



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:54 PM UTC

PDB ID : 1I4L / pdb_00001i4l
Title : CRYSTAL STRUCTURE ANALYSIS OF RAC1-GDP IN COMPLEX WITH ARFAPTIN (P41)
Authors : Tarricone, C.; Xiao, B.; Justin, N.; Gamblin, S.J.; Smerdon, S.J.
Deposited on : 2001-02-22
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 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

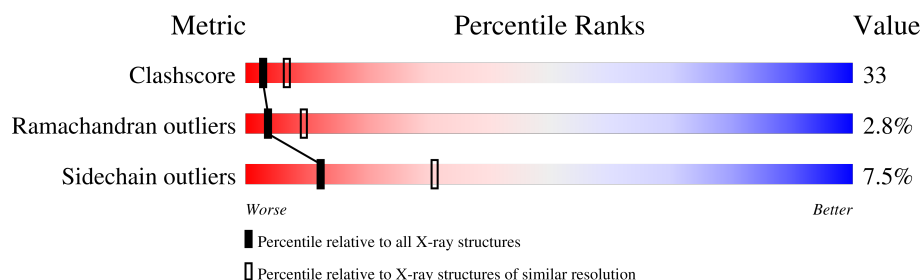
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 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	224	
1	B	224	
2	D	192	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4449 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 ARFAPTIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1479	936	251	288	4			
1	B	178	Total	C	N	O	S	0	0	0
			1434	912	241	277	4			

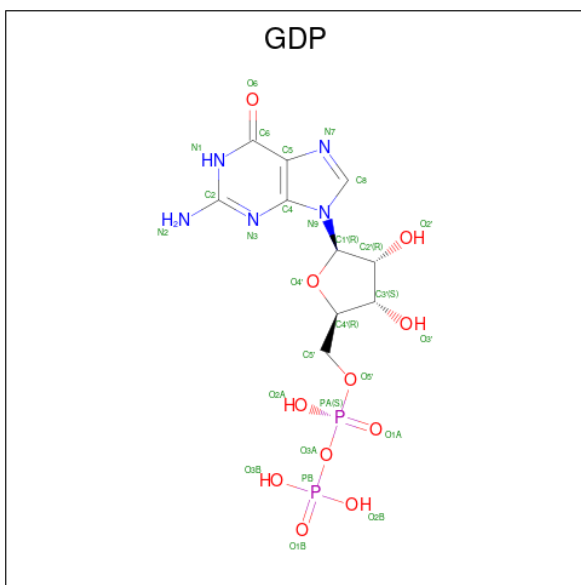
- Molecule 2 is a protein called RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	177	Total	C	N	O	S	0	0	0
			1381	887	228	258	8			

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

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

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 5 is water.

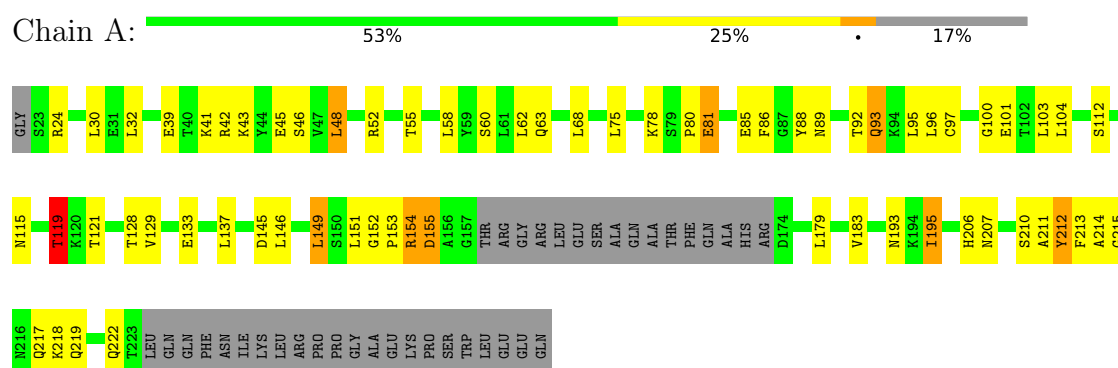
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	71	Total O 71 71	0	0
5	B	36	Total O 36 36	0	0
5	D	19	Total O 19 19	0	0

