	0	1344	54	0
1	D	1373	0	1347	25	0
1	E	1401	0	1368	27	0
1	F	1392	0	1360	51	0
1	G	1382	0	1353	57	0
1	H	1382	0	1355	56	0
2	A	6	0	10	0	0
2	B	6	0	10	1	0
2	C	6	0	10	0	0
2	D	6	0	10	1	0
2	E	6	0	10	0	0
2	F	6	0	10	2	0
2	G	6	0	10	1	0
2	H	6	0	10	1	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	H	5	0	0	0	0
4	B	4	0	3	1	0
4	C	4	0	3	0	0
4	E	4	0	3	0	0
4	H	4	0	3	3	0
5	A	41	0	0	1	0
5	B	36	0	0	1	0
5	C	47	0	0	3	0
5	D	53	0	0	0	0
5	E	29	0	0	0	0
5	F	36	0	0	0	0
5	G	9	0	0	0	0
5	H	31	0	0	1	0
All	All	11436	0	10918	343	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 16.

All (343) 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:F:95:GLN:HG2	1:F:109:PRO:HG3	1.34	1.09
1:A:95:GLN:HG2	1:A:109:PRO:HG3	1.34	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:ARG:HB2	1:F:102:ARG:HH21	1.26	0.99
1:D:195:LYS:HE2	1:D:197:ALA:HB2	1.48	0.96
1:F:102:ARG:HB2	1:F:102:ARG:NH2	1.84	0.91
1:B:130:PRO:HG2	1:B:133:CYS:SG	2.10	0.91
1:C:146:THR:HG23	1:C:149:HIS:H	1.36	0.90
1:C:40:ARG:NH2	1:C:107:THR:HG21	1.88	0.89
1:F:195:LYS:HE2	1:F:197:ALA:HB2	1.56	0.87
1:E:95:GLN:HG2	1:E:109:PRO:HG3	1.59	0.85
1:G:61:THR:HG22	1:G:62:CYS:H	1.41	0.84
1:B:176:ILE:H	1:B:176:ILE:HD12	1.44	0.83
1:G:49:ASN:HD21	1:G:51:LYS:HB2	1.43	0.82
1:G:95:GLN:HG2	1:G:109:PRO:HG3	1.60	0.82
1:C:130:PRO:HG2	1:C:133:CYS:SG	2.19	0.81
1:A:130:PRO:HG2	1:A:133:CYS:SG	2.22	0.80
1:G:49:ASN:HD21	1:G:51:LYS:CB	1.95	0.80
1:H:73:CYS:HB3	1:H:82:ILE:HD13	1.65	0.79
1:C:140:ARG:HB2	1:C:143:VAL:HG12	1.65	0.78
1:A:103:LYS:HE2	1:C:43:MET:HE1	1.65	0.78
1:C:40:ARG:HH22	1:C:107:THR:HG21	1.48	0.75
1:H:180:ARG:HG2	1:H:180:ARG:HH11	1.51	0.75
1:C:61:THR:HG22	1:C:62:CYS:H	1.51	0.74
1:B:176:ILE:HD12	1:B:176:ILE:N	2.02	0.74
1:G:61:THR:HG22	1:G:62:CYS:N	2.04	0.73
1:G:70:LEU:O	1:G:74:GLN:HG3	1.89	0.72
1:B:91:PRO:HB3	1:B:113:ILE:HD12	1.73	0.71
1:C:143:VAL:CG2	1:C:145:GLU:HG2	2.21	0.70
1:D:95:GLN:HB3	1:D:109:PRO:HG3	1.74	0.70
1:D:130:PRO:HG2	1:D:133:CYS:SG	2.33	0.69
1:B:71:GLN:O	1:B:75:GLU:HG3	1.93	0.69
1:D:175:GLY:HA2	2:D:2:BU4:H4A	1.74	0.69
1:F:130:PRO:HG2	1:F:133:CYS:SG	2.34	0.68
1:B:102:ARG:HD2	1:D:103:LYS:O	1.93	0.68
1:C:140:ARG:HB2	1:C:143:VAL:CG1	2.24	0.67
1:E:130:PRO:HG2	1:E:133:CYS:SG	2.34	0.67
1:B:97:TRP:H	1:B:107:THR:HG22	1.60	0.67
1:A:74:GLN:HG2	1:A:82:ILE:HB	1.78	0.66
1:B:190:ALA:H	2:B:7:BU4:H2	1.61	0.65
1:F:99:LYS:HD3	1:F:102:ARG:NH2	2.12	0.65
1:H:71:GLN:O	1:H:75:GLU:HG3	1.97	0.65
1:C:143:VAL:HG22	1:C:145:GLU:HG2	1.77	0.65
1:H:143:VAL:CG2	1:H:145:GLU:HG2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LYS:HE2	1:C:43:MET:CE	2.28	0.64
1:A:49:ASN:OD1	1:A:51:LYS:N	2.31	0.64
1:C:60:LYS:HE3	1:C:75:GLU:OE2	1.96	0.64
