



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2023 – 10:49 AM EDT

PDB ID : 2ZJV
Title : Crystal Structure of Lymnaea stagnalis Acetylcholine Binding Protein (Ls-AChBP) Complexed with Clothianidin
Authors : Okajima, T.; Ihara, M.; Yamashita, A.; Oda, T.; Morimoto, T.; Matsuda, K.
Deposited on : 2008-03-10
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 : 2.36
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) : 2.36

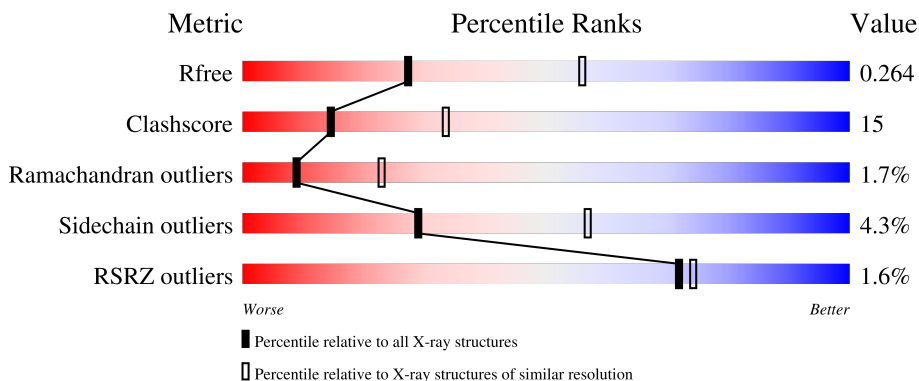
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 $\leq 5\%$. 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	214	 2% (poor fit), 67% (0 outliers), 28% (1 outlier), 3% (2 outliers), 0% (3+ outliers)
1	B	214	 0% (poor fit), 60% (0 outliers), 36% (1 outlier), 3% (2 outliers), 1% (3+ outliers)
1	C	214	 3% (poor fit), 62% (0 outliers), 32% (1 outlier), 3% (2 outliers), 0% (3+ outliers)
1	D	214	 0% (poor fit), 68% (0 outliers), 26% (1 outlier), 5% (2 outliers), 1% (3+ outliers)
1	E	214	 0% (poor fit), 64% (0 outliers), 31% (1 outlier), 5% (2 outliers), 0% (3+ outliers)

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8621 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
			Total	C	N	O	S			
1	A	208	1655	1032	285	333	5	0	0	0
1	B	208	1659	1034	285	335	5	0	0	0
1	C	207	1655	1032	285	333	5	0	1	0
1	D	208	1655	1032	285	333	5	0	0	0
1	E	208	1663	1037	288	333	5	0	1	0

There are 30 discrepancies between the modelled and reference sequences:

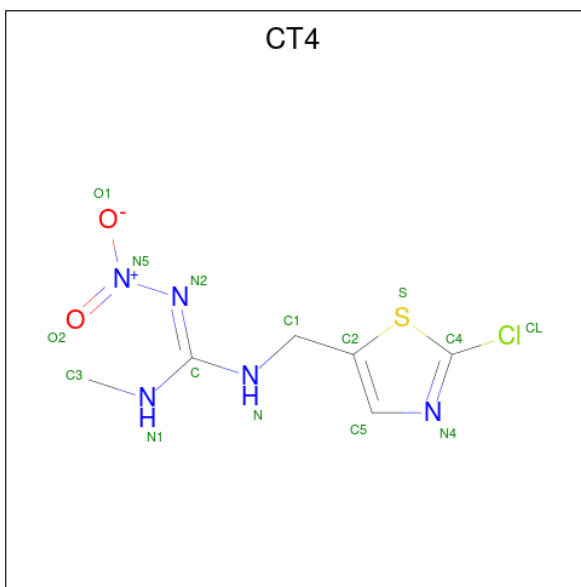
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLU	ALA	engineered mutation	UNP P58154
A	-2	ALA	CYS	engineered mutation	UNP P58154
A	-1	GLU	LEU	engineered mutation	UNP P58154
A	0	ALA	SER	engineered mutation	UNP P58154
A	1	ALA	LEU	engineered mutation	UNP P58154
A	66	ASP	ASN	engineered mutation	UNP P58154
B	-3	GLU	ALA	engineered mutation	UNP P58154
B	-2	ALA	CYS	engineered mutation	UNP P58154
B	-1	GLU	LEU	engineered mutation	UNP P58154
B	0	ALA	SER	engineered mutation	UNP P58154
B	1	ALA	LEU	engineered mutation	UNP P58154
B	66	ASP	ASN	engineered mutation	UNP P58154
C	-3	GLU	ALA	engineered mutation	UNP P58154
C	-2	ALA	CYS	engineered mutation	UNP P58154
C	-1	GLU	LEU	engineered mutation	UNP P58154
C	0	ALA	SER	engineered mutation	UNP P58154
C	1	ALA	LEU	engineered mutation	UNP P58154
C	66	ASP	ASN	engineered mutation	UNP P58154
D	-3	GLU	ALA	engineered mutation	UNP P58154

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	ALA	CYS	engineered mutation	UNP P58154
D	-1	GLU	LEU	engineered mutation	UNP P58154
D	0	ALA	SER	engineered mutation	UNP P58154
D	1	ALA	LEU	engineered mutation	UNP P58154
D	66	ASP	ASN	engineered mutation	UNP P58154
E	-3	GLU	ALA	engineered mutation	UNP P58154
E	-2	ALA	CYS	engineered mutation	UNP P58154
E	-1	GLU	LEU	engineered mutation	UNP P58154
E	0	ALA	SER	engineered mutation	UNP P58154
E	1	ALA	LEU	engineered mutation	UNP P58154
E	66	ASP	ASN	engineered mutation	UNP P58154