3 Residue-property plots [i](#)

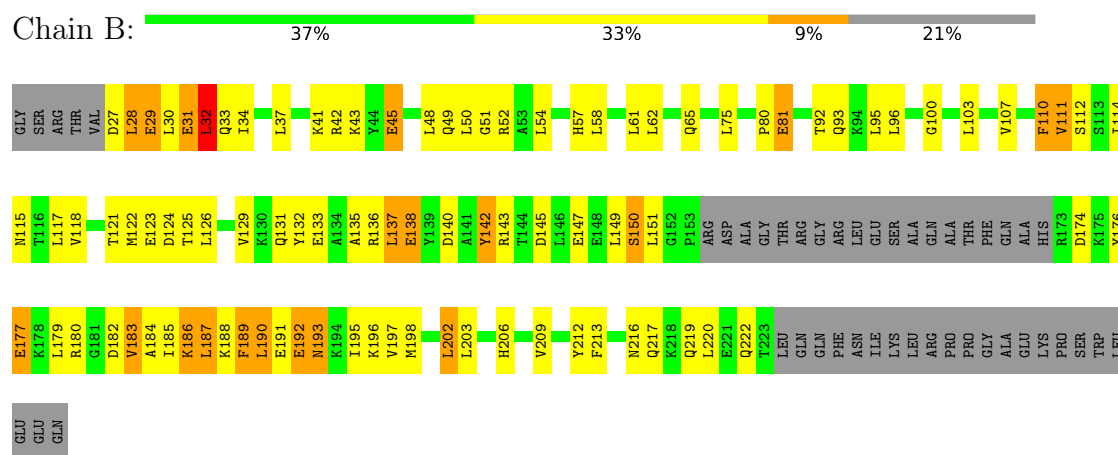
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

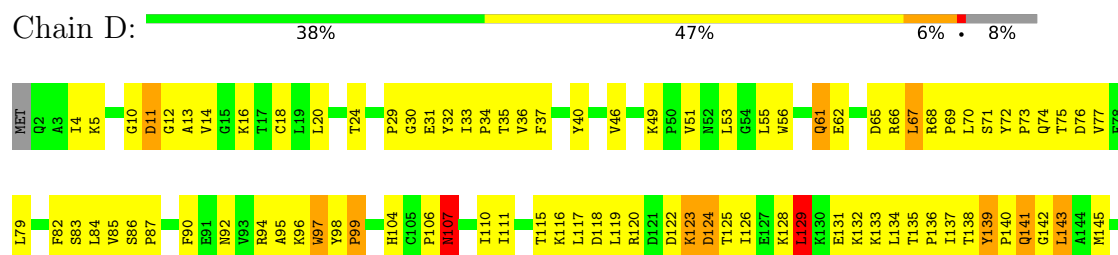
• Molecule 1: ARFAPTIN 2



• Molecule 1: ARFAPTIN 2



• Molecule 2: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE 1





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	112.38Å 112.38Å 68.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.258 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4449	wwPDB-VP
Average B, all atoms (Å ²)	62.0	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: MG, GDP

