



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:16 pm BST

PDB ID : 2BR7
Title : Crystal Structure of Acetylcholine-binding Protein (AChBP) from *Aplysia californica* in complex with HEPES
Authors : Celie, P.H.N.; Kasheverov, I.E.; Mordvintsev, D.Y.; Hogg, R.C.; Van Nierop, P.; Van Elk, R.; Van Rossum-Fikkert, S.E.; Zhmak, M.N.; Bertrand, D.; Tsetlin, V.; Sixma, T.K.; Smit, A.B.
Deposited on : 2005-05-03
Resolution : 3.00 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) : 1.13
EDS : 2.11
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) : 2.11

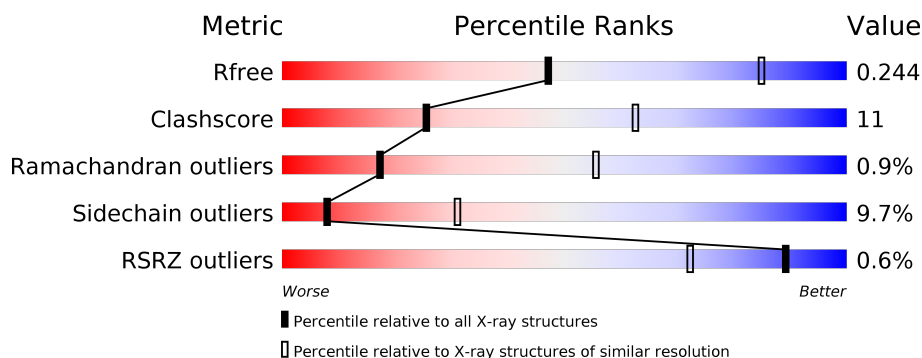
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	217	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 24%, green 67%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 67% 24% 6% </div> </div>
1	B	217	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 23%, green 68%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 68% 23% 6% </div> </div>
1	C	217	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 24%, green 66%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 66% 24% 5% 6% </div> </div>
1	D	217	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 19%, green 72%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 72% 19% 6% </div> </div>
1	E	217	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 23%, green 67%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 67% 23% 5% 6% </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8289 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called SOLUBLE ACETYLCHOLINE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	B	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	C	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	D	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	E	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	VAL	ALA	conflict	UNP Q8WSF8
A	136	VAL	ALA	conflict	UNP Q8WSF8
B	41	VAL	ALA	conflict	UNP Q8WSF8
B	136	VAL	ALA	conflict	UNP Q8WSF8
C	41	VAL	ALA	conflict	UNP Q8WSF8
C	136	VAL	ALA	conflict	UNP Q8WSF8
D	41	VAL	ALA	conflict	UNP Q8WSF8
D	136	VAL	ALA	conflict	UNP Q8WSF8
E	41	VAL	ALA	conflict	UNP Q8WSF8
E	136	VAL	ALA	conflict	UNP Q8WSF8

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



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

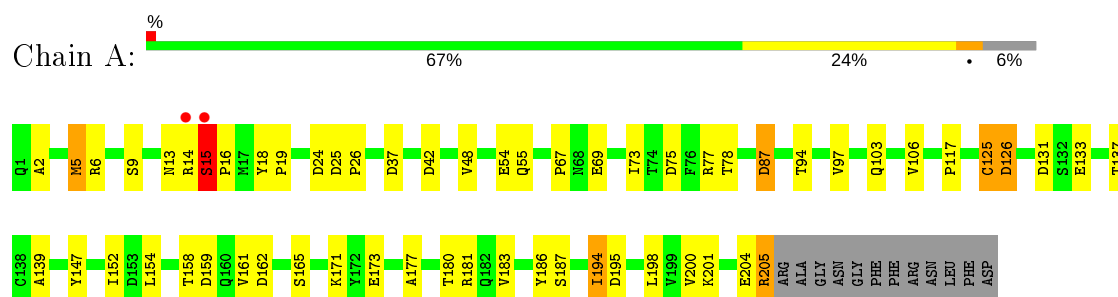
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	12	Total	O	0	0
			12	12		
3	C	9	Total	O	0	0
			9	9		
3	D	10	Total	O	0	0
			10	10		
3	E	12	Total	O	0	0
			12	12		