- Molecule 2 is 1-[(2-chloro-1,3-thiazol-5-yl)methyl]-3-methyl-2-nitroguanidine (three-letter code: CT4) (formula: C₆H₈ClN₅O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
2	A	1	Total	C	Cl	N	O	S	0	0
			15	6	1	5	2	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			15	6	1	5	2	1		
2	C	1	Total	C	Cl	N	O	S	0	0
			15	6	1	5	2	1		
2	D	1	Total	C	Cl	N	O	S	0	0
			15	6	1	5	2	1		
2	E	1	Total	C	Cl	N	O	S	0	0
			15	6	1	5	2	1		

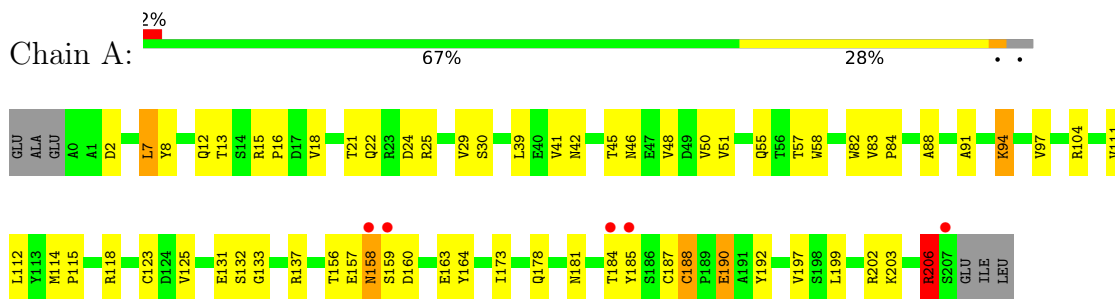
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	47	Total O 47 47	0	0
3	B	51	Total O 51 51	0	0
3	C	49	Total O 49 49	0	0
3	D	53	Total O 53 53	0	0
3	E	59	Total O 59 59	0	0

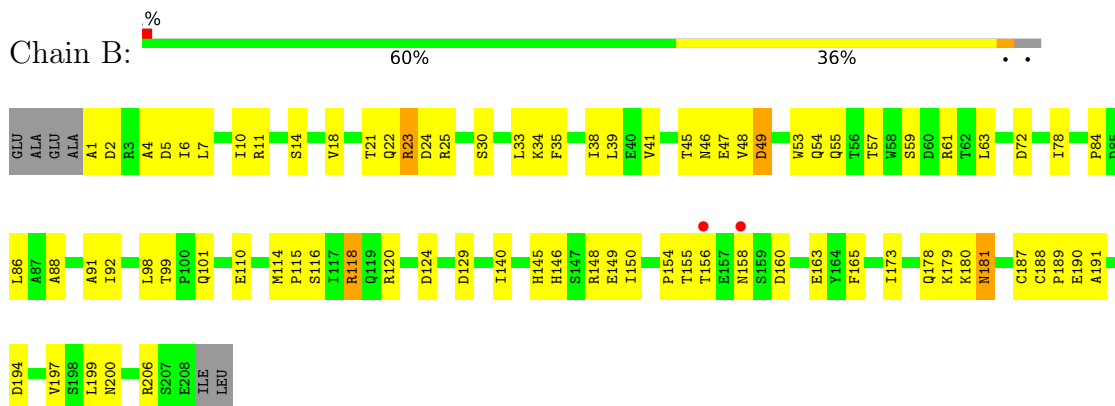
3 Residue-property plots [i](#)

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.

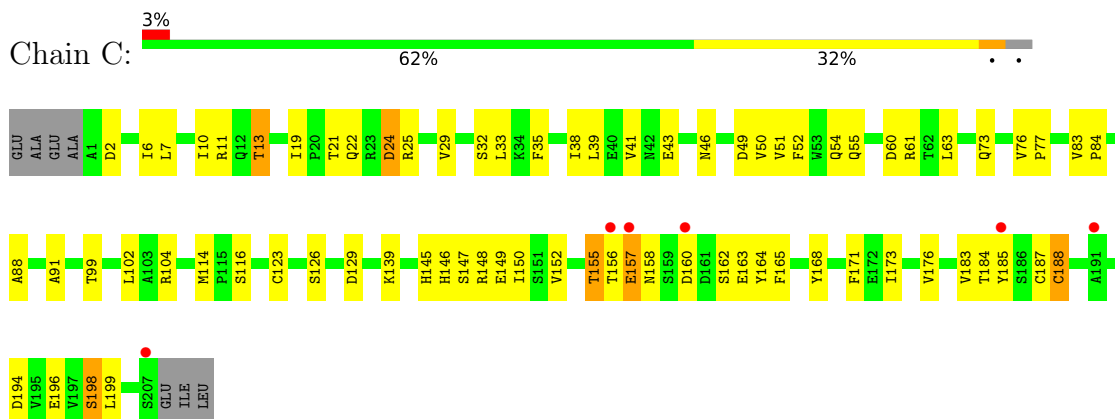
- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein

