Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:34 pm BST

PDB ID	:	1I9B
Title	:	X-RAY STRUCTURE OF ACETYLCHOLINE BINDING PROTEIN (ACHBP)
Authors	:	Brejc, K.; van Dijk, W.J.; Klaassen, R.; Schuurmans, M.; van der Oost, J.; Smit, A.B.; Sixma, T.K.
Deposited on	:	2001-03-18
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 following versions of software and data (see references ⓘ) were used in the production of this report:

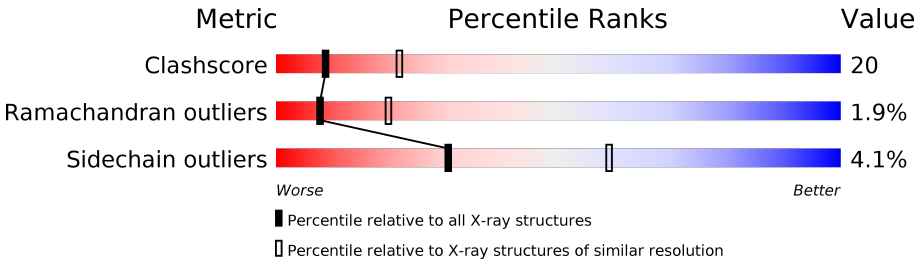
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 on 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	217	62% 29% • 6%
1	B	217	63% 29% • 6%
1	C	217	61% 29% 5% 6%
1	D	217	59% 31% • 6%
1	E	217	57% 34% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8299 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

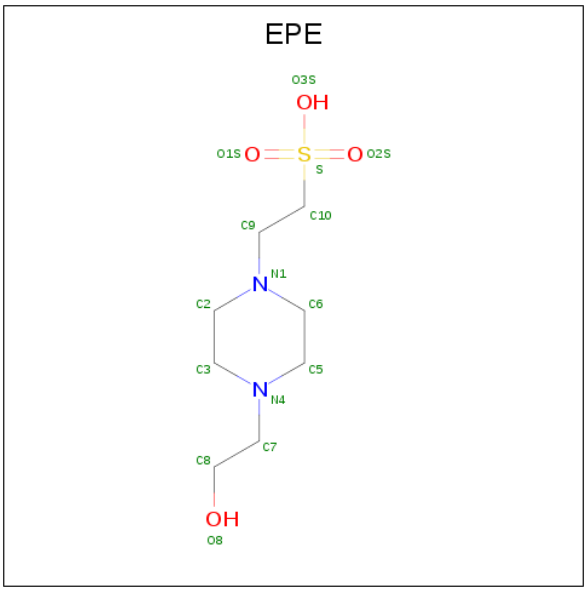
- Molecule 1 is a protein called ACETYLCHOLINE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1639	1026	280	328	5			
1	B	205	Total	C	N	O	S	0	0	0
			1639	1026	280	328	5			
1	C	205	Total	C	N	O	S	0	0	0
			1639	1026	280	328	5			
1	D	205	Total	C	N	O	S	0	0	0
			1639	1026	280	328	5			
1	E	205	Total	C	N	O	S	0	0	0
			1639	1026	280	328	5			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	2	Total	Ca	0	1
			3	3		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	E	3	Total	Ca	0	1
			4	4		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 15 8 2 4 1	0	0
3	B	1	Total C N O S 15 8 2 4 1	0	0
3	C	1	Total C N O S 15 8 2 4 1	0	0
3	D	1	Total C N O S 15 8 2 4 1	0	0
3	E	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 4 is water.

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

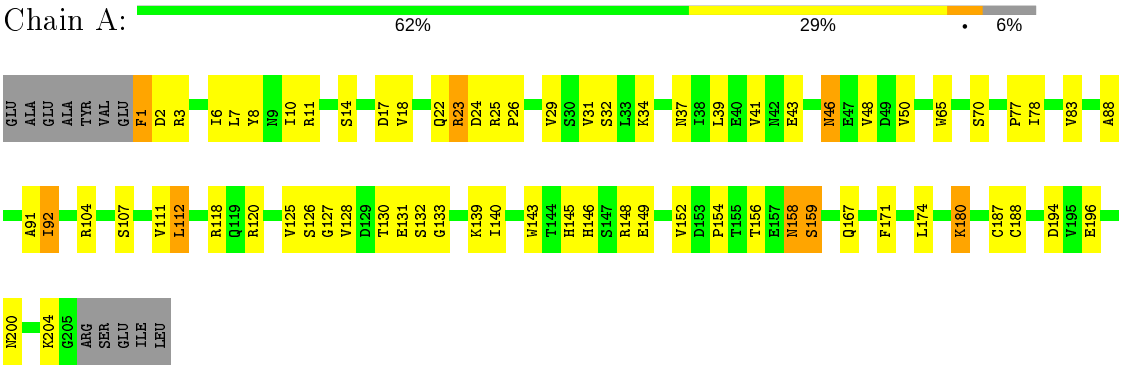
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

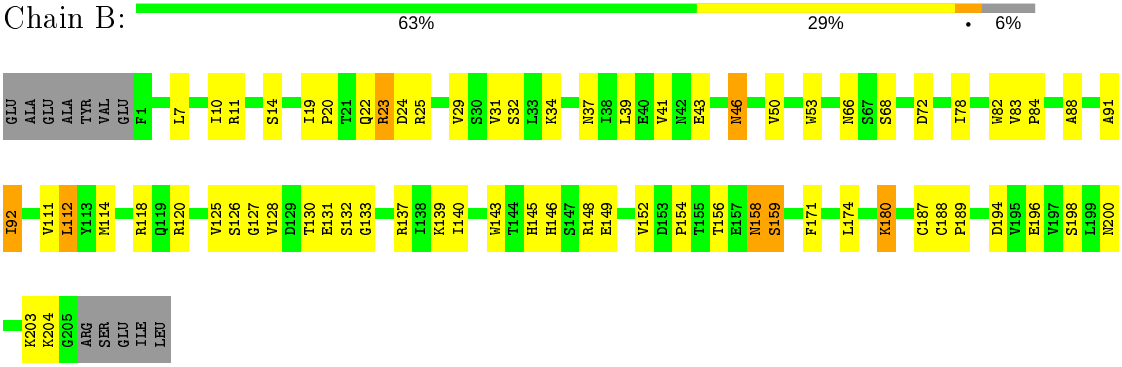
- Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain A:



