



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 10:28 pm BST

PDB ID : 1ADJ
Title : HISTIDYL-TRNA SYNTHETASE IN COMPLEX WITH HISTIDINE
Authors : Cusack, S.; Aberg, A.
Deposited on : 1997-02-18
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)
Xtrriage (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

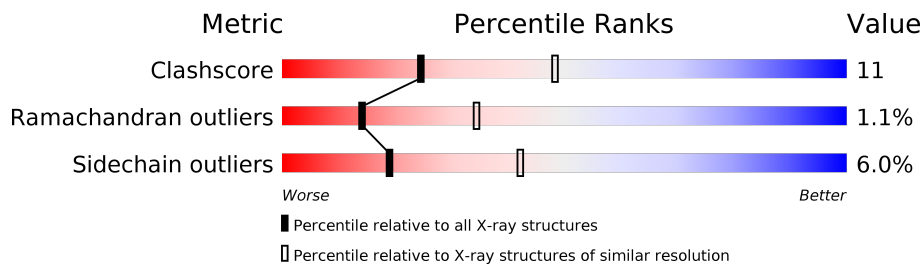
1 Overall quality at a glance

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	421	
1	B	421	
1	C	421	
1	D	421	

2 Entry composition [i](#)

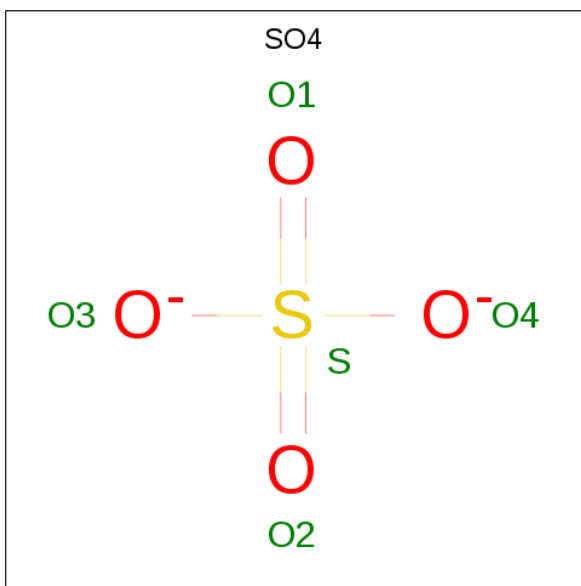
There are 4 unique types of molecules in this entry. The entry contains 13538 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HISTIDYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	420	Total 3309	C 2092	N 598	O 610	S 9	0	0	0
1	B	420	Total 3309	C 2092	N 598	O 610	S 9	0	0	0
1	C	420	Total 3309	C 2092	N 598	O 610	S 9	0	0	0
1	D	420	Total 3309	C 2092	N 598	O 610	S 9	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



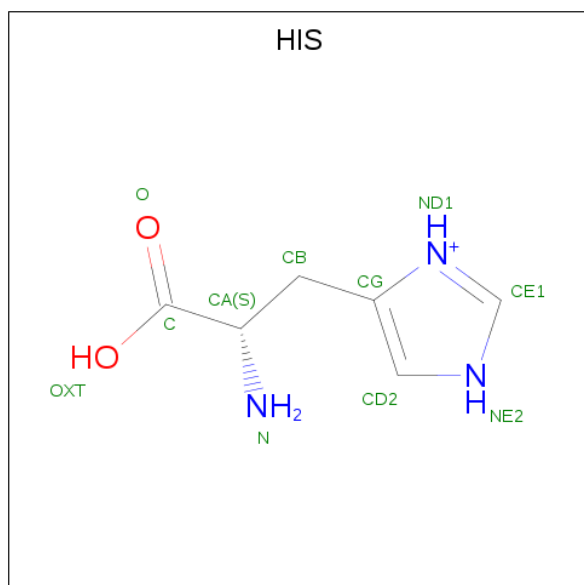
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is HISTIDINE (three-letter code: HIS) (formula: C₆H₁₀N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	6	3	2		
3	B	1	Total	C	N	O	0	0
			11	6	3	2		
3	C	1	Total	C	N	O	0	0
			11	6	3	2		
3	D	1	Total	C	N	O	0	0
			11	6	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	67	Total	O	0	0
			67	67		
4	B	91	Total	O	0	0
			91	91		
4	C	40	Total	O	0	0
			40	40		

Continued on next page...

Continued from previous page...

