



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:54 PM UTC

PDB ID : 2GMV / pdb_00002gmv
Title : PEPCK complex with a GTP-competitive inhibitor
Authors : Dunten, P.
Deposited on : 2006-04-07
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 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

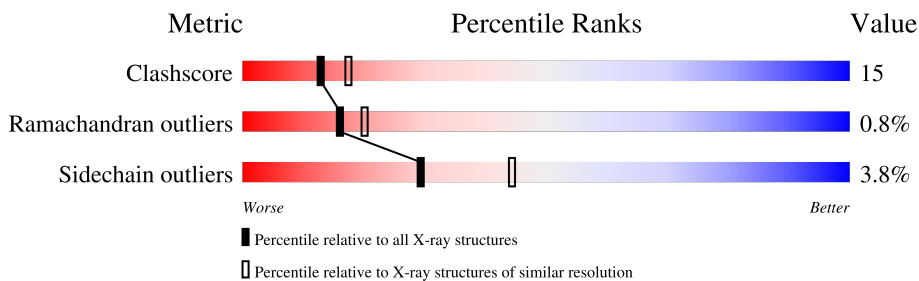
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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	A	625	 75% 21% . .
1	B	625	 59% 34% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9624 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 Phosphoenolpyruvate carboxykinase, cytosolic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	0	0
			4715	3009	806	865	35			
1	B	602	Total	C	N	O	S	0	0	0
			4715	3009	806	865	35			

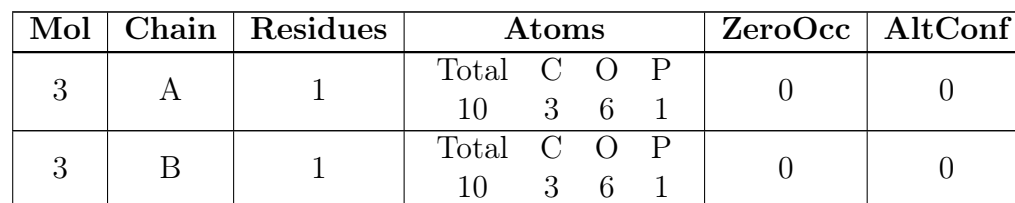
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P35558
A	-1	GLU	-	cloning artifact	UNP P35558
A	0	LEU	-	cloning artifact	UNP P35558
A	184	LEU	VAL	variant	UNP P35558
A	267	VAL	ILE	variant	UNP P35558
A	586	ASP	GLU	variant	UNP P35558
A	597	VAL	GLU	variant	UNP P35558
B	-2	GLY	-	cloning artifact	UNP P35558
B	-1	GLU	-	cloning artifact	UNP P35558
B	0	LEU	-	cloning artifact	UNP P35558
B	184	LEU	VAL	variant	UNP P35558
B	267	VAL	ILE	variant	UNP P35558
B	586	ASP	GLU	variant	UNP P35558
B	597	VAL	GLU	variant	UNP P35558

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

- Molecule 3 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: C₃H₅O₆P).



- # UN8

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	0	0
			40	27	1	7	4	1		

- Molecule 5 is water.

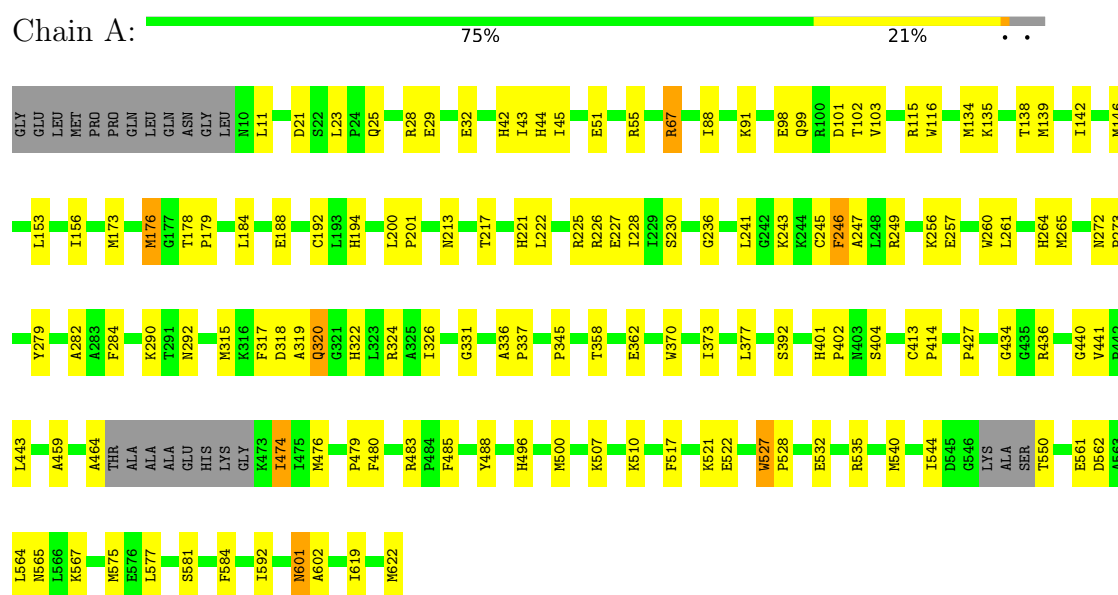
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	107	Total 107	O 107	0	0
5	B	25	Total 25	O 25	0	0