1:G:195:LYS:HE2	1:G:197:ALA:HB2	1.79	0.64
1:G:130:PRO:HG2	1:G:133:CYS:SG	2.38	0.64
1:B:174:CYS:HB3	1:B:180:ARG:NH2	2.13	0.64
1:G:149:HIS:O	1:G:153:VAL:HG23	1.99	0.63
1:H:46:ASN:HB3	1:H:49:ASN:OD1	1.98	0.63
1:B:176:ILE:H	1:B:176:ILE:CD1	2.10	0.63
1:G:180:ARG:HG2	1:G:180:ARG:HH11	1.64	0.63
1:G:43:MET:CE	1:G:97:TRP:HA	2.29	0.63
1:F:91:PRO:HB3	1:F:113:ILE:HD12	1.81	0.63
1:B:90:GLN:OE1	4:B:208:ACT:H2	1.98	0.62
1:A:61:THR:HG22	1:A:62:CYS:N	2.13	0.62
1:B:97:TRP:H	1:B:107:THR:CG2	2.13	0.62
1:G:198:ALA:HB2	1:H:126:ALA:HA	1.82	0.62
1:A:28:LEU:HD12	1:A:47:VAL:HB	1.81	0.62
1:B:91:PRO:HB3	1:B:113:ILE:CD1	2.30	0.62
1:A:90:GLN:HB3	1:A:201:GLU:HG2	1.81	0.62
1:D:70:LEU:O	1:D:74:GLN:HG3	2.00	0.62
1:C:109:PRO:O	1:C:110:HIS:HD2	1.82	0.62
1:C:141:MET:HE3	1:F:93:THR:HB	1.80	0.62
1:G:70:LEU:O	1:G:70:LEU:HD12	2.00	0.61
1:C:61:THR:HG22	1:C:62:CYS:N	2.14	0.61
1:E:26:ALA:HB3	1:E:28:LEU:HD13	1.83	0.61
1:B:174:CYS:CB	1:B:180:ARG:NH2	2.63	0.61
1:G:46:ASN:HB3	1:G:49:ASN:OD1	2.00	0.60
1:C:164:ASN:HB2	1:C:189:LEU:HD23	1.83	0.60
1:B:174:CYS:HB3	1:B:180:ARG:HH21	1.67	0.59
1:F:150:TRP:HB3	1:F:182:VAL:HB	1.83	0.59
1:G:66:LYS:HB3	1:G:176:ILE:HG13	1.84	0.59
1:G:66:LYS:HD2	1:G:66:LYS:N	2.16	0.59
1:G:86:VAL:HA	1:G:177:ASP:OD1	2.03	0.59
1:A:61:THR:HG22	1:A:62:CYS:H	1.67	0.59
1:A:95:GLN:CG	1:A:109:PRO:HG3	2.23	0.59
1:H:164:ASN:HB2	1:H:189:LEU:HD23	1.83	0.59
1:F:137:HIS:ND1	1:F:139:GLU:OE1	2.25	0.59
1:H:46:ASN:HB2	1:H:53:ASP:OD2	2.02	0.59
1:H:133:CYS:HB3	1:H:186:CYS:O	2.03	0.59
1:H:97:TRP:H	1:H:107:THR:HG22	1.68	0.58
1:E:180:ARG:HG2	1:E:180:ARG:HH11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:ILE:HD12	1:E:176:ILE:N	2.19	0.58
1:D:150:TRP:HB3	1:D:182:VAL:HB	1.85	0.58
1:F:70:LEU:O	1:F:74:GLN:HG3	2.04	0.57
1:E:71:GLN:O	1:E:75:GLU:HG3	2.04	0.57
1:E:91:PRO:HB3	1:E:113:ILE:HD13	1.86	0.57
1:F:96:ASN:OD1	1:H:103:LYS:HE2	2.05	0.57
1:G:95:GLN:CG	1:G:109:PRO:HG3	2.31	0.57
1:E:65:THR:O	1:E:69:ILE:HG13	2.05	0.57
1:G:29:LEU:HD11	1:H:71:GLN:HG2	1.87	0.57
1:H:97:TRP:H	1:H:107:THR:CG2	2.16	0.57
1:G:61:THR:CG2	1:G:62:CYS:H	2.15	0.56
1:C:146:THR:HG22	5:C:229:HOH:O	2.04	0.56
1:C:131:ASP:O	1:C:132:LYS:HB2	2.05	0.56
1:G:140:ARG:HB2	1:G:143:VAL:HG12	1.87	0.56
1:G:93:THR:HG22	1:H:180:ARG:HE	1.71	0.56
5:C:214:HOH:O	1:F:51:LYS:HG2	2.05	0.56
1:B:65:THR:O	1:B:69:ILE:HG13	2.05	0.56
1:F:86:VAL:HA	1:F:177:ASP:OD1	2.05	0.56
1:G:102:ARG:NH2	1:G:102:ARG:HB2	2.21	0.56
1:E:34:ILE:HD13	1:E:34:ILE:H	1.69	0.56
1:A:67:GLU:O	1:A:71:GLN:HG3	2.06	0.56
1:C:82:ILE:HD13	1:C:117:CYS:HB3	1.88	0.56
1:C:176:ILE:HD12	1:C:176:ILE:N	2.21	0.56
1:F:180:ARG:HG2	1:F:180:ARG:HH21	1.71	0.56
1:H:140:ARG:HB2	1:H:143:VAL:CG1	2.35	0.56