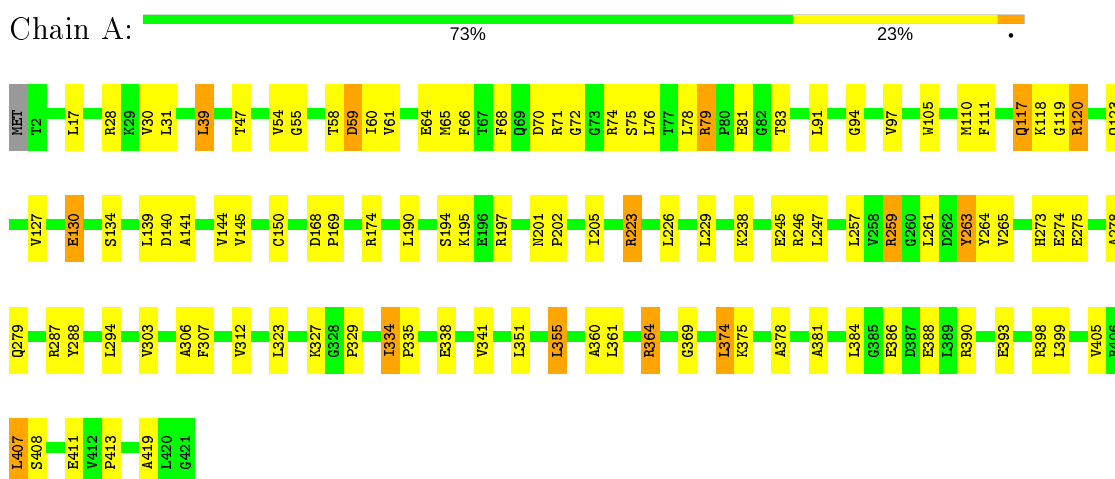
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	40	Total	O	0	0
			40	40		

3 Residue-property plots [i](#)

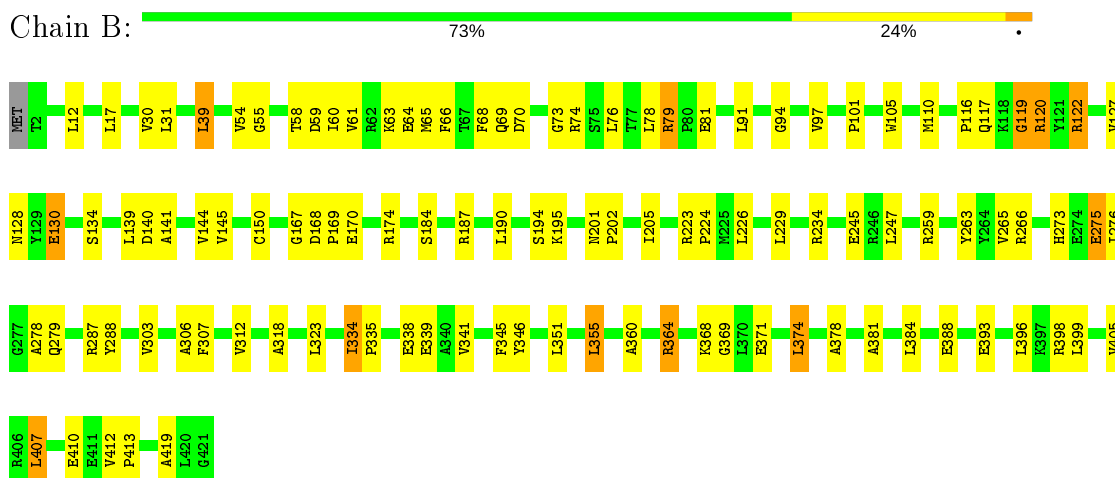
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

