



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2021 – 07:03 am BST

PDB ID : 7OIS
Title : mPI3Kd in complex with compound 7
Authors : Petersen, J.
Deposited on : 2021-05-12
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
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) : 2.23.1

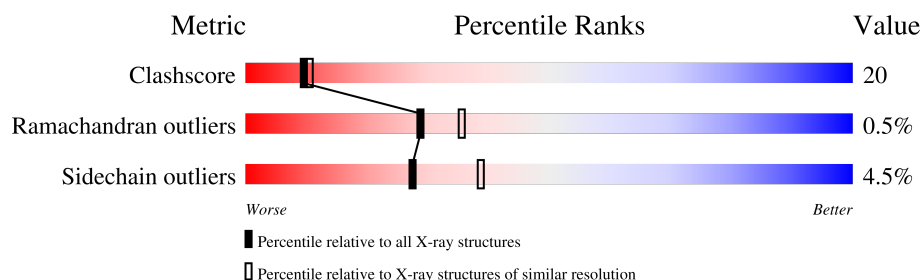
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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	AAA	1084	<div>55% 20% • 24%</div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8250 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	827	Total	C	N	O	S	3	1	0
			6678	4281	1131	1211	55			

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-39	MET	-	initiating methionine	UNP O35904
AAA	-38	SER	-	expression tag	UNP O35904
AAA	-37	TYR	-	expression tag	UNP O35904
AAA	-36	HIS	-	expression tag	UNP O35904
AAA	-35	ASN	-	expression tag	UNP O35904
AAA	-34	HIS	-	expression tag	UNP O35904
AAA	-33	ASN	-	expression tag	UNP O35904
AAA	-32	HIS	-	expression tag	UNP O35904
AAA	-31	ASN	-	expression tag	UNP O35904
AAA	-30	HIS	-	expression tag	UNP O35904
AAA	-29	ASN	-	expression tag	UNP O35904
AAA	-28	HIS	-	expression tag	UNP O35904
AAA	-27	ASN	-	expression tag	UNP O35904
AAA	-26	HIS	-	expression tag	UNP O35904
AAA	-25	ASN	-	expression tag	UNP O35904
AAA	-24	ASP	-	expression tag	UNP O35904
AAA	-23	TYR	-	expression tag	UNP O35904
AAA	-22	ASP	-	expression tag	UNP O35904
AAA	-21	ILE	-	expression tag	UNP O35904
AAA	-20	PRO	-	expression tag	UNP O35904
AAA	-19	THR	-	expression tag	UNP O35904
AAA	-18	THR	-	expression tag	UNP O35904
AAA	-17	GLU	-	expression tag	UNP O35904
AAA	-16	ASN	-	expression tag	UNP O35904
AAA	-15	LEU	-	expression tag	UNP O35904
AAA	-14	TYR	-	expression tag	UNP O35904

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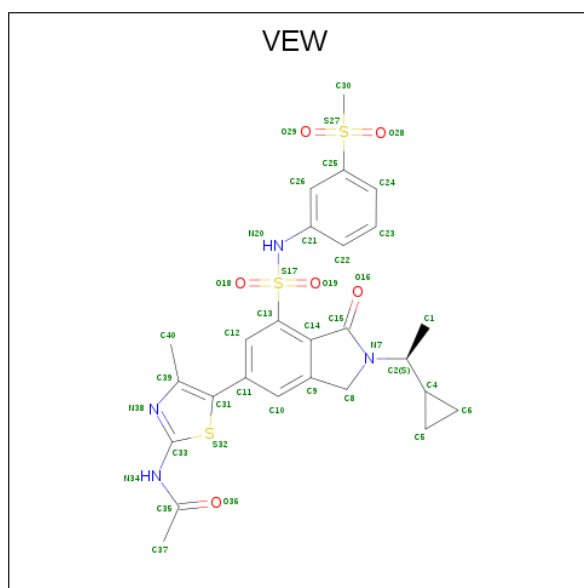
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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-13	PHE	-	expression tag	UNP O35904
AAA	-12	GLN	-	expression tag	UNP O35904
AAA	-11	GLY	-	expression tag	UNP O35904
AAA	-10	ALA	-	expression tag	UNP O35904
AAA	-9	MET	-	expression tag	UNP O35904
AAA	-8	ASP	-	expression tag	UNP O35904
AAA	-7	LEU	-	expression tag	UNP O35904
AAA	99	GLU	-	insertion	UNP O35904
AAA	100	ASN	-	insertion	UNP O35904
AAA	101	LEU	-	insertion	UNP O35904
AAA	102	TYR	-	insertion	UNP O35904
AAA	103	PHE	-	insertion	UNP O35904
AAA	104	GLN	-	insertion	UNP O35904
AAA	105	GLY	-	insertion	UNP O35904
AAA	510A	GLN	-	insertion	UNP O35904