3 Residue-property plots

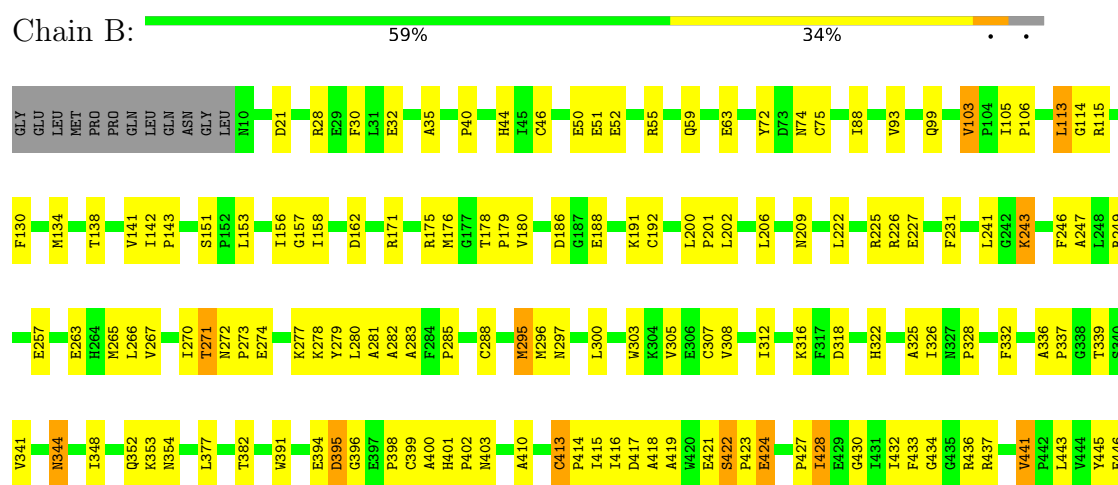
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

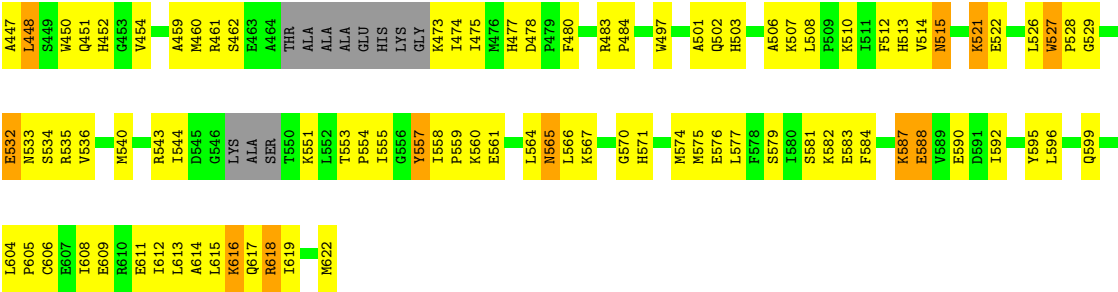
Note EDS was not executed.

- Molecule 1: Phosphoenolpyruvate carboxykinase, cytosolic



- Molecule 1: Phosphoenolpyruvate carboxykinase, cytosolic





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	128.01Å 66.13Å 137.36Å 90.00° 145.09° 90.00°	Depositor
Resolution (Å)	39.31 – 2.30	Depositor
% Data completeness (in resolution range)	75.7 (39.31-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX, REFMAC 5.1.24	Depositor
R, R_{free}	0.217 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9624	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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: UN8, MN, PEP

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	0.42	0/4836	0.82	5/6549 (0.1%)
1	B	0.38	0/4836	0.87	11/6549 (0.2%)
All	All	0.40	0/9672	0.84	16/13098 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	ASN	CA-C-N	6.68	126.19	119.24
1	B	344	ASN	C-N-CA	6.68	126.19	119.24
1	A	527	TRP	CA-C-N	6.59	126.28	119.56
1	A	527	TRP	C-N-CA	6.59	126.28	119.56
1	A	601	ASN	CB-CA-C	-5.80	109.34	117.23
1	B	413	CYS	CA-C-N	5.58	125.04	119.24
1	B	413	CYS	C-N-CA	5.58	125.04	119.24
1	B	527	TRP	CA-C-N	5.35	125.02	119.56
1	B	527	TRP	C-N-CA	5.35	125.02	119.56
1	B	441	VAL	CA-C-N	5.31	125.25	119.78
1	B	441	VAL	C-N-CA	5.31	125.25	119.78
1	B	587	LYS	N-CA-C	-5.21	105.69	111.36
1	B	422	SER	CA-C-N	5.17	124.97	119.28
1	B	422	SER	C-N-CA	5.17	124.97	119.28
1	A	441	VAL	CA-C-N	5.04	125.03	119.89
1	A	441	VAL	C-N-CA	5.04	125.03	119.89