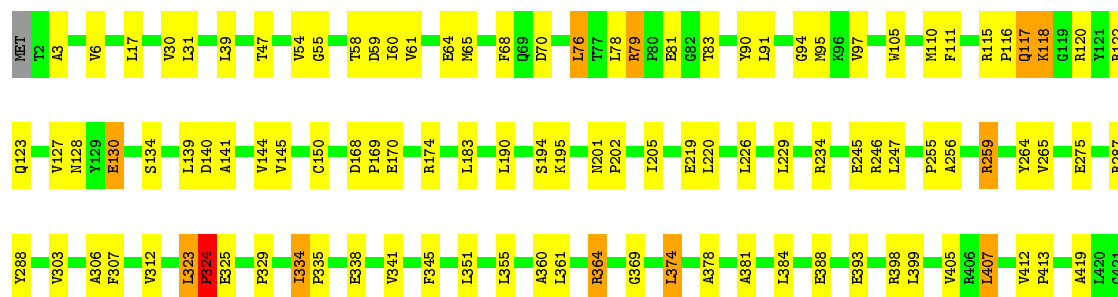


- Molecule 1: HISTIDYL-TRNA SYNTHETASE



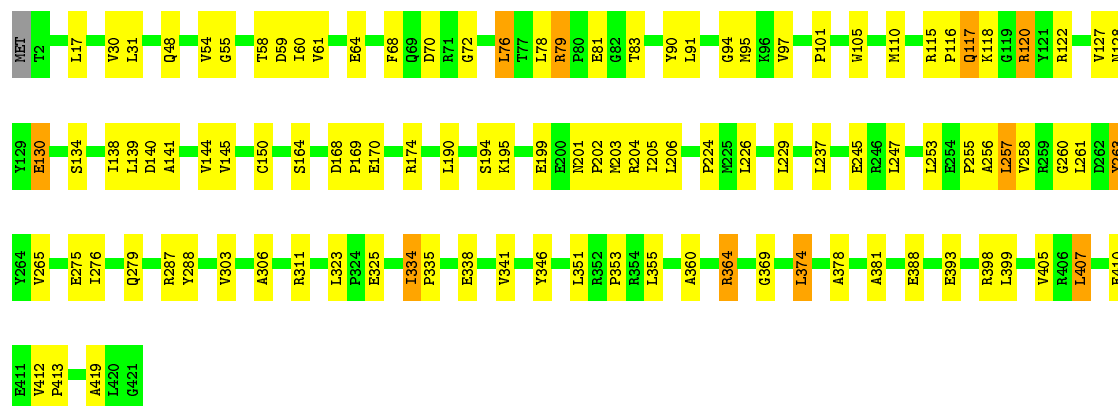
- Molecule 1: HISTIDYL-TRNA SYNTHETASE





- Molecule 1: HISTIDYL-TRNA SYNTHETASE

Chain D: 74% 23%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	171.30Å 214.70Å 49.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	99.0 (20.00-2.70)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.217 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13538	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

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: SO4

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	0.36	0/3371	0.62	1/4543 (0.0%)
1	B	0.37	0/3371	0.61	1/4543 (0.0%)
1	C	0.36	0/3371	0.62	0/4543
1	D	0.36	0/3371	0.61	0/4543
All	All	0.36	0/13484	0.61	2/18172 (0.0%)

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	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	39	LEU	CA-CB-CG	5.23	127.32	115.30
1	B	39	LEU	CA-CB-CG	5.13	127.09	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	324	PRO	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	3309	0	3339	82	0
1	B	3309	0	3339	78	0
1	C	3309	0	3339	74	0
1	D	3309	0	3339	75	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	11	0	6	1	0
3	B	11	0	6	0	0
3	C	11	0	6	1	0
3	D	11	0	6	1	0
4	A	67	0	0	6	0
4	B	91	0	0	6	0
4	C	40	0	0	5	0
4	D	40	0	0	2	0
All	All	13538	0	13380	290	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 11.