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total Na 1 1	0	0

- Molecule 3 is N-[5-[2-[(1S)-1-cyclopropylethyl]-7-[(3-methylsulfonylphenyl)sulfamoyl]-1-oxidanilidene-3H-isindol-5-yl]-4-methyl-1,3-thiazol-2-yl]ethanamide (three-letter code: VEW) (formula: C₂₆H₂₈N₄O₆S₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	S	0	0
			39	26	4	6	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1532	Total	O	0	0
			1532	1532		

ARG
GLN

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.90Å 64.96Å 116.14Å 90.00° 103.59° 90.00°	Depositor
Resolution (Å)	31.02 – 2.30	Depositor
% Data completeness (in resolution range)	99.9 (31.02-2.30)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.208 , 0.306	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8250	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: NA, VEW

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	AAA	0.68	0/6824	0.77	1/9207 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	AAA	912	PHE	CB-CA-C	6.55	123.50	110.40

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	AAA	6678	0	6656	258	1
2	AAA	1	0	0	0	0
3	AAA	39	0	0	4	0
4	AAA	1532	0	0	187	4
All	All	8250	0	6656	261	5

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 20.

All (261) 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:AAA:900:MET:SD	4:AAA:2359:HOH:O	1.96	1.20
1:AAA:900:MET:SD	4:AAA:1624:HOH:O	1.98	1.19
1:AAA:900:MET:CG	4:AAA:2359:HOH:O	1.90	1.16
1:AAA:900:MET:HG2	4:AAA:2359:HOH:O	1.44	1.15
1:AAA:910:ILE:HG13	4:AAA:2101:HOH:O	1.48	1.13
1:AAA:495:ILE:HD11	1:AAA:562:ALA:HB1	1.37	1.05
1:AAA:886:THR:HG22	4:AAA:2525:HOH:O	1.59	1.02
1:AAA:658:PRO:O	4:AAA:1201:HOH:O	1.82	0.96
1:AAA:932:PHE:HE1	4:AAA:2107:HOH:O	1.50	0.93
1:AAA:355:CYS:SG	4:AAA:1776:HOH:O	2.27	0.93
1:AAA:468:ALA:O	4:AAA:1202:HOH:O	1.87	0.92
1:AAA:900:MET:CE	4:AAA:2359:HOH:O	2.13	0.92
1:AAA:538:VAL:HG13	4:AAA:1225:HOH:O	1.69	0.91
1:AAA:898:ASN:HB3	4:AAA:1836:HOH:O	1.71	0.90
1:AAA:424:MET:SD	4:AAA:1224:HOH:O	2.29	0.90
1:AAA:790:THR:HG22	4:AAA:1959:HOH:O	1.75	0.87
1:AAA:620:LYS:HE2	4:AAA:1585:HOH:O	1.75	0.85
1:AAA:349:HIS:HE1	4:AAA:2136:HOH:O	1.59	0.84
1:AAA:379:ILE:HG22	4:AAA:1776:HOH:O	1.77	0.83
1:AAA:899:ILE:HD11	4:AAA:2031:HOH:O	1.78	0.83
1:AAA:418:ILE:HD13	4:AAA:1215:HOH:O	1.77	0.83
1:AAA:884:VAL:HG22	4:AAA:2107:HOH:O	1.77	0.83
1:AAA:197:GLU:OE2	4:AAA:1203:HOH:O	1.97	0.82
1:AAA:354:LEU:HD22	4:AAA:2048:HOH:O	1.79	0.82
1:AAA:799:VAL:HG13	4:AAA:1266:HOH:O	1.79	0.81
1:AAA:173:PRO:C	4:AAA:1292:HOH:O	2.16	0.81
1:AAA:655:MET:SD	4:AAA:1498:HOH:O	2.37	0.81
1:AAA:616:VAL:HA	4:AAA:1531:HOH:O	1.80	0.81
1:AAA:143:MET:SD	4:AAA:2139:HOH:O	2.39	0.81
1:AAA:545:ALA:HB3	4:AAA:1225:HOH:O	1.82	0.78