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	4715	0	4658	83	0
1	B	4715	0	4658	206	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	2	0	0
3	B	10	0	2	0	0
4	A	40	0	28	1	0
5	A	107	0	0	1	0
5	B	25	0	0	0	0
All	All	9624	0	9348	284	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (284) 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:448:LEU:HD21	1:B:618:ARG:NH1	1.68	1.09
1:B:448:LEU:HD21	1:B:618:ARG:HH12	1.20	0.98
1:B:272:ASN:HB2	1:B:273:PRO:HD2	1.46	0.95
1:B:295:MET:HA	1:B:415:ILE:HD11	1.53	0.90
1:B:527:TRP:CD1	1:B:529:GLY:HA2	2.09	0.87
1:B:437:ARG:HB2	1:B:515:ASN:HD21	1.38	0.86
1:B:613:LEU:HA	1:B:616:LYS:HB3	1.55	0.86
1:A:319:ALA:HB1	1:B:423:PRO:HB2	1.56	0.85
1:B:543:ARG:HA	1:B:543:ARG:HH11	1.41	0.85
1:B:434:GLY:HA2	1:B:513:HIS:NE2	1.93	0.83
1:B:437:ARG:HB2	1:B:515:ASN:ND2	1.94	0.81
1:B:604:LEU:HD12	1:B:605:PRO:HD2	1.63	0.80
1:B:272:ASN:CB	1:B:273:PRO:HD2	2.12	0.78
1:B:583:GLU:O	1:B:587:LYS:HG2	1.82	0.78
1:B:265:MET:HG2	1:B:283:ALA:HB2	1.69	0.75
1:A:257:GLU:HB3	1:B:188:GLU:HG3	1.70	0.73
1:B:460:MET:HG3	1:B:480:PHE:H	1.53	0.73
1:B:527:TRP:HD1	1:B:529:GLY:HA2	1.53	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:LYS:HD3	1:B:558:ILE:HD11	1.70	0.72
1:B:554:PRO:HB3	1:B:618:ARG:O	1.90	0.72
1:B:501:ALA:HA	1:B:508:LEU:HD11	1.71	0.72
1:B:443:LEU:HD13	1:B:577:LEU:HD21	1.73	0.71
1:B:206:LEU:HD23	1:B:209:ASN:HA	1.73	0.70
1:B:271:THR:HG22	1:B:272:ASN:H	1.55	0.70
1:B:527:TRP:CD1	1:B:529:GLY:H	2.10	0.70
1:B:153:LEU:HD12	1:B:326:ILE:HG23	1.73	0.70
1:B:175:ARG:HH21	1:B:421:GLU:HG3	1.54	0.70
1:A:21:ASP:HA	1:A:28:ARG:HH12	1.56	0.69
1:B:142:ILE:HG23	1:B:176:MET:HG3	1.74	0.69
1:B:551:LYS:HB3	1:B:558:ILE:HG13	1.74	0.69
1:B:153:LEU:HD21	1:B:316:LYS:HB3	1.74	0.68
1:A:102:THR:HG22	1:A:103:VAL:HG13	1.76	0.68
1:B:307:CYS:O	1:B:416:ILE:HD12	1.94	0.67
1:B:510:LYS:HE3	1:B:544:ILE:HA	1.76	0.67
1:B:527:TRP:CD1	1:B:529:GLY:CA	2.78	0.67
1:B:559:PRO:HB2	1:B:564:LEU:HD11	1.76	0.66
1:B:613:LEU:HA	1:B:616:LYS:CB	2.25	0.66
1:A:345:PRO:HD2	5:A:771:HOH:O	1.96	0.66
1:A:51:GLU:HG3	1:A:55:ARG:NH1	2.11	0.65
1:B:451:GLN:O	1:B:611:GLU:HG3	1.97	0.65
1:A:243:LYS:O	1:A:247:ALA:HB3	1.97	0.65
1:B:609:GLU:O	1:B:612:ILE:HB	1.97	0.64
1:B:271:THR:HA	1:B:277:LYS:HA	1.80	0.64
1:B:332:PHE:CE1	1:B:410:ALA:HA	2.33	0.64
1:B:30:PHE:CE1	1:B:191:LYS:HB3	2.34	0.63
1:B:134:MET:HG2	1:B:162:ASP:HB3	1.80	0.63
1:A:21:ASP:HA	1:A:28:ARG:NH1	2.14	0.63
1:A:153:LEU:HB2	1:A:326:ILE:HD13	1.81	0.62
1:B:336:ALA:HB3	1:B:337:PRO:HD3	1.82	0.61
1:A:459:ALA:HB1	1:A:592:ILE:HD13	1.82	0.61
1:B:543:ARG:HA	1:B:543:ARG:NH1	2.12	0.60
1:B:555:ILE:HG22	1:B:615:LEU:HD11	1.82	0.60
1:B:280:LEU:HD22	1:B:432:ILE:HD11	1.83	0.60
1:B:175:ARG:NH2	1:B:421:GLU:HG3	2.17	0.60
1:B:437:ARG:HG3	1:B:441:VAL:HG21	1.84	0.60
1:A:318:ASP:OD2	1:A:324:ARG:HD2	2.02	0.60
1:A:188:GLU:HG2	1:B:257:GLU:HB3	1.83	0.59
1:B:448:LEU:CD2	1:B:618:ARG:HH12	2.04	0.59
1:A:134:MET:SD	1:A:139:MET:HE3	2.42	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:MET:HG3	1:B:344:ASN:HD21	1.66	0.59
1:B:454:VAL:HG12	1:B:608:ILE:HD11	1.85	0.59
1:B:273:PRO:HD3	1:B:303:TRP:NE1	2.18	0.59
1:A:619:ILE:O	1:A:622:MET:HG2	2.03	0.59
1:B:344:ASN:O	1:B:348:ILE:HG12	2.03	0.59
1:B:434:GLY:HA2	1:B:513:HIS:CE1	2.38	0.59
1:B:434:GLY:HA2	1:B:513:HIS:CD2	2.37	0.58
1:A:436:ARG:HG3	1:A:517:PHE:CG	2.38	0.58
1:B:99:GLN:HG2	1:B:105:ILE:HD11	1.84	0.58
1:B:595:TYR:CE1	1:B:599:GLN:HG3	2.38	0.58
1:B:510:LYS:CE	1:B:544:ILE:HA	2.33	0.58
1:A:292:ASN:HB3	4:A:703:UN8:C23	2.34	0.57
1:B:459:ALA:HB1	1:B:592:ILE:HD13	1.85	0.57
1:B:151:SER:HB2	1:B:423:PRO:HA	1.86	0.57
1:B:527:TRP:CD1	1:B:529:GLY:N	2.72	0.57
1:B:283:ALA:O	1:B:460:MET:HE1	2.04	0.57
1:B:564:LEU:HD12	1:B:574:MET:HE1	1.86	0.57
1:B:582:LYS:HE3	1:B:619:ILE:O	2.05	0.56
1:A:370:TRP:CD1	1:A:373:ILE:HB	2.40	0.56
1:B:513:HIS:CE1	1:B:514:VAL:O	2.59	0.56
1:B:134:MET:HE2	1:B:162:ASP:HB3	1.88	0.56
1:A:246:PHE:C	1:A:246:PHE:HD1	2.14	0.56
1:A:153:LEU:HD12	1:A:326:ILE:HG23	1.88	0.56
1:A:246:PHE:C	1:A:246:PHE:CD1	2.85	0.55
1:B:503:HIS:O	1:B:506:ALA:HB2	2.06	0.55
1:A:496:HIS:HB2	1:B:186:ASP:OD2	2.07	0.55
1:B:295:MET:HA	1:B:415:ILE:CD1	2.31	0.55
1:B:446:GLU:HB3	1:B:557:TYR:HD1	1.70	0.55
1:B:441:VAL:HG23	1:B:584:PHE:CZ	2.42	0.54
1:B:247:ALA:HB1	1:B:312:ILE:HG21	1.90	0.54
1:A:565:ASN:OD1	1:A:567:LYS:HG3	2.07	0.54
