



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:20 PM UTC

PDB ID : 1QS0 / pdb_00001qs0
Title : Crystal Structure of Pseudomonas Putida 2-oxoisovalerate Dehydrogenase
(Branched-Chain Alpha-Keto Acid Dehydrogenase, E1B)
Authors : Aevarsson, A.; Seger, K.; Turley, S.; Sokatch, J.R.; Hol, W.G.J.
Deposited on : 1999-06-24
Resolution : 2.40 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

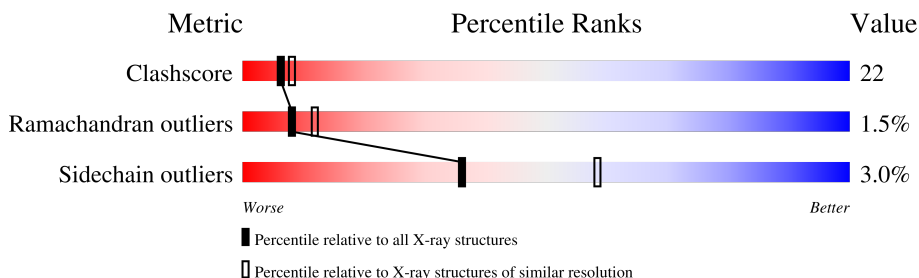
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	407	
2	B	338	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5999 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 2-OXOISOVALERATE DEHYDROGENASE ALPHA-SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	407	3165	1983	568	598	4	12	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	MSE	MET	modified residue	UNP P09060
A	84	MSE	MET	modified residue	UNP P09060
A	94	MSE	MET	modified residue	UNP P09060
A	103	MSE	MET	modified residue	UNP P09060
A	107	MSE	MET	modified residue	UNP P09060
A	128	MSE	MET	modified residue	UNP P09060
A	140	MSE	MET	modified residue	UNP P09060
A	149	MSE	MET	modified residue	UNP P09060
A	169	MSE	MET	modified residue	UNP P09060
A	196	MSE	MET	modified residue	UNP P09060
A	389	MSE	MET	modified residue	UNP P09060
A	397	MSE	MET	modified residue	UNP P09060

- Molecule 2 is a protein called 2-OXOISOVALERATE DEHYDROGENASE BETA-SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	338	2602	1652	441	492	7	10	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	MSE	MET	modified residue	UNP P09061
B	8	MSE	MET	modified residue	UNP P09061
B	16	MSE	MET	modified residue	UNP P09061
B	19	MSE	MET	modified residue	UNP P09061

Continued on next page...

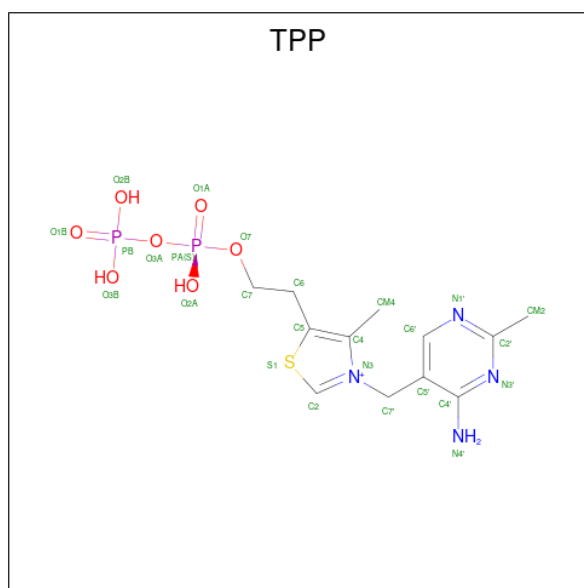
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	72	MSE	MET	modified residue	UNP P09061
B	100	MSE	MET	modified residue	UNP P09061
B	119	MSE	MET	modified residue	UNP P09061
B	138	MSE	MET	modified residue	UNP P09061
B	149	MSE	MET	modified residue	UNP P09061
B	337	MSE	MET	modified residue	UNP P09061

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

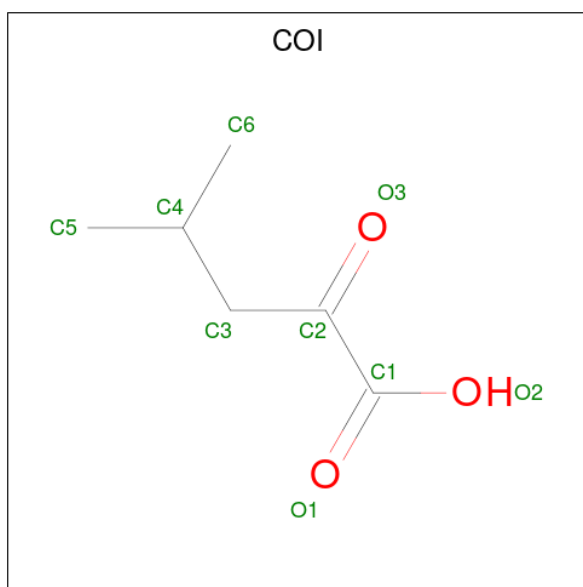
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0