1:AAA:589:ASP:OD1	4:AAA:1204:HOH:O	2.01	0.78
1:AAA:664:PHE:CZ	4:AAA:1585:HOH:O	2.36	0.77
1:AAA:418:ILE:HG21	4:AAA:1215:HOH:O	1.83	0.77
1:AAA:394:LEU:HD22	4:AAA:2625:HOH:O	1.84	0.76
1:AAA:1023:LEU:HB2	4:AAA:1537:HOH:O	1.84	0.76
1:AAA:664:PHE:CE2	4:AAA:1585:HOH:O	2.38	0.76
1:AAA:886:THR:O	4:AAA:1205:HOH:O	2.02	0.76
1:AAA:380:SER:HG	1:AAA:382:CYS:HG	1.23	0.75
1:AAA:743:GLU:HG2	4:AAA:1391:HOH:O	1.87	0.74
1:AAA:803:GLN:HG3	4:AAA:1266:HOH:O	1.88	0.74
1:AAA:139:PHE:CZ	4:AAA:2220:HOH:O	2.41	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AAA:1102:VEW:C23	4:AAA:2101:HOH:O	2.35	0.73
1:AAA:906:GLN:HB3	4:AAA:1304:HOH:O	1.88	0.73
1:AAA:546:LEU:HA	4:AAA:2318:HOH:O	1.87	0.73
1:AAA:668:MET:CE	4:AAA:1258:HOH:O	2.36	0.73
1:AAA:661:ALA:HB1	4:AAA:1498:HOH:O	1.90	0.71
1:AAA:274:LEU:HD22	4:AAA:1254:HOH:O	1.90	0.71
1:AAA:799:VAL:CG1	4:AAA:1266:HOH:O	2.35	0.71
1:AAA:795:GLN:OE1	4:AAA:1207:HOH:O	2.08	0.71
1:AAA:332:LYS:NZ	4:AAA:1215:HOH:O	2.23	0.71
1:AAA:847:THR:O	4:AAA:1206:HOH:O	2.08	0.70
1:AAA:941:VAL:HG12	4:AAA:1440:HOH:O	1.90	0.70
1:AAA:955:ARG:NH1	4:AAA:1216:HOH:O	2.23	0.70
1:AAA:894:ARG:HD3	4:AAA:2031:HOH:O	1.92	0.69
1:AAA:751:PHE:CE2	4:AAA:2518:HOH:O	2.44	0.69
1:AAA:912:PHE:CB	1:AAA:913:GLY:HA3	2.23	0.69
1:AAA:620:LYS:O	4:AAA:1208:HOH:O	2.09	0.68
1:AAA:747:GLU:OE2	4:AAA:1210:HOH:O	2.12	0.68
1:AAA:358:VAL:HG22	1:AAA:377:PHE:CE1	2.28	0.68
1:AAA:969:ARG:CZ	4:AAA:1326:HOH:O	2.40	0.68
1:AAA:951:GLU:OE1	4:AAA:1209:HOH:O	2.10	0.68
1:AAA:751:PHE:HE2	4:AAA:2518:HOH:O	1.75	0.68
1:AAA:135:GLU:OE1	4:AAA:1211:HOH:O	2.12	0.67
1:AAA:365:VAL:HG22	4:AAA:1381:HOH:O	1.94	0.67
1:AAA:633:LEU:CD1	4:AAA:1531:HOH:O	2.41	0.67
1:AAA:884:VAL:HA	4:AAA:2107:HOH:O	1.93	0.67
1:AAA:549:LEU:HG	1:AAA:564:MET:CE	2.24	0.67
1:AAA:965:THR:HB	4:AAA:1326:HOH:O	1.93	0.67
1:AAA:724:TYR:HA	4:AAA:1780:HOH:O	1.94	0.67
1:AAA:556:ASN:HA	4:AAA:2048:HOH:O	1.94	0.67
1:AAA:397:VAL:HG12	4:AAA:2331:HOH:O	1.95	0.66
1:AAA:881:GLY:HA2	4:AAA:1901:HOH:O	1.95	0.66
1:AAA:339:MET:N	4:AAA:1230:HOH:O	2.29	0.65
1:AAA:494:LEU:C	1:AAA:495:ILE:HD12	2.17	0.65
1:AAA:571:TRP:CH2	4:AAA:2318:HOH:O	2.49	0.65
1:AAA:425:LEU:HA	4:AAA:1719:HOH:O	1.96	0.64
1:AAA:962:ARG:NE	4:AAA:1213:HOH:O	2.20	0.64
1:AAA:794:ILE:HD12	4:AAA:1959:HOH:O	1.97	0.64
1:AAA:976:HIS:HE1	4:AAA:2273:HOH:O	1.80	0.63
1:AAA:907:LEU:C	1:AAA:907:LEU:HD23	2.19	0.63
1:AAA:655:MET:CE	4:AAA:1498:HOH:O	2.46	0.63
1:AAA:633:LEU:HD11	4:AAA:1531:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:328:ILE:HB	1:AAA:472:VAL:HG23	1.82	0.62
1:AAA:761:ILE:HG12	4:AAA:1212:HOH:O	1.99	0.62
1:AAA:385:PRO:HD3	4:AAA:2048:HOH:O	1.99	0.62
1:AAA:794:ILE:HG22	4:AAA:2088:HOH:O	2.00	0.62
1:AAA:675:SER:HB3	4:AAA:1697:HOH:O	2.00	0.61