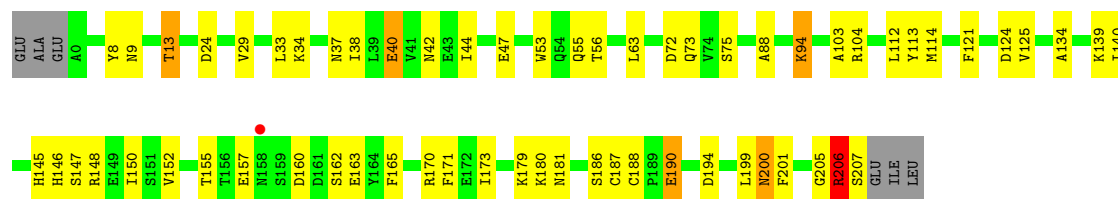


- Molecule 1: Acetylcholine-binding protein



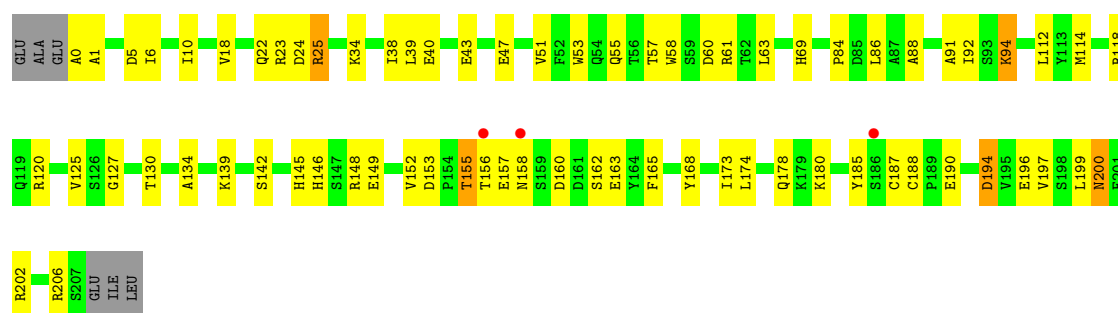
- Molecule 1: Acetylcholine-binding protein

Chain D:  68% 26%



- Molecule 1: Acetylcholine-binding protein

Chain E:  64% 31%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	74.56Å 74.56Å 351.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.26 – 2.70 39.61 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.26-2.70) 99.9 (39.61-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 2.69Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.202 , 0.270 0.196 , 0.264	Depositor DCC
R_{free} test set	1272 reflections (4.22%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtrriage
Anisotropy	0.492	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.125 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8621	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: CT4

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	0.41	0/1691	0.63	0/2307
1	B	0.41	0/1695	0.61	0/2312
1	C	0.40	0/1694	0.62	0/2311
1	D	0.41	0/1691	0.62	0/2307
1	E	0.44	0/1702	0.64	0/2321
All	All	0.42	0/8473	0.62	0/11558

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1655	0	1596	47	0
1	B	1659	0	1597	62	0
1	C	1655	0	1597	58	0
1	D	1655	0	1596	49	0
1	E	1663	0	1609	51	0
2	A	15	0	8	1	0
2	B	15	0	8	0	0
2	C	15	0	8	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	15	0	8	2	0
2	E	15	0	8	1	0
3	A	47	0	0	2	0
3	B	51	0	0	5	0
3	C	49	0	0	1	0
3	D	53	0	0	1	0
3	E	59	0	0	1	0
All	All	8621	0	8035	253	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 15.