All (290) 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:B:334:ILE:HD12	1:B:369:GLY:HA3	1.37	1.05
1:D:334:ILE:HD12	1:D:369:GLY:HA3	1.36	1.05
1:A:334:ILE:HD12	1:A:369:GLY:HA3	1.38	1.03
1:C:334:ILE:HD12	1:C:369:GLY:HA3	1.41	1.01
1:C:79:ARG:HD3	1:C:110:MET:SD	2.08	0.93
1:A:79:ARG:HD3	1:A:110:MET:SD	2.09	0.93
1:D:79:ARG:HD3	1:D:110:MET:SD	2.11	0.90
1:B:79:ARG:HD3	1:B:110:MET:SD	2.14	0.88
1:B:168:ASP:HA	1:B:265:VAL:HG23	1.58	0.84
1:C:226:LEU:HD12	1:C:255:PRO:HA	1.63	0.81
1:D:54:VAL:HG12	1:D:58:THR:HG21	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:VAL:HG12	1:C:58:THR:HG21	1.65	0.79
1:B:54:VAL:HG12	1:B:58:THR:HG21	1.65	0.77
1:A:190:LEU:HD22	1:A:205:ILE:HD11	1.67	0.77
1:A:54:VAL:HG12	1:A:58:THR:HG21	1.66	0.76
1:D:190:LEU:HD22	1:D:205:ILE:HD11	1.68	0.76
1:C:190:LEU:HD22	1:C:205:ILE:HD11	1.67	0.76
1:B:94:GLY:O	1:B:97:VAL:HG22	1.86	0.75
1:D:94:GLY:O	1:D:97:VAL:HG22	1.87	0.74
1:B:190:LEU:HD22	1:B:205:ILE:HD11	1.68	0.74
1:A:68:PHE:HB3	1:B:68:PHE:HB3	1.68	0.74
1:D:204:ARG:HH12	1:D:260:GLY:HA2	1.54	0.73
1:C:174:ARG:HD2	4:C:425:HOH:O	1.88	0.73
1:A:83:THR:HG1	3:A:423:HIS:N	1.86	0.72
1:A:47:THR:HB	4:A:488:HOH:O	1.90	0.71
1:C:141:ALA:O	1:C:145:VAL:HG23	1.91	0.70
1:C:83:THR:HG1	3:C:423:HIS:N	1.89	0.70
1:D:116:PRO:HB3	4:D:452:HOH:O	1.93	0.69
1:A:294:LEU:HD21	1:D:199:GLU:HG3	1.76	0.67
1:C:259:ARG:HG2	1:C:264:TYR:CE2	2.28	0.67
1:A:28:ARG:HD3	4:A:438:HOH:O	1.93	0.67
1:A:259:ARG:HG2	1:A:264:TYR:CE2	2.31	0.66
1:A:141:ALA:O	1:A:145:VAL:HG23	1.96	0.66
1:D:141:ALA:O	1:D:145:VAL:HG23	1.95	0.66
1:B:202:PRO:O	1:B:205:ILE:HG22	1.96	0.65
1:C:361:LEU:HD12	1:D:101:PRO:HD3	1.77	0.65
1:B:141:ALA:O	1:B:145:VAL:HG23	1.96	0.65
1:D:202:PRO:O	1:D:205:ILE:HG22	1.96	0.65
1:A:202:PRO:O	1:A:205:ILE:HG22	1.97	0.64
1:C:30:VAL:HG21	1:C:150:CYS:SG	2.38	0.64
1:C:202:PRO:O	1:C:205:ILE:HG22	1.97	0.63
1:A:30:VAL:HG21	1:A:150:CYS:SG	2.40	0.62
1:A:223:ARG:HB2	1:A:223:ARG:HH11	1.64	0.61
1:B:30:VAL:HG21	1:B:150:CYS:SG	2.41	0.61
1:D:30:VAL:HG21	1:D:150:CYS:SG	2.41	0.60
1:C:94:GLY:O	1:C:97:VAL:HG22	2.01	0.60
1:D:83:THR:HG1	3:D:423:HIS:N	1.99	0.60
1:C:405:VAL:HG12	1:C:407:LEU:HD22	1.84	0.60
1:A:361:LEU:HD12	1:B:101:PRO:HD3	1.85	0.59
1:B:55:GLY:O	1:B:58:THR:HG22	2.03	0.59
1:B:70:ASP:HB3	1:B:73:GLY:O	2.03	0.58
1:D:203:MET:O	1:D:258:VAL:HG21	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:PRO:HA	4:B:496:HOH:O	2.03	0.58
1:D:70:ASP:HB2	1:D:76:LEU:HD22	1.85	0.58
1:B:68:PHE:HE2	1:B:78:LEU:HD13	1.69	0.58
1:A:174:ARG:HD2	4:A:444:HOH:O	2.04	0.58
1:A:68:PHE:HE2	1:A:78:LEU:HD13	1.69	0.58
1:B:388:GLU:HB2	1:B:393:GLU:O	2.04	0.57
1:B:405:VAL:HG12	1:B:407:LEU:HD22	1.86	0.57
1:D:55:GLY:O	1:D:58:THR:HG22	2.05	0.57
1:A:388:GLU:HB2	1:A:393:GLU:O	2.05	0.57
1:C:388:GLU:HB2	1:C:393:GLU:O	2.04	0.57
1:A:55:GLY:O	1:A:58:THR:HG22	2.04	0.57
1:C:68:PHE:HE2	1:C:78:LEU:HD13	1.70	0.57
1:D:388:GLU:HB2	1:D:393:GLU:O	2.05	0.57
1:A:361:LEU:HD11	1:B:139:LEU:HD21	1.87	0.56
1:D:68:PHE:HE2	1:D:78:LEU:HD13	1.70	0.56
1:C:116:PRO:HA	4:C:443:HOH:O	2.04	0.56
1:A:381:ALA:HB2	1:A:399:LEU:HD21	1.88	0.56
1:B:410:GLU:O	1:B:413:PRO:HD2	2.06	0.56
1:A:386:GLU:HG3	1:A:390:ARG:HE	1.71	0.56
1:C:55:GLY:O	1:C:58:THR:HG22	2.05	0.56
1:C:381:ALA:HB2	1:C:399:LEU:HD21	1.89	0.55