- Molecule 5 is 2-OXO-4-METHYLPENTANOIC ACID (CCD ID: COI) (formula: C₆H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

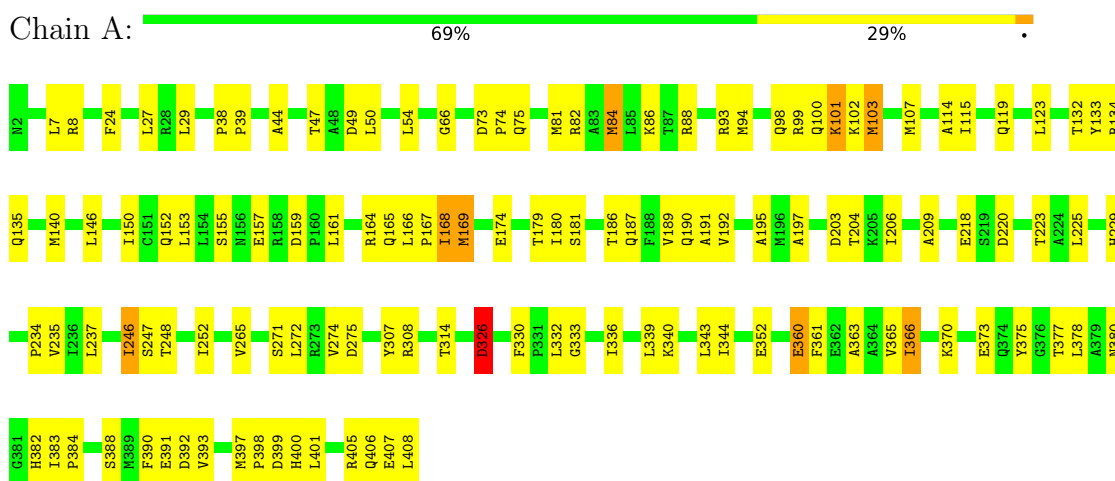
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	129	Total	O	0	0
			129	129		
6	B	68	Total	O	0	0
			68	68		

3 Residue-property plots

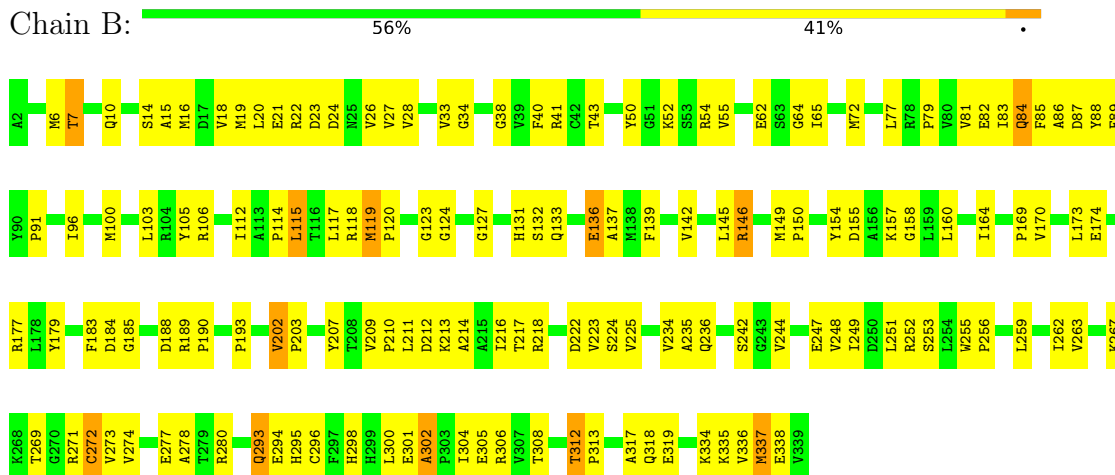
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: 2-OXISOVALERATE DEHYDROGENASE ALPHA-SUBUNIT



• Molecule 2: 2-OXISOVALERATE DEHYDROGENASE BETA-SUBUNIT



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.34Å 101.34Å 381.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40	Depositor
% Data completeness (in resolution range)	95.9 (40.00-2.40)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.218 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5999	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TPP, COI, MG

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	0.53	2/3225 (0.1%)	0.94	9/4355 (0.2%)
2	B	0.52	2/2660 (0.1%)	0.92	3/3608 (0.1%)
All	All	0.53	4/5885 (0.1%)	0.93	12/7963 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	MSE	CG-SE	-6.30	1.76	1.95
2	B	337	MSE	CG-SE	-5.22	1.79	1.95
2	B	119	MSE	CG-SE	-5.18	1.79	1.95
1	A	103	MSE	CG-SE	-5.12	1.80	1.95

