



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2017 – 04:23 pm GMT

PDB ID : 4BPQ
Title : Structure and substrate induced conformational changes of the secondary citrate-sodium symporter CitS revealed by electron crystallography
Authors : Kebbel, F.; Kurz, M.; Arbeit, M.; Gruetter, M.G.; Stahlberg, H.
Deposited on : 2013-05-27
Resolution : 6.00 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29102

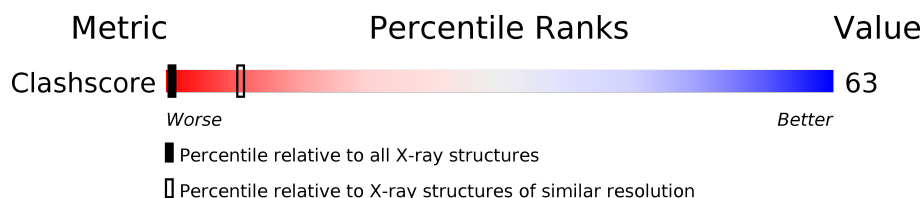
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 6.00 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))
Clashscore	112137	1017 (8.20-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	318	 66% 26% • •
1	B	318	 67% 29% •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3110 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 CITRATE\;SODIUM SYMPORTER.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	0	0	0
			1520	912	304	304			
1	B	318	Total	C	N	O	0	0	0
			1590	954	318	318			

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 6.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-6.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	2DX	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3110	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	22
1	B	4	24
All	All	8	46

There are no bond length outliers.

There are no bond angle outliers.

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	278	UNK	CA
1	A	291	UNK	CA
1	A	341	UNK	CA
1	A	382	UNK	CA
1	B	276	UNK	CA
1	B	289	UNK	CA
1	B	339	UNK	CA
1	B	403	UNK	CA

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	UNK	Mainchain
1	A	107	UNK	Mainchain
1	A	135	UNK	Mainchain
1	A	136	UNK	Mainchain
1	A	171	UNK	Mainchain

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Mol	Chain	Res	Type	Group
1	A	172	UNK	Mainchain
1	A	207	UNK	Mainchain
1	A	208	UNK	Mainchain
1	A	250	UNK	Mainchain
1	A	251	UNK	Mainchain
1	A	281	UNK	Mainchain
1	A	282	UNK	Mainchain
1	A	311	UNK	Mainchain
1	A	312	UNK	Mainchain
1	A	356	UNK	Mainchain
1	A	357	UNK	Mainchain
1	A	402	UNK	Mainchain
1	A	404	UNK	Mainchain
1	A	46	UNK	Mainchain
1	A	47	UNK	Mainchain
1	A	8	UNK	Mainchain
1	A	9	UNK	Mainchain
1	B	104	UNK	Mainchain
1	B	105	UNK	Mainchain
1	B	133	UNK	Mainchain
1	B	134	UNK	Mainchain
1	B	169	UNK	Mainchain
1	B	170	UNK	Mainchain
1	B	205	UNK	Mainchain
1	B	206	UNK	Mainchain
1	B	248	UNK	Mainchain
1	B	249	UNK	Mainchain
1	B	279	UNK	Mainchain
1	B	280	UNK	Mainchain
1	B	309	UNK	Mainchain
1	B	310	UNK	Mainchain
1	B	354	UNK	Mainchain
1	B	355	UNK	Mainchain
1	B	377	UNK	Mainchain
1	B	378	UNK	Mainchain
1	B	423	UNK	Mainchain
1	B	425	UNK	Mainchain
1	B	46	UNK	Mainchain
1	B	47	UNK	Mainchain
1	B	8	UNK	Mainchain
1	B	9	UNK	Mainchain

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	1520	0	327	126	0
1	B	1590	0	342	135	0
All	All	3110	0	669	237	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 63.