1:H:157:THR:O	1:H:161:LYS:HE2	2.05	0.55
1:H:140:ARG:HB2	1:H:143:VAL:HG12	1.87	0.55
1:D:137:HIS:HD2	1:D:139:GLU:OE1	1.90	0.55
1:E:87:GLU:HG3	1:E:115:TYR:CE2	2.41	0.55
1:G:140:ARG:CB	1:G:143:VAL:HG12	2.36	0.55
1:B:96:ASN:HA	1:B:107:THR:HG22	1.88	0.55
1:B:180:ARG:HH21	1:B:180:ARG:CG	2.20	0.55
1:C:171:LEU:O	1:C:179:PHE:HB3	2.07	0.55
1:H:172:LEU:HB2	1:H:180:ARG:HB2	1.87	0.55
1:H:144:CYS:HB2	1:H:180:ARG:HH12	1.73	0.54
1:H:67:GLU:O	1:H:71:GLN:HG3	2.07	0.54
1:A:90:GLN:CB	1:A:201:GLU:HG2	2.37	0.54
1:A:28:LEU:CD1	1:A:47:VAL:HB	2.38	0.53
1:D:140:ARG:HB2	1:D:143:VAL:HG13	1.89	0.53
1:F:49:ASN:OD1	1:F:51:LYS:N	2.40	0.53
1:B:164:ASN:HB2	1:B:189:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:ASP:O	1:E:132:LYS:HB2	2.08	0.53
1:H:155:LYS:CE	4:H:6:ACT:H3	2.39	0.53
1:A:70:LEU:O	1:A:74:GLN:HG3	2.09	0.53
1:E:133:CYS:HB3	1:E:186:CYS:O	2.09	0.53
1:H:155:LYS:NZ	4:H:6:ACT:H3	2.24	0.53
1:A:41:LEU:HD13	1:A:58:GLY:HA2	1.90	0.52
1:G:102:ARG:HB2	1:G:102:ARG:HH21	1.75	0.52
1:G:150:TRP:HB3	1:G:182:VAL:HB	1.92	0.52
1:H:143:VAL:HG22	1:H:145:GLU:HG2	1.91	0.52
1:C:65:THR:O	1:C:69:ILE:HG12	2.09	0.51
1:A:93:THR:HG23	1:A:111:PHE:CD1	2.44	0.51
1:G:93:THR:CG2	1:H:180:ARG:HE	2.23	0.51
1:B:67:GLU:O	1:B:71:GLN:HG3	2.11	0.51
1:G:102:ARG:HD2	1:G:104:GLN:HG3	1.93	0.51
1:G:40:ARG:HH21	1:G:106:LYS:HE2	1.76	0.51
1:A:66:LYS:HB3	1:A:176:ILE:HG22	1.92	0.51
1:G:99:LYS:HD2	1:G:102:ARG:NH1	2.25	0.51
1:A:104:GLN:NE2	1:C:103:LYS:O	2.43	0.51
1:C:40:ARG:CZ	1:C:99:LYS:HG3	2.41	0.51
1:B:131:ASP:O	1:B:132:LYS:HB2	2.11	0.50
1:C:96:ASN:HB3	1:C:105:CYS:O	2.11	0.50
1:E:66:LYS:HB3	1:E:176:ILE:HG22	1.93	0.50
1:C:70:LEU:O	1:C:70:LEU:HD12	2.11	0.50
1:C:133:CYS:HB3	1:C:186:CYS:O	2.12	0.50
1:G:29:LEU:HD11	1:H:71:GLN:CG	2.42	0.50
1:E:46:ASN:OD1	1:E:49:ASN:ND2	2.45	0.50
1:G:136:LEU:HB2	1:G:184:PHE:CZ	2.47	0.50
1:H:77:TYR:HB2	1:H:82:ILE:HD11	1.93	0.50
1:G:91:PRO:HD2	1:G:201:GLU:HG3	1.93	0.49
1:G:61:THR:CG2	1:G:62:CYS:N	2.74	0.49
1:C:73:CYS:HB3	1:C:82:ILE:HD13	1.94	0.49
1:D:191:ILE:O	1:D:194:ARG:HG2	2.13	0.49
1:F:191:ILE:CD1	1:F:196:LEU:HG	2.43	0.49
1:C:63:ILE:HG22	1:C:65:THR:H	1.77	0.49
1:C:145:GLU:HG3	1:C:149:HIS:CD2	2.48	0.49
1:F:33:GLN:HG3	1:F:52:TRP:CH2	2.48	0.49
1:H:143:VAL:HG22	1:H:144:CYS:N	2.28	0.49
1:B:39:GLY:O	1:B:40:ARG:HD3	2.13	0.49
1:D:163:THR:HB	1:D:187:CYS:O	2.12	0.49
1:F:200:LEU:C	1:F:201:GLU:HG2	2.33	0.49
1:B:140:ARG:HB3	1:B:143:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:29:LEU:HB2	1:H:47:VAL:O	2.12	0.49
1:A:199:ALA:C	1:A:200:LEU:HG	2.33	0.49
1:A:200:LEU:HB2	1:A:201:GLU:HG3	1.94	0.49
1:B:79:GLU:OE2	1:D:60:LYS:NZ	2.35	0.49
1:H:131:ASP:O	1:H:132:LYS:HB2	2.11	0.49