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	GLY	N-CA-C	7.59	124.61	111.78
1	A	157	GLU	N-CA-C	-6.98	104.64	113.01
1	A	393	VAL	N-CA-C	-6.38	104.28	110.72
1	A	66	GLY	CA-C-N	6.23	126.13	119.28
1	A	66	GLY	C-N-CA	6.23	126.13	119.28
1	A	115	ILE	N-CA-C	6.05	116.17	110.30
2	B	170	VAL	N-CA-C	5.62	115.95	107.75
1	A	326	ASP	N-CA-C	5.42	117.63	111.02
1	A	39	PRO	N-CA-C	-5.37	103.36	111.41
1	A	102	LYS	N-CA-C	-5.32	106.29	112.89
2	B	202	VAL	N-CA-C	5.18	113.78	107.61
2	B	7	THR	N-CA-C	-5.05	103.27	110.59

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	3165	0	3075	109	1
2	B	2602	0	2532	148	0
3	A	1	0	0	0	0
4	A	26	0	16	0	0
5	B	8	0	9	2	0
6	A	129	0	0	10	0
6	B	68	0	0	12	0
All	All	5999	0	5632	254	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 22.

All (254) 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:377:THR:HG22	1:A:378:LEU:H	1.24	1.01
2:B:280:ARG:HG2	2:B:308:THR:OG1	1.66	0.96
1:A:165:GLN:HG2	1:A:169:MSE:HB3	1.55	0.88
1:A:47:THR:HG21	1:A:271:SER:H	1.36	0.88
2:B:146:ARG:HB2	2:B:146:ARG:HH11	1.36	0.87
1:A:167:PRO:O	1:A:168:ILE:HG12	1.74	0.87
2:B:19:MSE:HA	2:B:19:MSE:HE2	1.60	0.84
2:B:65:ILE:HG23	2:B:81:VAL:HG21	1.60	0.84
2:B:23:ASP:HB3	2:B:26:VAL:HG23	1.60	0.81
2:B:87:ASP:OD1	2:B:133:GLN:HG2	1.82	0.79
2:B:123:GLY:HA2	2:B:132:SER:HB2	1.65	0.78
1:A:94:MSE:HE1	1:A:150:ILE:HG23	1.63	0.78
1:A:86:LYS:HG2	1:A:140:MSE:HE3	1.66	0.78
1:A:377:THR:HG22	1:A:378:LEU:N	2.00	0.76
2:B:19:MSE:HE1	2:B:22:ARG:HD3	1.68	0.75
1:A:165:GLN:CG	1:A:169:MSE:HB3	2.17	0.75
1:A:380:ASN:HB3	1:A:382:HIS:ND1	2.02	0.75
2:B:317:ALA:HB3	2:B:318:GLN:NE2	2.03	0.74
1:A:195:ALA:HB2	1:A:235:VAL:HG22	1.69	0.74
2:B:223:VAL:HG22	2:B:271:ARG:HG3	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:MSE:CE	1:A:153:LEU:HD12	2.20	0.72
1:A:94:MSE:HE3	1:A:103:MSE:HE1	1.72	0.72
1:A:94:MSE:HE2	1:A:153:LEU:HD12	1.73	0.71
2:B:6:MSE:HB3	2:B:10:GLN:HB2	1.73	0.70
2:B:202:VAL:HB	6:B:560:HOH:O	1.90	0.70
1:A:352:GLU:N	1:A:352:GLU:OE1	2.23	0.70
2:B:52:LYS:HD3	6:B:548:HOH:O	1.92	0.70
2:B:62:GLU:HG2	2:B:88:TYR:O	1.91	0.69
1:A:186:THR:O	1:A:190:GLN:HG3	1.93	0.69
2:B:218:ARG:O	2:B:247:GLU:HA	1.93	0.69
2:B:271:ARG:NH1	2:B:337:MSE:HA	2.08	0.68
2:B:271:ARG:HH11	2:B:337:MSE:HA	1.59	0.68
2:B:269:THR:HG22	2:B:271:ARG:H	1.57	0.67
1:A:390:PHE:HB3	1:A:397:MSE:HE3	1.76	0.67
2:B:127:GLY:O	2:B:131:HIS:HB2	1.95	0.67
1:A:44:ALA:O	1:A:47:THR:HG22	1.93	0.67
2:B:146:ARG:HD3	2:B:211:LEU:HD13	1.77	0.67
2:B:72:MSE:HE3	2:B:77:LEU:HD13	1.77	0.65
2:B:223:VAL:HA	2:B:269:THR:HG21	1.78	0.65
2:B:184:ASP:O	2:B:234:VAL:HG22	1.97	0.64
2:B:217:THR:HG21	2:B:236:GLN:NE2	2.13	0.64
1:A:218:GLU:HG3	6:A:517:HOH:O	1.98	0.63
1:A:98:GLN:HG3	1:A:314:THR:HG21	1.81	0.63
2:B:72:MSE:HE3	2:B:77:LEU:CD1	2.29	0.62
2:B:177:ARG:HD3	2:B:183:PHE:CD2	2.34	0.62
2:B:255:TRP:HA	2:B:256:PRO:C	2.23	0.62
2:B:280:ARG:HG2	2:B:308:THR:HG1	1.65	0.62
1:A:399:ASP:CG	6:A:599:HOH:O	2.41	0.62
1:A:195:ALA:CB	1:A:235:VAL:HG22	2.30	0.62