All (237) 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:73:UNK:CB	1:B:417:UNK:HA	1.08	1.51
1:A:396:UNK:CA	1:B:72:UNK:CB	1.84	1.51
1:A:396:UNK:HA	1:B:72:UNK:CB	1.05	1.49
1:A:73:UNK:CB	1:B:417:UNK:CA	1.93	1.47
1:A:101:UNK:CB	1:A:257:UNK:C	1.95	1.44
1:B:99:UNK:CB	1:B:255:UNK:C	1.95	1.43
1:A:101:UNK:CA	1:A:257:UNK:O	1.74	1.35
1:B:99:UNK:CA	1:B:255:UNK:O	1.74	1.34
1:B:203:UNK:O	1:B:207:UNK:CB	1.77	1.33
1:A:133:UNK:O	1:A:137:UNK:CB	1.76	1.32
1:B:131:UNK:O	1:B:135:UNK:CB	1.76	1.32
1:A:205:UNK:O	1:A:209:UNK:CB	1.77	1.32
1:B:375:UNK:O	1:B:379:UNK:CB	1.83	1.26
1:B:352:UNK:O	1:B:356:UNK:CB	1.83	1.26
1:A:354:UNK:O	1:A:358:UNK:CB	1.83	1.24
1:A:309:UNK:O	1:A:313:UNK:CB	1.86	1.23
1:B:307:UNK:O	1:B:311:UNK:CB	1.86	1.22
1:A:134:UNK:O	1:A:138:UNK:CB	1.89	1.20
1:B:132:UNK:O	1:B:136:UNK:CB	1.89	1.19
1:B:44:UNK:O	1:B:48:UNK:CB	1.91	1.19
1:A:44:UNK:O	1:A:48:UNK:CB	1.91	1.17
1:B:216:UNK:CB	1:B:318:UNK:CB	2.22	1.17
1:A:218:UNK:CB	1:A:320:UNK:CB	2.22	1.16
1:A:113:UNK:HA	1:A:294:UNK:CB	1.76	1.16
1:A:208:UNK:N	1:A:306:UNK:CB	2.04	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:UNK:O	1:A:210:UNK:CB	1.95	1.14
1:B:111:UNK:HA	1:B:292:UNK:CB	1.76	1.14
1:B:204:UNK:O	1:B:208:UNK:CB	1.95	1.14
1:A:403:UNK:O	1:A:405:UNK:N	1.82	1.13
1:A:396:UNK:CB	1:B:72:UNK:CB	2.25	1.13
1:B:206:UNK:N	1:B:304:UNK:CB	2.04	1.12
1:B:424:UNK:O	1:B:426:UNK:N	1.82	1.12
1:A:6:UNK:O	1:A:10:UNK:CB	2.01	1.09
1:B:6:UNK:O	1:B:10:UNK:CB	2.01	1.08
1:A:208:UNK:C	1:A:309:UNK:CB	2.33	1.07
1:B:206:UNK:C	1:B:307:UNK:CB	2.33	1.06
1:A:101:UNK:CB	1:A:257:UNK:O	0.75	1.05
1:B:205:UNK:CB	1:B:304:UNK:CB	2.35	1.05
1:A:207:UNK:CB	1:A:306:UNK:CB	2.35	1.05
1:A:310:UNK:O	1:A:314:UNK:CB	2.05	1.05
1:B:99:UNK:CB	1:B:255:UNK:O	0.76	1.05
1:B:308:UNK:O	1:B:312:UNK:CB	2.05	1.04
1:A:104:UNK:O	1:A:108:UNK:CB	2.08	1.02
1:B:102:UNK:O	1:B:106:UNK:CB	2.08	1.01
1:B:376:UNK:O	1:B:380:UNK:CB	2.11	0.99
1:A:355:UNK:O	1:A:359:UNK:CB	2.11	0.99
1:B:353:UNK:O	1:B:357:UNK:CB	2.11	0.98