1:B:180:ARG:HH21	1:B:180:ARG:HG3	1.78	0.49
1:D:131:ASP:O	1:D:132:LYS:HB2	2.13	0.49
1:A:195:LYS:HE2	1:A:197:ALA:HB2	1.95	0.48
1:C:40:ARG:O	1:C:61:THR:HG23	2.13	0.48
1:C:145:GLU:OE2	5:C:229:HOH:O	2.20	0.48
1:F:175:GLY:HA2	2:F:4:BU4:H4A	1.95	0.48
1:A:93:THR:HG23	1:A:111:PHE:HD1	1.76	0.48
1:F:66:LYS:HG2	1:F:177:ASP:HB3	1.96	0.48
1:B:90:GLN:HA	1:B:90:GLN:NE2	2.27	0.48
1:C:57:SER:O	1:C:59:THR:HG23	2.13	0.48
1:C:95:GLN:HG2	1:C:109:PRO:HG3	1.94	0.48
1:C:109:PRO:O	1:C:110:HIS:CD2	2.66	0.48
1:B:172:LEU:HB2	1:B:180:ARG:HB2	1.95	0.48
1:H:34:ILE:C	1:H:34:ILE:HD12	2.34	0.48
1:C:72:TYR:O	1:C:76:VAL:HG22	2.13	0.48
1:G:87:GLU:HG3	1:G:115:TYR:CE2	2.49	0.48
1:H:155:LYS:HE3	4:H:6:ACT:H3	1.94	0.48
1:C:176:ILE:HD12	1:C:176:ILE:H	1.79	0.48
1:G:29:LEU:N	1:G:29:LEU:HD22	2.29	0.48
1:G:171:LEU:O	1:G:179:PHE:HB3	2.13	0.48
1:C:137:HIS:HD2	1:C:139:GLU:OE1	1.97	0.48
1:C:143:VAL:HG22	1:C:144:CYS:N	2.28	0.48
1:F:194:ARG:H	1:F:194:ARG:HD2	1.79	0.48
1:D:55:ASP:OD1	1:D:60:LYS:HB2	2.13	0.47
1:F:28:LEU:HG	1:F:47:VAL:HG11	1.96	0.47
1:G:180:ARG:HG2	1:G:180:ARG:NH1	2.28	0.47
1:A:30:ALA:HB3	1:A:47:VAL:HA	1.96	0.47
1:A:52:TRP:CE2	1:A:94:ILE:HD11	2.49	0.47
1:D:34:ILE:C	1:D:34:ILE:HD12	2.35	0.47
1:F:34:ILE:HD13	1:F:117:CYS:SG	2.55	0.47
1:F:200:LEU:N	1:F:200:LEU:HD23	2.29	0.47
1:A:49:ASN:OD1	1:A:50:GLY:N	2.46	0.47
1:B:150:TRP:HB3	1:B:182:VAL:HB	1.97	0.47
1:G:131:ASP:O	1:G:132:LYS:HB2	2.13	0.47
1:G:156:GLU:O	1:G:160:GLU:HG3	2.15	0.47
1:G:32:PRO:HB2	1:G:77:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:GLU:HG3	1:H:149:HIS:CD2	2.49	0.47
1:F:34:ILE:HG12	1:F:72:TYR:HD2	1.80	0.47
1:C:172:LEU:HB2	1:C:180:ARG:HB2	1.96	0.46
1:H:65:THR:O	1:H:69:ILE:HG13	2.16	0.46
1:H:130:PRO:HG2	1:H:133:CYS:SG	2.55	0.46
1:F:176:ILE:HD13	2:F:4:BU4:O3	2.16	0.46
1:H:108:HIS:O	1:H:110:HIS:ND1	2.49	0.46
1:H:56:PRO:HD2	5:H:12:HOH:O	2.16	0.46
1:H:140:ARG:CB	1:H:143:VAL:HG12	2.45	0.46
1:D:142:ASP:OD2	1:F:138:GLN:NE2	2.48	0.46
1:H:156:GLU:O	1:H:160:GLU:HG3	2.16	0.46
1:B:143:VAL:HG12	1:B:145:GLU:HG2	1.98	0.45
1:C:42:ASN:HD21	1:C:63:ILE:CD1	2.29	0.45
1:E:91:PRO:CB	1:E:113:ILE:HD13	2.46	0.45
1:A:55:ASP:HA	1:A:56:PRO:HD3	1.82	0.45
1:B:96:ASN:HB3	1:B:105:CYS:O	2.16	0.45
1:G:170:MET:HB3	1:G:179:PHE:CG	2.51	0.45
1:B:83:THR:O	1:B:84:ASN:HB2	2.16	0.45
1:G:49:ASN:CG	1:G:50:GLY:N	2.69	0.45
1:B:66:LYS:HB3	1:B:176:ILE:HG22	1.97	0.45
1:D:156:GLU:OE1	1:F:134:LYS:HE3	2.17	0.45
1:A:108:HIS:O	1:A:108:HIS:ND1	2.49	0.45
1:B:137:HIS:HD2	1:B:139:GLU:OE1	1.99	0.45
1:H:37:PHE:CE2	1:H:110:HIS:NE2	2.85	0.45
1:E:99:LYS:O	1:E:100:ARG:C	2.56	0.45
1:E:171:LEU:O	1:E:179:PHE:HB3	2.17	0.45
1:G:89:ASN:N	1:H:121:GLU:OE1	2.37	0.45