1:A:181:SER:HB3	6:A:503:HOH:O	2.00	0.61
1:A:189:VAL:HG23	1:A:220:ASP:HB3	1.81	0.61
2:B:222:ASP:O	2:B:269:THR:HG23	2.01	0.61
1:A:49:ASP:HB2	6:A:585:HOH:O	1.99	0.61
1:A:94:MSE:CE	1:A:103:MSE:HE1	2.30	0.61
1:A:390:PHE:CB	1:A:397:MSE:HE3	2.30	0.61
2:B:301:GLU:O	2:B:302:ALA:HB2	2.01	0.61
2:B:223:VAL:HG23	2:B:337:MSE:SE	2.51	0.60
2:B:65:ILE:CG2	2:B:81:VAL:HG21	2.30	0.60
1:A:377:THR:CG2	1:A:378:LEU:H	2.07	0.60
2:B:259:LEU:HD21	2:B:295:HIS:CE1	2.37	0.60
2:B:188:ASP:O	2:B:190:PRO:HD3	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ILE:HD12	1:A:370:LYS:HE2	1.84	0.58
1:A:192:VAL:HA	1:A:235:VAL:HG21	1.85	0.58
2:B:38:GLY:HA2	6:B:509:HOH:O	2.02	0.58
1:A:398:PRO:HD2	1:A:401:LEU:HD12	1.85	0.58
2:B:65:ILE:HG23	2:B:81:VAL:CG2	2.30	0.58
1:A:29:LEU:HD22	1:A:54:LEU:HD22	1.86	0.57
1:A:99:ARG:C	1:A:101:LYS:H	2.11	0.57
1:A:275:ASP:OD2	1:A:332:LEU:HD22	2.04	0.57
2:B:27:VAL:HG11	2:B:72:MSE:HE1	1.85	0.57
2:B:158:GLY:HA3	2:B:209:VAL:HG23	1.86	0.57
2:B:118:ARG:HH11	2:B:174:GLU:CD	2.13	0.57
1:A:82:ARG:HD3	6:A:557:HOH:O	2.05	0.57
2:B:96:ILE:HG23	2:B:100:MSE:CE	2.34	0.56
2:B:123:GLY:CA	2:B:132:SER:HB2	2.35	0.56
1:A:248:THR:HG23	1:A:252:ILE:HD12	1.87	0.56
2:B:20:LEU:HD21	2:B:55:VAL:CG2	2.35	0.56
2:B:251:LEU:HD22	2:B:262:ILE:HD11	1.86	0.56
2:B:263:VAL:HG13	2:B:296:CYS:SG	2.45	0.56
2:B:334:LYS:O	2:B:338:GLU:HG3	2.06	0.56
2:B:96:ILE:HG23	2:B:100:MSE:HE2	1.86	0.56
2:B:81:VAL:CG1	2:B:117:LEU:HD22	2.35	0.56
1:A:407:GLU:O	1:A:407:GLU:HG2	2.06	0.55
1:A:47:THR:HG21	1:A:271:SER:N	2.15	0.55
1:A:397:MSE:HE1	1:A:405:ARG:HB2	1.87	0.55
2:B:119:MSE:HE2	2:B:173:LEU:HD21	1.89	0.55
2:B:19:MSE:HA	2:B:19:MSE:CE	2.34	0.55
2:B:81:VAL:HG12	2:B:117:LEU:HD22	1.89	0.55
1:A:107:MSE:HB2	6:A:548:HOH:O	2.06	0.54
1:A:223:THR:HG21	2:B:64:GLY:CA	2.37	0.54
1:A:339:LEU:O	1:A:343:LEU:HB2	2.06	0.54
2:B:23:ASP:HB3	2:B:26:VAL:CG2	2.35	0.54
1:A:223:THR:HG21	2:B:64:GLY:HA2	1.88	0.54
2:B:14:SER:O	2:B:18:VAL:HG23	2.07	0.54
1:A:38:PRO:HG3	1:A:50:LEU:HD11	1.89	0.53
2:B:112:ILE:HG13	2:B:114:PRO:HD3	1.90	0.53
1:A:152:GLN:HA	1:A:159:ASP:OD2	2.08	0.53
1:A:246:ILE:HG22	1:A:247:SER:N	2.23	0.53
5:B:502:COI:C1	5:B:502:COI:H53	2.39	0.53
1:A:94:MSE:HE2	1:A:150:ILE:HG12	1.89	0.53
1:A:134:ARG:NH2	1:A:308:ARG:HD2	2.23	0.53
2:B:222:ASP:HB3	2:B:337:MSE:CE	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:502:COI:O1	5:B:502:COI:H62	2.07	0.53
2:B:203:PRO:HD2	2:B:207:TYR:CE2	2.43	0.52
1:A:380:ASN:C	1:A:382:HIS:H	2.16	0.52
2:B:119:MSE:HE2	2:B:173:LEU:CD2	2.40	0.52
2:B:223:VAL:HA	2:B:269:THR:CG2	2.40	0.52
1:A:155:SER:O	1:A:384:PRO:HD3	2.10	0.52
2:B:19:MSE:CE	2:B:22:ARG:HD3	2.39	0.52
1:A:166:LEU:HG	1:A:167:PRO:HD2	1.92	0.52
2:B:33:VAL:HG13	2:B:43:THR:HG21	1.91	0.52
1:A:94:MSE:HE3	1:A:153:LEU:HD12	1.91	0.52
1:A:159:ASP:OD1	1:A:161:LEU:N	2.40	0.52
2:B:216:ILE:CD1	2:B:249:ILE:HG12	2.41	0.51
2:B:28:VAL:O	2:B:55:VAL:HA	2.10	0.51
1:A:229:HIS:CE1	6:A:553:HOH:O	2.64	0.51
2:B:335:LYS:HA	2:B:338:GLU:OE2	2.11	0.51