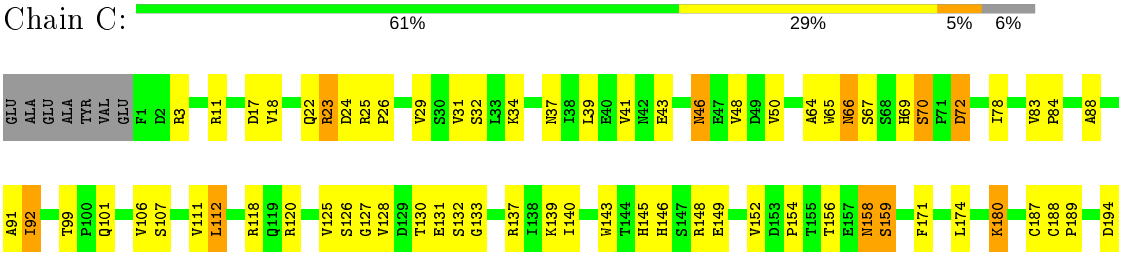
- Molecule 1: ACETYLCHOLINE BINDING PROTEIN

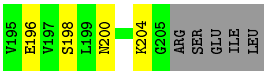
Chain B:



- Molecule 1: ACETYLCHOLINE BINDING PROTEIN

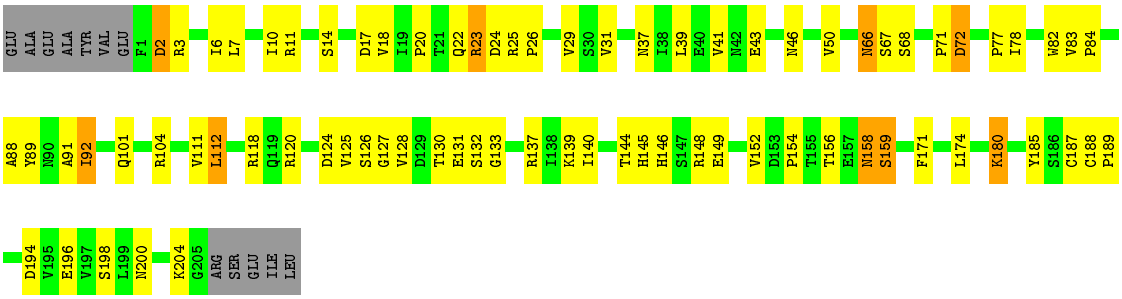
Chain C:





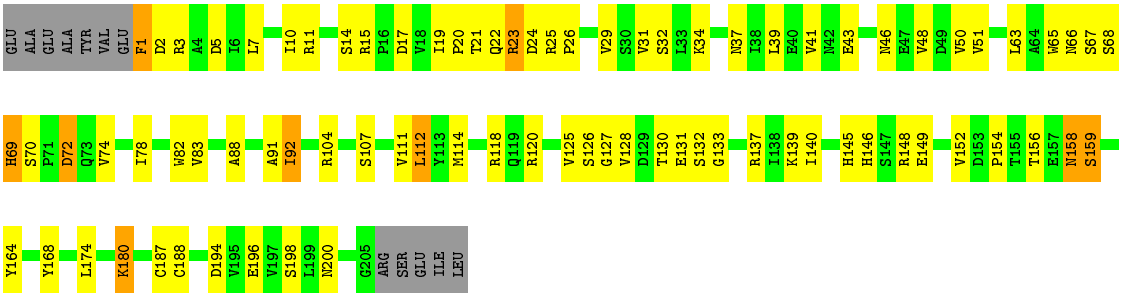
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain D:



• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain E:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	141.66Å 141.66Å 120.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.70	Depositor
% Data completeness (in resolution range)	97.8 (19.97-2.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.260 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8299	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.48	0/1676	0.67	0/2287
1	B	0.48	0/1676	0.68	0/2287
1	C	0.49	0/1676	0.68	0/2287
1	D	0.51	0/1676	0.68	0/2287
1	E	0.50	0/1676	0.68	0/2287
All	All	0.49	0/8380	0.68	0/11435

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	1639	0	1579	65	0
1	B	1639	0	1579	64	0
1	C	1639	0	1579	78	0
1	D	1639	0	1579	82	0
1	E	1639	0	1579	86	1
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	4	0	0	0	0
3	A	15	0	18	4	0
3	B	15	0	18	2	0
3	C	15	0	18	1	0
3	D	15	0	18	5	0
3	E	15	0	18	1	0
4	A	5	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
All	All	8299	0	7985	333	1

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 20.