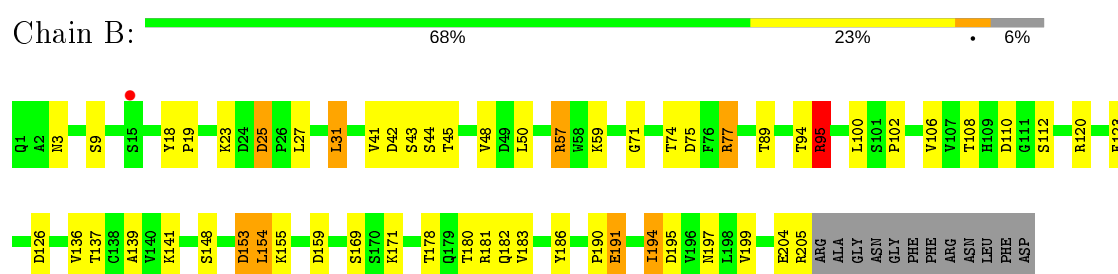
3 Residue-property plots

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 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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

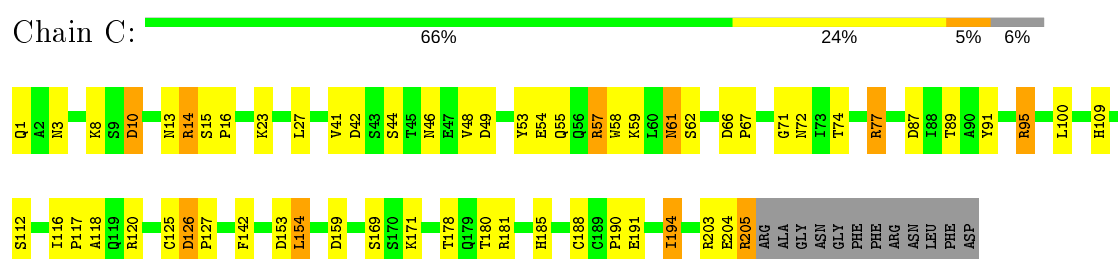
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



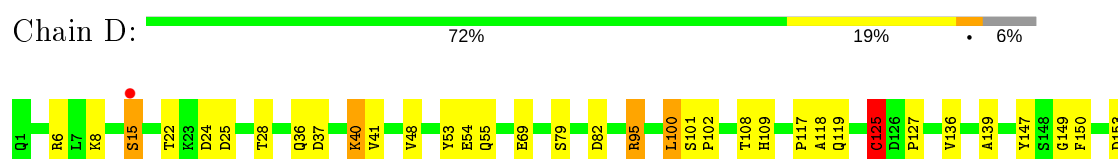
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR





• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	204.20 Å 204.20 Å 204.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.84 – 3.00 19.83 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.84-3.00) 100.0 (19.83-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.98 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.174 , 0.249 0.172 , 0.244	Depositor DCC
R_{free} test set	1430 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8289	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.57	0/1676	0.89	8/2287 (0.3%)
1	B	0.62	0/1676	0.92	5/2287 (0.2%)
1	C	0.64	0/1676	0.93	7/2287 (0.3%)
1	D	0.61	0/1676	0.88	4/2287 (0.2%)
1	E	0.58	0/1676	0.88	6/2287 (0.3%)
All	All	0.61	0/8380	0.90	30/11435 (0.3%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	49	ASP	CB-CG-OD2	7.13	124.72	118.30
1	B	25	ASP	CB-CG-OD2	6.51	124.16	118.30
1	B	153	ASP	CB-CG-OD2	6.47	124.12	118.30
1	D	25	ASP	CB-CG-OD2	6.42	124.08	118.30
1	B	95	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	195	ASP	CB-CG-OD2	6.15	123.84	118.30
1	C	87	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	37	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	162	ASP	CB-CG-OD2	6.05	123.75	118.30
1	E	75	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	42	ASP	CB-CG-OD2	5.96	123.66	118.30
1	C	42	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	126	ASP	CB-CG-OD2	5.86	123.57	118.30
1	D	195	ASP	CB-CG-OD2	5.79	123.51	118.30
1	C	153	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	110	ASP	CB-CG-OD2	5.67	123.40	118.30
1	E	110	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	87	ASP	CB-CG-OD2	5.52	123.26	118.30
1	C	159	ASP	CB-CG-OD2	5.47	123.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	25	ASP	CB-CG-OD2	5.36	123.12	118.30
1	E	126	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	159	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	126	ASP	CB-CG-OD2	5.22	122.99	118.30
1	A	126	ASP	CB-CG-OD2	5.21	122.99	118.30
1	E	49	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	25	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	82	ASP	CB-CG-OD2	5.15	122.93	118.30
1	E	24	ASP	CB-CG-OD2	5.09	122.88	118.30
1	D	24	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	10	ASP	CB-CG-OD2	5.02	122.82	118.30