1:B:277:UNK:O	1:B:281:UNK:CB	2.12	0.97
1:A:279:UNK:O	1:A:283:UNK:CB	2.12	0.96
1:A:113:UNK:CA	1:A:294:UNK:CB	2.43	0.95
1:B:111:UNK:CA	1:B:292:UNK:CB	2.43	0.95
1:A:73:UNK:CB	1:B:417:UNK:CB	2.44	0.93
1:B:246:UNK:O	1:B:250:UNK:CB	2.17	0.93
1:A:80:UNK:CA	1:B:426:UNK:CB	2.47	0.93
1:A:248:UNK:O	1:A:252:UNK:CB	2.17	0.93
1:B:48:UNK:CB	1:B:378:UNK:CB	2.48	0.92
1:A:48:UNK:CB	1:A:357:UNK:CB	2.48	0.92
1:A:80:UNK:CB	1:B:426:UNK:CB	2.49	0.90
1:B:55:UNK:CB	1:B:360:UNK:CB	2.49	0.90
1:A:218:UNK:C	1:A:320:UNK:CB	2.51	0.89
1:B:216:UNK:C	1:B:318:UNK:CB	2.51	0.88
1:B:45:UNK:O	1:B:49:UNK:CB	2.21	0.88
1:A:45:UNK:O	1:A:49:UNK:CB	2.21	0.87
1:A:396:UNK:CB	1:B:72:UNK:N	2.37	0.87
1:A:216:UNK:HA	1:A:351:UNK:C	2.06	0.86
1:B:214:UNK:HA	1:B:372:UNK:C	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:UNK:HA	1:A:351:UNK:CA	2.06	0.85
1:A:216:UNK:HA	1:A:351:UNK:O	1.77	0.85
1:B:214:UNK:HA	1:B:372:UNK:CA	2.07	0.84
1:B:214:UNK:HA	1:B:372:UNK:O	1.77	0.84
1:A:80:UNK:HA	1:B:426:UNK:CB	2.09	0.82
1:B:202:UNK:O	1:B:304:UNK:CB	2.28	0.81
1:A:204:UNK:O	1:A:306:UNK:CB	2.28	0.80
1:A:113:UNK:CB	1:A:294:UNK:CB	2.61	0.79
1:A:403:UNK:O	1:A:404:UNK:C	2.31	0.79
1:B:111:UNK:CB	1:B:292:UNK:CB	2.61	0.79
1:A:73:UNK:N	1:B:417:UNK:CB	2.47	0.78
1:A:7:UNK:O	1:A:11:UNK:CB	2.33	0.77
1:B:7:UNK:O	1:B:11:UNK:CB	2.33	0.77
1:B:424:UNK:O	1:B:425:UNK:C	2.31	0.77
1:A:396:UNK:CB	1:B:72:UNK:CA	2.63	0.75
1:A:133:UNK:C	1:A:137:UNK:CB	2.66	0.74
1:B:131:UNK:C	1:B:135:UNK:CB	2.66	0.72
1:A:405:UNK:CB	1:B:79:UNK:CA	2.68	0.70
1:B:422:UNK:C	1:B:424:UNK:H2	2.05	0.69
1:B:103:UNK:O	1:B:107:UNK:CB	2.41	0.69
1:B:424:UNK:C	1:B:426:UNK:N	2.56	0.69
1:A:401:UNK:C	1:A:403:UNK:H2	2.05	0.68
1:A:105:UNK:O	1:A:109:UNK:CB	2.41	0.68
1:A:403:UNK:O	1:A:406:UNK:N	2.27	0.68
1:B:203:UNK:C	1:B:207:UNK:CB	2.69	0.68
1:B:424:UNK:O	1:B:427:UNK:N	2.27	0.68
1:A:205:UNK:C	1:A:209:UNK:CB	2.69	0.67
1:B:307:UNK:O	1:B:311:UNK:N	2.27	0.67
1:A:309:UNK:O	1:A:313:UNK:CA	2.43	0.67