1:C:40:ARG:HH22	1:C:107:THR:CG2	2.25	0.45
1:D:93:THR:HG23	1:D:111:PHE:CD2	2.52	0.45
1:E:140:ARG:HB2	1:E:143:VAL:CG1	2.47	0.45
1:E:176:ILE:N	1:E:176:ILE:CD1	2.79	0.45
1:F:95:GLN:CG	1:F:109:PRO:HG3	2.25	0.44
1:A:92:VAL:HG22	1:A:93:THR:N	2.32	0.44
1:D:144:CYS:SG	1:D:178:LYS:HB3	2.57	0.44
1:H:107:THR:HG23	1:H:108:HIS:N	2.32	0.44
1:A:187:CYS:HA	1:A:188:PRO:HD3	1.83	0.44
1:B:72:TYR:O	1:B:76:VAL:HG22	2.18	0.44
1:C:40:ARG:HD3	1:C:98:CYS:O	2.16	0.44
1:E:143:VAL:CG2	1:E:145:GLU:HG2	2.48	0.44
1:F:163:THR:HB	1:F:187:CYS:O	2.18	0.44
1:G:49:ASN:ND2	1:G:51:LYS:HB2	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:143:VAL:CG2	1:H:144:CYS:N	2.81	0.44
1:B:36:MET:HG2	1:B:42:ASN:OD1	2.17	0.44
1:B:45:MET:SD	1:B:50:GLY:O	2.75	0.44
1:B:174:CYS:CB	1:B:180:ARG:HH21	2.28	0.44
1:C:149:HIS:O	1:C:153:VAL:HG23	2.18	0.44
1:G:37:PHE:CE2	1:G:110:HIS:CD2	3.05	0.44
1:G:55:ASP:HA	1:G:56:PRO:HD3	1.86	0.44
1:H:34:ILE:HD12	1:H:34:ILE:O	2.18	0.44
1:H:180:ARG:HH11	1:H:180:ARG:CG	2.22	0.44
1:A:152:THR:O	1:A:156:GLU:HG3	2.18	0.44
1:D:140:ARG:CB	1:D:143:VAL:HG13	2.48	0.44
1:H:164:ASN:ND2	1:H:165:LEU:N	2.66	0.44
1:F:191:ILE:N	1:F:191:ILE:HD12	2.33	0.44
1:G:43:MET:HE2	1:G:97:TRP:HA	2.00	0.43
1:B:97:TRP:N	1:B:107:THR:HG22	2.29	0.43
1:G:89:ASN:OD1	1:G:147:HIS:HE1	2.02	0.43
1:F:55:ASP:HA	1:F:56:PRO:HD3	1.83	0.43
1:F:91:PRO:HB3	1:F:113:ILE:CD1	2.47	0.43
1:A:61:THR:CG2	1:A:62:CYS:N	2.80	0.43
1:A:194:ARG:H	1:A:194:ARG:HG2	1.65	0.43
1:C:126:ALA:HA	1:F:198:ALA:HB2	2.01	0.43
1:F:99:LYS:HD3	1:F:102:ARG:HH21	1.81	0.43
1:F:200:LEU:N	1:F:200:LEU:CD2	2.81	0.43
1:B:77:TYR:HB3	1:B:80:LEU:HD12	2.01	0.43
1:F:29:LEU:CD2	1:F:29:LEU:N	2.82	0.43
1:F:187:CYS:HA	1:F:188:PRO:HD3	1.88	0.43
1:F:74:GLN:HG2	1:F:82:ILE:HB	2.00	0.43
1:A:52:TRP:CD1	1:A:94:ILE:HG12	2.54	0.42
1:C:63:ILE:N	1:C:63:ILE:HD12	2.34	0.42
1:B:145:GLU:HG3	1:B:149:HIS:CD2	2.54	0.42
1:H:180:ARG:HG2	1:H:180:ARG:NH1	2.26	0.42
1:F:29:LEU:N	1:F:29:LEU:HD22	2.33	0.42
1:H:37:PHE:CZ	1:H:110:HIS:CD2	3.07	0.42
1:H:149:HIS:O	1:H:153:VAL:HG23	2.19	0.42
1:A:95:GLN:HE21	1:A:109:PRO:HG3	1.84	0.42
1:D:171:LEU:O	1:D:179:PHE:HB3	2.20	0.42
1:H:180:ARG:CG	1:H:180:ARG:NH1	2.81	0.42
1:B:53:ASP:HA	5:B:218:HOH:O	2.19	0.42
1:B:90:GLN:HE21	1:B:91:PRO:HD2	1.84	0.42
1:B:109:PRO:O	1:B:110:HIS:CD2	2.72	0.42
1:B:192:GLU:OE2	1:B:192:GLU:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LEU:O	1:B:179:PHE:HB3	2.20	0.42
1:C:42:ASN:HD21	1:C:63:ILE:HD11	1.85	0.42
1:F:40:ARG:NH1	1:F:40:ARG:HG2	2.35	0.42
1:D:33:GLN:HG3	1:D:52:TRP:CH2	2.54	0.42
1:F:40:ARG:HG2	1:F:40:ARG:HH11	1.84	0.42
1:H:171:LEU:O	1:H:179:PHE:HB3	2.20	0.42
1:A:95:GLN:HE21	1:A:109:PRO:CG	2.33	0.41