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	1636	0	1572	28	0
1	B	1636	0	1572	43	0
1	C	1636	0	1572	37	1
1	D	1636	0	1572	30	0
1	E	1636	0	1572	42	0
2	A	15	0	18	2	0
2	B	15	0	18	2	0
2	C	15	0	18	1	0
2	D	15	0	18	0	0
3	A	6	0	0	0	0
3	B	12	0	0	3	0
3	C	9	0	0	2	0
3	D	10	0	0	1	0
3	E	12	0	0	2	0
All	All	8289	0	7932	172	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 11.

All (172) 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:15:SER:HB3	1:A:16:PRO:CD	1.80	1.10
1:A:15:SER:CB	1:A:16:PRO:HD3	1.92	0.99
1:B:57:ARG:HH11	1:B:57:ARG:HG3	1.28	0.98
1:E:3:ASN:C	1:E:3:ASN:HD22	1.68	0.96
1:E:95:ARG:HH11	1:E:95:ARG:CG	1.82	0.93
1:A:15:SER:HB3	1:A:16:PRO:HD3	0.96	0.92
1:B:154:LEU:HB2	1:B:194:ILE:HD11	1.54	0.89
1:D:191:GLU:HB2	1:D:192:PRO:HD2	1.55	0.89
1:A:131:ASP:HB3	1:A:204:GLU:OE2	1.76	0.85
1:B:95:ARG:HH11	1:B:95:ARG:HG3	1.43	0.82
1:A:154:LEU:HB3	1:A:194:ILE:HD11	1.62	0.81
1:C:95:ARG:HG2	1:C:95:ARG:HH11	1.46	0.81
1:E:3:ASN:ND2	1:E:3:ASN:C	2.31	0.80
1:E:154:LEU:H	1:E:194:ILE:HD11	1.46	0.79
1:E:95:ARG:HH11	1:E:95:ARG:HG3	1.48	0.78
1:B:148:SER:CB	1:B:191:GLU:HG2	2.13	0.77
1:C:185:HIS:HE1	3:C:2009:HOH:O	1.71	0.74
1:E:95:ARG:HH11	1:E:95:ARG:HG2	1.51	0.74
1:E:35:LEU:HD11	1:E:50:LEU:HD22	1.68	0.73
1:B:25:ASP:HB2	3:B:2001:HOH:O	1.88	0.72
1:B:77:ARG:CG	1:B:77:ARG:HH11	2.01	0.72
1:C:77:ARG:HG3	1:C:77:ARG:HH11	1.55	0.72
1:B:190:PRO:HG2	1:B:191:GLU:OE1	1.90	0.71
1:C:77:ARG:CG	1:C:77:ARG:HH11	2.02	0.70
1:B:41:VAL:HG22	1:B:48:VAL:HG22	1.74	0.69
1:A:161:VAL:HB	1:A:177:ALA:HB1	1.73	0.69
1:E:45:THR:O	1:E:46:ASN:HB2	1.94	0.66
1:A:6:ARG:NH2	1:A:69:GLU:O	2.29	0.65
1:D:37:ASP:OD1	1:D:170:SER:HB2	1.97	0.65
1:B:148:SER:HB2	1:B:191:GLU:HG2	1.76	0.64
1:E:95:ARG:NH1	1:E:95:ARG:HG3	2.10	0.63
1:E:154:LEU:N	1:E:194:ILE:HD11	2.13	0.63
1:E:35:LEU:CD1	1:E:50:LEU:HD22	2.29	0.63
1:B:57:ARG:NH1	1:B:57:ARG:HG3	2.07	0.63
1:A:2:ALA:HA	1:A:5:MET:HB2	1.81	0.62
1:D:154:LEU:HB2	1:D:194:ILE:HG22	1.81	0.61
1:E:154:LEU:HB2	1:E:194:ILE:CD1	2.30	0.61
1:D:28:THR:HG23	1:D:153:ASP:HB3	1.82	0.60