All (333) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ASN:ND2	1:D:68:SER:H	1.64	0.94
1:E:125:VAL:O	1:E:128:VAL:HG23	1.72	0.89
1:A:125:VAL:O	1:A:128:VAL:HG23	1.72	0.89
1:D:125:VAL:O	1:D:128:VAL:HG23	1.72	0.88
1:C:88:ALA:HA	1:C:140:ILE:HG22	1.55	0.87
1:B:125:VAL:O	1:B:128:VAL:HG23	1.76	0.86
1:E:88:ALA:HA	1:E:140:ILE:HG22	1.58	0.85
1:D:88:ALA:HA	1:D:140:ILE:HG22	1.58	0.84
1:C:125:VAL:O	1:C:128:VAL:HG23	1.77	0.84
1:B:88:ALA:HA	1:B:140:ILE:HG22	1.60	0.82
3:D:1053:EPE:H92	1:E:114:MET:SD	2.22	0.79
1:A:171:PHE:O	1:A:204:LYS:HE3	1.82	0.79
1:E:67:SER:HA	1:E:70:SER:OG	1.83	0.79
1:A:88:ALA:HA	1:A:140:ILE:HG22	1.63	0.79
1:D:22:GLN:O	1:D:25:ARG:HB2	1.85	0.77
1:A:46:ASN:ND2	1:A:125:VAL:H	1.85	0.75
1:C:46:ASN:ND2	1:C:125:VAL:H	1.84	0.75
1:B:154:PRO:HD3	1:B:180:LYS:HB3	1.69	0.75
1:A:22:GLN:O	1:A:25:ARG:HB2	1.88	0.74
1:D:154:PRO:HD3	1:D:180:LYS:HB3	1.67	0.74
1:E:154:PRO:HD3	1:E:180:LYS:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:PRO:HD3	1:C:180:LYS:HB3	1.71	0.73
1:B:46:ASN:ND2	1:B:125:VAL:H	1.87	0.73
1:E:22:GLN:O	1:E:25:ARG:HB2	1.88	0.73
1:C:22:GLN:O	1:C:25:ARG:HB2	1.89	0.72
1:B:22:GLN:O	1:B:25:ARG:HB2	1.88	0.72
1:A:1:PHE:HB2	1:A:70:SER:OG	1.91	0.71
1:A:154:PRO:HD3	1:A:180:LYS:HB3	1.70	0.71
1:E:46:ASN:ND2	1:E:125:VAL:H	1.89	0.71
1:D:149:GLU:CD	1:E:104:ARG:HH22	1.95	0.70
1:B:46:ASN:HD22	1:B:125:VAL:HB	1.58	0.69
1:D:2:ASP:O	1:D:6:ILE:HG13	1.93	0.69
1:D:46:ASN:ND2	1:D:125:VAL:H	1.91	0.68
1:D:130:THR:HG22	1:D:132:SER:H	1.59	0.68
1:C:130:THR:HG22	1:C:132:SER:H	1.57	0.68
1:E:130:THR:HG22	1:E:132:SER:H	1.57	0.68
1:D:66:ASN:C	1:D:66:ASN:HD22	1.98	0.67
1:A:130:THR:HG22	1:A:132:SER:H	1.60	0.66
1:C:17:ASP:O	1:D:7:LEU:HD13	1.95	0.66
1:B:130:THR:HG22	1:B:132:SER:H	1.61	0.66
1:C:66:ASN:HD22	1:C:67:SER:H	1.44	0.64
1:C:66:ASN:HD22	1:C:67:SER:N	1.94	0.64
1:E:174:LEU:HB2	1:E:200:ASN:ND2	2.13	0.63
1:E:3:ARG:HD3	1:E:74:VAL:HG12	1.81	0.63
1:E:125:VAL:HG13	1:E:128:VAL:HG21	1.81	0.62
1:E:3:ARG:CD	1:E:74:VAL:HG12	2.29	0.62
1:D:72:ASP:N	1:D:72:ASP:OD1	2.28	0.62
1:A:46:ASN:HD22	1:A:125:VAL:HB	1.65	0.61
1:D:174:LEU:HB2	1:D:200:ASN:ND2	2.16	0.61
1:A:118:ARG:NH1	1:E:92:ILE:HG23	2.16	0.60
1:D:66:ASN:HD22	1:D:67:SER:N	1.99	0.60
1:C:125:VAL:HG13	1:C:128:VAL:HG21	1.84	0.60
1:C:69:HIS:O	1:C:70:SER:HB3	2.01	0.59
1:D:66:ASN:HD22	1:D:68:SER:H	1.50	0.59
1:E:31:VAL:HG11	1:E:140:ILE:HD11	1.84	0.59
1:B:125:VAL:HG13	1:B:128:VAL:HG21	1.85	0.59
1:C:174:LEU:HB2	1:C:200:ASN:ND2	2.18	0.59
1:A:127:GLY:O	1:A:133:GLY:HA2	2.03	0.59
1:B:31:VAL:HG11	1:B:140:ILE:HD11	1.83	0.59
1:B:127:GLY:O	1:B:130:THR:HB	2.03	0.58
1:A:174:LEU:HB2	1:A:200:ASN:ND2	2.19	0.58
1:A:125:VAL:HG13	1:A:128:VAL:HG21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ASN:HD21	1:D:68:SER:CB	2.16	0.58
1:A:41:VAL:HG11	1:A:128:VAL:HG21	1.85	0.58
1:C:11:ARG:HH11	1:C:11:ARG:HG3	1.68	0.58
1:D:125:VAL:HG13	1:D:128:VAL:HG21	1.85	0.58
1:E:127:GLY:O	1:E:133:GLY:HA2	2.04	0.58
1:D:31:VAL:HG11	1:D:140:ILE:HD11	1.87	0.57
1:D:185:TYR:HB3	1:E:164:TYR:OH	2.03	0.57
1:C:41:VAL:HG11	1:C:128:VAL:HG21	1.86	0.57
1:D:88:ALA:HB3	1:D:91:ALA:HB2	1.86	0.57
1:B:92:ILE:HG23	1:C:118:ARG:NH1	2.18	0.57
1:E:130:THR:HG22	1:E:132:SER:N	2.20	0.57
1:B:174:LEU:HB2	1:B:200:ASN:ND2	2.20	0.57
1:A:23:ARG:HH11	1:A:23:ARG:HG2	1.70	0.57
1:C:46:ASN:HD22	1:C:125:VAL:HB	1.70	0.57
1:C:127:GLY:O	1:C:133:GLY:HA2	2.05	0.57
1:D:46:ASN:HD22	1:D:125:VAL:HB	1.70	0.56
1:C:130:THR:HG22	1:C:132:SER:N	2.20	0.56
1:E:127:GLY:O	1:E:130:THR:HB	2.06	0.56
1:C:88:ALA:HB3	1:C:91:ALA:HB2	1.86	0.56
1:A:127:GLY:O	1:A:130:THR:HB	2.05	0.56