1:A:398:PRO:HB2	1:A:400:HIS:CE1	2.46	0.50
1:A:132:THR:H	1:A:135:GLN:NE2	2.10	0.50
2:B:273:VAL:HG22	2:B:336:VAL:HG11	1.94	0.50
2:B:16:MSE:O	2:B:20:LEU:HB2	2.12	0.50
2:B:259:LEU:O	2:B:263:VAL:HG23	2.11	0.50
2:B:269:THR:HG22	2:B:271:ARG:N	2.24	0.50
2:B:223:VAL:HG22	2:B:271:ARG:CG	2.40	0.50
2:B:123:GLY:HA2	2:B:132:SER:CB	2.40	0.50
1:A:161:LEU:HB2	6:A:541:HOH:O	2.12	0.49
1:A:361:PHE:O	1:A:365:VAL:HG23	2.12	0.49
2:B:82:GLU:HG2	2:B:83:ILE:N	2.25	0.49
2:B:277:GLU:HG3	6:B:557:HOH:O	2.12	0.49
2:B:7:THR:OG1	2:B:10:GLN:HG3	2.12	0.49
1:A:169:MSE:HE2	1:A:180:ILE:HG21	1.94	0.49
1:A:340:LYS:O	1:A:344:ILE:HG13	2.13	0.49
2:B:216:ILE:HD13	2:B:249:ILE:HG12	1.95	0.49
1:A:81:MSE:HE2	1:A:339:LEU:HG	1.95	0.48
2:B:81:VAL:HG12	2:B:117:LEU:CD2	2.43	0.48
2:B:89:PHE:CD1	2:B:89:PHE:C	2.91	0.48
2:B:105:TYR:HB2	6:B:538:HOH:O	2.13	0.48
2:B:19:MSE:HE2	2:B:22:ARG:HB3	1.96	0.48
2:B:85:PHE:HB2	2:B:88:TYR:CD1	2.49	0.48
2:B:118:ARG:NH1	2:B:174:GLU:OE1	2.47	0.47
2:B:146:ARG:HB2	2:B:146:ARG:NH1	2.16	0.47
2:B:218:ARG:HG2	6:B:559:HOH:O	2.13	0.47
2:B:212:ASP:OD1	2:B:256:PRO:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:SER:HB2	2:B:106:ARG:NH1	2.28	0.47
1:A:360:GLU:HG3	1:A:361:PHE:N	2.30	0.47
1:A:388:SER:HA	1:A:391:GLU:OE2	2.14	0.47
1:A:93:ARG:HG3	1:A:365:VAL:HG11	1.97	0.47
1:A:383:ILE:HB	1:A:384:PRO:CD	2.45	0.47
2:B:15:ALA:HB3	2:B:160:LEU:HD23	1.96	0.47
2:B:251:LEU:C	2:B:253:SER:H	2.22	0.47
1:A:73:ASP:OD2	1:A:75:GLN:HB2	2.15	0.46
1:A:406:GLN:C	1:A:408:LEU:H	2.22	0.46
2:B:225:VAL:HB	2:B:248:VAL:HA	1.97	0.46
2:B:27:VAL:CB	2:B:72:MSE:HE1	2.46	0.46
2:B:142:VAL:HB	2:B:145:LEU:HD12	1.98	0.46
2:B:223:VAL:HG11	2:B:273:VAL:HG23	1.97	0.46
2:B:251:LEU:O	2:B:252:ARG:HB2	2.14	0.46
2:B:27:VAL:CG1	2:B:72:MSE:HE1	2.46	0.46
2:B:72:MSE:HG2	2:B:77:LEU:HD12	1.98	0.46
2:B:120:PRO:HA	2:B:174:GLU:O	2.15	0.46
1:A:397:MSE:CE	1:A:405:ARG:HB2	2.46	0.46
2:B:296:CYS:O	2:B:300:LEU:HB2	2.16	0.46
2:B:65:ILE:CG2	2:B:81:VAL:CG2	2.93	0.45
2:B:84:GLN:HG3	6:B:565:HOH:O	2.16	0.45
2:B:273:VAL:HA	2:B:305:GLU:O	2.17	0.45
1:A:133:TYR:HE1	1:A:134:ARG:HH11	1.63	0.45
1:A:191:ALA:CB	1:A:209:ALA:HB2	2.46	0.45
2:B:224:SER:O	2:B:272:CYS:HA	2.17	0.45
2:B:312:THR:HG23	2:B:313:PRO:O	2.16	0.45
1:A:195:ALA:CB	1:A:235:VAL:CG2	2.94	0.45
2:B:136:GLU:HG2	2:B:137:ALA:N	2.32	0.45
1:A:225:LEU:HD23	1:A:237:LEU:HD13	1.99	0.45
2:B:21:GLU:HB2	2:B:50:TYR:OH	2.16	0.45
1:A:27:LEU:HD23	6:A:561:HOH:O	2.17	0.45
1:A:81:MSE:HE1	1:A:340:LYS:N	2.32	0.44
1:A:248:THR:CG2	1:A:252:ILE:HB	2.48	0.44
1:A:84:MSE:SE	1:A:114:ALA:HB2	2.67	0.44
2:B:189:ARG:O	2:B:190:PRO:C	2.61	0.44
1:A:274:VAL:HG12	1:A:275:ASP:N	2.32	0.44
2:B:40:PHE:O	2:B:41:ARG:HB2	2.16	0.44
2:B:6:MSE:CG	6:B:560:HOH:O	2.66	0.44
2:B:112:ILE:HG12	6:B:524:HOH:O	2.17	0.44
2:B:263:VAL:O	2:B:267:LYS:HB2	2.18	0.44
2:B:137:ALA:HB3	6:B:508:HOH:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:TYR:OH	1:A:326:ASP:HB3	2.18	0.44
1:A:94:MSE:CE	1:A:150:ILE:HG12	2.47	0.44
1:A:123:LEU:HD22	1:A:206:ILE:HD11	2.00	0.44