5:A:216:HOH:O	1:C:53:ASP:HA	2.20	0.41
1:C:124:SER:O	1:F:166:HIS:HE1	2.02	0.41
1:H:190:ALA:H	2:H:8:BU4:C3	2.33	0.41
1:A:65:THR:O	1:A:69:ILE:HG13	2.20	0.41
1:C:143:VAL:HG21	1:C:145:GLU:HG2	1.99	0.41
1:F:33:GLN:HG3	1:F:52:TRP:HH2	1.85	0.41
1:F:39:GLY:O	1:F:40:ARG:NH1	2.53	0.41
1:H:83:THR:O	1:H:84:ASN:HB2	2.19	0.41
1:B:143:VAL:CG1	1:B:145:GLU:HG2	2.51	0.41
1:D:95:GLN:O	1:D:96:ASN:HB2	2.21	0.41
1:E:34:ILE:HD11	1:E:115:TYR:HB2	2.03	0.41
1:F:94:ILE:HB	1:F:97:TRP:CZ2	2.56	0.41
1:H:147:HIS:HD2	1:H:170:MET:CE	2.33	0.41
1:A:33:GLN:HB2	1:A:115:TYR:O	2.21	0.41
1:C:143:VAL:O	1:C:180:ARG:HG2	2.21	0.41
1:G:60:LYS:HG3	1:G:72:TYR:HE1	1.86	0.41
1:H:164:ASN:ND2	1:H:165:LEU:H	2.17	0.41
1:D:187:CYS:HA	1:D:188:PRO:HD3	1.87	0.41
1:H:179:PHE:CD1	1:H:179:PHE:N	2.89	0.41
1:G:81:GLN:O	1:G:83:THR:HG23	2.21	0.41
1:B:37:PHE:CZ	1:B:110:HIS:CE1	3.09	0.41
1:C:184:PHE:CD1	1:C:184:PHE:N	2.89	0.41
1:D:33:GLN:HG2	1:D:45:MET:HB2	2.02	0.41
1:E:83:THR:O	1:E:84:ASN:HB2	2.19	0.41
1:F:180:ARG:HG2	1:F:180:ARG:NH2	2.35	0.41
1:F:184:PHE:CD1	1:F:184:PHE:N	2.89	0.41
1:G:55:ASP:OD1	1:G:56:PRO:HD2	2.21	0.41
1:G:175:GLY:N	2:G:3:BU4:H2	2.35	0.41
1:H:150:TRP:HB3	1:H:182:VAL:HB	2.01	0.41
1:A:61:THR:CG2	1:A:62:CYS:H	2.32	0.41
1:B:138:GLN:NE2	1:B:153:VAL:HG11	2.36	0.41
1:B:180:ARG:NH2	1:B:180:ARG:CG	2.80	0.41
1:C:61:THR:CG2	1:C:62:CYS:H	2.28	0.41
1:F:75:GLU:O	1:F:78:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:92:VAL:HG22	1:G:93:THR:N	2.36	0.41
1:G:140:ARG:HB3	1:G:143:VAL:HG12	2.03	0.40
1:G:66:LYS:HB3	1:G:176:ILE:CG1	2.51	0.40
1:G:99:LYS:HB3	1:G:102:ARG:HB3	2.02	0.40
1:A:90:GLN:NE2	1:E:121:GLU:OE1	2.51	0.40
1:A:163:THR:HB	1:A:187:CYS:O	2.22	0.40
1:E:34:ILE:CD1	1:E:115:TYR:HB2	2.51	0.40
1:E:41:LEU:HD13	1:E:58:GLY:HA2	2.03	0.40
1:E:96:ASN:HB3	1:E:105:CYS:O	2.20	0.40
1:F:39:GLY:C	1:F:40:ARG:HH11	2.25	0.40
1:B:187:CYS:HB3	1:B:188:PRO:CD	2.52	0.40
1:C:108:HIS:O	1:C:110:HIS:CD2	2.75	0.40
1:E:46:ASN:CG	1:E:49:ASN:HD21	2.25	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	173/191 (91%)	164 (95%)	8 (5%)	1 (1%)	25 50
1	B	171/191 (90%)	160 (94%)	11 (6%)	0	100 100
1	C	172/191 (90%)	160 (93%)	12 (7%)	0	100 100
1	D	171/191 (90%)	165 (96%)	6 (4%)	0	100 100
1	E	175/191 (92%)	162 (93%)	13 (7%)	0	100 100
1	F	173/191 (91%)	165 (95%)	7 (4%)	1 (1%)	25 50
1	G	172/191 (90%)	161 (94%)	9 (5%)	2 (1%)	13 32
1	H	173/191 (91%)	161 (93%)	12 (7%)	0	100 100
All	All	1380/1528 (90%)	1298 (94%)	78 (6%)	4 (0%)	41 66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	201	GLU
1	A	201	GLU
1	G	198	ALA
1	G	176	ILE

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	156/169 (92%)	150 (96%)	6 (4%)	33	62