All (253) 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:E:22:GLN:HE22	1:E:61:ARG:HG3	1.31	0.94
1:B:160:ASP:HB3	1:B:163:GLU:HB2	1.50	0.91
1:D:179:LYS:HG2	1:D:180:LYS:H	1.36	0.91
1:E:173:ILE:HD12	1:E:199:LEU:HD11	1.53	0.88
1:C:22:GLN:HE22	1:C:61:ARG:HG3	1.38	0.87
1:A:7:LEU:HD13	1:E:18:VAL:HG22	1.55	0.87
1:D:160:ASP:HB3	1:D:163:GLU:HB2	1.58	0.84
1:B:22:GLN:NE2	1:B:61:ARG:HG3	1.93	0.83
1:E:22:GLN:HE22	1:E:61:ARG:CG	1.93	0.82
1:C:10:ILE:HG23	1:C:63:LEU:HD22	1.63	0.80
1:D:173:ILE:HD12	1:D:199:LEU:HD11	1.66	0.77
1:C:88:ALA:HB3	1:C:91:ALA:HB2	1.69	0.75
1:A:160:ASP:HB3	1:A:163:GLU:HB2	1.69	0.73
1:E:146:HIS:CD2	1:E:190:GLU:HG3	2.24	0.72
1:A:50:VAL:HG12	1:A:51:VAL:N	2.06	0.71
1:E:0:ALA:HB2	1:E:69:HIS:HB2	1.71	0.71
1:A:25:ARG:HG2	1:A:25:ARG:HH11	1.56	0.71
1:E:6:ILE:O	1:E:10:ILE:HG12	1.93	0.69
1:C:22:GLN:HE22	1:C:61:ARG:CG	2.06	0.69
1:B:39:LEU:HD12	1:B:118:ARG:HE	1.58	0.67
1:A:173:ILE:HD12	1:A:199:LEU:HD11	1.77	0.67
1:C:160:ASP:HB3	1:C:163:GLU:HB2	1.77	0.67
1:C:173:ILE:HD12	1:C:199:LEU:HD11	1.75	0.67
1:B:22:GLN:CD	1:B:61:ARG:HG3	2.14	0.66
1:B:1:ALA:HB1	1:B:5:ASP:HB2	1.79	0.64
1:D:146:HIS:CE1	1:D:148:ARG:HB2	2.33	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HB3	3:B:313:HOH:O	1.98	0.63
1:E:88:ALA:HB3	1:E:91:ALA:HB2	1.79	0.63
1:D:55:GLN:HB2	1:D:114:MET:CE	2.29	0.63
1:B:206:ARG:HB2	3:B:328:HOH:O	1.98	0.62
1:A:187:CYS:SG	1:A:188:CYS:N	2.72	0.62
1:C:43:GLU:OE2	1:C:126:SER:HA	1.99	0.62
1:C:187:CYS:SG	1:C:188:CYS:N	2.72	0.62
1:C:77:PRO:HA	1:C:102:LEU:HD23	1.81	0.61
1:D:55:GLN:HB2	1:D:114:MET:HE2	1.82	0.60
1:E:173:ILE:CD1	1:E:199:LEU:HD11	2.28	0.60
1:B:173:ILE:HD12	1:B:199:LEU:HD11	1.83	0.60
1:B:34:LYS:HB2	1:B:53:TRP:HB2	1.84	0.60
1:B:10:ILE:HG23	1:B:63:LEU:HD22	1.83	0.59
1:A:25:ARG:HG2	1:A:25:ARG:NH1	2.17	0.59
1:A:188:CYS:HB2	1:A:190:GLU:HG2	1.84	0.59
1:E:22:GLN:O	1:E:25:ARG:HG2	2.03	0.59
1:B:146:HIS:CE1	1:B:148:ARG:HB2	2.37	0.58
1:A:15:ARG:HH12	1:B:4:ALA:HB1	1.68	0.58
1:B:148:ARG:NH2	1:B:191:ALA:H	2.00	0.58
1:B:6:ILE:O	1:B:10:ILE:HG13	2.04	0.58
1:C:184:THR:HG22	1:C:185:TYR:N	2.19	0.57
1:B:118:ARG:HG2	1:B:118:ARG:HH11	1.69	0.57
1:E:148:ARG:NH2	1:E:190:GLU:HB3	2.20	0.57
1:B:21:THR:HG23	1:B:25:ARG:O	2.04	0.57
1:D:187:CYS:SG	1:D:188:CYS:N	2.78	0.57
1:D:179:LYS:HG2	1:D:180:LYS:N	2.14	0.57
1:E:148:ARG:HH21	1:E:190:GLU:HB3	1.69	0.57
1:B:1:ALA:HB1	1:B:5:ASP:CB	2.34	0.57
1:B:10:ILE:O	1:B:14:SER:HB3	2.05	0.56
1:B:39:LEU:HD12	1:B:118:ARG:NE	2.19	0.56
1:A:50:VAL:CG1	1:A:51:VAL:N	2.69	0.56
1:A:192:TYR:CZ	2:A:301:CT4:H1A	2.41	0.56
1:B:39:LEU:O	1:B:41:VAL:HG23	2.06	0.56
1:B:99:THR:HG23	1:B:116:SER:HB3	1.87	0.56
1:B:35:PHE:N	3:B:324:HOH:O	2.37	0.56
1:A:58:TRP:CZ2	1:A:111:VAL:HG11	2.41	0.56
1:B:187:CYS:SG	1:B:188:CYS:N	2.79	0.55
1:D:9:ASN:O	1:D:13:THR:HG23	2.07	0.55
1:E:47:GLU:HB3	1:E:120[B]:ARG:HD3	1.89	0.55
1:B:78:ILE:HG23	1:B:101:GLN:O	2.06	0.55
1:C:173:ILE:CD1	1:C:199:LEU:HD11	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:HIS:CE1	1:C:148:ARG:HB2	2.42	0.55
1:D:38:ILE:HG13	1:D:165:PHE:CE1	2.43	0.54
1:B:88:ALA:HB3	1:B:91:ALA:HB2	1.90	0.54
1:E:34:LYS:HB2	1:E:53:TRP:HB2	1.89	0.54
1:E:139:LYS:HG2	1:E:196:GLU:HG2	1.89	0.54
1:B:45:THR:O	1:B:46:ASN:HB2	2.08	0.54
1:B:92:ILE:HD11	1:B:120:ARG:HG2	1.90	0.54
1:C:73:GLN:HB3	1:C:104:ARG:HH12	1.72	0.54
1:D:188:CYS:HB3	1:D:190:GLU:OE2	2.07	0.54
1:B:41:VAL:HG13	1:B:48:VAL:HG12	1.90	0.53
1:D:124:ASP:HB2	1:E:168:TYR:CE1	2.43	0.53
1:E:34:LYS:HE3	3:E:340:HOH:O	2.09	0.53
1:E:188:CYS:HB3	1:E:190:GLU:OE2	2.09	0.53
1:A:55:GLN:HA	1:A:114:MET:HG3	1.91	0.53
1:A:21:THR:HG23	1:A:25:ARG:O	2.08	0.52
1:C:157:GLU:O	1:C:157:GLU:HG3	2.08	0.52
1:A:41:VAL:HG22	1:A:48:VAL:HG12	1.91	0.52
1:E:178:GLN:HG2	1:E:197:VAL:HG13	1.92	0.52
3:A:314:HOH:O	1:E:94:LYS:HG2	2.08	0.52