1:AAA:895:HIS:O	1:AAA:898:ASN:OD1	2.18	0.61
1:AAA:900:MET:HE3	4:AAA:2359:HOH:O	1.85	0.61
1:AAA:590:CYS:SG	4:AAA:1521:HOH:O	2.09	0.60
1:AAA:617:GLN:HE21	1:AAA:984:ALA:HA	1.66	0.60
3:AAA:1102:VEW:C37	3:AAA:1102:VEW:S32	2.89	0.60
1:AAA:762:MET:HB3	4:AAA:1302:HOH:O	2.02	0.60
1:AAA:912:PHE:HB2	1:AAA:913:GLY:HA3	1.83	0.60
1:AAA:979:ALA:HB2	4:AAA:2256:HOH:O	2.01	0.60
1:AAA:662:LEU:HD11	4:AAA:2663:HOH:O	2.02	0.59
1:AAA:454:ASN:N	4:AAA:1247:HOH:O	2.34	0.59
1:AAA:759:LEU:O	4:AAA:1212:HOH:O	2.17	0.59
1:AAA:349:HIS:CE1	4:AAA:2136:HOH:O	2.41	0.59
1:AAA:898:ASN:HA	4:AAA:2101:HOH:O	2.02	0.59
1:AAA:785:ARG:NH1	4:AAA:1231:HOH:O	2.29	0.58
1:AAA:956:PHE:N	4:AAA:1248:HOH:O	2.35	0.58
1:AAA:665:GLY:N	4:AAA:1258:HOH:O	2.36	0.58
1:AAA:728:LEU:HG	4:AAA:1780:HOH:O	2.03	0.58
1:AAA:154:ARG:NE	4:AAA:1257:HOH:O	2.36	0.58
1:AAA:495:ILE:O	1:AAA:497:GLU:N	2.36	0.58
1:AAA:756:MET:HE3	4:AAA:2294:HOH:O	2.02	0.58
1:AAA:549:LEU:HG	1:AAA:564:MET:HE3	1.84	0.58
1:AAA:620:LYS:CE	4:AAA:1585:HOH:O	2.43	0.58
3:AAA:1102:VEW:C33	4:AAA:1624:HOH:O	2.51	0.57
1:AAA:720:ARG:NH1	4:AAA:1261:HOH:O	2.38	0.57
1:AAA:328:ILE:HB	1:AAA:472:VAL:CG2	2.34	0.57
1:AAA:814:GLY:HA3	4:AAA:1932:HOH:O	2.05	0.57
1:AAA:758:PRO:HD3	4:AAA:2018:HOH:O	2.05	0.57
1:AAA:332:LYS:HA	4:AAA:1871:HOH:O	2.04	0.56
1:AAA:367:SER:CB	1:AAA:368:GLU:C	2.73	0.56
1:AAA:172:GLU:HG3	1:AAA:263:CYS:SG	2.46	0.56
1:AAA:223:LYS:O	1:AAA:226:THR:OG1	2.22	0.56
1:AAA:617:GLN:NE2	1:AAA:984:ALA:HA	2.21	0.56
1:AAA:391:CYS:HB2	4:AAA:1535:HOH:O	2.06	0.55
1:AAA:339:MET:N	4:AAA:1273:HOH:O	2.39	0.55
1:AAA:550:LEU:O	1:AAA:553:THR:HG23	2.07	0.55
1:AAA:685:GLN:HG3	4:AAA:1720:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:358:VAL:HG12	4:AAA:2426:HOH:O	2.06	0.55
1:AAA:728:LEU:HD23	4:AAA:1813:HOH:O	2.06	0.54
1:AAA:209:THR:HB	1:AAA:257:CYS:HB3	1.88	0.54
1:AAA:663:ARG:HD2	4:AAA:1735:HOH:O	2.07	0.54
1:AAA:567:LEU:HD12	4:AAA:1969:HOH:O	2.06	0.54
1:AAA:367:SER:HB2	1:AAA:368:GLU:C	2.28	0.54
1:AAA:173:PRO:HB3	4:AAA:1266:HOH:O	2.07	0.54
1:AAA:661:ALA:CB	4:AAA:1498:HOH:O	2.50	0.54
1:AAA:495:ILE:HD11	1:AAA:562:ALA:CB	2.24	0.53
1:AAA:248:GLU:HG3	4:AAA:2034:HOH:O	2.07	0.53
1:AAA:495:ILE:C	1:AAA:497:GLU:H	2.11	0.52
1:AAA:666:LEU:HD21	4:AAA:2663:HOH:O	2.09	0.52
1:AAA:957:ARG:NH1	4:AAA:1279:HOH:O	2.41	0.52
1:AAA:1023:LEU:HD23	4:AAA:1343:HOH:O	2.09	0.52
1:AAA:539:GLN:NE2	1:AAA:570:SER:OG	2.42	0.52
1:AAA:624:TYR:HB3	4:AAA:1265:HOH:O	2.08	0.52
1:AAA:170:GLN:N	4:AAA:1286:HOH:O	2.43	0.52
1:AAA:475:LEU:HD22	4:AAA:2414:HOH:O	2.08	0.52
1:AAA:349:HIS:HB2	1:AAA:354:LEU:HD21	1.93	0.51
1:AAA:380:SER:OG	1:AAA:382:CYS:SG	2.42	0.51
1:AAA:367:SER:HB3	1:AAA:368:GLU:O	2.11	0.51
1:AAA:969:ARG:NE	4:AAA:1290:HOH:O	2.44	0.50
1:AAA:894:ARG:HB3	4:AAA:2031:HOH:O	2.12	0.50