1:B:613:LEU:HD23	1:B:616:LYS:HE3	1.90	0.54
1:B:282:ALA:HB2	1:B:432:ILE:HB	1.88	0.53
1:A:178:THR:N	1:A:179:PRO:CD	2.71	0.53
1:B:448:LEU:HD21	1:B:618:ARG:CZ	2.35	0.53
1:B:575:MET:O	1:B:579:SER:HB3	2.08	0.53
1:A:142:ILE:CG2	1:A:176:MET:HG3	2.38	0.53
1:B:296:MET:HE3	1:B:305:VAL:HG21	1.90	0.53
1:B:430:GLY:HA2	1:B:510:LYS:O	2.09	0.53
1:B:581:SER:OG	1:B:584:PHE:HB3	2.09	0.53
1:B:588:GLU:C	1:B:590:GLU:H	2.18	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:VAL:HG12	1:B:308:VAL:HB	1.91	0.52
1:B:441:VAL:HG23	1:B:584:PHE:HZ	1.74	0.52
1:B:243:LYS:O	1:B:247:ALA:HB3	2.09	0.52
1:B:105:ILE:HG23	1:B:106:PRO:HD2	1.91	0.52
1:A:188:GLU:CG	1:B:257:GLU:HB3	2.39	0.51
1:A:222:LEU:N	1:A:222:LEU:HD12	2.24	0.51
1:B:265:MET:CG	1:B:283:ALA:HB2	2.40	0.51
1:B:93:VAL:HG12	1:B:115:ARG:NH1	2.25	0.51
1:B:51:GLU:HB3	1:B:55:ARG:HH12	1.76	0.51
1:B:272:ASN:CB	1:B:273:PRO:CD	2.86	0.51
1:B:551:LYS:NZ	1:B:561:GLU:HB2	2.26	0.51
1:A:535:ARG:HD3	1:A:565:ASN:O	2.11	0.51
1:A:44:HIS:C	1:A:44:HIS:CD2	2.89	0.50
1:B:74:ASN:O	1:B:354:ASN:HA	2.11	0.50
1:B:564:LEU:CD1	1:B:574:MET:HE1	2.41	0.50
1:B:46:CYS:HA	1:B:52:GLU:OE2	2.12	0.50
1:A:25:GLN:O	1:A:29:GLU:HG3	2.12	0.50
1:B:202:LEU:HD11	1:B:206:LEU:HD13	1.94	0.50
1:A:156:ILE:HD12	1:A:184:LEU:HB2	1.94	0.50
1:B:200:LEU:HA	1:B:201:PRO:C	2.36	0.50
1:B:460:MET:HB2	1:B:478:ASP:O	2.12	0.50
1:B:419:ALA:HB1	1:B:422:SER:HB2	1.94	0.49
1:A:23:LEU:HD11	1:A:45:ILE:HD11	1.93	0.49
1:B:312:ILE:HG22	1:B:328:PRO:HG3	1.95	0.49
1:B:450:TRP:C	1:B:452:HIS:N	2.69	0.49
1:B:297:ASN:C	1:B:297:ASN:HD22	2.19	0.49
1:B:341:VAL:HA	1:B:348:ILE:HG13	1.95	0.49
1:B:249:ARG:HG3	1:B:249:ARG:HH11	1.78	0.48
1:A:99:GLN:HA	1:A:116:TRP:CD1	2.48	0.48
1:A:336:ALA:HB3	1:A:337:PRO:HD3	1.95	0.48
1:B:617:GLN:C	1:B:619:ILE:H	2.21	0.48
1:A:11:LEU:HD23	1:A:32:GLU:HG2	1.95	0.48
1:A:440:GLY:HA3	1:A:584:PHE:CZ	2.48	0.48
1:B:394:GLU:C	1:B:396:GLY:H	2.22	0.47
1:B:555:ILE:HA	1:B:615:LEU:CD1	2.44	0.47
1:A:401:HIS:CD2	1:A:402:PRO:HD2	2.49	0.47
1:B:613:LEU:CA	1:B:616:LYS:HB3	2.36	0.47
1:B:527:TRP:HH2	1:B:535:ARG:HD2	1.79	0.47
1:A:228:ILE:HG21	1:A:245:CYS:HB3	1.96	0.47
1:A:249:ARG:HG2	1:A:485:PHE:O	2.15	0.47
1:A:261:LEU:HG	1:A:500:MET:HE2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ILE:HD13	1:A:474:ILE:HA	1.72	0.47
1:A:284:PHE:CE2	1:A:434:GLY:HA3	2.51	0.46
1:B:527:TRP:CH2	1:B:535:ARG:HD2	2.49	0.46
1:B:587:LYS:O	1:B:590:GLU:HB2	2.15	0.46
1:A:221:HIS:NE2	1:A:249:ARG:HD2	2.30	0.46
1:B:532:GLU:OE1	1:B:532:GLU:HA	2.11	0.46
1:B:582:LYS:HD2	1:B:622:MET:C	2.40	0.46
1:A:142:ILE:HG23	1:A:176:MET:HG3	1.97	0.46
1:A:320:GLN:OE1	1:A:320:GLN:HA	2.16	0.46
1:B:88:ILE:HG23	1:B:88:ILE:O	2.15	0.46
1:A:135:LYS:HD2	1:A:135:LYS:HA	1.83	0.46
1:B:206:LEU:CD2	1:B:209:ASN:HA	2.42	0.46
1:B:433:PHE:O	1:B:514:VAL:HG22	2.16	0.46
1:B:605:PRO:O	1:B:608:ILE:HB	2.14	0.46
1:B:614:ALA:HB1	1:B:618:ARG:NH1	2.31	0.46
1:B:50:GLU:HG3	1:B:171:ARG:NH2	2.31	0.46
1:B:141:VAL:O	1:B:143:PRO:HD3	2.16	0.46
1:B:192:CYS:HB3	1:B:241:LEU:HD12	1.97	0.46
1:A:527:TRP:HA	1:A:528:PRO:HD2	1.75	0.46
1:B:559:PRO:HB3	1:B:564:LEU:HD21	1.98	0.46
1:A:443:LEU:HB2	1:A:577:LEU:HD11	1.97	0.46
1:B:249:ARG:HG3	1:B:249:ARG:NH1	2.31	0.46
1:B:300:LEU:HD21	1:B:535:ARG:NH1	2.31	0.46
1:A:532:GLU:HA	1:A:532:GLU:OE1	2.16	0.45
1:A:213:ASN:C	1:A:213:ASN:HD22	2.24	0.45
1:B:247:ALA:HB3	1:B:312:ILE:HD13	1.98	0.45
1:A:564:LEU:HD12	1:A:564:LEU:HA	1.80	0.45
1:A:67:ARG:HD3	1:A:362:GLU:OE1	2.17	0.45
1:B:157:GLY:O	1:B:158:ILE:HD13	2.16	0.45
1:A:91:LYS:HG2	1:A:217:THR:O	2.17	0.45
1:B:51:GLU:CB	1:B:55:ARG:HH12	2.28	0.45
1:B:527:TRP:HA	1:B:528:PRO:HD2	1.78	0.45
1:A:260:TRP:HB2	1:A:315:MET:O	2.17	0.45
1:A:320:GLN:O	1:A:507:LYS:HE2	2.17	0.44
1:B:461:ARG:NH1	1:B:588:GLU:OE1	2.50	0.44
1:B:526:LEU:HD11	1:B:576:GLU:OE2	2.16	0.44
1:B:559:PRO:CB	1:B:564:LEU:HD21	2.46	0.44
1:B:574:MET:HE3	1:B:574:MET:HB3	1.75	0.44
1:B:564:LEU:O	1:B:566:LEU:HG	2.17	0.44
1:B:588:GLU:C	1:B:590:GLU:N	2.73	0.44
1:A:88:ILE:HD13	1:A:91:LYS:HD3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:HIS:CD2	1:A:290:LYS:NZ	2.86	0.44
1:B:273:PRO:HG2	1:B:274:GLU:OE1	2.17	0.44
1:B:543:ARG:NH1	1:B:543:ARG:CA	2.79	0.44
1:A:115:ARG:NH1	1:A:115:ARG:HB3	2.33	0.44
1:B:21:ASP:HA	1:B:28:ARG:NH1	2.32	0.44
1:B:59:GLN:O	1:B:63:GLU:HG2	2.17	0.44