1:E:154:LEU:HB2	1:E:194:ILE:HD11	1.82	0.60
1:A:18:TYR:CD1	1:A:19:PRO:HD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:VAL:HB	1:A:177:ALA:CB	2.31	0.60
1:C:169:SER:HA	1:C:205:ARG:NH2	2.17	0.59
1:E:3:ASN:ND2	1:E:3:ASN:O	2.20	0.59
1:D:95:ARG:NH1	1:E:98:GLN:OE1	2.34	0.59
1:E:41:VAL:HG22	1:E:48:VAL:HG22	1.85	0.58
1:C:55:GLN:HE21	1:C:57:ARG:CD	2.17	0.58
1:E:154:LEU:O	1:E:181:ARG:HD2	2.03	0.57
1:C:95:ARG:CG	1:C:95:ARG:HH11	2.16	0.57
1:D:117:PRO:HB2	1:D:119:GLN:HE21	1.70	0.57
1:C:27:LEU:HD11	1:C:58:TRP:HB2	1.87	0.57
1:B:77:ARG:HH11	1:B:77:ARG:HG3	1.70	0.56
1:D:41:VAL:HG22	1:D:48:VAL:HG22	1.87	0.56
1:A:48:VAL:HG21	1:A:125:CYS:SG	2.45	0.56
1:A:154:LEU:CB	1:A:194:ILE:HD11	2.34	0.55
1:B:182:GLN:NE2	1:B:197:ASN:HB2	2.21	0.55
1:C:3:ASN:ND2	1:C:71:GLY:HA3	2.22	0.55
1:C:91:TYR:CE2	2:C:1206:EPE:H22	2.42	0.55
1:E:23:LYS:HZ2	1:E:150:PHE:HD2	1.55	0.55
1:E:36:GLN:NE2	1:E:53:TYR:CE1	2.75	0.55
1:B:95:ARG:HD2	3:B:2005:HOH:O	2.06	0.54
1:B:148:SER:HB3	1:B:191:GLU:HG2	1.87	0.54
1:B:77:ARG:HH11	1:B:77:ARG:HG2	1.72	0.54
1:D:161:VAL:HG21	1:D:198:LEU:HD11	1.90	0.54
1:E:95:ARG:NH1	1:E:95:ARG:CG	2.51	0.53
1:D:149:GLY:HA2	1:D:194:ILE:HD12	1.91	0.53
1:E:14:ARG:HD3	3:E:2001:HOH:O	2.09	0.53
1:A:54:GLU:O	1:A:117:PRO:HD2	2.09	0.53
1:C:61:ASN:H	1:C:61:ASN:ND2	2.07	0.53
1:A:186:TYR:CE1	2:A:1206:EPE:H101	2.44	0.52
1:E:123:PHE:HD2	3:E:2008:HOH:O	1.92	0.52
1:C:154:LEU:O	1:C:181:ARG:HD2	2.10	0.52
1:E:55:GLN:HG3	1:E:116:ILE:HG12	1.92	0.52
1:B:171:LYS:HA	1:B:205:ARG:HD2	1.91	0.52
1:B:148:SER:CB	1:B:191:GLU:CG	2.85	0.51
1:A:103:GLN:NE2	1:A:103:GLN:HA	2.25	0.51
1:B:57:ARG:HH11	1:B:57:ARG:CG	2.10	0.51
1:D:154:LEU:HB2	1:D:194:ILE:CG2	2.40	0.51
1:C:185:HIS:CE1	3:C:2009:HOH:O	2.53	0.51
1:B:94:THR:O	1:C:120:ARG:HD2	2.11	0.50
1:A:94:THR:O	1:B:120:ARG:HD2	2.11	0.50
1:B:136:VAL:HG22	1:B:137:THR:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ARG:CD	3:B:2005:HOH:O	2.59	0.50
1:E:167:TYR:CZ	1:E:169:SER:HB2	2.47	0.49
1:B:77:ARG:CG	1:B:77:ARG:NH1	2.68	0.49
1:B:194:ILE:HD12	1:B:195:ASP:N	2.27	0.49
1:D:41:VAL:HG13	1:D:127:PRO:HG3	1.94	0.49