1:AAA:495:ILE:C	1:AAA:497:GLU:N	2.64	0.50
1:AAA:360:SER:HB2	4:AAA:1592:HOH:O	2.12	0.50
1:AAA:367:SER:HB3	1:AAA:368:GLU:HB3	1.93	0.50
1:AAA:495:ILE:HD12	1:AAA:495:ILE:N	2.27	0.49
1:AAA:680:LYS:NZ	4:AAA:1295:HOH:O	2.44	0.49
1:AAA:389:ARG:NH2	4:AAA:1224:HOH:O	2.44	0.49
1:AAA:491:ILE:O	1:AAA:495:ILE:CD1	2.60	0.49
1:AAA:756:MET:HE2	1:AAA:780:ASN:O	2.11	0.49
1:AAA:786:GLN:HE22	1:AAA:988:GLU:CD	2.16	0.49
1:AAA:253:ASN:HB3	4:AAA:2199:HOH:O	2.13	0.49
1:AAA:545:ALA:HA	4:AAA:1641:HOH:O	2.11	0.49
1:AAA:889:LEU:HB2	4:AAA:1205:HOH:O	2.12	0.49
1:AAA:833:THR:HG22	4:AAA:2359:HOH:O	2.14	0.48
1:AAA:759:LEU:O	1:AAA:777:ILE:HA	2.13	0.48
1:AAA:792:GLN:HB3	4:AAA:1925:HOH:O	2.12	0.48
1:AAA:437:ARG:HB2	4:AAA:2352:HOH:O	2.12	0.48
1:AAA:962:ARG:NH2	4:AAA:1213:HOH:O	2.46	0.48
1:AAA:316:LEU:HD12	1:AAA:317:TRP:CD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:136:VAL:HG13	4:AAA:2663:HOH:O	2.14	0.48
1:AAA:688:ALA:HA	4:AAA:1813:HOH:O	2.13	0.48
1:AAA:192:VAL:HG13	1:AAA:272:PRO:HB2	1.95	0.48
1:AAA:389:ARG:HB3	4:AAA:2290:HOH:O	2.14	0.48
1:AAA:475:LEU:HD13	4:AAA:2352:HOH:O	2.14	0.48
1:AAA:684:LYS:HE3	4:AAA:1430:HOH:O	2.14	0.48
1:AAA:935:THR:HB	1:AAA:938:PHE:CD2	2.49	0.48
1:AAA:291:ASN:ND2	4:AAA:1305:HOH:O	2.46	0.47
1:AAA:628:GLU:HG2	4:AAA:1952:HOH:O	2.13	0.47
1:AAA:709:PRO:HA	4:AAA:1380:HOH:O	2.14	0.47
1:AAA:691:LYS:HE3	4:AAA:1450:HOH:O	2.15	0.47
1:AAA:725:MET:HE3	4:AAA:1221:HOH:O	2.14	0.47
1:AAA:247:HIS:HB2	1:AAA:738:SER:HA	1.96	0.47
1:AAA:550:LEU:HA	1:AAA:553:THR:CG2	2.44	0.47
1:AAA:154:ARG:HD2	1:AAA:165:TYR:CZ	2.49	0.47
1:AAA:633:LEU:HD13	4:AAA:1531:HOH:O	2.09	0.47
1:AAA:154:ARG:CD	4:AAA:1257:HOH:O	2.63	0.46
1:AAA:386:ARG:HG3	1:AAA:387:MET:HE2	1.96	0.46
1:AAA:389:ARG:NE	4:AAA:1224:HOH:O	2.48	0.46
1:AAA:828:VAL:CG1	1:AAA:902:ARG:HD3	2.45	0.46
1:AAA:832:ASP:HB2	4:AAA:2238:HOH:O	2.15	0.46
1:AAA:803:GLN:CG	4:AAA:1266:HOH:O	2.54	0.46
1:AAA:961:GLU:O	1:AAA:965:THR:HG23	2.15	0.46
1:AAA:213:PRO:O	1:AAA:217:MET:HG3	2.16	0.46
1:AAA:250:LEU:HB2	4:AAA:1254:HOH:O	2.16	0.46
1:AAA:803:GLN:CD	4:AAA:1266:HOH:O	2.54	0.46
1:AAA:387:MET:HE3	1:AAA:590:CYS:HB3	1.96	0.46
1:AAA:888:VAL:HG21	1:AAA:967:LEU:HD12	1.97	0.46
1:AAA:490:LYS:NZ	4:AAA:1321:HOH:O	2.49	0.45
1:AAA:109:VAL:N	4:AAA:1330:HOH:O	2.50	0.45
1:AAA:511:LEU:HD23	1:AAA:530:LEU:HD22	1.98	0.45
1:AAA:194:VAL:HG21	1:AAA:216:LEU:CD2	2.46	0.45
1:AAA:555:TRP:HB2	4:AAA:2008:HOH:O	2.17	0.45
1:AAA:715:MET:O	1:AAA:719:MET:HG3	2.16	0.45
1:AAA:365:VAL:HG11	4:AAA:1472:HOH:O	2.16	0.45
1:AAA:391:CYS:HB3	4:AAA:1256:HOH:O	2.17	0.44
1:AAA:485:PHE:HB2	4:AAA:1715:HOH:O	2.17	0.44
1:AAA:984:ALA:HB3	1:AAA:986:LEU:HD13	1.99	0.44
1:AAA:216:LEU:HD12	1:AAA:256:LEU:HD11	2.00	0.44
1:AAA:757:LYS:HE3	4:AAA:2518:HOH:O	2.17	0.44