1:E:92:ILE:HD11	1:E:120[B]:ARG:CD	2.38	0.52
1:E:162:SER:HB2	1:E:165:PHE:HB3	1.92	0.52
1:A:125:VAL:HG12	1:A:125:VAL:O	2.08	0.52
1:C:22:GLN:O	1:C:25:ARG:HG2	2.09	0.52
1:C:99:THR:HG23	1:C:116:SER:HB3	1.92	0.52
1:C:55:GLN:HG3	1:C:114:MET:HE3	1.92	0.51
1:D:8:TYR:N	1:D:8:TYR:CD1	2.78	0.51
1:B:18:VAL:HG23	1:C:7:LEU:HD23	1.91	0.51
1:C:39:LEU:HB2	1:C:49:ASP:HB3	1.92	0.51
1:A:15:ARG:NH1	1:B:4:ALA:HB1	2.25	0.51
1:E:152:VAL:HG21	1:E:194:ASP:HA	1.93	0.51
1:C:24:ASP:OD1	1:C:24:ASP:O	2.28	0.51
1:C:32:SER:HB3	1:C:55:GLN:HB3	1.94	0.50
1:C:184:THR:HG22	1:C:185:TYR:H	1.76	0.50
1:A:8:TYR:O	1:A:12:GLN:HG2	2.11	0.50
1:C:38:ILE:HG13	1:C:165:PHE:HE1	1.76	0.50
1:A:22:GLN:OE1	1:A:22:GLN:HA	2.12	0.50
1:A:39:LEU:HD13	1:A:118:ARG:CZ	2.42	0.50
1:E:174:LEU:HD11	1:E:202:ARG:HD3	1.94	0.49
1:D:152:VAL:O	1:D:180:LYS:HE3	2.12	0.49
1:A:184:THR:HG22	1:A:185:TYR:N	2.28	0.49
1:E:127:GLY:HA2	1:E:130:THR:HG23	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:GLN:NE2	1:E:61:ARG:HG3	2.14	0.49
1:D:205:GLY:C	1:D:207:SER:H	2.16	0.49
1:E:173:ILE:HD12	1:E:199:LEU:CD1	2.36	0.48
1:A:83:VAL:HG13	1:A:84:PRO:HD2	1.94	0.48
1:B:145:HIS:HB2	1:B:150:ILE:HD12	1.96	0.48
1:C:176:VAL:HA	1:C:198:SER:O	2.13	0.48
1:C:139:LYS:HG2	1:C:196:GLU:HG2	1.95	0.48
1:C:50:VAL:HG12	1:C:51:VAL:N	2.28	0.48
1:A:46:ASN:HB3	1:A:123:CYS:O	2.14	0.48
1:D:42:ASN:OD1	1:D:44:ILE:HB	2.14	0.48
1:A:137:ARG:HG3	1:A:137:ARG:HH11	1.79	0.47
1:C:21:THR:HG23	1:C:25:ARG:O	2.14	0.47
1:C:60:ASP:OD2	1:C:63:LEU:HG	2.14	0.47
1:D:34:LYS:HB2	1:D:53:TRP:HB2	1.96	0.47
1:C:19:ILE:HG23	1:C:19:ILE:O	2.15	0.47
1:C:22:GLN:NE2	1:C:61:ARG:HG3	2.19	0.47
1:D:206:ARG:H	1:D:206:ARG:HE	1.63	0.47
1:B:178:GLN:HG2	1:B:197:VAL:HG22	1.97	0.47
1:B:146:HIS:CE1	1:B:149:GLU:HG3	2.50	0.47
1:C:33:LEU:HD22	1:C:52:PHE:CD2	2.49	0.47
1:E:92:ILE:HD11	1:E:120[B]:ARG:HD2	1.95	0.47
1:E:55:GLN:HA	1:E:114:MET:HG3	1.96	0.47
1:D:201:PHE:N	1:D:201:PHE:CD1	2.83	0.46
1:E:22:GLN:HG2	1:E:25:ARG:HH12	1.78	0.46
1:E:57:THR:HG22	1:E:58:TRP:N	2.31	0.46
1:A:16:PRO:HA	1:A:82:TRP:HA	1.97	0.46
1:B:84:PRO:HB2	1:B:86:LEU:HG	1.97	0.46
1:D:152:VAL:HG21	1:D:194:ASP:HA	1.96	0.46
1:B:7:LEU:HB3	3:B:302:HOH:O	2.14	0.46
1:B:11:ARG:HG3	1:B:11:ARG:HH11	1.80	0.46
1:D:162:SER:HB3	1:D:173:ILE:HB	1.98	0.46
2:C:301:CT4:CL	1:D:112:LEU:O	2.70	0.46
1:C:7:LEU:HD11	1:C:11:ARG:CZ	2.46	0.46
1:A:16:PRO:HA	1:A:82:TRP:CA	2.46	0.46
1:D:145:HIS:HB2	1:D:150:ILE:HD12	1.97	0.46
1:B:124:ASP:HB2	1:C:168:TYR:CE1	2.51	0.46
1:C:145:HIS:HB2	1:C:150:ILE:HD12	1.98	0.46
1:E:153:ASP:OD2	1:E:180:LYS:HD2	2.15	0.46
1:A:30:SER:HB2	1:A:57:THR:HB	1.97	0.46
1:B:158:ASN:HB2	3:B:326:HOH:O	2.16	0.46
1:D:88:ALA:HB1	1:D:121:PHE:HE1	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ASP:O	1:B:6:ILE:HG13	2.16	0.45
1:D:146:HIS:CD2	1:D:190:GLU:HG3	2.51	0.45
1:B:33:LEU:HD11	1:B:140:ILE:HD11	1.97	0.45
1:A:112:LEU:O	2:E:301:CT4:CL	2.72	0.45
1:D:88:ALA:HA	1:D:139:LYS:O	2.16	0.45
1:D:29:VAL:O	1:D:152:VAL:HA	2.17	0.45
1:B:59:SER:HB2	1:B:110:GLU:OE2	2.16	0.45
1:A:158:ASN:N	1:A:158:ASN:HD22	2.15	0.45
1:E:38:ILE:HG13	1:E:165:PHE:HE1	1.82	0.45
1:E:187:CYS:SG	1:E:188:CYS:N	2.90	0.44
1:E:55:GLN:HG3	1:E:114:MET:HE2	1.98	0.44
1:B:38:ILE:HD11	1:B:199:LEU:HD21	1.99	0.44
1:D:112:LEU:HD12	1:D:113:TYR:N	2.32	0.44
1:D:134:ALA:O	1:D:200:ASN:HA	2.18	0.44
1:D:165:PHE:CE1	1:D:173:ILE:HD11	2.52	0.44
1:A:29:VAL:HA	1:A:57:THR:O	2.16	0.44
1:C:6:ILE:O	1:C:10:ILE:HG12	2.17	0.44
1:C:29:VAL:O	1:C:152:VAL:HA	2.18	0.44
1:C:149:GLU:CD	1:D:104:ARG:HH22	2.20	0.44
1:D:181:ASN:HB2	1:D:194:ASP:OD1	2.17	0.44
2:D:301:CT4:CL	1:E:112:LEU:O	2.72	0.44
1:E:125:VAL:HG12	1:E:125:VAL:O	2.17	0.44
1:B:189:PRO:HD2	1:B:190:GLU:OE2	2.18	0.44
1:D:187:CYS:HB3	2:D:301:CT4:O1	2.17	0.44
1:E:51:VAL:HG22	1:E:118:ARG:HG3	1.99	0.44