1:E:46:ASN:HD22	1:E:125:VAL:HB	1.70	0.56
1:B:149:GLU:OE2	1:C:3:ARG:NH2	2.38	0.56
1:C:127:GLY:O	1:C:130:THR:HB	2.06	0.56
1:C:145:HIS:HD2	1:C:149:GLU:OE1	1.89	0.56
1:D:130:THR:HG22	1:D:132:SER:N	2.21	0.56
1:D:66:ASN:HD21	1:D:68:SER:H	1.49	0.56
1:C:31:VAL:HG11	1:C:140:ILE:HD11	1.88	0.55
1:A:130:THR:HG22	1:A:132:SER:N	2.21	0.55
1:A:88:ALA:HB3	1:A:91:ALA:HB2	1.87	0.55
1:D:41:VAL:HG11	1:D:128:VAL:HG21	1.88	0.55
1:C:146:HIS:HD2	1:C:148:ARG:H	1.54	0.55
1:D:185:TYR:HD2	1:E:164:TYR:HE1	1.54	0.55
1:E:88:ALA:HB3	1:E:91:ALA:HB2	1.88	0.55
1:C:72:ASP:O	1:C:106:VAL:HA	2.06	0.55
1:E:1:PHE:N	1:E:1:PHE:CD1	2.71	0.55
1:E:1:PHE:HB2	1:E:5:ASP:HB2	1.88	0.54
1:D:66:ASN:C	1:D:66:ASN:ND2	2.60	0.54
1:B:146:HIS:HD2	1:B:148:ARG:H	1.55	0.54
1:A:39:LEU:CD2	1:E:92:ILE:HD11	2.38	0.54
1:B:88:ALA:HB3	1:B:91:ALA:HB2	1.88	0.54
1:B:127:GLY:O	1:B:133:GLY:HA2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:THR:HG22	1:B:132:SER:N	2.22	0.54
1:D:127:GLY:O	1:D:130:THR:HB	2.07	0.54
1:C:23:ARG:HH11	1:C:23:ARG:HG2	1.73	0.54
1:A:77:PRO:HG2	1:E:17:ASP:OD1	2.08	0.54
1:D:23:ARG:HH11	1:D:23:ARG:HG2	1.73	0.53
1:D:92:ILE:HG22	1:D:120:ARG:HB2	1.90	0.53
1:E:23:ARG:HG2	1:E:23:ARG:HH11	1.73	0.53
1:E:11:ARG:HG3	1:E:11:ARG:HH11	1.74	0.53
1:D:92:ILE:HD11	1:E:39:LEU:CD2	2.39	0.53
1:D:145:HIS:HD2	1:D:149:GLU:OE1	1.92	0.53
1:B:23:ARG:HH11	1:B:23:ARG:HG2	1.73	0.53
1:A:2:ASP:O	1:A:6:ILE:HG13	2.09	0.53
1:E:125:VAL:HG13	1:E:128:VAL:CG2	2.38	0.53
1:B:145:HIS:HD2	1:B:149:GLU:OE1	1.92	0.52
1:D:11:ARG:HH11	1:D:11:ARG:HG3	1.74	0.52
1:B:41:VAL:HG11	1:B:128:VAL:HG21	1.91	0.52
1:C:11:ARG:NH1	1:C:11:ARG:HG3	2.24	0.52
1:E:145:HIS:HD2	1:E:149:GLU:OE1	1.93	0.52
1:D:17:ASP:O	1:E:7:LEU:HD13	2.09	0.52
1:E:3:ARG:HH11	1:E:3:ARG:HG3	1.74	0.52
1:B:66:ASN:ND2	1:B:68:SER:OG	2.41	0.52
1:D:144:THR:HA	3:D:1053:EPE:O1S	2.10	0.52
1:B:92:ILE:HG22	1:B:120:ARG:HB2	1.92	0.52
1:A:26:PRO:HG3	1:A:148:ARG:O	2.10	0.52
1:B:143:TRP:CH2	1:C:99:THR:HG21	2.44	0.52
1:C:67:SER:HA	1:C:70:SER:OG	2.10	0.52
1:A:104:ARG:HH22	1:E:149:GLU:CD	2.14	0.52
1:C:92:ILE:HG23	1:D:118:ARG:NH1	2.25	0.51
1:A:92:ILE:HG22	1:A:120:ARG:HB2	1.93	0.51
1:A:39:LEU:HD22	1:E:92:ILE:HD11	1.92	0.51
1:A:145:HIS:HD2	1:A:149:GLU:OE1	1.94	0.51
1:A:31:VAL:HG11	1:A:140:ILE:HD11	1.92	0.51
1:E:92:ILE:HG22	1:E:120:ARG:HB2	1.93	0.51
1:A:3:ARG:HD2	1:E:21:THR:HG21	1.92	0.51
1:E:146:HIS:HD2	1:E:148:ARG:H	1.57	0.51
1:D:127:GLY:O	1:D:133:GLY:HA2	2.11	0.51
1:C:18:VAL:HG22	1:D:7:LEU:HD12	1.91	0.51
1:C:92:ILE:HG22	1:C:120:ARG:HB2	1.93	0.51
1:E:41:VAL:HG11	1:E:128:VAL:HG21	1.91	0.51
1:C:149:GLU:CD	1:D:104:ARG:HH22	2.13	0.51
1:C:171:PHE:O	1:C:204:LYS:HE3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:VAL:HG22	1:E:7:LEU:HD12	1.92	0.51
1:C:125:VAL:HG13	1:C:128:VAL:CG2	2.41	0.51
1:C:149:GLU:OE2	1:D:3:ARG:NH2	2.42	0.50
1:A:7:LEU:HD13	1:E:17:ASP:O	2.12	0.50
1:D:66:ASN:HD21	1:D:68:SER:HB3	1.76	0.50
1:D:26:PRO:HG3	1:D:148:ARG:O	2.12	0.50
1:A:3:ARG:NH2	1:E:149:GLU:OE2	2.45	0.50
1:B:125:VAL:HG13	1:B:128:VAL:CG2	2.42	0.49
1:B:187:CYS:SG	1:B:188:CYS:N	2.85	0.49
1:A:17:ASP:O	1:B:7:LEU:HD13	2.12	0.49
1:D:146:HIS:HD2	1:D:148:ARG:H	1.59	0.49
1:E:63:LEU:O	1:E:65:TRP:HE3	1.96	0.49
1:A:125:VAL:HG13	1:A:128:VAL:CG2	2.42	0.49
1:D:29:VAL:O	1:D:152:VAL:HA	2.13	0.49
1:A:146:HIS:HD2	1:A:148:ARG:H	1.59	0.49
1:D:149:GLU:OE2	1:E:3:ARG:NH2	2.45	0.49
1:A:37:ASN:O	1:A:50:VAL:HG23	2.12	0.49
1:E:65:TRP:CZ3	1:E:107:SER:HA	2.48	0.49
1:B:143:TRP:CZ2	3:B:1051:EPE:H62	2.48	0.49
1:E:187:CYS:SG	1:E:188:CYS:N	2.86	0.49
1:A:65:TRP:CZ3	1:A:107:SER:HA	2.47	0.48
1:E:3:ARG:NE	1:E:74:VAL:HG12	2.27	0.48