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	0.54	0/1498	0.93	6/2015 (0.3%)
1	B	0.43	0/1453	0.97	7/1954 (0.4%)
2	D	0.37	0/1411	1.01	11/1920 (0.6%)
All	All	0.46	0/4362	0.97	24/5889 (0.4%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	61	GLN	OE1-CD-NE2	-9.76	112.84	122.60
1	A	101	GLU	N-CA-C	-9.40	101.94	113.41
1	B	184	ALA	N-CA-C	-8.61	102.58	113.43
2	D	143	LEU	N-CA-C	-6.78	104.01	112.90
1	B	189	PHE	N-CA-C	-6.73	96.46	110.80
2	D	61	GLN	CG-CD-NE2	6.63	126.34	116.40
1	A	212	TYR	N-CA-C	-6.40	106.19	112.97
2	D	33	ILE	CA-C-N	6.19	126.22	119.90
2	D	33	ILE	C-N-CA	6.19	126.22	119.90
2	D	97	TRP	N-CA-C	6.18	117.71	110.97
1	B	32	LEU	N-CA-C	-6.00	98.02	110.80
1	A	119	THR	N-CA-C	5.99	117.81	111.28
1	B	28	LEU	N-CA-C	5.97	117.46	111.07
2	D	142	GLY	N-CA-C	-5.94	99.11	113.18
2	D	141	GLN	N-CA-C	-5.91	103.63	111.02
1	B	45	GLU	N-CA-C	-5.84	103.62	112.04
2	D	139	TYR	N-CA-C	-5.79	104.87	112.75
1	B	190	LEU	N-CA-C	-5.67	106.40	113.55
1	B	192	GLU	N-CA-C	-5.45	105.42	111.36
1	A	211	ALA	N-CA-C	-5.41	106.52	113.01
2	D	129	LEU	N-CA-C	-5.31	105.57	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	LEU	N-CA-C	-5.26	107.00	113.41
2	D	24	THR	N-CA-C	5.21	117.87	111.82
1	A	215	GLY	N-CA-C	-5.16	108.92	115.31

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	1479	0	1485	57	0
1	B	1434	0	1448	127	0
2	D	1381	0	1397	118	0
3	D	1	0	0	0	0
4	D	28	0	12	2	0
5	A	71	0	0	5	0
5	B	36	0	0	14	0
5	D	19	0	0	9	0
All	All	4449	0	4342	282	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 33.