1:E:155:THR:O	1:E:157:GLU:HG2	2.17	0.44
1:A:94:LYS:N	1:B:98:LEU:HD22	2.33	0.44
1:A:133:GLY:HA3	1:A:202:ARG:HB3	2.00	0.44
1:B:1:ALA:HB1	1:B:5:ASP:OD2	2.17	0.44
1:C:39:LEU:O	1:C:41:VAL:HG23	2.17	0.44
1:A:88:ALA:HB3	1:A:91:ALA:HB2	1.99	0.44
1:B:55:GLN:HG3	1:B:114:MET:HE3	2.00	0.43
1:B:54:GLN:O	1:B:115:PRO:HD2	2.18	0.43
1:C:46:ASN:HB3	1:C:123:CYS:O	2.18	0.43
1:D:33:LEU:HD11	1:D:140:ILE:CD1	2.49	0.43
1:E:1:ALA:HB1	1:E:5:ASP:HB2	1.99	0.43
1:A:203:LYS:HD3	3:A:339:HOH:O	2.18	0.43
1:C:183:VAL:HG23	1:C:194:ASP:OD2	2.19	0.43
1:D:33:LEU:HD11	1:D:140:ILE:HD12	2.00	0.43
1:E:43:GLU:HG3	1:E:125:VAL:HG12	1.99	0.43
1:E:160:ASP:O	1:E:163:GLU:HB2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:PHE:CD1	1:D:171:PHE:N	2.87	0.43
1:A:164:TYR:CZ	1:E:185:TYR:HD2	2.37	0.43
1:B:165:PHE:CE1	1:B:173:ILE:HD11	2.54	0.43
1:C:38:ILE:HG13	1:C:165:PHE:CE1	2.53	0.43
1:C:83:VAL:HG13	1:C:84:PRO:HD2	2.01	0.43
1:D:38:ILE:HG13	1:D:165:PHE:HE1	1.81	0.43
1:A:206:ARG:HH11	1:A:206:ARG:HG2	1.84	0.43
1:C:162:SER:HB3	1:C:173:ILE:HB	2.01	0.43
1:A:158:ASN:H	1:A:158:ASN:ND2	2.16	0.43
1:D:94:LYS:HB2	1:D:94:LYS:NZ	2.34	0.43
1:B:47:GLU:OE2	1:C:39:LEU:HD22	2.19	0.42
1:B:118:ARG:HG2	1:B:118:ARG:NH1	2.32	0.42
1:E:84:PRO:HB2	1:E:86:LEU:HG	2.00	0.42
1:C:155:THR:C	1:C:157:GLU:H	2.23	0.42
1:B:148:ARG:HH22	1:B:191:ALA:H	1.66	0.42
1:D:155:THR:C	1:D:157:GLU:H	2.23	0.42
1:E:134:ALA:O	1:E:200:ASN:HA	2.19	0.42
1:B:39:LEU:HB2	1:B:49:ASP:HB3	2.01	0.42
1:B:129:ASP:OD1	1:B:206:ARG:HD2	2.19	0.42
1:C:164:TYR:HB2	3:C:317:HOH:O	2.19	0.42
1:D:13:THR:OG1	1:D:63:LEU:HD23	2.20	0.42
1:B:22:GLN:O	1:B:23:ARG:C	2.57	0.42
1:C:73:GLN:HB3	1:C:104:ARG:NH1	2.35	0.42
1:C:152:VAL:HG21	1:C:194:ASP:HA	2.02	0.42
1:A:50:VAL:HG12	1:A:51:VAL:H	1.84	0.42
1:B:18:VAL:CG2	1:C:7:LEU:HD23	2.50	0.42
1:C:54:GLN:O	1:C:114:MET:HA	2.20	0.42
1:C:146:HIS:HE1	1:C:148:ARG:HB2	1.84	0.42
1:C:176:VAL:HG22	1:C:199:LEU:HD12	2.02	0.41
1:E:142:SER:OG	1:E:145:HIS:HB2	2.20	0.41
1:A:39:LEU:CD1	1:A:118:ARG:CZ	2.98	0.41
1:A:42:ASN:HB3	1:A:45:THR:OG1	2.21	0.41
1:D:55:GLN:HB2	1:D:114:MET:HE3	2.00	0.41
1:D:170:ARG:HB2	1:D:171:PHE:CE1	2.54	0.41
1:A:125:VAL:O	1:A:125:VAL:CG1	2.68	0.41
1:C:2:ASP:O	1:C:6:ILE:HG12	2.20	0.41
1:C:139:LYS:HG2	1:C:196:GLU:CG	2.51	0.41
1:B:30:SER:HB3	1:B:155:THR:OG1	2.20	0.41
1:C:76:VAL:HA	1:C:77:PRO:HD3	1.92	0.41
1:D:47:GLU:OE2	1:E:39:LEU:HD23	2.20	0.41
1:D:94:LYS:NZ	1:D:94:LYS:CB	2.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:PRO:O	1:B:156:THR:N	2.53	0.41
1:B:154:PRO:HB2	1:B:178:GLN:HE21	1.85	0.41
1:B:180:LYS:O	1:B:181:ASN:ND2	2.53	0.41
1:A:158:ASN:N	1:A:158:ASN:ND2	2.69	0.41
1:D:206:ARG:HE	1:D:206:ARG:N	2.19	0.41
1:D:125:VAL:O	1:D:125:VAL:HG12	2.21	0.41
1:D:94:LYS:H	1:D:94:LYS:HG2	1.70	0.41
1:C:35:PHE:CD1	1:C:50:VAL:HG11	2.56	0.41
1:C:171:PHE:CD1	1:C:171:PHE:N	2.89	0.41
1:D:75:SER:HA	1:D:103:ALA:O	2.21	0.41
1:E:60:ASP:HB3	1:E:63:LEU:HD12	2.03	0.41
1:E:146:HIS:CE1	1:E:149:GLU:HG3	2.56	0.41
1:A:178:GLN:HG2	1:A:197:VAL:HG13	2.03	0.40
1:A:104:ARG:HH22	1:E:149:GLU:CD	2.24	0.40
1:D:37:ASN:HB2	3:D:322:HOH:O	2.22	0.40
1:A:157:GLU:O	1:A:159:SER:N	2.54	0.40
1:B:179:LYS:HE3	1:B:181:ASN:ND2	2.37	0.40
1:B:181:ASN:HD22	1:B:181:ASN:HA	1.62	0.40
1:E:22:GLN:CG	1:E:25:ARG:HH12	2.34	0.40
1:A:18:VAL:HG22	1:B:7:LEU:HD13	2.04	0.40
1:A:97:VAL:HG13	1:A:115:PRO:HB2	2.02	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	206/214 (96%)	196 (95%)	7 (3%)	3 (2%)	10	26
1	B	206/214 (96%)	190 (92%)	14 (7%)	2 (1%)	15	37
1	C	206/214 (96%)	185 (90%)	17 (8%)	4 (2%)	8	20
1	D	206/214 (96%)	188 (91%)	13 (6%)	5 (2%)	6	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	207/214 (97%)	195 (94%)	9 (4%)	3 (1%)	11	28
All	All	1031/1070 (96%)	954 (92%)	60 (6%)	17 (2%)	9	24