1:A:309:UNK:O	1:A:313:UNK:N	2.27	0.67
1:A:405:UNK:CB	1:B:79:UNK:CB	2.73	0.67
1:B:307:UNK:O	1:B:311:UNK:CA	2.43	0.67
1:A:101:UNK:HA	1:A:257:UNK:O	1.91	0.66
1:A:52:UNK:CB	1:A:353:UNK:CB	2.74	0.66
1:B:131:UNK:O	1:B:135:UNK:CA	2.44	0.66
1:B:52:UNK:CB	1:B:374:UNK:CB	2.74	0.66
1:A:216:UNK:HA	1:A:351:UNK:HA	1.78	0.66
1:A:403:UNK:C	1:A:405:UNK:N	2.56	0.65
1:B:278:UNK:O	1:B:282:UNK:CB	2.45	0.65
1:B:218:UNK:N	1:B:372:UNK:CB	2.59	0.65
1:A:280:UNK:O	1:A:284:UNK:CB	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:UNK:CA	1:A:351:UNK:O	2.44	0.64
1:B:203:UNK:O	1:B:207:UNK:CA	2.45	0.64
1:A:133:UNK:O	1:A:137:UNK:CA	2.44	0.64
1:B:214:UNK:CA	1:B:372:UNK:O	2.44	0.64
1:A:220:UNK:N	1:A:351:UNK:CB	2.59	0.64
1:A:80:UNK:C	1:B:426:UNK:CB	2.76	0.64
1:A:212:UNK:HA	1:A:313:UNK:CB	2.27	0.64
1:B:210:UNK:HA	1:B:311:UNK:CB	2.27	0.64
1:B:134:UNK:O	1:B:135:UNK:C	2.46	0.63
1:B:214:UNK:HA	1:B:372:UNK:HA	1.78	0.63
1:A:205:UNK:O	1:A:209:UNK:CA	2.46	0.63
1:A:136:UNK:O	1:A:137:UNK:C	2.46	0.62
1:A:216:UNK:CA	1:A:351:UNK:C	2.78	0.62
1:A:216:UNK:CB	1:A:351:UNK:O	2.48	0.62
1:B:214:UNK:CB	1:B:372:UNK:O	2.48	0.62
1:A:103:UNK:N	1:A:260:UNK:CB	2.63	0.61
1:B:214:UNK:CA	1:B:372:UNK:C	2.78	0.61
1:A:208:UNK:O	1:A:209:UNK:C	2.48	0.61
1:A:309:UNK:C	1:A:313:UNK:CB	2.76	0.61
1:B:206:UNK:O	1:B:207:UNK:C	2.48	0.61
1:A:208:UNK:CA	1:A:309:UNK:CB	2.79	0.61
1:A:405:UNK:CB	1:B:79:UNK:HA	2.29	0.61
1:B:247:UNK:O	1:B:251:UNK:CB	2.49	0.61
1:A:396:UNK:CA	1:B:72:UNK:CA	2.74	0.61
1:B:101:UNK:N	1:B:258:UNK:CB	2.63	0.60
1:B:206:UNK:CA	1:B:307:UNK:CB	2.79	0.60
1:A:249:UNK:O	1:A:253:UNK:CB	2.49	0.60
1:A:208:UNK:O	1:A:309:UNK:CB	2.51	0.59
1:A:211:UNK:CB	1:A:310:UNK:HA	2.33	0.59
1:B:167:UNK:O	1:B:171:UNK:CB	2.50	0.59
1:B:99:UNK:HA	1:B:255:UNK:O	1.91	0.59
1:B:307:UNK:C	1:B:311:UNK:CB	2.76	0.58
1:B:209:UNK:CB	1:B:308:UNK:HA	2.33	0.58
1:A:169:UNK:O	1:A:173:UNK:CB	2.51	0.58
1:B:217:UNK:N	1:B:372:UNK:CB	2.67	0.58
1:B:206:UNK:O	1:B:307:UNK:CB	2.51	0.57