All (282) 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)
2:D:61:GLN:OE1	5:D:215:HOH:O	1.74	1.05
1:A:55:THR:HG22	2:D:56:TRP:HH2	1.25	1.01
2:D:87:PRO:HA	2:D:137:ILE:HD11	1.48	0.92
2:D:92:ASN:HA	2:D:95:ALA:HB3	1.53	0.88
2:D:129:LEU:HD13	2:D:136:PRO:HD3	1.59	0.84
1:B:183:VAL:O	1:B:187:LEU:HB2	1.77	0.84
1:B:95:LEU:HD21	1:B:219:GLN:HB2	1.58	0.84
1:B:188:LYS:HB3	1:B:188:LYS:NZ	1.94	0.82
2:D:46:VAL:HG21	2:D:173:ILE:HG21	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ALA:HA	1:B:217:GLN:NE2	1.94	0.81
2:D:139:TYR:HB3	2:D:140:PRO:HD3	1.60	0.81
1:B:132:TYR:HE1	1:B:180:ARG:HH21	1.29	0.81
2:D:166:LYS:HB3	5:D:209:HOH:O	1.81	0.80
1:A:95:LEU:HD11	1:A:219:GLN:NE2	1.97	0.79
1:B:95:LEU:HD21	1:B:219:GLN:CB	2.13	0.78
2:D:11:ASP:H	2:D:97:TRP:HE1	1.31	0.77
1:B:33:GLN:NE2	1:B:188:LYS:HG3	2.00	0.77
1:B:136:ARG:CZ	1:B:137:LEU:HD11	2.16	0.75
1:B:48:LEU:HD21	1:B:115:ASN:HD22	1.51	0.75
1:B:143:ARG:HB3	1:B:143:ARG:HH11	1.50	0.74
1:A:55:THR:HG22	2:D:56:TRP:CH2	2.16	0.72
1:B:65:GLN:HG2	1:B:93:GLN:HE21	1.53	0.72
1:B:198:MET:O	1:B:202:LEU:HB2	1.89	0.72
1:A:210:SER:HB2	1:B:220:LEU:HD21	1.70	0.72
2:D:125:THR:O	2:D:129:LEU:HB2	1.89	0.72
2:D:83:SER:HB3	2:D:86:SER:HB3	1.73	0.71
2:D:69:PRO:HA	2:D:72:TYR:CD2	2.26	0.71
1:A:154:ARG:C	1:A:154:ARG:HD2	2.16	0.70
1:B:33:GLN:HE21	1:B:187:LEU:HD22	1.54	0.70
2:D:116:LYS:HE2	4:D:200:GDP:C4	2.28	0.69
1:B:31:GLU:HA	5:B:256:HOH:O	1.92	0.69
1:B:188:LYS:HB3	1:B:188:LYS:HZ2	1.56	0.68
2:D:67:LEU:HD23	2:D:67:LEU:H	1.57	0.68
2:D:155:LEU:HD12	2:D:168:VAL:HA	1.76	0.68
1:A:219:GLN:HA	1:A:222:GLN:HB3	1.74	0.68
1:B:143:ARG:HB3	1:B:143:ARG:NH1	2.10	0.67
2:D:153:LYS:HB2	2:D:153:LYS:NZ	2.09	0.67
2:D:68:ARG:HB3	2:D:69:PRO:HD3	1.77	0.67
1:B:137:LEU:HD12	1:B:137:LEU:H	1.59	0.66
2:D:94:ARG:HE	2:D:145:MET:HE1	1.61	0.66
2:D:135:THR:OG1	2:D:136:PRO:HD2	1.94	0.66
1:A:95:LEU:HD11	1:A:219:GLN:HE21	1.61	0.65
1:A:206:HIS:HE1	1:B:92:THR:OG1	1.79	0.65
2:D:51:VAL:HA	5:D:203:HOH:O	1.95	0.65
2:D:158:SER:HB3	2:D:161:THR:OG1	1.95	0.65
2:D:49:LYS:HG2	5:D:202:HOH:O	1.95	0.65
2:D:11:ASP:N	2:D:97:TRP:HE1	1.96	0.64
2:D:123:LYS:H	2:D:123:LYS:HD2	1.61	0.64
1:B:95:LEU:HD11	1:B:219:GLN:OE1	1.98	0.64
1:A:60:SER:HB3	1:B:57:HIS:CD2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASN:O	1:A:119:THR:HB	1.98	0.63
2:D:139:TYR:HE1	2:D:143:LEU:HD13	1.63	0.63
2:D:116:LYS:HB3	5:D:208:HOH:O	1.99	0.63
2:D:98:TYR:CE1	2:D:149:ILE:HG23	2.34	0.63