1:B:424:GLU:CD	1:B:424:GLU:H	2.25	0.44
1:A:336:ALA:O	1:A:337:PRO:C	2.59	0.44
1:B:103:VAL:CG1	1:B:114:GLY:HA3	2.47	0.44
1:B:50:GLU:HG3	1:B:171:ARG:HH22	1.82	0.44
1:B:443:LEU:HD21	1:B:536:VAL:HG21	2.00	0.44
1:B:278:LYS:HD3	1:B:544:ILE:CD1	2.48	0.44
1:B:417:ASP:OD1	1:B:418:ALA:N	2.51	0.44
1:B:619:ILE:O	1:B:622:MET:HG2	2.17	0.44
1:B:178:THR:N	1:B:179:PRO:CD	2.80	0.43
1:B:535:ARG:HD3	1:B:565:ASN:O	2.17	0.43
1:B:615:LEU:O	1:B:619:ILE:HG13	2.18	0.43
1:A:317:PHE:HA	1:A:322:HIS:O	2.18	0.43
1:B:222:LEU:N	1:B:222:LEU:HD12	2.34	0.43
1:A:601:ASN:HB3	1:A:602:ALA:H	1.60	0.43
1:B:416:ILE:HD12	1:B:416:ILE:HA	1.89	0.43
1:B:436:ARG:O	1:B:437:ARG:HD2	2.18	0.43
1:B:615:LEU:HG	1:B:619:ILE:HD11	2.01	0.43
1:A:42:HIS:C	1:A:43:ILE:HD12	2.43	0.43
1:B:266:LEU:O	1:B:281:ALA:HA	2.18	0.43
1:B:483:ARG:N	1:B:484:PRO:CD	2.82	0.43
1:B:510:LYS:HD2	1:B:512:PHE:HZ	1.84	0.43
1:A:225:ARG:HB3	1:A:227:GLU:OE2	2.18	0.43
1:A:358:THR:O	1:A:404:SER:HB2	2.18	0.43
1:B:130:PHE:CZ	1:B:231:PHE:HB2	2.54	0.43
1:B:553:THR:HB	1:B:554:PRO:CD	2.49	0.43
1:B:246:PHE:CD1	1:B:246:PHE:C	2.97	0.43
1:B:285:PRO:HG3	1:B:462:SER:HB2	2.01	0.43
1:B:391:TRP:CD2	1:B:399:CYS:HB3	2.53	0.43
1:B:401:HIS:CE1	1:B:403:ASN:HB3	2.54	0.43
1:A:23:LEU:HD11	1:A:45:ILE:CD1	2.49	0.43
1:A:192:CYS:HB3	1:A:241:LEU:HD12	2.01	0.43
1:B:44:HIS:CD2	1:B:44:HIS:C	2.96	0.43
1:B:339:THR:HG22	1:B:348:ILE:CD1	2.49	0.43
1:B:398:PRO:HB2	1:B:400:ALA:O	2.18	0.43
1:B:267:VAL:CG1	1:B:308:VAL:HB	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:LEU:HB2	1:B:577:LEU:HD11	2.01	0.42
1:B:521:LYS:HG3	1:B:522:GLU:N	2.34	0.42
1:B:533:ASN:C	1:B:535:ARG:N	2.77	0.42
1:B:272:ASN:HB2	1:B:303:TRP:CZ2	2.53	0.42
1:B:35:ALA:O	1:B:40:PRO:HD2	2.19	0.42
1:B:225:ARG:O	1:B:227:GLU:HG3	2.18	0.42
1:A:540:MET:O	1:A:544:ILE:HG13	2.19	0.42
1:B:113:LEU:HD11	1:B:599:GLN:HB3	2.01	0.42
1:B:156:ILE:HD13	1:B:180:VAL:HG13	2.01	0.42
1:B:401:HIS:CG	1:B:402:PRO:HD2	2.54	0.42
1:B:450:TRP:C	1:B:452:HIS:H	2.28	0.42
1:B:461:ARG:HG2	1:B:477:HIS:ND1	2.34	0.42
1:A:11:LEU:HA	1:A:11:LEU:HD12	1.77	0.42
1:B:246:PHE:C	1:B:246:PHE:HD1	2.27	0.42
1:B:446:GLU:CG	1:B:447:ALA:N	2.81	0.42
1:B:571:HIS:CD2	1:B:571:HIS:C	2.98	0.42
1:A:146:MET:HE2	1:A:247:ALA:HB2	2.02	0.42
1:A:256:LYS:HD2	1:A:488:TYR:CE1	2.54	0.42
1:A:173:MET:HE1	1:A:331:GLY:O	2.19	0.42
1:A:483:ARG:HG2	1:A:483:ARG:HH11	1.84	0.42
1:B:510:LYS:HD2	1:B:512:PHE:CZ	2.55	0.42
1:A:200:LEU:HA	1:A:201:PRO:C	2.45	0.41
1:A:194:HIS:HA	1:A:230:SER:O	2.20	0.41
1:B:270:ILE:O	1:B:270:ILE:HG23	2.20	0.41
1:B:592:ILE:O	1:B:596:LEU:HG	2.20	0.41
1:A:221:HIS:ND1	1:A:221:HIS:N	2.68	0.41
1:A:265:MET:HA	1:A:282:ALA:O	2.20	0.41
1:B:72:TYR:HB2	1:B:75:CYS:HB2	2.02	0.41
1:B:325:ALA:HB2	1:B:428:ILE:HG13	2.03	0.41
1:B:437:ARG:CB	1:B:515:ASN:HD21	2.22	0.41
1:B:606:CYS:C	1:B:608:ILE:H	2.27	0.41
1:A:176:MET:HE3	1:A:176:MET:HB3	1.61	0.41
1:A:279:TYR:HB2	1:A:427:PRO:O	2.21	0.41
1:B:460:MET:HG3	1:B:480:PHE:N	2.29	0.41
1:B:588:GLU:OE1	1:B:588:GLU:HA	2.19	0.41
1:A:413:CYS:HA	1:A:414:PRO:HD2	1.88	0.41
1:A:479:PRO:O	1:A:480:PHE:HB2	2.21	0.41
1:B:446:GLU:HG3	1:B:447:ALA:H	1.85	0.41
1:B:512:PHE:CB	1:B:540:MET:HE2	2.50	0.41
1:B:532:GLU:C	1:B:534:SER:N	2.78	0.41
1:B:551:LYS:HZ2	1:B:561:GLU:HB2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:PRO:HG2	1:B:608:ILE:CG1	2.51	0.41
1:A:464:ALA:HB3	1:A:476:MET:HE2	2.01	0.41
1:B:348:ILE:O	1:B:352:GLN:HG2	2.21	0.41
1:B:445:TYR:CE2	1:B:513:HIS:HB3	2.56	0.41
1:A:98:GLU:HB2	1:A:101:ASP:OD2	2.21	0.41
1:B:461:ARG:HG2	1:B:477:HIS:CE1	2.56	0.41
1:A:272:ASN:HB2	1:A:273:PRO:CD	2.50	0.40
1:B:279:TYR:HB2	1:B:427:PRO:O	2.20	0.40
1:B:295:MET:CA	1:B:415:ILE:HD11	2.36	0.40
1:B:477:HIS:CD2	1:B:595:TYR:CG	3.09	0.40
1:B:318:ASP:OD1	1:B:322:HIS:N	2.54	0.40
1:B:339:THR:HG22	1:B:348:ILE:HD11	2.03	0.40
1:B:437:ARG:HD2	1:B:437:ARG:HA	1.76	0.40
1:B:501:ALA:HB3	1:B:502:GLN:NE2	2.36	0.40
1:A:561:GLU:O	1:A:562:ASP:HB2	2.22	0.40
1:B:413:CYS:HA	1:B:414:PRO:HD3	1.91	0.40
1:B:535:ARG:NH1	1:B:565:ASN:O	2.53	0.40
1:B:543:ARG:CZ	1:B:543:ARG:HB3	2.52	0.40
1:B:263:GLU:CD	1:B:497:TRP:HZ2	2.29	0.40
1:B:533:ASN:C	1:B:535:ARG:H	2.28	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	596/625 (95%)	571 (96%)	24 (4%)	1 (0%)	43	55
1	B	596/625 (95%)	539 (90%)	49 (8%)	8 (1%)	9	10
All	All	1192/1250 (95%)	1110 (93%)	73 (6%)	9 (1%)	16	20