1:C:181:ARG:HG2	1:C:194:ILE:CD1	2.43	0.48
1:A:15:SER:CB	1:A:16:PRO:CD	2.69	0.48
1:D:95:ARG:HD3	3:D:2004:HOH:O	2.14	0.48
1:B:186:TYR:CE1	2:B:1206:EPE:H101	2.49	0.47
1:D:139:ALA:HA	1:D:198:LEU:O	2.14	0.47
1:D:147:TYR:CE1	1:E:77:ARG:HG3	2.48	0.47
1:D:154:LEU:HD23	1:D:196:VAL:HG23	1.96	0.47
1:D:6:ARG:NH2	1:D:69:GLU:O	2.48	0.47
1:C:48:VAL:HG21	1:C:125:CYS:SG	2.55	0.47
1:E:54:GLU:O	1:E:116:ILE:HA	2.14	0.47
1:B:50:LEU:HG	1:B:123:PHE:HE1	1.79	0.46
1:B:3:ASN:ND2	1:B:71:GLY:HA3	2.30	0.46
1:C:41:VAL:HG22	1:C:48:VAL:HG22	1.98	0.46
1:D:125:CYS:HA	1:E:167:TYR:OH	2.15	0.46
1:E:33:PHE:CE1	1:E:54:GLU:HG3	2.50	0.46
1:A:77:ARG:HD3	1:E:147:TYR:CE1	2.50	0.46
1:B:31:LEU:HD22	1:B:154:LEU:HG	1.97	0.46
1:D:101:SER:HB2	1:D:102:PRO:CD	2.46	0.46
1:B:141:LYS:HE3	1:B:182:GLN:NE2	2.31	0.46
1:E:171:LYS:HA	1:E:205:ARG:HG2	1.96	0.46
1:C:95:ARG:NH1	1:C:95:ARG:CG	2.76	0.46
1:E:77:ARG:HD3	1:E:106:VAL:HB	1.98	0.46
1:C:77:ARG:CG	1:C:77:ARG:NH1	2.70	0.45
1:D:154:LEU:O	1:D:181:ARG:HD2	2.16	0.45
1:A:87:ASP:HB2	1:B:102:PRO:HG2	1.99	0.45
1:B:18:TYR:CD1	1:B:19:PRO:HD2	2.52	0.45
1:C:10:ASP:HA	1:C:14:ARG:HB2	1.98	0.45
1:A:126:ASP:OD2	1:B:205:ARG:NH2	2.42	0.45
1:B:43:SER:O	1:C:171:LYS:HE3	2.16	0.45
1:E:144:SER:OG	1:E:147:TYR:HB2	2.17	0.45
1:E:183:VAL:HG23	1:E:194:ILE:HG22	1.99	0.44
1:D:180:THR:O	1:D:196:VAL:HA	2.17	0.44
2:A:1206:EPE:H51	2:A:1206:EPE:H81	1.60	0.44
1:B:77:ARG:NH1	1:B:77:ARG:HG2	2.30	0.44
1:A:9:SER:O	1:A:13:ASN:HB2	2.18	0.44
1:E:48:VAL:HG21	1:E:125:CYS:SG	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ASP:O	1:B:45:THR:O	2.36	0.43
1:E:54:GLU:O	1:E:117:PRO:HD2	2.18	0.43
1:B:154:LEU:H	1:B:194:ILE:HG12	1.84	0.43
1:E:95:ARG:NH1	1:E:95:ARG:HG2	2.25	0.43
1:C:203:ARG:HG3	1:C:204:GLU:O	2.18	0.43
1:A:161:VAL:HG21	1:A:198:LEU:HD13	2.00	0.43
1:B:95:ARG:NH1	1:B:95:ARG:HG3	2.20	0.43
1:E:126:ASP:HA	1:E:127:PRO:HD3	1.87	0.43
1:B:3:ASN:HD22	1:B:71:GLY:HA3	1.84	0.43
1:C:54:GLU:O	1:C:117:PRO:HD2	2.19	0.43
1:C:59:LYS:HA	1:C:112:SER:HA	2.01	0.43
1:E:21:PRO:HD2	1:E:147:TYR:CZ	2.53	0.43