1:A:95:LEU:HD21	1:A:219:GLN:HG3	1.81	0.62
1:B:133:GLU:HG2	1:B:136:ARG:HE	1.63	0.62
2:D:139:TYR:CE1	2:D:143:LEU:HD22	2.34	0.62
1:B:180:ARG:O	1:B:183:VAL:HG12	1.99	0.62
2:D:98:TYR:CD1	2:D:149:ILE:HG23	2.35	0.62
2:D:172:ALA:O	2:D:176:VAL:HG23	2.00	0.62
1:A:128:THR:HG22	1:A:183:VAL:HG12	1.81	0.61
2:D:20:LEU:HD22	2:D:55:LEU:HD13	1.81	0.61
2:D:177:LEU:HD22	2:D:177:LEU:H	1.64	0.61
2:D:119:LEU:HB2	5:D:208:HOH:O	1.99	0.61
1:B:143:ARG:O	1:B:147:GLU:HB2	2.01	0.61
1:B:143:ARG:HH11	1:B:143:ARG:CB	2.13	0.61
1:B:33:GLN:NE2	1:B:187:LEU:HD13	2.15	0.60
2:D:10:GLY:HA2	2:D:97:TRP:NE1	2.16	0.60
2:D:53:LEU:HD12	5:D:216:HOH:O	2.00	0.60
1:B:61:LEU:HG	1:B:65:GLN:HE21	1.66	0.60
1:B:129:VAL:O	1:B:133:GLU:HG3	2.02	0.60
1:B:136:ARG:NH2	1:B:137:LEU:HD11	2.16	0.60
2:D:164:GLY:O	2:D:168:VAL:HG23	2.01	0.60
1:B:132:TYR:CE2	1:B:136:ARG:HD3	2.36	0.59
1:B:187:LEU:HD22	1:B:188:LYS:HG3	1.83	0.59
1:B:192:GLU:O	1:B:196:LYS:HG3	2.02	0.59
1:A:85:GLU:HB3	1:B:202:LEU:HD23	1.85	0.59
1:B:129:VAL:HG21	5:B:274:HOH:O	2.02	0.59
1:A:41:LYS:O	1:A:45:GLU:HG3	2.03	0.59
1:B:132:TYR:O	1:B:136:ARG:HB2	2.03	0.59
2:D:72:TYR:N	2:D:73:PRO:HD2	2.18	0.59
1:A:58:LEU:HD21	1:A:103:LEU:HG	1.85	0.58
1:B:65:GLN:HG2	1:B:93:GLN:NE2	2.16	0.58
2:D:153:LYS:HB2	2:D:153:LYS:HZ2	1.67	0.58
1:B:112:SER:O	1:B:115:ASN:HB3	2.02	0.58
1:B:177:GLU:O	1:B:180:ARG:HB3	2.02	0.58
2:D:12:GLY:O	2:D:13:ALA:HB3	2.03	0.58
2:D:117:LEU:HD11	2:D:120:ARG:HH11	1.69	0.58
1:A:55:THR:HG23	1:A:104:LEU:HD11	1.85	0.57
2:D:29:PRO:C	2:D:31:GLU:H	2.13	0.57
1:A:24:ARG:HD3	5:A:254:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:O	1:B:65:GLN:HG3	2.05	0.57
1:B:117:LEU:O	1:B:122:MET:HG3	2.04	0.57
1:B:137:LEU:HD12	1:B:137:LEU:N	2.20	0.57
1:A:214:ALA:HA	1:B:217:GLN:HE22	1.67	0.56
2:D:85:VAL:HG22	2:D:119:LEU:O	2.04	0.56
2:D:11:ASP:O	2:D:14:VAL:HG13	2.05	0.56
1:B:126:LEU:HA	5:B:274:HOH:O	2.04	0.56
2:D:4:ILE:HD13	2:D:51:VAL:HG13	1.87	0.56
1:A:78:LYS:HD2	1:B:43:LYS:HE3	1.88	0.56
2:D:56:TRP:CE3	2:D:71:SER:HB2	2.41	0.56
1:A:89:ASN:OD1	1:B:206:HIS:HB2	2.06	0.55
1:A:222:GLN:O	1:A:222:GLN:HG2	2.06	0.55
2:D:123:LYS:HD3	5:D:205:HOH:O	2.06	0.55
1:B:34:ILE:HB	5:B:256:HOH:O	2.06	0.55
2:D:36:VAL:HG12	2:D:37:PHE:CD1	2.42	0.55
1:B:121:THR:HG22	1:B:190:LEU:CD1	2.36	0.55
1:B:180:ARG:C	1:B:183:VAL:HG12	2.31	0.55
1:A:86:PHE:CD2	1:B:202:LEU:HD21	2.41	0.55
2:D:120:ARG:HH21	2:D:138:THR:HA	1.71	0.55