1	B	153/169 (90%)	151 (99%)	2 (1%)	69	87
1	C	153/169 (90%)	147 (96%)	6 (4%)	32	61
1	D	154/169 (91%)	145 (94%)	9 (6%)	20	43
1	E	156/169 (92%)	150 (96%)	6 (4%)	33	62
1	F	156/169 (92%)	148 (95%)	8 (5%)	24	50
1	G	155/169 (92%)	149 (96%)	6 (4%)	32	61
1	H	154/169 (91%)	146 (95%)	8 (5%)	23	49
All	All	1237/1352 (92%)	1186 (96%)	51 (4%)	30	59

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	GLU
1	A	93	THR
1	A	111	PHE
1	A	141	MET
1	A	196	LEU
1	A	200	LEU
1	B	111	PHE
1	B	194	ARG
1	C	40	ARG
1	C	90	GLN

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Mol	Chain	Res	Type
1	C	108	HIS
1	C	119	VAL
1	C	140	ARG
1	C	194	ARG
1	D	75	GLU
1	D	79	GLU
1	D	93	THR
1	D	109	PRO
1	D	111	PHE
1	D	139	GLU
1	D	143	VAL
1	D	172	LEU
1	D	194	ARG
1	E	34	ILE
1	E	108	HIS
1	E	111	PHE
1	E	142	ASP
1	E	162	SER
1	E	194	ARG
1	F	48	GLN
1	F	79	GLU
1	F	93	THR
1	F	111	PHE
1	F	194	ARG
1	F	196	LEU
1	F	200	LEU
1	F	201	GLU
1	G	66	LYS
1	G	79	GLU
1	G	102	ARG
1	G	111	PHE
1	G	172	LEU
1	G	194	ARG
1	H	28	LEU
1	H	29	LEU
1	H	65	THR
1	H	93	THR
1	H	107	THR
1	H	108	HIS
1	H	142	ASP
1	H	194	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	95	GLN
1	A	137	HIS
1	A	151	HIS
1	B	33	GLN
1	B	110	HIS
1	B	137	HIS
1	B	138	GLN
1	B	147	HIS
1	B	151	HIS
1	C	110	HIS
1	C	137	HIS
1	C	147	HIS
1	C	151	HIS
1	D	81	GLN
1	D	108	HIS
1	D	137	HIS
1	D	138	GLN
1	D	151	HIS
1	D	164	ASN
1	E	33	GLN
1	E	49	ASN
1	E	81	GLN
1	E	90	GLN
1	E	110	HIS
1	E	137	HIS
1	E	151	HIS
1	F	44	HIS
1	F	149	HIS
1	F	151	HIS
1	F	166	HIS
1	G	33	GLN
1	G	81	GLN
1	G	108	HIS
1	G	138	GLN
1	G	147	HIS
1	G	149	HIS
1	G	151	HIS
1	G	166	HIS
1	H	95	GLN
1	H	137	HIS
1	H	147	HIS

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Mol	Chain	Res	Type
1	H	164	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

17 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	BU4	C	5	-	5,5,5	0.39	0	5,5,5	0.37	0
2	BU4	D	2	-	5,5,5	0.48	0	5,5,5	0.56	0
4	ACT	E	9	-	3,3,3	0.84	0	3,3,3	0.83	0
3	SO4	D	5	-	4,4,4	0.29	0	6,6,6	0.17	0
2	BU4	F	4	-	5,5,5	0.53	0	5,5,5	1.10	1 (20%)
3	SO4	E	4	-	4,4,4	0.29	0	6,6,6	0.23	0
4	ACT	C	8	-	3,3,3	0.86	0	3,3,3	0.81	0
2	BU4	A	1	-	5,5,5	0.43	0	5,5,5	0.45	0
3	SO4	B	2	-	4,4,4	0.31	0	6,6,6	0.31	0
3	SO4	H	1	-	4,4,4	0.30	0	6,6,6	0.21	0
2	BU4	E	6	-	5,5,5	0.40	0	5,5,5	0.48	0
2	BU4	H	8	-	5,5,5	0.42	0	5,5,5	0.79	0
4	ACT	H	6	-	3,3,3	0.78	0	3,3,3	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BU4	G	3	-	5,5,5	0.48	0	5,5,5	0.43	0
3	SO4	C	3	-	4,4,4	0.23	0	6,6,6	0.24	0
2	BU4	B	7	-	5,5,5	0.38	0	5,5,5	0.26	0
4	ACT	B	208	-	3,3,3	0.83	0	3,3,3	0.71	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	BU4	C	5	-	-	1/3/3/3	-
2	BU4	D	2	-	-	1/3/3/3	-
2	BU4	F	4	-	-	2/3/3/3	-