1:A:71:ARG:HB3	4:B:456:HOH:O	2.06	0.55
1:A:71:ARG:NH2	1:B:63:LYS:HD2	2.22	0.55
1:D:164:SER:HB3	1:D:257:LEU:HB2	1.89	0.55
1:D:224:PRO:HB3	1:D:255:PRO:HA	1.89	0.54
1:A:405:VAL:HG12	1:A:407:LEU:HD22	1.88	0.54
1:A:246:ARG:HG2	1:B:346:TYR:CZ	2.42	0.54
1:C:70:ASP:HB2	1:C:76:LEU:HD22	1.90	0.54
1:C:130:GLU:HG3	1:C:288:TYR:OH	2.08	0.54
1:A:130:GLU:HG3	1:A:288:TYR:OH	2.06	0.54
1:B:381:ALA:HB2	1:B:399:LEU:HD21	1.89	0.54
1:B:338:GLU:O	1:B:341:VAL:HG22	2.08	0.54
1:D:405:VAL:HG12	1:D:407:LEU:HD22	1.89	0.54
1:A:94:GLY:O	1:A:97:VAL:HG22	2.08	0.54
1:A:119:GLY:O	1:A:120:ARG:HB2	2.08	0.53
1:B:168:ASP:HB3	1:B:169:PRO:HD2	1.90	0.53
1:C:68:PHE:HB3	1:D:68:PHE:HB3	1.90	0.53
1:C:190:LEU:O	1:C:195:LYS:HE3	2.08	0.53
1:B:174:ARG:NH2	4:B:501:HOH:O	2.41	0.53
1:C:338:GLU:O	1:C:341:VAL:HG22	2.08	0.53
1:D:190:LEU:O	1:D:195:LYS:HE3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:VAL:O	1:B:306:ALA:HA	2.08	0.53
1:B:374:LEU:HD12	1:B:399:LEU:HD13	1.91	0.53
1:D:381:ALA:HB2	1:D:399:LEU:HD21	1.91	0.53
1:A:190:LEU:O	1:A:195:LYS:HE3	2.09	0.53
1:C:374:LEU:HD12	1:C:399:LEU:HD13	1.90	0.52
1:B:190:LEU:O	1:B:195:LYS:HE3	2.09	0.52
1:D:226:LEU:HD23	1:D:229:LEU:HD11	1.91	0.52
1:D:130:GLU:HG3	1:D:288:TYR:OH	2.07	0.52
1:D:194:SER:HB3	1:D:205:ILE:HG13	1.91	0.52
1:B:273:HIS:CE1	1:B:275:GLU:HB2	2.45	0.52
1:C:226:LEU:HD23	1:C:229:LEU:HD11	1.91	0.52
1:A:398:ARG:NH2	1:A:419:ALA:HB1	2.25	0.52
1:D:120:ARG:HB3	4:D:438:HOH:O	2.09	0.52
1:B:12:LEU:HA	4:B:458:HOH:O	2.10	0.51
1:B:130:GLU:HG3	1:B:288:TYR:OH	2.09	0.51
1:C:194:SER:HB3	1:C:205:ILE:HG13	1.91	0.51
1:D:127:VAL:O	1:D:306:ALA:HA	2.10	0.51
1:A:127:VAL:O	1:A:306:ALA:HA	2.10	0.51
1:B:194:SER:HB3	1:B:205:ILE:HG13	1.91	0.51
1:D:265:VAL:O	1:D:287:ARG:HB3	2.10	0.51
1:A:194:SER:HB3	1:A:205:ILE:HG13	1.91	0.51
1:A:247:LEU:HD11	1:B:345:PHE:CE2	2.45	0.51
1:D:398:ARG:NH2	1:D:419:ALA:HB1	2.26	0.51
1:A:327:LYS:HE2	4:A:451:HOH:O	2.09	0.51
1:C:60:ILE:HA	1:C:64:GLU:HB2	1.93	0.51
1:D:60:ILE:HA	1:D:64:GLU:HB2	1.93	0.50
1:C:140:ASP:O	1:C:144:VAL:HG23	2.11	0.50
1:C:127:VAL:O	1:C:306:ALA:HA	2.11	0.50
1:B:265:VAL:O	1:B:287:ARG:HB3	2.10	0.50
1:B:140:ASP:O	1:B:144:VAL:HG23	2.11	0.50
1:B:60:ILE:HA	1:B:64:GLU:HB2	1.94	0.50
1:D:338:GLU:O	1:D:341:VAL:HG22	2.12	0.50
1:A:60:ILE:HA	1:A:64:GLU:HB2	1.94	0.50
1:D:261:LEU:HD22	1:D:263:TYR:CZ	2.47	0.50
1:A:168:ASP:HB3	1:A:169:PRO:HD2	1.94	0.50
1:A:278:ALA:O	1:A:279:GLN:HB2	2.12	0.49
1:A:265:VAL:O	1:A:287:ARG:HB3	2.11	0.49
1:C:168:ASP:HB3	1:C:169:PRO:HD2	1.93	0.49
1:C:30:VAL:CG2	1:C:150:CYS:SG	3.00	0.49
1:B:398:ARG:NH2	1:B:419:ALA:HB1	2.27	0.49
1:C:398:ARG:NH2	1:C:419:ALA:HB1	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LEU:HD12	1:A:399:LEU:HD13	1.95	0.49
1:B:226:LEU:HD23	1:B:229:LEU:HD11	1.95	0.49
1:B:168:ASP:HA	1:B:265:VAL:CG2	2.36	0.48
1:D:374:LEU:HD12	1:D:399:LEU:HD13	1.95	0.48
1:D:140:ASP:O	1:D:144:VAL:HG23	2.14	0.48
1:C:265:VAL:O	1:C:287:ARG:HB3	2.13	0.48
1:A:70:ASP:O	1:A:72:GLY:N	2.47	0.48
1:C:360:ALA:HB1	1:C:364:ARG:NH1	2.29	0.48
1:A:68:PHE:HB3	1:B:68:PHE:CB	2.41	0.47
1:C:234:ARG:HG2	4:C:463:HOH:O	2.13	0.47
1:D:224:PRO:HB3	1:D:255:PRO:CA	2.44	0.47
1:A:134:SER:HB3	1:A:139:LEU:HD11	1.97	0.47
1:A:140:ASP:O	1:A:144:VAL:HG23	2.15	0.47
1:D:204:ARG:HA	1:D:258:VAL:HG11	1.96	0.47