1:A:146:LEU:O	1:A:150:ILE:HG13	2.18	0.44
1:A:380:ASN:C	1:A:382:HIS:N	2.75	0.44
2:B:15:ALA:HB2	2:B:157:LYS:HG3	1.99	0.44
1:A:94:MSE:HE3	1:A:103:MSE:CE	2.44	0.43
1:A:167:PRO:C	1:A:168:ILE:HG23	2.43	0.43
1:A:229:HIS:HE1	6:A:553:HOH:O	1.97	0.43
2:B:293:GLN:NE2	2:B:293:GLN:C	2.76	0.43
2:B:154:TYR:HA	2:B:202:VAL:HG22	2.00	0.43
1:A:166:LEU:HG	1:A:167:PRO:CD	2.49	0.43
1:A:330:PHE:CE2	1:A:332:LEU:HB2	2.54	0.43
2:B:155:ASP:OD2	2:B:252:ARG:NH1	2.52	0.43
1:A:88:ARG:CZ	1:A:336:ILE:HD12	2.49	0.43
2:B:298:HIS:C	2:B:300:LEU:H	2.27	0.43
1:A:377:THR:CG2	1:A:378:LEU:N	2.71	0.43
1:A:373:GLU:C	1:A:375:TYR:H	2.28	0.42
2:B:118:ARG:NH1	2:B:174:GLU:CD	2.76	0.42
2:B:223:VAL:HG22	2:B:271:ARG:CD	2.49	0.42
1:A:164:ARG:NH1	1:A:392:ASP:HB2	2.34	0.42
2:B:100:MSE:HG2	2:B:169:PRO:HB3	2.00	0.42
2:B:225:VAL:HG11	2:B:235:ALA:HB1	2.00	0.42
1:A:169:MSE:HE2	1:A:180:ILE:CG2	2.49	0.42
2:B:86:ALA:CB	2:B:119:MSE:HE3	2.49	0.42
1:A:203:ASP:OD1	1:A:204:THR:N	2.43	0.42
1:A:223:THR:CG2	2:B:64:GLY:CA	2.97	0.42
2:B:118:ARG:HD2	2:B:174:GLU:OE2	2.20	0.42
2:B:242:SER:C	2:B:244:VAL:H	2.27	0.42
2:B:259:LEU:HD21	2:B:295:HIS:HE1	1.79	0.42
1:A:167:PRO:O	1:A:168:ILE:CG1	2.58	0.42
1:A:383:ILE:HB	1:A:384:PRO:HD2	2.02	0.42
2:B:6:MSE:HG3	6:B:560:HOH:O	2.18	0.42
2:B:19:MSE:HE2	2:B:22:ARG:CB	2.49	0.42
2:B:115:LEU:N	2:B:115:LEU:HD23	2.34	0.42
2:B:149:MSE:HG3	2:B:173:LEU:HB2	2.01	0.42
2:B:318:GLN:CD	2:B:318:GLN:H	2.27	0.42
1:A:187:GLN:H	1:A:187:GLN:CD	2.28	0.42
2:B:83:ILE:O	2:B:84:GLN:C	2.63	0.41
1:A:73:ASP:HA	1:A:74:PRO:HD3	1.88	0.41
2:B:127:GLY:C	2:B:131:HIS:HB2	2.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:PHE:CE2	2:B:185:GLY:HA2	2.56	0.41
1:A:47:THR:CG2	1:A:265:VAL:HG22	2.50	0.41
1:A:397:MSE:HE1	1:A:405:ARG:HD3	2.01	0.41
2:B:18:VAL:HG12	2:B:19:MSE:HE3	2.01	0.41
2:B:301:GLU:O	2:B:302:ALA:CB	2.66	0.41
1:A:99:ARG:C	1:A:101:LYS:N	2.78	0.41
1:A:152:GLN:HA	1:A:159:ASP:CG	2.46	0.41
1:A:195:ALA:HB1	1:A:234:PRO:HG2	2.03	0.41
2:B:294:GLU:HG2	2:B:295:HIS:HD2	1.86	0.41
2:B:20:LEU:HD12	2:B:54:ARG:NH1	2.36	0.41
2:B:77:LEU:O	2:B:79:PRO:HD3	2.20	0.41
1:A:225:LEU:CD2	1:A:237:LEU:HD13	2.51	0.41
2:B:24:ASP:HA	2:B:54:ARG:NH2	2.36	0.41
2:B:274:VAL:O	2:B:306:ARG:HA	2.21	0.41
1:A:363:ALA:O	1:A:366:ILE:HG22	2.20	0.41
2:B:43:THR:HG23	6:B:564:HOH:O	2.19	0.41
2:B:119:MSE:HE1	2:B:139:PHE:HE1	1.86	0.41
2:B:124:GLY:HA2	2:B:319:GLU:OE2	2.20	0.41
2:B:160:LEU:O	2:B:164:ILE:HG13	2.20	0.41
2:B:223:VAL:CG2	2:B:337:MSE:SE	3.18	0.41
2:B:189:ARG:H	2:B:189:ARG:HG2	1.67	0.40
1:A:133:TYR:HE1	1:A:134:ARG:NH1	2.19	0.40
1:A:191:ALA:HB3	1:A:209:ALA:HB2	2.04	0.40
2:B:210:PRO:CG	2:B:213:LYS:HD2	2.51	0.40
1:A:197:ALA:HB2	2:B:72:MSE:HG2	2.04	0.40
1:A:252:ILE:O	1:A:252:ILE:HG22	2.21	0.40
2:B:62:GLU:HB2	2:B:91:PRO:HB2	2.03	0.40
2:B:150:PRO:HD2	2:B:173:LEU:O	2.21	0.40
2:B:272:CYS:SG	2:B:304:ILE:HG23	2.60	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:A:360:GLU:OE2	1:A:360:GLU:OE2[7_545]	1.68	0.52