1:AAA:780:ASN:HA	1:AAA:821:ARG:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:342:VAL:HA	4:AAA:1399:HOH:O	2.17	0.44
1:AAA:616:VAL:O	1:AAA:619:LEU:HB2	2.18	0.44
1:AAA:471:LEU:CG	4:AAA:2625:HOH:O	2.66	0.44
1:AAA:1020:ASN:HA	4:AAA:1343:HOH:O	2.17	0.44
1:AAA:549:LEU:HG	1:AAA:564:MET:HE1	1.98	0.44
1:AAA:584:ASP:OD1	4:AAA:1214:HOH:O	2.21	0.43
1:AAA:713:GLU:O	1:AAA:717:MET:HG3	2.18	0.43
1:AAA:969:ARG:NH1	4:AAA:1326:HOH:O	2.49	0.43
1:AAA:619:LEU:HD23	1:AAA:629:LEU:HD23	2.00	0.43
1:AAA:779:LYS:N	4:AAA:1237:HOH:O	2.51	0.43
1:AAA:799:VAL:HG12	4:AAA:1266:HOH:O	2.13	0.43
1:AAA:154:ARG:HD2	1:AAA:165:TYR:CE2	2.53	0.43
1:AAA:119:LEU:HD11	4:AAA:2674:HOH:O	2.18	0.43
1:AAA:489:GLU:O	1:AAA:493:GLU:HB2	2.19	0.43
1:AAA:211:ASP:O	1:AAA:256:LEU:HG	2.19	0.43
1:AAA:453:LEU:HG	4:AAA:1219:HOH:O	2.18	0.43
1:AAA:471:LEU:HG	4:AAA:2625:HOH:O	2.18	0.43
1:AAA:434:THR:HG21	1:AAA:477:GLU:HA	2.01	0.42
1:AAA:691:LYS:NZ	4:AAA:1351:HOH:O	2.52	0.42
1:AAA:139:PHE:CE1	4:AAA:2220:HOH:O	2.70	0.42
1:AAA:834:ILE:HD12	1:AAA:855:LEU:HD11	2.01	0.42
1:AAA:430:ASP:HA	4:AAA:1715:HOH:O	2.20	0.42
1:AAA:434:THR:HA	1:AAA:435:GLY:HA2	1.88	0.42
1:AAA:912:PHE:HB3	1:AAA:913:GLY:HA3	2.00	0.42
1:AAA:339:MET:O	1:AAA:365:VAL:HG23	2.19	0.42
1:AAA:386:ARG:HG3	1:AAA:387:MET:CE	2.48	0.42
1:AAA:437:ARG:NH2	4:AAA:1358:HOH:O	2.53	0.42
1:AAA:495:ILE:HG12	1:AAA:563:GLN:HA	2.02	0.42
1:AAA:884:VAL:CG2	4:AAA:2107:HOH:O	2.53	0.42
1:AAA:1016:ARG:HB3	4:AAA:1279:HOH:O	2.19	0.42
1:AAA:494:LEU:HD21	4:AAA:2165:HOH:O	2.20	0.42
1:AAA:912:PHE:CD2	4:AAA:1226:HOH:O	2.71	0.42
1:AAA:226:THR:HG22	4:AAA:2681:HOH:O	2.19	0.42
1:AAA:495:ILE:O	1:AAA:497:GLU:O	2.37	0.42
1:AAA:493:GLU:HG2	4:AAA:1896:HOH:O	2.19	0.42
1:AAA:367:SER:HB3	1:AAA:368:GLU:C	2.39	0.42
1:AAA:459:VAL:HG11	4:AAA:1224:HOH:O	2.19	0.42
1:AAA:666:LEU:HD22	4:AAA:1667:HOH:O	2.20	0.42
1:AAA:894:ARG:NH2	4:AAA:1369:HOH:O	2.53	0.42
1:AAA:705:LYS:HD3	4:AAA:1401:HOH:O	2.18	0.41
1:AAA:744:VAL:HG12	4:AAA:1221:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:440:TYR:CG	1:AAA:465:THR:HG22	2.55	0.41
1:AAA:912:PHE:CB	1:AAA:913:GLY:CA	2.97	0.41
1:AAA:872:ILE:HG23	4:AAA:1440:HOH:O	2.20	0.41
1:AAA:912:PHE:CE2	4:AAA:1226:HOH:O	2.57	0.41
1:AAA:894:ARG:HG3	4:AAA:2508:HOH:O	2.20	0.41
1:AAA:982:ARG:NH2	1:AAA:991:CYS:HA	2.36	0.41
1:AAA:728:LEU:CD2	4:AAA:1813:HOH:O	2.66	0.41
1:AAA:117:ILE:HD11	4:AAA:1781:HOH:O	2.21	0.41
1:AAA:815:CYS:SG	3:AAA:1102:VEW:C5	3.09	0.41
1:AAA:965:THR:CB	4:AAA:1326:HOH:O	2.60	0.41
1:AAA:626:ASP:HB3	4:AAA:2438:HOH:O	2.21	0.40
1:AAA:663:ARG:NH1	4:AAA:1281:HOH:O	2.41	0.40
1:AAA:708:LYS:N	1:AAA:709:PRO:CD	2.84	0.40
1:AAA:790:THR:N	4:AAA:1275:HOH:O	2.54	0.40
1:AAA:282:ILE:HG22	4:AAA:1827:HOH:O	2.21	0.40