1:A:215:UNK:HA	1:A:317:UNK:HA	1.87	0.57
1:A:219:UNK:N	1:A:351:UNK:CB	2.67	0.57
1:A:354:UNK:O	1:A:358:UNK:CA	2.52	0.56
1:B:213:UNK:HA	1:B:315:UNK:HA	1.86	0.56
1:A:73:UNK:CA	1:B:417:UNK:CB	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:UNK:O	1:B:356:UNK:CA	2.52	0.55
1:A:405:UNK:CB	1:B:79:UNK:O	2.55	0.55
1:B:217:UNK:CA	1:B:372:UNK:CB	2.82	0.55
1:B:355:UNK:O	1:B:356:UNK:C	2.53	0.55
1:B:6:UNK:O	1:B:10:UNK:N	2.40	0.55
1:A:104:UNK:O	1:A:108:UNK:N	2.40	0.55
1:B:58:UNK:O	1:B:361:UNK:O	2.24	0.55
1:A:80:UNK:O	1:B:426:UNK:CB	2.54	0.55
1:A:6:UNK:O	1:A:10:UNK:N	2.40	0.55
1:B:102:UNK:O	1:B:106:UNK:N	2.40	0.55
1:B:277:UNK:O	1:B:281:UNK:N	2.40	0.55
1:B:375:UNK:O	1:B:379:UNK:CA	2.52	0.54
1:A:219:UNK:CA	1:A:351:UNK:CB	2.82	0.54
1:A:44:UNK:O	1:A:48:UNK:N	2.40	0.54
1:B:213:UNK:HA	1:B:315:UNK:CA	2.38	0.54
1:A:248:UNK:O	1:A:252:UNK:N	2.41	0.54
1:A:279:UNK:O	1:A:283:UNK:N	2.40	0.54
1:B:44:UNK:O	1:B:48:UNK:N	2.40	0.54
1:A:357:UNK:O	1:A:358:UNK:C	2.53	0.53
1:A:364:UNK:C	1:A:383:UNK:O	2.56	0.53
1:B:378:UNK:O	1:B:379:UNK:C	2.53	0.53
1:A:354:UNK:O	1:A:358:UNK:N	2.42	0.53
1:B:246:UNK:O	1:B:250:UNK:N	2.41	0.53
1:A:215:UNK:HA	1:A:317:UNK:CA	2.38	0.53
1:B:375:UNK:O	1:B:379:UNK:N	2.42	0.53
1:B:385:UNK:C	1:B:404:UNK:O	2.56	0.53
1:B:352:UNK:O	1:B:356:UNK:N	2.42	0.52
1:A:405:UNK:CB	1:B:79:UNK:C	2.87	0.52
1:B:55:UNK:CA	1:B:360:UNK:CB	2.87	0.52
1:A:218:UNK:CA	1:A:320:UNK:CB	2.88	0.51
1:A:47:UNK:O	1:A:48:UNK:C	2.56	0.51
1:A:401:UNK:C	1:A:403:UNK:N	2.68	0.50
1:B:47:UNK:O	1:B:48:UNK:C	2.56	0.50
1:B:216:UNK:CA	1:B:318:UNK:CB	2.88	0.50
1:A:7:UNK:O	1:A:11:UNK:N	2.45	0.50
1:B:7:UNK:O	1:B:11:UNK:N	2.45	0.50
1:A:105:UNK:O	1:A:109:UNK:N	2.45	0.49
1:B:9:UNK:O	1:B:10:UNK:C	2.59	0.49
1:B:103:UNK:O	1:B:107:UNK:N	2.45	0.49
1:A:9:UNK:O	1:A:10:UNK:C	2.59	0.49
1:B:247:UNK:O	1:B:251:UNK:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:UNK:O	1:B:282:UNK:N	2.45	0.49
1:B:352:UNK:C	1:B:356:UNK:CB	2.82	0.49