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	565	ASN
1	A	236	GLY
1	B	448	LEU
1	B	618	ARG
1	B	243	LYS
1	B	271	THR
1	B	515	ASN
1	B	395	ASP
1	B	570	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	A	507/523 (97%)	492 (97%)	15 (3%)	36	53
1	B	507/523 (97%)	483 (95%)	24 (5%)	23	35
All	All	1014/1046 (97%)	975 (96%)	39 (4%)	29	44

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	138	THR
1	A	176	MET
1	A	226	ARG
1	A	246	PHE
1	A	320	GLN
1	A	377	LEU
1	A	392	SER
1	A	474	ILE
1	A	510	LYS
1	A	521	LYS
1	A	522	GLU
1	A	550	THR
1	A	575	MET
1	A	581	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	32	GLU
1	B	103	VAL
1	B	113	LEU
1	B	138	THR
1	B	226	ARG
1	B	288	CYS
1	B	295	MET
1	B	353	LYS
1	B	377	LEU
1	B	382	THR
1	B	395	ASP
1	B	424	GLU
1	B	428	ILE
1	B	473	LYS
1	B	474	ILE
1	B	475	ILE
1	B	507	LYS
1	B	521	LYS
1	B	532	GLU
1	B	557	TYR
1	B	560	LYS
1	B	567	LYS
1	B	588	GLU
1	B	616	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	213	ASN
1	A	297	ASN
1	A	322	HIS
1	A	352	GLN
1	A	621	GLN
1	B	10	ASN
1	B	44	HIS
1	B	209	ASN
1	B	213	ASN
1	B	238	ASN
1	B	297	ASN
1	B	320	GLN
1	B	346	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	502	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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$
4	UN8	A	703	-	43,44,44	1.72	11 (25%)	56,64,64	2.92	20 (35%)
3	PEP	A	702	-	9,9,9	1.28	1 (11%)	11,13,13	1.98	4 (36%)
3	PEP	B	702	-	9,9,9	1.37	1 (11%)	11,13,13	2.91	6 (54%)