All (5) 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:AAA:714:MET:SD	1:AAA:714:MET:SD[2_555]	1.63	0.57
4:AAA:1450:HOH:O	4:AAA:1808:HOH:O[2_555]	2.00	0.20
4:AAA:1609:HOH:O	4:AAA:2241:HOH:O[4_445]	2.12	0.08
4:AAA:1825:HOH:O	4:AAA:2151:HOH:O[3_545]	2.17	0.03
4:AAA:2475:HOH:O	4:AAA:2628:HOH:O[3_455]	2.18	0.02

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	AAA	806/1084 (74%)	768 (95%)	34 (4%)	4 (0%)	29	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	496	THR
1	AAA	893	ASP
1	AAA	367	SER
1	AAA	913	GLY

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	AAA	734/962 (76%)	701 (96%)	33 (4%)	27	39

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	111	LYS
1	AAA	188	ARG
1	AAA	203	PHE
1	AAA	206	GLN
1	AAA	216	LEU
1	AAA	223	LYS
1	AAA	226	THR
1	AAA	316	LEU
1	AAA	332	LYS
1	AAA	340	LYS
1	AAA	352	GLU
1	AAA	356	LYS
1	AAA	367	SER
1	AAA	374	ARG
1	AAA	415	ASP
1	AAA	423	LEU
1	AAA	436	GLU
1	AAA	472	VAL
1	AAA	475	LEU
1	AAA	497	GLU
1	AAA	517	ARG

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Mol	Chain	Res	Type
1	AAA	523	LEU
1	AAA	553	THR
1	AAA	560	ASP
1	AAA	634	LEU
1	AAA	659	SER
1	AAA	816	LEU
1	AAA	841	LYS
1	AAA	843	ASN
1	AAA	855	LEU
1	AAA	895	HIS
1	AAA	915	PHE
1	AAA	962	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
3	VEW	AAA	1102	-	37,43,43	1.16	4 (10%)	45,67,67	3.76	13 (28%)

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
3	VEW	AAA	1102	-	-	10/31/47/47	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	1102	VEW	C10-C9	-2.68	1.34	1.39
3	AAA	1102	VEW	C33-N34	2.65	1.41	1.36
3	AAA	1102	VEW	C12-C13	-2.64	1.35	1.39
3	AAA	1102	VEW	C21-N20	-2.43	1.39	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	1102	VEW	C9-C8-N7	16.36	107.63	102.18
3	AAA	1102	VEW	C8-N7-C15	-11.73	108.30	113.12
3	AAA	1102	VEW	O28-S27-C25	-8.89	101.00	108.25
3	AAA	1102	VEW	C37-C35-N34	4.73	121.92	114.98
3	AAA	1102	VEW	O29-S27-C25	4.26	111.72	108.25
3	AAA	1102	VEW	O29-S27-O28	3.85	124.55	117.92
3	AAA	1102	VEW	O16-C15-C14	-3.56	124.02	129.09
3	AAA	1102	VEW	C2-N7-C15	3.41	126.56	122.91
3	AAA	1102	VEW	O36-C35-C37	-3.36	115.81	122.06
3	AAA	1102	VEW	C13-S17-N20	2.89	110.65	107.27
3	AAA	1102	VEW	C11-C10-C9	-2.88	117.59	121.90
3	AAA	1102	VEW	C12-C13-C14	-2.63	117.93	120.72
3	AAA	1102	VEW	C21-C26-C25	2.51	120.78	118.89