1:A:280:UNK:O	1:A:284:UNK:N	2.45	0.49
1:A:107:UNK:O	1:A:108:UNK:C	2.61	0.49
1:A:274:UNK:CB	1:B:164:UNK:H2	2.26	0.49
1:A:45:UNK:O	1:A:49:UNK:N	2.46	0.48
1:B:105:UNK:O	1:B:106:UNK:C	2.61	0.48
1:B:45:UNK:O	1:B:49:UNK:N	2.46	0.48
1:A:249:UNK:O	1:A:253:UNK:N	2.46	0.48
1:B:310:UNK:O	1:B:311:UNK:C	2.61	0.48
1:B:280:UNK:O	1:B:281:UNK:C	2.62	0.48
1:A:44:UNK:O	1:A:48:UNK:CA	2.58	0.47
1:B:167:UNK:O	1:B:171:UNK:N	2.47	0.47
1:B:203:UNK:O	1:B:207:UNK:N	2.47	0.47
1:A:362:UNK:O	1:A:385:UNK:C	2.60	0.47
1:B:44:UNK:O	1:B:48:UNK:CA	2.58	0.47
1:A:169:UNK:O	1:A:173:UNK:N	2.47	0.47
1:B:249:UNK:O	1:B:250:UNK:C	2.63	0.47
1:B:353:UNK:O	1:B:357:UNK:N	2.48	0.47
1:B:376:UNK:O	1:B:380:UNK:N	2.48	0.47
1:A:205:UNK:O	1:A:209:UNK:N	2.47	0.47
1:A:355:UNK:O	1:A:359:UNK:N	2.48	0.47
1:A:251:UNK:O	1:A:252:UNK:C	2.63	0.47
1:A:282:UNK:O	1:A:283:UNK:C	2.62	0.47
1:A:312:UNK:O	1:A:313:UNK:C	2.61	0.47
1:B:375:UNK:C	1:B:379:UNK:CB	2.82	0.47
1:A:354:UNK:C	1:A:358:UNK:CB	2.82	0.46
1:B:422:UNK:C	1:B:424:UNK:N	2.68	0.46
1:B:58:UNK:C	1:B:361:UNK:O	2.64	0.46
1:B:383:UNK:O	1:B:406:UNK:C	2.60	0.46
1:A:73:UNK:CA	1:B:417:UNK:CA	2.84	0.44
1:A:133:UNK:O	1:A:137:UNK:N	2.50	0.44
1:B:131:UNK:O	1:B:135:UNK:N	2.50	0.44
1:A:212:UNK:CA	1:A:313:UNK:CB	2.96	0.43
1:A:403:UNK:O	1:A:405:UNK:CA	2.64	0.43
1:B:206:UNK:CB	1:B:307:UNK:CB	2.96	0.43
1:A:170:UNK:O	1:A:174:UNK:N	2.52	0.43
1:A:208:UNK:CB	1:A:309:UNK:CB	2.96	0.43
1:B:168:UNK:O	1:B:172:UNK:N	2.51	0.43
1:B:204:UNK:O	1:B:208:UNK:N	2.53	0.42
1:B:210:UNK:CA	1:B:311:UNK:CB	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:UNK:O	1:A:210:UNK:N	2.53	0.42
1:B:308:UNK:O	1:B:312:UNK:N	2.53	0.42
1:A:310:UNK:O	1:A:314:UNK:N	2.53	0.41
1:B:424:UNK:O	1:B:426:UNK:CA	2.64	0.41
1:A:73:UNK:CB	1:B:417:UNK:C	2.88	0.41
1:A:401:UNK:O	1:A:403:UNK:N	2.54	0.40
1:A:172:UNK:O	1:A:173:UNK:C	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

There are no ligands in this entry.

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.