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	E	40	GLU
1	B	24	ASP
1	D	24	ASP
1	E	156	THR
1	D	186	SER
1	E	158	ASN
1	A	156	THR
1	B	23	ARG
1	C	155	THR
1	C	156	THR
1	C	157	GLU
1	D	40	GLU
1	C	147	SER
1	A	206	ARG
1	D	147	SER
1	D	206	ARG

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	192/197 (98%)	181 (94%)	11 (6%)	20	44
1	B	193/197 (98%)	186 (96%)	7 (4%)	35	64
1	C	193/197 (98%)	187 (97%)	6 (3%)	40	69
1	D	192/197 (98%)	183 (95%)	9 (5%)	26	54
1	E	193/197 (98%)	185 (96%)	8 (4%)	30	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	963/985 (98%)	922 (96%)	41 (4%)	29 57

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	7	LEU
1	A	13	THR
1	A	24	ASP
1	A	94	LYS
1	A	131	GLU
1	A	132	SER
1	A	181	ASN
1	A	188	CYS
1	A	190	GLU
1	A	206	ARG
1	B	49	ASP
1	B	57	THR
1	B	72	ASP
1	B	118	ARG
1	B	181	ASN
1	B	194	ASP
1	B	200	ASN
1	C	13	THR
1	C	24	ASP
1	C	129	ASP
1	C	158	ASN
1	C	188	CYS
1	C	198	SER
1	D	13	THR
1	D	40	GLU
1	D	56	THR
1	D	72	ASP
1	D	73	GLN
1	D	94	LYS
1	D	190	GLU
1	D	200	ASN
1	D	206	ARG
1	E	23	ARG
1	E	24	ASP
1	E	25	ARG
1	E	94	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	155	THR
1	E	194	ASP
1	E	200	ASN
1	E	206	ARG