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	1102	VEW	C24-C25-S27-C30
3	AAA	1102	VEW	C26-C25-S27-C30

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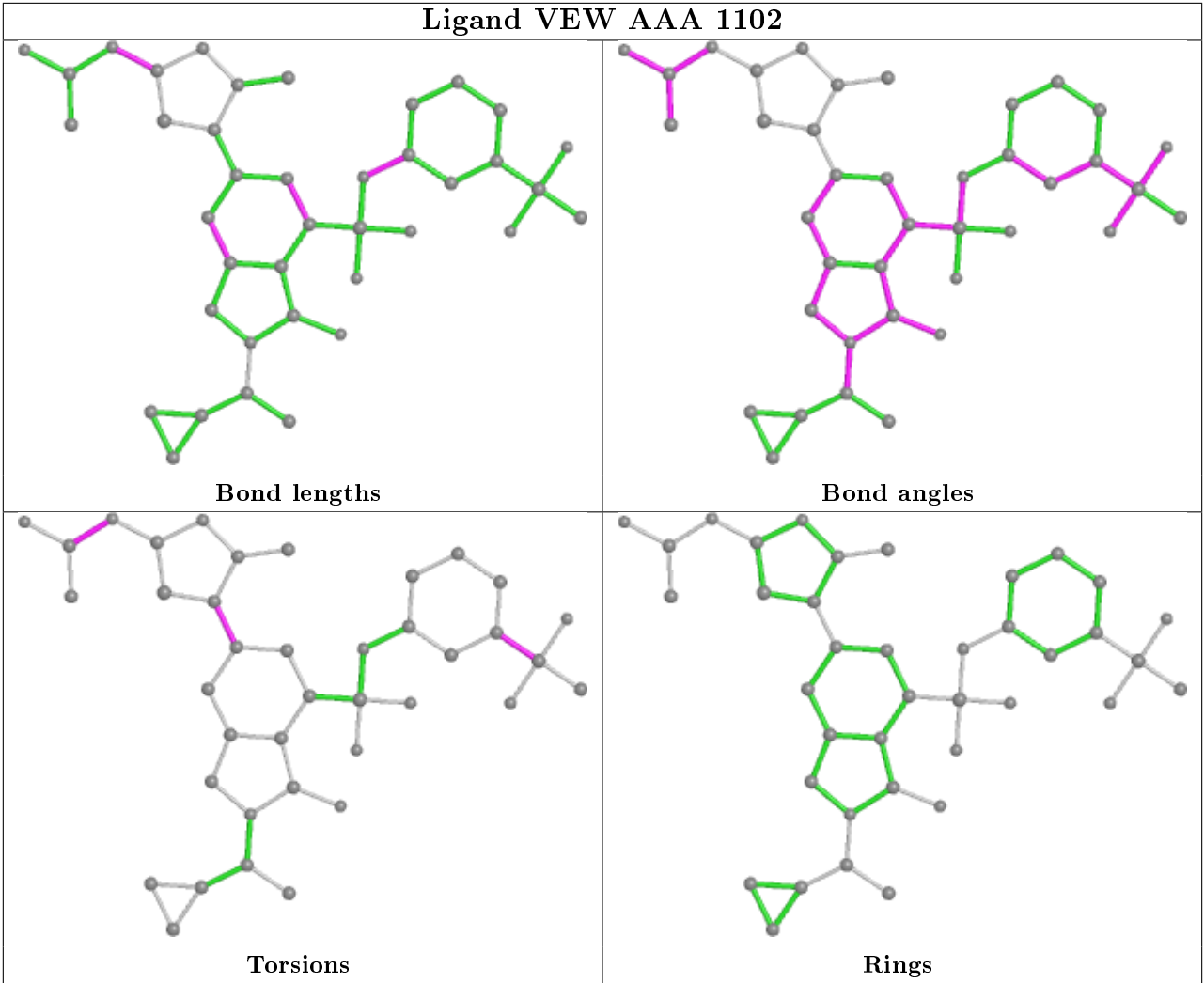
Mol	Chain	Res	Type	Atoms
3	AAA	1102	VEW	C24-C25-S27-O28
3	AAA	1102	VEW	C26-C25-S27-O28
3	AAA	1102	VEW	C37-C35-N34-C33
3	AAA	1102	VEW	O36-C35-N34-C33
3	AAA	1102	VEW	C26-C25-S27-O29
3	AAA	1102	VEW	C24-C25-S27-O29
3	AAA	1102	VEW	C12-C11-C31-C39
3	AAA	1102	VEW	C10-C11-C31-C39

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	1102	VEW	4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AAA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AAA	497:GLU	C	509:GLU	N	22.95

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.