1:B:139:ALA:HB2	1:B:199:VAL:HG22	2.01	0.42
1:D:100:LEU:HB2	1:D:118:ALA:O	2.19	0.42
1:A:173:GLU:HB2	1:A:205:ARG:HG3	2.00	0.42
1:D:170:SER:O	1:D:205:ARG:NH1	2.52	0.42
1:D:36:GLN:OE1	1:D:53:TYR:CE1	2.73	0.42
1:D:150:PHE:CE2	1:D:191:GLU:HB2	2.55	0.42
1:D:161:VAL:HG21	1:D:198:LEU:CD1	2.49	0.42
1:E:18:TYR:HA	1:E:19:PRO:HD3	1.91	0.42
1:A:137:THR:OG1	1:A:201:LYS:HG3	2.19	0.42
1:C:13:ASN:C	1:C:15:SER:H	2.24	0.42
1:C:46:ASN:HD22	1:C:46:ASN:HA	1.67	0.42
1:C:89:THR:O	1:C:142:PHE:HA	2.20	0.42
1:E:154:LEU:HB2	1:E:194:ILE:HD12	2.02	0.42
1:C:191:GLU:CD	1:C:191:GLU:H	2.24	0.41
1:C:15:SER:HA	1:C:16:PRO:HD3	1.91	0.41
1:C:53:TYR:HB3	1:C:118:ALA:HA	2.03	0.41
1:D:200:VAL:O	1:D:200:VAL:HG23	2.21	0.41
1:A:24:ASP:O	1:A:26:PRO:HD3	2.19	0.41
1:B:153:ASP:OD1	1:B:181:ARG:NH1	2.54	0.41
1:D:108:THR:HG22	1:D:109:HIS:N	2.35	0.41
1:C:188:CYS:HB3	1:D:55:GLN:HE22	1.85	0.41
1:A:147:TYR:CD2	1:A:152:ILE:HD12	2.56	0.41
1:A:73:ILE:HG22	1:A:75:ASP:O	2.21	0.41
1:B:59:LYS:HA	1:B:112:SER:HA	2.03	0.41
1:B:75:ASP:HB3	1:B:108:THR:HA	2.02	0.41
1:A:139:ALA:HA	1:A:198:LEU:O	2.21	0.41
1:C:71:GLY:O	1:C:72:ASN:HB2	2.21	0.41
1:B:27:LEU:HA	1:B:27:LEU:HD12	1.84	0.41
1:C:3:ASN:HD22	1:C:71:GLY:HA3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:GLU:O	1:D:117:PRO:HD2	2.20	0.41
1:E:31:LEU:HD12	1:E:31:LEU:HA	1.81	0.41
1:C:41:VAL:HG13	1:C:127:PRO:HG3	2.02	0.40
1:D:40:LYS:HG3	1:D:41:VAL:N	2.35	0.40
2:B:1206:EPE:H102	2:B:1206:EPE:H22	1.90	0.40
1:E:159:ASP:HB3	1:E:179:GLN:O	2.21	0.40
1:C:66:ASP:HA	1:C:67:PRO:HD3	1.98	0.40
1:C:126:ASP:OD1	1:C:126:ASP:C	2.59	0.40
1:C:55:GLN:HE21	1:C:57:ARG:HD3	1.86	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:C:109:HIS:CE1	1:C:185:HIS:CE1[9_555]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	193 (95%)	7 (3%)	3 (2%)	10	42
1	B	203/217 (94%)	189 (93%)	13 (6%)	1 (0%)	29	68
1	C	203/217 (94%)	191 (94%)	11 (5%)	1 (0%)	29	68
1	D	203/217 (94%)	191 (94%)	10 (5%)	2 (1%)	15	53
1	E	203/217 (94%)	185 (91%)	16 (8%)	2 (1%)	15	53
All	All	1015/1085 (94%)	949 (94%)	57 (6%)	9 (1%)	17	55