1:D:37:ASN:O	1:D:50:VAL:HG23	2.14	0.48
1:C:158:ASN:O	1:C:159:SER:C	2.51	0.48
3:A:1050:EPE:HO8	1:B:53:TRP:HH2	1.60	0.47
1:E:37:ASN:O	1:E:50:VAL:HG23	2.14	0.47
1:D:144:THR:HG22	3:D:1053:EPE:O1S	2.14	0.47
1:C:92:ILE:HD11	1:D:39:LEU:CD2	2.44	0.47
1:C:187:CYS:SG	1:C:188:CYS:N	2.87	0.47
1:C:92:ILE:HD11	1:D:39:LEU:HD22	1.97	0.47
1:D:11:ARG:NH1	1:D:11:ARG:HG3	2.30	0.47
1:D:125:VAL:HG13	1:D:128:VAL:CG2	2.43	0.47
1:B:11:ARG:HG3	1:B:11:ARG:HH11	1.80	0.47
1:E:11:ARG:NH1	1:E:11:ARG:HG3	2.29	0.47
1:A:158:ASN:O	1:A:159:SER:C	2.53	0.47
1:C:29:VAL:O	1:C:152:VAL:HA	2.15	0.47
1:A:29:VAL:O	1:A:152:VAL:HA	2.14	0.47
1:B:37:ASN:O	1:B:50:VAL:HG23	2.15	0.47
1:C:37:ASN:O	1:C:50:VAL:HG23	2.15	0.47
1:D:43:GLU:CG	1:D:126:SER:HA	2.44	0.47
1:D:88:ALA:CA	1:D:140:ILE:HG22	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LYS:HG2	1:C:196:GLU:HG3	1.96	0.46
1:C:88:ALA:CA	1:C:140:ILE:HG22	2.36	0.46
1:D:92:ILE:HD11	1:E:39:LEU:HD22	1.98	0.46
1:A:10:ILE:O	1:A:14:SER:HB2	2.16	0.46
1:D:187:CYS:SG	1:D:188:CYS:N	2.88	0.46
1:B:92:ILE:HD11	1:C:39:LEU:HD22	1.98	0.46
1:E:26:PRO:HG3	1:E:148:ARG:O	2.15	0.46
1:E:78:ILE:HG23	1:E:83:VAL:HG21	1.98	0.46
1:E:139:LYS:HG2	1:E:196:GLU:HG3	1.97	0.46
1:E:39:LEU:HD12	1:E:118:ARG:CZ	2.46	0.46
1:A:39:LEU:HD11	1:E:92:ILE:HG12	1.96	0.46
1:A:1:PHE:CB	1:A:70:SER:OG	2.62	0.46
1:D:180:LYS:C	1:D:180:LYS:HD3	2.36	0.46
1:B:10:ILE:O	1:B:14:SER:HB2	2.16	0.46
1:B:29:VAL:O	1:B:152:VAL:HA	2.16	0.46
1:B:188:CYS:HA	1:B:189:PRO:HD3	1.70	0.46
1:B:46:ASN:ND2	1:B:125:VAL:HB	2.27	0.46
1:E:48:VAL:O	1:E:120:ARG:HA	2.16	0.46
1:A:111:VAL:C	1:A:112:LEU:HD13	2.36	0.45
1:D:43:GLU:CD	1:D:126:SER:HA	2.36	0.45
1:E:111:VAL:C	1:E:112:LEU:HD13	2.37	0.45
1:A:92:ILE:HD11	1:B:39:LEU:CD2	2.46	0.45
1:D:139:LYS:HE2	1:D:194:ASP:OD1	2.17	0.45
1:B:158:ASN:O	1:B:159:SER:C	2.55	0.45
1:D:130:THR:CG2	1:D:131:GLU:N	2.80	0.45
1:E:67:SER:C	1:E:69:HIS:H	2.20	0.45
1:A:11:ARG:HH11	1:A:11:ARG:HG3	1.80	0.45
1:A:180:LYS:HD3	1:A:180:LYS:C	2.36	0.45
1:D:78:ILE:HA	1:D:78:ILE:HD13	1.82	0.45
1:A:43:GLU:CG	1:A:126:SER:HA	2.47	0.45
3:A:1050:EPE:O3S	1:B:114:MET:HB3	2.16	0.45
1:C:64:ALA:HA	1:C:107:SER:O	2.16	0.45
1:D:124:ASP:HB2	1:E:168:TYR:CE1	2.52	0.45
1:B:32:SER:OG	1:B:34:LYS:HE2	2.16	0.45
1:A:130:THR:CG2	1:A:131:GLU:N	2.80	0.44
1:A:139:LYS:HG2	1:A:196:GLU:HG3	1.97	0.44
1:D:149:GLU:OE2	1:E:104:ARG:NH2	2.45	0.44
1:E:67:SER:O	1:E:69:HIS:N	2.50	0.44
1:A:143:TRP:CE2	3:A:1050:EPE:H62	2.52	0.44
1:A:78:ILE:HA	1:A:78:ILE:HD13	1.79	0.44
1:B:139:LYS:HG2	1:B:196:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:TRP:O	3:C:1052:EPE:N1	2.50	0.44
1:C:43:GLU:CG	1:C:126:SER:HA	2.48	0.44
1:E:39:LEU:CD1	1:E:118:ARG:CZ	2.96	0.44
1:E:158:ASN:O	1:E:159:SER:C	2.56	0.44
1:A:48:VAL:O	1:A:120:ARG:HA	2.17	0.44
1:C:48:VAL:O	1:C:120:ARG:HA	2.17	0.44
1:D:139:LYS:HG2	1:D:196:GLU:HG3	1.99	0.44
1:B:11:ARG:HG3	1:B:11:ARG:NH1	2.33	0.44
1:D:188:CYS:HA	1:D:189:PRO:HD3	1.69	0.44
1:E:180:LYS:HD3	1:E:180:LYS:C	2.38	0.44
1:B:92:ILE:HD11	1:C:39:LEU:CD2	2.48	0.44
1:E:10:ILE:O	1:E:14:SER:HB2	2.17	0.44
1:C:180:LYS:HD3	1:C:180:LYS:C	2.38	0.44
1:C:188:CYS:HA	1:C:189:PRO:HD3	1.71	0.44
1:B:139:LYS:HE2	1:B:194:ASP:OD1	2.17	0.43
1:E:43:GLU:CG	1:E:126:SER:HA	2.48	0.43
1:D:130:THR:HG22	1:D:131:GLU:N	2.33	0.43
1:A:139:LYS:HE2	1:A:194:ASP:OD1	2.18	0.43
1:D:158:ASN:O	1:D:159:SER:C	2.56	0.43
1:A:118:ARG:HH11	1:E:92:ILE:HG23	1.81	0.43
1:C:111:VAL:C	1:C:112:LEU:HD13	2.39	0.43
1:E:130:THR:CG2	1:E:131:GLU:N	2.81	0.43
1:C:139:LYS:HE2	1:C:194:ASP:OD1	2.18	0.43
1:C:158:ASN:O	1:C:159:SER:O	2.37	0.43
1:D:10:ILE:O	1:D:14:SER:HB2	2.18	0.43