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
4	UN8	A	703	-	-	0/21/23/23	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEP	A	702	-	-	4/9/9/9	-
3	PEP	B	702	-	-	2/9/9/9	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	UN8	S1-N4	4.74	1.70	1.62
4	A	703	UN8	C55-C54	4.53	1.43	1.37
4	A	703	UN8	C52-N51	2.94	1.43	1.38
4	A	703	UN8	C52-N53	2.71	1.43	1.38
4	A	703	UN8	C14-N15	2.66	1.40	1.36
4	A	703	UN8	O1-S1	-2.31	1.40	1.43
4	A	703	UN8	C2-N5	2.29	1.40	1.37
3	B	702	PEP	O2'-C1	2.28	1.36	1.30
4	A	703	UN8	C3-N5	2.24	1.41	1.35
4	A	703	UN8	C54-N13	2.20	1.40	1.36
4	A	703	UN8	C55-C56	2.19	1.46	1.42
4	A	703	UN8	C9-C8	2.10	1.42	1.39
3	A	702	PEP	O2'-C1	2.07	1.36	1.30

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	UN8	N53-C54-N13	10.05	130.69	125.53
4	A	703	UN8	C55-C54-N13	-7.42	109.30	112.39
4	A	703	UN8	C3-N7-C1	6.83	109.67	103.39
4	A	703	UN8	N51-C52-N53	6.06	123.14	115.75
4	A	703	UN8	N5-C3-N7	-5.86	110.42	112.66
3	B	702	PEP	O2-C2-C3	-5.75	113.87	124.85
4	A	703	UN8	O1-S1-N4	-4.94	99.05	107.35
4	A	703	UN8	C52-N53-C54	-4.37	116.60	119.59
3	B	702	PEP	O2'-C1-O1	-4.06	114.23	123.90
4	A	703	UN8	C17-N51-C56	4.01	123.37	117.72
4	A	703	UN8	C2-N5-C3	-3.90	105.17	106.71
4	A	703	UN8	O1-S1-O2	3.90	126.97	119.82
4	A	703	UN8	C56-N51-C52	-3.90	120.82	125.62
4	A	703	UN8	C7-C8-C9	-3.81	113.99	119.04
3	B	702	PEP	O1-C1-C2	3.76	127.46	121.79
3	A	702	PEP	O2'-C1-O1	-3.75	114.98	123.90
4	A	703	UN8	C17-N51-C52	-3.60	111.89	116.92
3	B	702	PEP	O2-P-O1P	3.28	119.96	109.47
3	A	702	PEP	O1-C1-C2	3.14	126.52	121.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	UN8	O58-C52-N51	-3.09	117.83	121.98
3	A	702	PEP	O2-P-O1P	3.06	119.28	109.47
3	B	702	PEP	C3-C2-C1	-2.58	117.97	122.73
4	A	703	UN8	O58-C52-N53	-2.45	118.68	121.98
3	B	702	PEP	O2'-C1-C2	2.40	118.00	113.91
4	A	703	UN8	C6-C7-C8	2.36	123.02	120.30
4	A	703	UN8	C30-C9-C8	2.14	122.77	120.30
3	A	702	PEP	O2'-C1-C2	2.13	117.55	113.91
4	A	703	UN8	C6-C5-C30	-2.06	115.17	118.23
4	A	703	UN8	C5-C16-C14	-2.05	109.38	113.62
4	A	703	UN8	C1-S1-N4	2.04	109.18	106.18