1:D:351:LEU:CD2	1:D:413:PRO:HG3	2.44	0.47
1:C:351:LEU:CD2	1:C:413:PRO:HG3	2.44	0.47
1:A:338:GLU:O	1:A:341:VAL:HG22	2.15	0.47
1:A:386:GLU:HG2	1:A:390:ARG:HH21	1.79	0.47
1:A:378:ALA:O	1:A:399:LEU:HD12	2.15	0.47
1:A:68:PHE:CB	1:B:68:PHE:HB3	2.41	0.47
1:C:117:GLN:O	1:C:118:LYS:HB2	2.14	0.47
1:D:378:ALA:O	1:D:399:LEU:HD12	2.15	0.47
1:A:226:LEU:HD23	1:A:229:LEU:HD11	1.96	0.47
1:A:351:LEU:CD2	1:A:413:PRO:HG3	2.45	0.47
1:A:294:LEU:CD2	1:D:199:GLU:HG3	2.43	0.47
1:D:226:LEU:HD11	1:D:253:LEU:CD2	2.44	0.46
1:C:246:ARG:HG2	1:D:346:TYR:CZ	2.50	0.46
1:D:407:LEU:N	1:D:407:LEU:HD23	2.31	0.46
1:B:278:ALA:O	1:B:279:GLN:HB2	2.14	0.46
1:C:47:THR:HG22	4:C:457:HOH:O	2.16	0.46
1:B:119:GLY:O	1:B:120:ARG:HG2	2.16	0.46
1:D:201:ASN:N	1:D:202:PRO:HD3	2.30	0.46
1:A:360:ALA:HB1	1:A:364:ARG:NH1	2.30	0.46
1:D:279:GLN:HB3	1:D:311:ARG:NH2	2.31	0.46
1:A:30:VAL:CG2	1:A:150:CYS:SG	3.03	0.46
1:A:408:SER:OG	1:A:411:GLU:HG3	2.16	0.46
1:A:58:THR:HG23	1:A:61:VAL:H	1.80	0.46
1:B:201:ASN:N	1:B:202:PRO:HD3	2.31	0.46
1:B:30:VAL:CG2	1:B:150:CYS:SG	3.04	0.46
1:D:30:VAL:CG2	1:D:150:CYS:SG	3.03	0.46
1:A:201:ASN:N	1:A:202:PRO:HD3	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:LYS:O	1:B:371:GLU:HB3	2.16	0.46
1:C:378:ALA:O	1:C:399:LEU:HD12	2.16	0.46
1:A:246:ARG:HG2	1:B:346:TYR:CE2	2.51	0.45
1:C:201:ASN:N	1:C:202:PRO:HD3	2.31	0.45
1:D:204:ARG:HH22	1:D:260:GLY:C	2.19	0.45
1:D:226:LEU:HD21	1:D:237:LEU:CD2	2.45	0.45
1:C:134:SER:HB3	1:C:139:LEU:HD11	1.98	0.45
1:C:334:ILE:HA	1:C:335:PRO:HD3	1.84	0.45
1:D:261:LEU:HD22	1:D:263:TYR:OH	2.17	0.45
1:B:145:VAL:HG21	1:B:247:LEU:HD13	1.99	0.45
1:B:360:ALA:HB1	1:B:364:ARG:NH1	2.32	0.45
1:D:410:GLU:O	1:D:413:PRO:HD2	2.17	0.45
1:A:273:HIS:CE1	1:A:275:GLU:HB2	2.52	0.45
1:B:407:LEU:HD23	1:B:407:LEU:N	2.31	0.45
1:B:351:LEU:CD2	1:B:413:PRO:HG3	2.47	0.45
1:D:117:GLN:O	1:D:118:LYS:HB2	2.17	0.45
1:D:360:ALA:HB1	1:D:364:ARG:NH1	2.31	0.45
1:C:219:GLU:HG3	1:C:220:LEU:N	2.33	0.44
1:C:255:PRO:HG2	1:C:256:ALA:H	1.81	0.44
1:C:30:VAL:HA	1:D:353:PRO:HB3	1.99	0.44
1:C:117:GLN:HG3	1:C:117:GLN:O	2.17	0.44
1:C:105:TRP:HA	1:C:128:ASN:O	2.18	0.44
1:D:334:ILE:HA	1:D:335:PRO:HD3	1.86	0.44
1:B:374:LEU:CD1	1:B:399:LEU:HD13	2.47	0.44
1:B:275:GLU:HB3	1:B:318:ALA:HB1	2.00	0.44
4:A:429:HOH:O	1:B:339:GLU:HA	2.18	0.44
1:D:351:LEU:HD23	1:D:413:PRO:HG3	2.00	0.44
1:A:117:GLN:O	1:A:117:GLN:HG3	2.18	0.44
1:C:30:VAL:HG23	1:C:31:LEU:HD13	2.00	0.44
1:D:412:VAL:HB	1:D:413:PRO:HD3	2.00	0.44
1:A:111:PHE:CE1	1:A:123:GLN:HG3	2.52	0.43
1:D:117:GLN:O	1:D:117:GLN:HG3	2.18	0.43
1:D:134:SER:HB3	1:D:139:LEU:HD11	2.00	0.43
1:D:206:LEU:HD13	1:D:256:ALA:CB	2.48	0.43
1:A:375:LYS:HD2	4:A:472:HOH:O	2.18	0.43
1:C:115:ARG:HA	1:C:116:PRO:HD2	1.84	0.43
1:D:145:VAL:HG21	1:D:247:LEU:HD13	2.00	0.43
1:A:30:VAL:HG23	1:A:31:LEU:HD13	1.99	0.43
1:D:105:TRP:HA	1:D:128:ASN:O	2.19	0.43
1:A:134:SER:HB3	1:A:139:LEU:CD1	2.49	0.43
1:B:58:THR:HG23	1:B:61:VAL:H	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:THR:HG23	1:C:61:VAL:H	1.82	0.43
1:D:170:GLU:HB3	1:D:174:ARG:NH1	2.33	0.43
1:B:120:ARG:HD3	1:B:120:ARG:HA	1.79	0.43
1:B:122:ARG:NH1	4:B:456:HOH:O	2.51	0.43
1:A:59:ASP:CG	1:A:197:ARG:HH21	2.21	0.43
1:B:334:ILE:HA	1:B:335:PRO:HD3	1.85	0.43