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	405/407 (100%)	371 (92%)	29 (7%)	5 (1%)	10	16
2	B	336/338 (99%)	297 (88%)	33 (10%)	6 (2%)	6	9
All	All	741/745 (100%)	668 (90%)	62 (8%)	11 (2%)	8	12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	ILE
1	A	101	LYS
1	A	246	ILE
2	B	84	GLN
2	B	214	ALA
1	A	24	PHE
2	B	34	GLY
1	A	100	GLN
2	B	193	PRO
2	B	278	ALA
2	B	302	ALA

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	326/314 (104%)	316 (97%)	10 (3%)	35	57
2	B	279/269 (104%)	271 (97%)	8 (3%)	37	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	605/583 (104%)	587 (97%)	18 (3%)	36 58

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	8	ARG
1	A	119	GLN
1	A	169	MSE
1	A	174	GLU
1	A	179	THR
1	A	272	LEU
1	A	326	ASP
1	A	360	GLU
1	A	366	ILE
2	B	103	LEU
2	B	115	LEU
2	B	136	GLU
2	B	146	ARG
2	B	179	TYR
2	B	272	CYS
2	B	293	GLN
2	B	312	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	61	GLN
1	A	98	GLN
1	A	124	ASN
1	A	135	GLN
1	A	165	GLN
1	A	229	HIS
1	A	241	ASN
1	A	341	GLN
1	A	355	GLN
1	A	369	GLN
2	B	84	GLN
2	B	180	ASN
2	B	236	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	293	GLN
2	B	295	HIS
2	B	298	HIS
2	B	316	HIS
2	B	318	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	COI	B	502	2	7,7,8	0.78	0	8,8,10	1.76	1 (12%)
4	TPP	A	500	3	26,27,27	1.58	6 (23%)	38,40,40	1.59	7 (18%)