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	E	46	ASN
1	A	14	ARG
1	E	5	MET
1	B	155	LYS
1	D	125	CYS
1	A	67	PRO
1	D	15	SER
1	C	190	PRO

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	188/197 (95%)	170 (90%)	18 (10%)	8	32
1	B	188/197 (95%)	168 (89%)	20 (11%)	6	26
1	C	188/197 (95%)	170 (90%)	18 (10%)	8	32
1	D	188/197 (95%)	175 (93%)	13 (7%)	15	48
1	E	188/197 (95%)	166 (88%)	22 (12%)	5	22
All	All	940/985 (95%)	849 (90%)	91 (10%)	8	31

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	15	SER
1	A	55	GLN
1	A	78	THR
1	A	97	VAL
1	A	106	VAL
1	A	125	CYS
1	A	133	GLU
1	A	158	THR
1	A	165	SER
1	A	171	LYS

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Mol	Chain	Res	Type
1	A	180	THR
1	A	181	ARG
1	A	183	VAL
1	A	187	SER
1	A	194	ILE
1	A	200	VAL
1	A	205	ARG
1	B	9	SER
1	B	23	LYS
1	B	31	LEU
1	B	44	SER
1	B	57	ARG
1	B	74	THR
1	B	77	ARG
1	B	89	THR
1	B	95	ARG
1	B	100	LEU
1	B	106	VAL
1	B	154	LEU
1	B	159	ASP
1	B	169	SER
1	B	178	THR
1	B	180	THR
1	B	183	VAL
1	B	191	GLU
1	B	194	ILE
1	B	204	GLU
1	C	1	GLN
1	C	8	LYS
1	C	14	ARG
1	C	23	LYS
1	C	44	SER
1	C	57	ARG
1	C	61	ASN
1	C	62	SER
1	C	74	THR
1	C	77	ARG
1	C	95	ARG
1	C	100	LEU
1	C	116	ILE
1	C	154	LEU
1	C	178	THR

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Mol	Chain	Res	Type
1	C	180	THR
1	C	194	ILE
1	C	205	ARG
1	D	8	LYS
1	D	15	SER
1	D	22	THR
1	D	40	LYS
1	D	79	SER
1	D	95	ARG
1	D	100	LEU
1	D	125	CYS
1	D	136	VAL
1	D	170	SER
1	D	178	THR
1	D	180	THR
1	D	191	GLU
1	E	1	GLN
1	E	3	ASN
1	E	5	MET
1	E	14	ARG
1	E	17	MET
1	E	24	ASP
1	E	40	LYS
1	E	89	THR
1	E	95	ARG
1	E	100	LEU
1	E	106	VAL
1	E	119	GLN
1	E	133	GLU
1	E	154	LEU
1	E	178	THR
1	E	182	GLN
1	E	184	GLN
1	E	186	TYR
1	E	191	GLU
1	E	194	ILE
1	E	200	VAL
1	E	205	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	36	GLN
1	A	46	ASN
1	A	103	GLN
1	A	182	GLN
1	B	46	ASN
1	B	182	GLN
1	C	13	ASN
1	C	36	GLN
1	C	46	ASN
1	C	55	GLN
1	C	61	ASN
1	C	185	HIS
1	D	46	ASN
1	D	103	GLN
1	D	119	GLN
1	D	182	GLN
1	D	197	ASN
1	E	3	ASN
1	E	36	GLN
1	E	56	GLN
1	E	184	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	EPE	A	1206	-	15,15,15	1.75	1 (6%)	18,20,20	2.99	10 (55%)
2	EPE	C	1206	-	15,15,15	1.58	1 (6%)	18,20,20	3.07	11 (61%)
2	EPE	B	1206	-	15,15,15	1.53	1 (6%)	18,20,20	2.75	8 (44%)
2	EPE	D	1206	-	15,15,15	1.65	1 (6%)	18,20,20	2.75	9 (50%)

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	EPE	A	1206	-	-	3/9/19/19	0/1/1/1
2	EPE	C	1206	-	-	6/9/19/19	0/1/1/1
2	EPE	B	1206	-	-	2/9/19/19	0/1/1/1
2	EPE	D	1206	-	-	7/9/19/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1206	EPE	C10-S	-6.30	1.68	1.77
2	D	1206	EPE	C10-S	-5.85	1.69	1.77
2	C	1206	EPE	C10-S	-5.52	1.69	1.77
2	B	1206	EPE	C10-S	-5.21	1.70	1.77