1:B:32:LEU:N	5:B:256:HOH:O	2.40	0.54
1:B:33:GLN:HG2	1:B:187:LEU:HD21	1.89	0.54
1:B:114:ILE:O	1:B:118:VAL:HG23	2.07	0.54
1:B:65:GLN:CG	1:B:93:GLN:HE21	2.19	0.54
1:B:93:GLN:HB2	5:B:263:HOH:O	2.07	0.54
1:B:61:LEU:HG	1:B:65:GLN:NE2	2.23	0.54
2:D:29:PRO:O	2:D:31:GLU:N	2.40	0.54
1:B:107:VAL:O	1:B:111:VAL:HG23	2.08	0.54
2:D:4:ILE:HD12	2:D:4:ILE:N	2.23	0.54
1:B:121:THR:HG22	1:B:190:LEU:HD13	1.88	0.53
1:A:24:ARG:CD	5:A:254:HOH:O	2.55	0.53
1:B:33:GLN:HG2	1:B:187:LEU:CD2	2.38	0.53
1:A:207:ASN:C	1:A:207:ASN:HD22	2.16	0.53
2:D:62:GLU:HA	2:D:65:ASP:OD2	2.09	0.53
1:B:95:LEU:HD21	1:B:219:GLN:HB3	1.90	0.53
1:B:103:LEU:O	1:B:107:VAL:HG23	2.09	0.53
1:A:62:LEU:HD11	1:A:100:GLY:HA3	1.91	0.53
1:B:48:LEU:HD12	1:B:111:VAL:HG13	1.90	0.53
2:D:5:LYS:HE3	2:D:56:TRP:CE2	2.44	0.53
2:D:128:LYS:HA	2:D:131:GLU:HB3	1.89	0.53
1:A:213:PHE:HE2	1:B:216:ASN:ND2	2.07	0.52
2:D:110:ILE:C	2:D:111:ILE:HD12	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:139:TYR:CD1	2:D:143:LEU:HD22	2.45	0.52
1:B:135:ALA:HA	1:B:138:GLU:HG2	1.92	0.52
1:B:140:ASP:HA	1:B:143:ARG:NH1	2.24	0.52
2:D:116:LYS:HG2	4:D:200:GDP:C6	2.45	0.52
1:B:49:GLN:OE1	1:B:49:GLN:HA	2.09	0.52
1:A:217:GLN:OE1	1:B:213:PHE:C	2.53	0.52
1:B:209:VAL:O	1:B:212:TYR:HB3	2.10	0.52
1:B:27:ASP:OD2	1:B:180:ARG:NH2	2.43	0.52
1:B:81:GLU:H	1:B:81:GLU:CD	2.17	0.52
2:D:139:TYR:CE1	2:D:143:LEU:HD13	2.44	0.52
1:A:212:TYR:CG	1:A:212:TYR:O	2.64	0.51
1:B:33:GLN:HE21	1:B:188:LYS:HG3	1.72	0.51
1:B:125:THR:O	1:B:129:VAL:HG23	2.11	0.51
2:D:36:VAL:HG12	2:D:37:PHE:CG	2.46	0.51
1:B:49:GLN:C	1:B:51:GLY:N	2.66	0.50
1:B:133:GLU:CG	1:B:136:ARG:HE	2.24	0.50
1:B:187:LEU:HD22	1:B:188:LYS:CG	2.41	0.50
1:B:198:MET:HE3	1:B:202:LEU:HD13	1.93	0.50
2:D:123:LYS:H	2:D:123:LYS:CD	2.21	0.50
2:D:124:ASP:H	2:D:126:ILE:HG22	1.76	0.50
2:D:94:ARG:NE	2:D:145:MET:HE1	2.24	0.50
1:B:138:GLU:O	1:B:142:TYR:HB2	2.11	0.50
1:A:112:SER:HB2	2:D:74:GLN:NE2	2.27	0.50
1:B:133:GLU:HA	1:B:136:ARG:CB	2.41	0.50
2:D:153:LYS:HG3	2:D:154:TYR:N	2.27	0.50
2:D:115:THR:O	2:D:116:LYS:HB2	2.12	0.50
2:D:14:VAL:CG2	2:D:16:LYS:HG3	2.42	0.50
2:D:4:ILE:HD13	2:D:51:VAL:CG1	2.41	0.49
2:D:123:LYS:HD2	2:D:123:LYS:N	2.25	0.49
2:D:177:LEU:HD22	2:D:177:LEU:N	2.27	0.49
2:D:77:VAL:CG2	2:D:111:ILE:HD13	2.42	0.49
1:A:62:LEU:HD11	1:A:100:GLY:C	2.38	0.49
1:B:62:LEU:HD21	1:B:100:GLY:HA3	1.93	0.49
2:D:123:LYS:O	2:D:124:ASP:HB2	2.13	0.49
1:A:48:LEU:O	1:A:52:ARG:HG3	2.12	0.49