1:B:154:PRO:CD	1:B:180:LYS:HB3	2.45	0.43
1:C:32:SER:OG	1:C:34:LYS:HE2	2.18	0.43
1:D:111:VAL:C	1:D:112:LEU:HD13	2.39	0.43
1:E:29:VAL:O	1:E:152:VAL:HA	2.18	0.43
1:E:78:ILE:HA	1:E:78:ILE:HD13	1.83	0.43
1:B:111:VAL:C	1:B:112:LEU:HD13	2.38	0.43
1:C:72:ASP:O	1:C:107:SER:N	2.51	0.43
1:D:92:ILE:HD11	1:E:39:LEU:HD21	2.01	0.43
1:C:43:GLU:HG3	1:C:125:VAL:HG12	2.01	0.43
1:C:17:ASP:OD1	1:D:77:PRO:HG2	2.19	0.43
1:B:130:THR:CG2	1:B:131:GLU:N	2.82	0.42
1:A:167:GLN:O	1:A:204:LYS:NZ	2.52	0.42
1:C:67:SER:C	1:C:69:HIS:N	2.73	0.42
1:D:89:TYR:CZ	3:D:1053:EPE:H81	2.54	0.42
1:A:171:PHE:CD1	1:A:171:PHE:N	2.87	0.42
1:B:92:ILE:HG23	1:C:118:ARG:HH11	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:PRO:HG3	1:C:148:ARG:O	2.20	0.42
1:B:143:TRP:CZ2	1:C:99:THR:HG21	2.54	0.42
1:D:171:PHE:O	1:D:204:LYS:HE3	2.20	0.42
1:E:137:ARG:HG2	1:E:198:SER:OG	2.19	0.42
1:B:78:ILE:HG23	1:B:83:VAL:HG21	2.02	0.42
1:E:32:SER:OG	1:E:34:LYS:HE2	2.20	0.42
1:A:78:ILE:HG23	1:A:83:VAL:HG21	2.02	0.42
1:B:180:LYS:HD3	1:B:180:LYS:C	2.40	0.42
1:C:43:GLU:CD	1:C:126:SER:HA	2.40	0.42
1:C:78:ILE:HD13	1:C:78:ILE:HA	1.80	0.42
1:A:187:CYS:SG	1:A:188:CYS:N	2.93	0.42
1:A:8:TYR:HB2	1:E:15:ARG:HH12	1.84	0.42
1:C:72:ASP:HB3	1:C:107:SER:OG	2.20	0.42
1:E:19:ILE:HA	1:E:20:PRO:HD3	1.82	0.42
1:A:11:ARG:HG3	1:A:11:ARG:NH1	2.34	0.42
1:C:130:THR:CG2	1:C:131:GLU:N	2.82	0.42
1:A:130:THR:HG22	1:A:131:GLU:N	2.34	0.42
1:A:158:ASN:O	1:A:159:SER:O	2.37	0.42
1:B:39:LEU:HD12	1:B:118:ARG:CZ	2.50	0.42
1:E:72:ASP:O	1:E:107:SER:N	2.48	0.42
1:E:88:ALA:CA	1:E:140:ILE:HG22	2.40	0.41
1:E:20:PRO:HD3	1:E:82:TRP:CD2	2.55	0.41
1:B:20:PRO:HD3	1:B:82:TRP:CD2	2.55	0.41
1:B:88:ALA:CA	1:B:140:ILE:HG22	2.41	0.41
1:C:171:PHE:CD1	1:C:171:PHE:N	2.87	0.41
1:D:171:PHE:N	1:D:171:PHE:CD1	2.88	0.41
1:E:188:CYS:SG	3:E:1054:EPE:H101	2.60	0.41
1:C:46:ASN:HD22	1:C:46:ASN:HA	1.67	0.41
1:B:171:PHE:N	1:B:171:PHE:CD1	2.89	0.41
1:E:43:GLU:CD	1:E:126:SER:HA	2.41	0.41
1:C:149:GLU:CD	1:D:3:ARG:HH12	2.24	0.41
1:C:69:HIS:O	1:C:70:SER:CB	2.66	0.41
1:D:20:PRO:HD3	1:D:82:TRP:CD2	2.56	0.41
1:A:65:TRP:CE2	1:A:107:SER:HB3	2.55	0.41
1:B:143:TRP:CH2	3:B:1051:EPE:H62	2.55	0.41
1:C:130:THR:HG22	1:C:131:GLU:N	2.36	0.41
1:D:137:ARG:HG2	1:D:198:SER:OG	2.21	0.41
1:A:25:ARG:HA	1:A:26:PRO:HD3	1.92	0.41
1:B:43:GLU:CG	1:B:126:SER:HA	2.51	0.41
1:B:203:LYS:HG2	1:B:204:LYS:N	2.35	0.41
1:D:83:VAL:HG13	1:D:84:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:GLU:HG3	1:E:125:VAL:HG12	2.03	0.41
1:A:43:GLU:HG3	1:A:125:VAL:HG12	2.03	0.41
1:C:78:ILE:HG12	1:C:101:GLN:O	2.19	0.41
1:B:130:THR:HG22	1:B:131:GLU:N	2.36	0.41
1:B:19:ILE:HA	1:B:20:PRO:HD3	1.82	0.41
1:D:78:ILE:HG12	1:D:101:GLN:O	2.20	0.41
1:E:50:VAL:HG22	1:E:51:VAL:N	2.36	0.41
1:C:137:ARG:HG2	1:C:198:SER:OG	2.20	0.41
1:C:66:ASN:ND2	1:C:67:SER:N	2.65	0.41
1:C:83:VAL:HG13	1:C:84:PRO:HD2	2.02	0.41
1:A:32:SER:OG	1:A:34:LYS:HE2	2.21	0.40
1:D:39:LEU:HD12	1:D:118:ARG:CZ	2.52	0.40
1:E:139:LYS:HE2	1:E:194:ASP:OD1	2.21	0.40
3:A:1050:EPE:O3S	1:B:114:MET:CB	2.70	0.40
1:B:78:ILE:HA	1:B:78:ILE:HD13	1.79	0.40
1:A:18:VAL:HG22	1:B:7:LEU:HD12	2.02	0.40
1:B:83:VAL:HG13	1:B:84:PRO:HD2	2.03	0.40
1:D:78:ILE:HG23	1:D:83:VAL:HG21	2.02	0.40
3:D:1053:EPE:C9	1:E:114:MET:HB3	2.51	0.40
1:E:130:THR:HG22	1:E:131:GLU:N	2.36	0.40
1:B:137:ARG:HG2	1:B:198:SER:OG	2.21	0.40
1:C:43:GLU:OE2	1:C:126:SER:HA	2.22	0.40
1:C:65:TRP:HD1	1:C:66:ASN:O	2.04	0.40
1:D:145:HIS:CD2	1:E:104:ARG:HH12	2.40	0.40
1:D:154:PRO:CD	1:D:180:LYS:HB3	2.45	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:HIS:CE1	1:E:69:HIS:CE1[8_665]	2.06	0.14