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1206	EPE	C5-N4-C3	7.26	125.17	108.83
2	A	1206	EPE	C6-N1-C2	5.96	122.25	108.83
2	B	1206	EPE	C5-N4-C3	5.77	121.81	108.83
2	D	1206	EPE	C6-N1-C2	5.31	120.78	108.83
2	A	1206	EPE	C7-N4-C5	5.05	124.16	111.23
2	C	1206	EPE	O1S-S-C10	4.99	112.92	106.92
2	B	1206	EPE	C9-N1-C2	4.80	123.50	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1206	EPE	C6-N1-C2	4.52	119.01	108.83
2	A	1206	EPE	C2-C3-N4	-4.46	101.49	110.64
2	C	1206	EPE	C9-N1-C6	4.46	122.63	111.23
2	D	1206	EPE	C7-N4-C5	4.23	122.06	111.23
2	D	1206	EPE	C5-N4-C3	4.12	118.10	108.83
2	C	1206	EPE	C9-N1-C2	3.81	120.98	111.23
2	B	1206	EPE	O1S-S-C10	3.74	111.42	106.92
2	A	1206	EPE	C6-C5-N4	-3.69	103.07	110.64
2	A	1206	EPE	C9-N1-C6	3.68	120.65	111.23
2	B	1206	EPE	C7-N4-C3	3.62	120.50	111.23
2	B	1206	EPE	O3S-S-C10	3.51	111.44	105.77
2	D	1206	EPE	O2S-S-C10	3.50	111.12	106.92
2	A	1206	EPE	C5-N4-C3	3.39	116.45	108.83
2	D	1206	EPE	C7-N4-C3	3.36	119.84	111.23
2	D	1206	EPE	C9-N1-C6	3.35	119.80	111.23
2	C	1206	EPE	C6-N1-C2	3.35	116.36	108.83
2	C	1206	EPE	C5-C6-N1	-3.28	103.91	110.64
2	D	1206	EPE	C9-N1-C2	3.19	119.39	111.23
2	A	1206	EPE	C7-N4-C3	3.15	119.30	111.23
2	A	1206	EPE	O2S-S-C10	3.13	110.68	106.92
2	D	1206	EPE	C6-C5-N4	-3.01	104.46	110.64
2	C	1206	EPE	C7-N4-C3	2.64	117.99	111.23
2	B	1206	EPE	C7-N4-C5	2.49	117.59	111.23
2	B	1206	EPE	C9-N1-C6	2.40	117.37	111.23
2	A	1206	EPE	O3S-S-C10	2.36	109.58	105.77
2	C	1206	EPE	C8-C7-N4	-2.35	104.95	113.40
2	D	1206	EPE	O3S-S-C10	2.32	109.52	105.77
2	A	1206	EPE	C9-N1-C2	2.29	117.10	111.23
2	C	1206	EPE	O2S-S-C10	2.28	109.66	106.92
2	C	1206	EPE	C7-N4-C5	2.18	116.80	111.23
2	C	1206	EPE	C3-C2-N1	-2.04	106.45	110.64

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1206	EPE	C8-C7-N4-C5
2	C	1206	EPE	C9-C10-S-O2S
2	C	1206	EPE	C9-C10-S-O3S
2	B	1206	EPE	C10-C9-N1-C2
2	D	1206	EPE	C10-C9-N1-C6
2	D	1206	EPE	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
2	D	1206	EPE	C9-C10-S-O3S
2	A	1206	EPE	N4-C7-C8-O8
2	C	1206	EPE	C10-C9-N1-C2
2	B	1206	EPE	C8-C7-N4-C5
2	D	1206	EPE	N4-C7-C8-O8
2	C	1206	EPE	C9-C10-S-O1S
2	D	1206	EPE	C9-C10-S-O1S
2	D	1206	EPE	C9-C10-S-O2S
2	A	1206	EPE	C10-C9-N1-C2
2	C	1206	EPE	C8-C7-N4-C5
2	C	1206	EPE	N4-C7-C8-O8
2	D	1206	EPE	C10-C9-N1-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1206	EPE	2	0
2	C	1206	EPE	1	0
2	B	1206	EPE	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	205/217 (94%)	-0.47	2 (0%) 82 59	26, 35, 54, 64	0
1	B	205/217 (94%)	-0.68	1 (0%) 91 75	23, 33, 48, 59	0
1	C	205/217 (94%)	-0.63	0 100 100	22, 33, 46, 58	0
1	D	205/217 (94%)	-0.60	1 (0%) 91 75	22, 33, 49, 63	0
1	E	205/217 (94%)	-0.50	2 (0%) 82 59	23, 33, 56, 67	0
All	All	1025/1085 (94%)	-0.58	6 (0%) 89 72	22, 33, 52, 67	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	SER	4.1
1	E	1	GLN	3.1
1	D	15	SER	2.7
1	A	14	ARG	2.4
1	E	14	ARG	2.4
1	B	15	SER	2.3

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. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
2	EPE	C	1206	15/15	0.79	0.34	84,88,90,90	0
2	EPE	B	1206	15/15	0.87	0.29	67,69,75,75	0
2	EPE	A	1206	15/15	0.93	0.19	38,41,51,51	0
2	EPE	D	1206	15/15	0.94	0.19	59,61,65,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.