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

Mol	Chain	Res	Type
1	A	145	HIS
1	A	158	ASN
1	A	181	ASN
1	A	200	ASN
1	B	178	GLN
1	B	181	ASN
1	B	200	ASN
1	C	22	GLN
1	C	158	ASN
1	C	181	ASN
1	D	12	GLN
1	D	55	GLN
1	D	119	GLN
1	D	158	ASN
1	D	178	GLN
1	D	181	ASN
1	D	200	ASN
1	E	9	ASN
1	E	22	GLN
1	E	55	GLN
1	E	158	ASN
1	E	200	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](#)

5 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	CT4	E	301	-	9,15,15	1.75	2 (22%)	5,19,19	5.24	3 (60%)
2	CT4	C	301	-	9,15,15	1.75	3 (33%)	5,19,19	5.60	3 (60%)
2	CT4	D	301	-	9,15,15	1.70	3 (33%)	5,19,19	5.77	3 (60%)
2	CT4	A	301	-	9,15,15	1.53	3 (33%)	5,19,19	5.76	3 (60%)
2	CT4	B	301	-	9,15,15	1.58	2 (22%)	5,19,19	6.18	3 (60%)

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	CT4	E	301	-	-	0/7/11/11	0/1/1/1
2	CT4	C	301	-	-	0/7/11/11	0/1/1/1
2	CT4	D	301	-	-	0/7/11/11	0/1/1/1
2	CT4	A	301	-	-	0/7/11/11	0/1/1/1
2	CT4	B	301	-	-	0/7/11/11	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	CT4	C-N2	-3.29	1.31	1.35
2	E	301	CT4	C-N1	2.95	1.39	1.33
2	C	301	CT4	C-N2	-2.92	1.32	1.35
2	C	301	CT4	C-N1	2.77	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CT4	C-N1	2.72	1.39	1.33
2	D	301	CT4	C-N1	2.69	1.39	1.33
2	D	301	CT4	C-N	2.61	1.39	1.34
2	B	301	CT4	C-N1	2.61	1.39	1.33
2	C	301	CT4	C1-C2	-2.49	1.48	1.51
2	D	301	CT4	C1-C2	-2.39	1.49	1.51
2	B	301	CT4	C-N	2.36	1.39	1.34
2	A	301	CT4	C-N	2.32	1.39	1.34
2	A	301	CT4	C-N2	-2.07	1.33	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	CT4	N-C-N1	-13.27	107.31	119.48
2	D	301	CT4	N-C-N1	-12.30	108.20	119.48
2	A	301	CT4	N-C-N1	-12.18	108.31	119.48
2	C	301	CT4	N-C-N1	-11.90	108.57	119.48
2	E	301	CT4	N-C-N1	-10.79	109.59	119.48
2	E	301	CT4	C3-N1-C	3.43	131.44	123.86
2	C	301	CT4	C3-N1-C	3.07	130.65	123.86
2	E	301	CT4	C5-C2-S	-3.01	109.01	112.00
2	A	301	CT4	C3-N1-C	2.94	130.35	123.86
2	D	301	CT4	C3-N1-C	2.86	130.18	123.86
2	A	301	CT4	C5-C2-S	-2.80	109.22	112.00
2	B	301	CT4	C5-C2-S	-2.71	109.30	112.00
2	B	301	CT4	C3-N1-C	2.68	129.79	123.86
2	D	301	CT4	C5-C2-S	-2.51	109.50	112.00
2	C	301	CT4	C5-C2-S	-2.39	109.62	112.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	CT4	1	0
2	C	301	CT4	1	0
2	D	301	CT4	2	0
2	A	301	CT4	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, 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	208/214 (97%)	-0.19	5 (2%) 59 60	16, 36, 79, 91	0
1	B	208/214 (97%)	-0.19	2 (0%) 82 83	21, 41, 70, 94	0
1	C	207/214 (96%)	-0.15	6 (2%) 51 52	18, 41, 78, 90	0
1	D	208/214 (97%)	-0.27	1 (0%) 91 92	16, 36, 68, 96	0
1	E	208/214 (97%)	-0.23	3 (1%) 75 77	16, 34, 70, 92	0
All	All	1039/1070 (97%)	-0.21	17 (1%) 72 74	16, 38, 75, 96	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	158	ASN	5.8
1	A	158	ASN	4.9
1	B	156	THR	3.9
1	E	156	THR	3.4
1	D	158	ASN	3.1
1	C	156	THR	3.1
1	C	157	GLU	2.7
1	B	158	ASN	2.6
1	C	207	SER	2.5
1	C	185	TYR	2.5
1	C	160	ASP	2.4
1	A	184	THR	2.4
1	A	207	SER	2.2
1	A	185	TYR	2.2
1	E	186	SER	2.2
1	A	159	SER	2.1
1	C	191	ALA	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, 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(Å ²)	Q<0.9
2	CT4	C	301	15/15	0.81	0.32	73,76,86,86	0
2	CT4	A	301	15/15	0.89	0.21	63,68,78,78	0
2	CT4	E	301	15/15	0.91	0.28	45,54,66,68	0
2	CT4	B	301	15/15	0.92	0.25	40,51,65,67	0
2	CT4	D	301	15/15	0.94	0.20	33,43,56,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.