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	203/217 (94%)	192 (95%)	8 (4%)	3 (2%)	10 26
1	B	203/217 (94%)	192 (95%)	8 (4%)	3 (2%)	10 26
1	C	203/217 (94%)	189 (93%)	10 (5%)	4 (2%)	7 19
1	D	203/217 (94%)	189 (93%)	10 (5%)	4 (2%)	7 19
1	E	203/217 (94%)	191 (94%)	7 (3%)	5 (2%)	5 14
All	All	1015/1085 (94%)	953 (94%)	43 (4%)	19 (2%)	8 20

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	SER
1	C	159	SER
1	D	159	SER
1	B	156	THR
1	B	159	SER
1	E	68	SER
1	E	159	SER
1	A	156	THR
1	A	158	ASN
1	B	158	ASN
1	C	156	THR
1	C	158	ASN
1	D	156	THR
1	D	158	ASN
1	E	156	THR
1	E	158	ASN
1	D	2	ASP
1	E	69	HIS
1	C	70	SER

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/201 (95%)	184 (96%)	7 (4%)	34	63
1	B	191/201 (95%)	184 (96%)	7 (4%)	34	63
1	C	191/201 (95%)	183 (96%)	8 (4%)	30	58
1	D	191/201 (95%)	183 (96%)	8 (4%)	30	58
1	E	191/201 (95%)	182 (95%)	9 (5%)	26	54
All	All	955/1005 (95%)	916 (96%)	39 (4%)	30	59