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
5	COI	B	502	2	-	3/5/5/8	-
4	TPP	A	500	3	-	2/17/17/17	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	TPP	PA-O3A	-3.52	1.55	1.59
4	A	500	TPP	C4'-N3'	3.48	1.39	1.35
4	A	500	TPP	C2'-N1'	3.28	1.39	1.34
4	A	500	TPP	C7'-N3	2.62	1.54	1.48
4	A	500	TPP	PB-O3B	-2.33	1.46	1.54
4	A	500	TPP	C5-C4	2.02	1.39	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	COI	C3-C2-C1	4.14	123.53	112.49
4	A	500	TPP	O3B-PB-O2B	4.10	123.19	107.80
4	A	500	TPP	CM2-C2'-N1'	3.88	121.33	117.20
4	A	500	TPP	C7'-N3-C4	2.87	129.95	122.36
4	A	500	TPP	PA-O7-C7	2.84	134.78	121.26
4	A	500	TPP	S1-C2-N3	2.60	115.59	112.30
4	A	500	TPP	N1'-C2'-N3'	-2.60	121.21	125.53
4	A	500	TPP	C7'-N3-C2	-2.30	118.69	123.48

There are no chirality outliers.

All (5) torsion outliers are listed below:

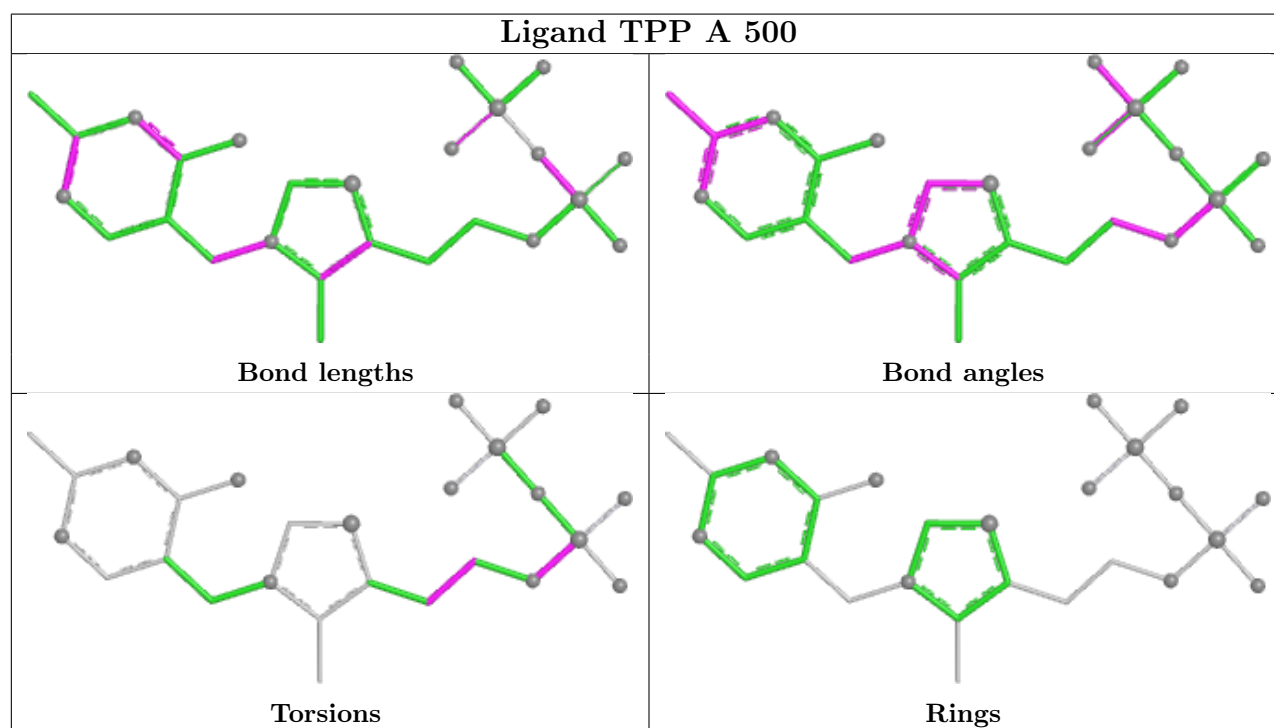
Mol	Chain	Res	Type	Atoms
5	B	502	COI	C1-C2-C3-C4
4	A	500	TPP	C7-O7-PA-O2A
5	B	502	COI	O2-C1-C2-C3
5	B	502	COI	O1-C1-C2-C3
4	A	500	TPP	C5-C6-C7-O7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	COI	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.