2	BU4	A	1	-	-	1/3/3/3	-
2	BU4	E	6	-	-	1/3/3/3	-
2	BU4	H	8	-	-	3/3/3/3	-
2	BU4	G	3	-	-	2/3/3/3	-
2	BU4	B	7	-	-	1/3/3/3	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	4	BU4	C1-C2-C3	2.42	120.67	114.04

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	5	BU4	O1-C1-C2-C3
2	F	4	BU4	C1-C2-C3-C4
2	G	3	BU4	O1-C1-C2-C3
2	H	8	BU4	O1-C1-C2-C3
2	H	8	BU4	C1-C2-C3-C4
2	D	2	BU4	O1-C1-C2-C3
2	A	1	BU4	C1-C2-C3-C4
2	B	7	BU4	C1-C2-C3-O3
2	E	6	BU4	C1-C2-C3-O3
2	F	4	BU4	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	G	3	BU4	C1-C2-C3-O3
2	H	8	BU4	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	BU4	1	0
2	F	4	BU4	2	0
2	H	8	BU4	1	0
4	H	6	ACT	3	0
2	G	3	BU4	1	0
2	B	7	BU4	1	0
4	B	208	ACT	1	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	175/191 (91%)	-0.29	2 (1%)	80	82	19, 41, 72, 86	14 (8%)
1	B	173/191 (90%)	-0.28	1 (0%)	89	91	26, 45, 66, 89	10 (5%)
1	C	174/191 (91%)	-0.26	1 (0%)	89	91	32, 46, 72, 87	10 (5%)
1	D	173/191 (90%)	-0.33	2 (1%)	79	80	21, 38, 66, 81	14 (8%)
1	E	177/191 (92%)	-0.21	5 (2%)	53	54	31, 49, 79, 100	16 (9%)
1	F	175/191 (91%)	-0.26	1 (0%)	89	91	25, 44, 75, 97	15 (8%)
1	G	174/191 (91%)	0.06	4 (2%)	60	62	36, 60, 89, 100	22 (12%)
1	H	175/191 (91%)	-0.27	3 (1%)	70	72	29, 48, 72, 89	17 (9%)
All	All	1396/1528 (91%)	-0.23	19 (1%)	75	77	19, 47, 75, 100	118 (8%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	202	HIS	6.0
1	F	202	HIS	3.8
1	B	108	HIS	3.6
1	E	108	HIS	3.3
1	G	143	VAL	3.2
1	D	29	LEU	3.0
1	G	121	GLU	2.7
1	G	140	ARG	2.6
1	H	143	VAL	2.5
1	A	202	HIS	2.5
1	G	107	THR	2.4
1	E	201	GLU	2.3
1	E	140	ARG	2.3
1	H	140	ARG	2.3
1	E	37	PHE	2.2
1	H	123	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	109	PRO	2.1
1	A	109	PRO	2.1
1	C	105	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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. 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	B-factors(Å^2)	Q<0.9
4	ACT	C	8	4/4	0.67	0.43	85,86,87,88	0
2	BU4	F	4	6/6	0.77	0.24	62,70,76,76	0
2	BU4	G	3	6/6	0.79	0.28	78,82,83,85	0
2	BU4	D	2	6/6	0.88	0.16	59,60,66,66	0
2	BU4	H	8	6/6	0.89	0.26	50,57,65,67	0
4	ACT	E	9	4/4	0.90	0.28	71,72,73,74	0
4	ACT	B	208	4/4	0.91	0.36	68,68,70,73	0
2	BU4	E	6	6/6	0.92	0.20	63,65,71,75	0
2	BU4	A	1	6/6	0.93	0.17	50,53,55,55	0
2	BU4	B	7	6/6	0.94	0.17	58,64,65,65	0
4	ACT	H	6	4/4	0.94	0.31	57,57,58,60	0
2	BU4	C	5	6/6	0.96	0.12	51,53,58,58	0
3	SO4	D	5	5/5	0.97	0.11	72,73,75,75	0
3	SO4	E	4	5/5	0.98	0.17	39,45,48,53	0
3	SO4	H	1	5/5	0.98	0.13	39,42,48,50	0
3	SO4	C	3	5/5	0.98	0.17	38,42,49,49	0
3	SO4	B	2	5/5	0.99	0.15	27,36,46,50	0

6.5 Other polymers (i)

There are no such residues in this entry.