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	PHE
1	A	23	ARG
1	A	24	ASP
1	A	46	ASN
1	A	92	ILE
1	A	112	LEU
1	A	180	LYS
1	B	23	ARG
1	B	24	ASP
1	B	46	ASN
1	B	72	ASP
1	B	92	ILE
1	B	112	LEU
1	B	180	LYS
1	C	23	ARG
1	C	24	ASP
1	C	46	ASN
1	C	66	ASN
1	C	72	ASP
1	C	92	ILE
1	C	112	LEU
1	C	180	LYS
1	D	23	ARG
1	D	24	ASP
1	D	66	ASN
1	D	71	PRO
1	D	72	ASP
1	D	92	ILE
1	D	112	LEU
1	D	180	LYS
1	E	1	PHE

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Mol	Chain	Res	Type
1	E	2	ASP
1	E	23	ARG
1	E	24	ASP
1	E	66	ASN
1	E	72	ASP
1	E	92	ILE
1	E	112	LEU
1	E	180	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	145	HIS
1	A	146	HIS
1	A	181	ASN
1	A	200	ASN
1	B	22	GLN
1	B	46	ASN
1	B	145	HIS
1	B	146	HIS
1	B	181	ASN
1	B	200	ASN
1	C	46	ASN
1	C	66	ASN
1	C	145	HIS
1	C	146	HIS
1	C	181	ASN
1	C	200	ASN
1	D	46	ASN
1	D	66	ASN
1	D	145	HIS
1	D	146	HIS
1	D	181	ASN
1	D	200	ASN
1	E	46	ASN
1	E	55	GLN
1	E	66	ASN
1	E	145	HIS
1	E	146	HIS
1	E	181	ASN
1	E	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 15 ligands modelled in this entry, 10 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
3	EPE	D	1053	-	15,15,15	0.93	0	18,20,20	1.14	2 (11%)
3	EPE	E	1054	-	15,15,15	0.95	0	18,20,20	1.42	2 (11%)
3	EPE	C	1052	-	15,15,15	1.13	1 (6%)	18,20,20	1.67	3 (16%)
3	EPE	B	1051	-	15,15,15	1.01	1 (6%)	18,20,20	1.64	4 (22%)
3	EPE	A	1050	-	15,15,15	0.94	0	18,20,20	1.42	3 (16%)

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
3	EPE	D	1053	-	-	3/9/19/19	0/1/1/1
3	EPE	E	1054	-	-	6/9/19/19	0/1/1/1
3	EPE	C	1052	-	-	2/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	B	1051	-	-	4/9/19/19	0/1/1/1
3	EPE	A	1050	-	-	2/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1052	EPE	C9-N1	2.59	1.53	1.47
3	B	1051	EPE	C2-N1	2.25	1.53	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1052	EPE	O3S-S-O2S	-4.25	100.90	111.27
3	B	1051	EPE	O3S-S-O2S	-3.98	101.54	111.27
3	A	1050	EPE	O3S-S-O2S	-3.87	101.81	111.27
3	C	1052	EPE	O3S-S-C10	3.72	111.78	105.77
3	E	1054	EPE	O3S-S-O2S	-3.66	102.33	111.27
3	D	1053	EPE	O3S-S-O2S	-3.11	103.68	111.27
3	B	1051	EPE	O3S-S-C10	2.68	110.10	105.77
3	B	1051	EPE	O2S-S-O1S	2.42	122.32	113.95
3	A	1050	EPE	O3S-S-C10	2.42	109.67	105.77
3	A	1050	EPE	O2S-S-O1S	2.35	122.09	113.95
3	C	1052	EPE	O2S-S-O1S	2.32	121.96	113.95
3	B	1051	EPE	C2-C3-N4	-2.26	106.00	110.64
3	D	1053	EPE	O2S-S-O1S	2.13	121.34	113.95
3	E	1054	EPE	O2S-S-O1S	2.09	121.17	113.95

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1052	EPE	C10-C9-N1-C2
3	C	1052	EPE	C10-C9-N1-C6
3	E	1054	EPE	C10-C9-N1-C2
3	E	1054	EPE	C10-C9-N1-C6
3	E	1054	EPE	C9-C10-S-O1S
3	E	1054	EPE	C9-C10-S-O2S
3	E	1054	EPE	C9-C10-S-O3S
3	D	1053	EPE	C10-C9-N1-C2
3	D	1053	EPE	S-C10-C9-N1
3	A	1050	EPE	C10-C9-N1-C2

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Mol	Chain	Res	Type	Atoms
3	B	1051	EPE	C10-C9-N1-C2
3	B	1051	EPE	C10-C9-N1-C6
3	B	1051	EPE	S-C10-C9-N1
3	E	1054	EPE	N4-C7-C8-O8
3	B	1051	EPE	C9-C10-S-O3S
3	D	1053	EPE	C10-C9-N1-C6
3	A	1050	EPE	C10-C9-N1-C6

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1053	EPE	5	0
3	E	1054	EPE	1	0
3	C	1052	EPE	1	0
3	B	1051	EPE	2	0
3	A	1050	EPE	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.