There are no chirality outliers.

All (6) torsion outliers are listed below:

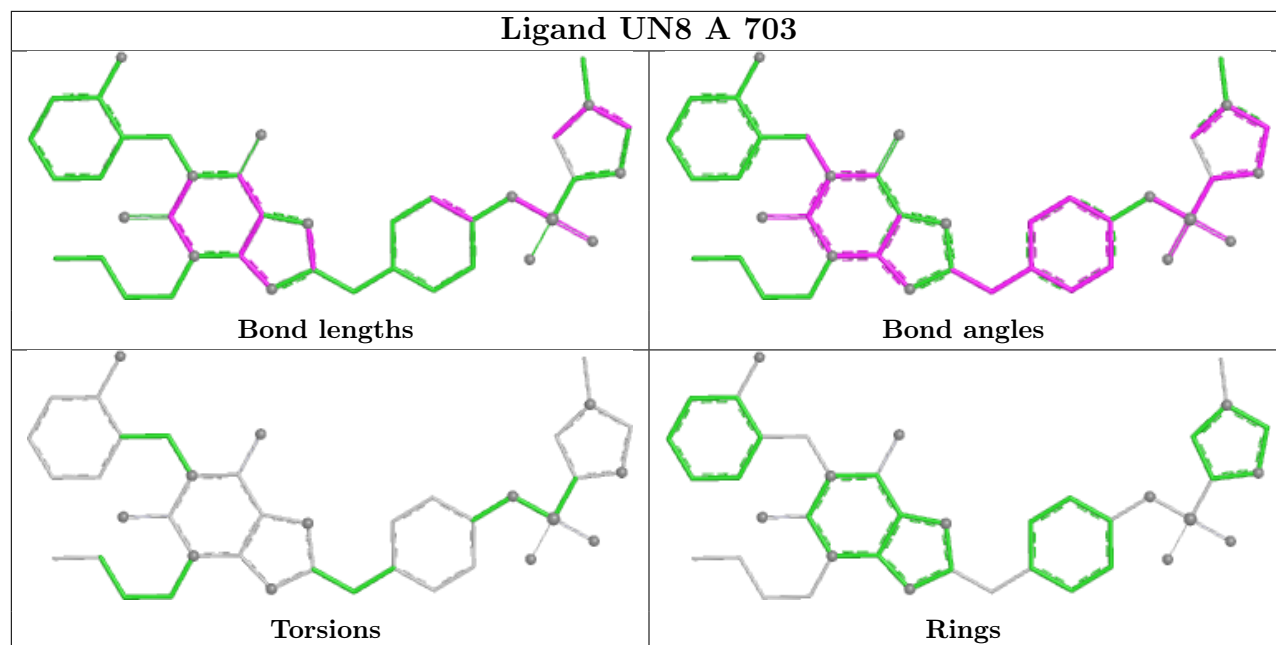
Mol	Chain	Res	Type	Atoms
3	A	702	PEP	O1-C1-C2-O2
3	A	702	PEP	O2'-C1-C2-C3
3	A	702	PEP	O2'-C1-C2-O2
3	B	702	PEP	O1-C1-C2-C3
3	B	702	PEP	O2'-C1-C2-C3
3	A	702	PEP	C2-O2-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	UN8	1	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.