1:C:111:PHE:CE1	1:C:123:GLN:HG3	2.54	0.43
1:C:145:VAL:HG21	1:C:247:LEU:HD13	2.01	0.43
1:B:105:TRP:HA	1:B:128:ASN:O	2.18	0.43
1:A:288:TYR:CD1	1:A:288:TYR:O	2.72	0.43
1:A:386:GLU:CG	1:A:390:ARG:HH21	2.32	0.43
1:A:78:LEU:HD11	1:B:78:LEU:HD11	2.01	0.42
1:B:170:GLU:HB3	1:B:174:ARG:NH1	2.34	0.42
1:C:324:PRO:HB2	1:C:325:GLU:H	1.61	0.42
1:B:60:ILE:O	1:B:65:MET:HG3	2.19	0.42
1:C:259:ARG:HH11	1:C:259:ARG:CG	2.32	0.42
1:C:60:ILE:O	1:C:65:MET:HG3	2.20	0.42
1:D:168:ASP:HB3	1:D:169:PRO:HD2	2.01	0.42
1:A:238:LYS:HD2	1:A:238:LYS:HA	1.93	0.42
1:A:47:THR:CG2	1:A:75:SER:HB3	2.49	0.42
1:C:307:PHE:CD1	1:C:312:VAL:HG21	2.53	0.42
1:C:323:LEU:HD12	1:C:323:LEU:HA	1.80	0.42
1:B:360:ALA:HB1	1:B:364:ARG:HH11	1.85	0.42
1:C:374:LEU:CD1	1:C:399:LEU:HD13	2.49	0.42
1:C:90:TYR:HA	1:C:95:MET:SD	2.60	0.42
1:B:223:ARG:NH2	4:B:446:HOH:O	2.52	0.42
1:C:288:TYR:CD1	1:C:288:TYR:O	2.73	0.42
1:C:407:LEU:HD23	1:C:407:LEU:N	2.34	0.42
1:D:58:THR:HG23	1:D:61:VAL:H	1.84	0.42
1:A:31:LEU:HD23	1:A:105:TRP:HB2	2.02	0.42
1:A:407:LEU:HD23	1:A:407:LEU:N	2.34	0.42
1:B:223:ARG:HA	1:B:224:PRO:HD3	1.74	0.42
1:C:329:PRO:O	1:C:378:ALA:HA	2.19	0.42
1:D:115:ARG:HA	1:D:116:PRO:HD2	1.83	0.42
1:A:329:PRO:O	1:A:378:ALA:HA	2.20	0.42
1:A:384:LEU:HD23	1:A:384:LEU:HA	1.90	0.42
1:C:79:ARG:CD	1:C:110:MET:SD	2.96	0.42
1:A:307:PHE:CD1	1:A:312:VAL:HG21	2.55	0.41
1:B:30:VAL:HG23	1:B:31:LEU:HD13	2.01	0.41
1:C:412:VAL:HB	1:C:413:PRO:HD3	2.00	0.41
1:C:384:LEU:HD23	1:C:384:LEU:HA	1.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:PHE:HB2	1:B:78:LEU:HB2	2.02	0.41
1:C:134:SER:HB3	1:C:139:LEU:CD1	2.50	0.41
1:A:145:VAL:HG21	1:A:247:LEU:HD13	2.01	0.41
1:A:261:LEU:HD22	1:A:263:TYR:CZ	2.55	0.41
1:A:60:ILE:O	1:A:65:MET:HG3	2.20	0.41
1:A:66:PHE:HB2	1:A:78:LEU:HB2	2.02	0.41
1:D:54:VAL:HG13	1:D:261:LEU:HD23	2.02	0.41
1:B:134:SER:HB3	1:B:139:LEU:HD11	2.02	0.41
1:B:412:VAL:HB	1:B:413:PRO:HD3	2.02	0.41
1:A:355:LEU:HD12	1:A:355:LEU:HA	1.94	0.41
1:D:30:VAL:HG23	1:D:31:LEU:HD13	2.02	0.41
1:B:384:LEU:HA	1:B:384:LEU:HD23	1.91	0.41
1:C:6:VAL:HG22	4:C:436:HOH:O	2.21	0.41
1:B:355:LEU:HA	1:B:355:LEU:HD12	1.94	0.41
1:C:351:LEU:HD23	1:C:413:PRO:HG3	2.01	0.41
1:C:3:ALA:HB2	1:D:48:GLN:HE21	1.86	0.41
1:D:134:SER:HB3	1:D:139:LEU:CD1	2.50	0.41
1:D:374:LEU:CD1	1:D:399:LEU:HD13	2.51	0.41
1:A:334:ILE:HA	1:A:335:PRO:HD3	1.84	0.41
1:B:167:GLY:O	1:B:266:ARG:N	2.53	0.41
1:C:183:LEU:HD13	1:C:205:ILE:HD13	2.02	0.41
1:D:90:TYR:HA	1:D:95:MET:SD	2.61	0.41
1:A:247:LEU:HD11	1:B:345:PHE:CZ	2.56	0.40
1:B:396:LEU:HD11	1:B:412:VAL:HG13	2.03	0.40
1:C:345:PHE:CD2	1:D:138:ILE:HG23	2.56	0.40
1:D:360:ALA:HB1	1:D:364:ARG:HH11	1.86	0.40
1:A:374:LEU:CD1	1:A:399:LEU:HD13	2.51	0.40
1:B:288:TYR:O	1:B:288:TYR:CD1	2.75	0.40
1:B:378:ALA:O	1:B:399:LEU:HD12	2.21	0.40
1:C:170:GLU:HB3	1:C:174:ARG:NH1	2.35	0.40
1:D:170:GLU:HB3	1:D:174:ARG:HH12	1.86	0.40
1:B:184:SER:O	1:B:187:ARG:HB2	2.21	0.40
1:B:307:PHE:CD1	1:B:312:VAL:HG21	2.55	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	418/421 (99%)	394 (94%)	20 (5%)	4 (1%)	15	37
1	B	418/421 (99%)	396 (95%)	16 (4%)	6 (1%)	11	28
1	C	418/421 (99%)	399 (96%)	15 (4%)	4 (1%)	15	37
1	D	418/421 (99%)	399 (96%)	14 (3%)	5 (1%)	13	32
All	All	1672/1684 (99%)	1588 (95%)	65 (4%)	19 (1%)	14	34

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	B	117	GLN
1	C	117	GLN
1	D	117	GLN
1	D	325	GLU
1	A	74	ARG
1	A	120	ARG
1	B	74	ARG
1	B	120	ARG
1	B	275	GLU
1	B	276	ILE
1	C	120	ARG
1	A	118	LYS
1	D	120	ARG
1	C	118	LYS
1	D	72	GLY
1	B	119	GLY
1	D	276	ILE
1	C	324	PRO

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	334/335 (100%)	313 (94%)	21 (6%)	18	40
1	B	334/335 (100%)	313 (94%)	21 (6%)	18	40
1	C	334/335 (100%)	315 (94%)	19 (6%)	20	44
1	D	334/335 (100%)	315 (94%)	19 (6%)	20	44
All	All	1336/1340 (100%)	1256 (94%)	80 (6%)	19	42

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	39	LEU
1	A	59	ASP
1	A	76	LEU
1	A	79	ARG
1	A	81	GLU
1	A	91	LEU
1	A	130	GLU
1	A	223	ARG
1	A	245	GLU
1	A	257	LEU
1	A	259	ARG
1	A	263	TYR
1	A	274	GLU
1	A	303	VAL
1	A	323	LEU
1	A	334	ILE
1	A	355	LEU
1	A	364	ARG
1	A	374	LEU
1	A	407	LEU
1	B	17	LEU
1	B	39	LEU
1	B	59	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	69	GLN
1	B	76	LEU
1	B	79	ARG
1	B	81	GLU
1	B	91	LEU
1	B	122	ARG
1	B	130	GLU
1	B	234	ARG
1	B	245	GLU
1	B	259	ARG
1	B	263	TYR
1	B	303	VAL
1	B	323	LEU
1	B	334	ILE
1	B	355	LEU
1	B	364	ARG
1	B	374	LEU
1	B	407	LEU
1	C	17	LEU
1	C	39	LEU
1	C	59	ASP
1	C	76	LEU
1	C	79	ARG
1	C	81	GLU
1	C	91	LEU
1	C	122	ARG
1	C	130	GLU
1	C	245	GLU
1	C	259	ARG
1	C	275	GLU
1	C	303	VAL
1	C	323	LEU
1	C	334	ILE
1	C	355	LEU
1	C	364	ARG
1	C	374	LEU
1	C	407	LEU
1	D	17	LEU
1	D	59	ASP
1	D	76	LEU
1	D	79	ARG
1	D	81	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	91	LEU
1	D	122	ARG
1	D	130	GLU
1	D	245	GLU
1	D	257	LEU
1	D	263	TYR
1	D	275	GLU
1	D	303	VAL
1	D	323	LEU
1	D	334	ILE
1	D	355	LEU
1	D	364	ARG
1	D	374	LEU
1	D	407	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	69	GLN
1	D	48	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](#)

8 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	SO4	C	422	-	4,4,4	0.36	0	6,6,6	0.43	0
2	SO4	D	422	-	4,4,4	0.46	0	6,6,6	0.36	0
2	SO4	A	422	-	4,4,4	0.46	0	6,6,6	0.35	0
2	SO4	B	422	-	4,4,4	0.31	0	6,6,6	0.41	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.