2:D:98:TYR:HB3	2:D:99:PRO:HD3	1.94	0.49
2:D:69:PRO:HB3	2:D:104:HIS:NE2	2.28	0.49
2:D:132:LYS:O	2:D:133:LYS:HB3	2.12	0.48
1:B:193:ASN:O	1:B:197:VAL:HG23	2.12	0.48
1:B:151:LEU:HD12	1:B:151:LEU:N	2.28	0.48
2:D:29:PRO:C	2:D:31:GLU:N	2.69	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:GLU:O	2:D:32:TYR:HB2	2.13	0.48
1:B:145:ASP:C	1:B:147:GLU:H	2.22	0.48
1:A:154:ARG:C	1:A:154:ARG:CD	2.85	0.48
2:D:118:ASP:C	2:D:120:ARG:H	2.22	0.48
2:D:90:PHE:CD2	2:D:137:ILE:HD12	2.49	0.48
2:D:139:TYR:HB3	2:D:140:PRO:CD	2.40	0.48
2:D:79:LEU:HD22	2:D:111:ILE:HB	1.96	0.47
1:A:39:GLU:OE2	1:A:42:ARG:NH2	2.44	0.47
2:D:18:CYS:SG	2:D:29:PRO:HG2	2.54	0.47
1:B:54:LEU:O	1:B:58:LEU:HB2	2.14	0.47
1:A:81:GLU:CD	1:A:81:GLU:H	2.17	0.47
1:B:33:GLN:HB3	1:B:187:LEU:HD11	1.97	0.47
2:D:96:LYS:HE2	2:D:97:TRP:CZ3	2.50	0.47
2:D:82:PHE:CE2	2:D:84:LEU:HD23	2.50	0.47
1:A:217:GLN:HG2	1:B:217:GLN:OE1	2.15	0.46
1:B:131:GLN:O	1:B:179:LEU:HD13	2.15	0.46
1:B:52:ARG:HB3	5:B:270:HOH:O	2.15	0.46
2:D:66:ARG:HD2	2:D:66:ARG:N	2.30	0.46
1:B:191:GLU:O	1:B:195:ILE:HG12	2.14	0.46
1:B:49:GLN:C	1:B:51:GLY:H	2.22	0.46
1:B:133:GLU:HA	1:B:136:ARG:HB2	1.97	0.46
2:D:18:CYS:SG	2:D:29:PRO:CG	3.04	0.46
2:D:129:LEU:HD13	2:D:136:PRO:CD	2.40	0.46
2:D:155:LEU:CD1	2:D:168:VAL:HA	2.43	0.46
1:B:126:LEU:HD12	5:B:274:HOH:O	2.16	0.46
2:D:111:ILE:HD12	2:D:111:ILE:N	2.31	0.46
1:A:68:LEU:N	1:B:50:LEU:HD13	2.31	0.46
2:D:128:LYS:O	2:D:131:GLU:HB3	2.16	0.46
1:B:27:ASP:O	1:B:31:GLU:HG2	2.16	0.46
1:B:41:LYS:HB2	1:B:122:MET:CE	2.46	0.46
2:D:67:LEU:HD23	2:D:67:LEU:N	2.28	0.45
1:B:133:GLU:CB	1:B:136:ARG:HE	2.30	0.45
1:B:198:MET:CE	1:B:202:LEU:HD13	2.46	0.45
2:D:11:ASP:N	2:D:97:TRP:NE1	2.63	0.45
2:D:129:LEU:HD22	2:D:134:LEU:C	2.42	0.45
1:A:153:PRO:O	1:A:154:ARG:HB3	2.17	0.45
1:B:110:PHE:CE1	1:B:114:ILE:HD11	2.51	0.45
1:A:206:HIS:CE1	1:B:92:THR:OG1	2.65	0.45
1:B:28:LEU:O	1:B:29:GLU:C	2.59	0.45
1:B:80:PRO:HD3	5:B:249:HOH:O	2.17	0.45
2:D:4:ILE:HG21	2:D:176:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:PRO:HA	2:D:72:TYR:CE2	2.51	0.45
1:A:62:LEU:HD11	1:A:100:GLY:CA	2.47	0.45
1:B:33:GLN:HE21	1:B:187:LEU:HD13	1.80	0.45
2:D:106:PRO:O	2:D:107:ASN:CG	2.60	0.45
1:A:63:GLN:HB3	2:D:37:PHE:CD1	2.53	0.44
1:B:133:GLU:O	1:B:136:ARG:HB3	2.18	0.44
1:B:149:LEU:O	1:B:150:SER:OG	2.29	0.44
2:D:53:LEU:HD21	2:D:55:LEU:HD21	1.98	0.44
2:D:117:LEU:HD12	2:D:120:ARG:HD2	1.98	0.44
1:B:32:LEU:O	1:B:32:LEU:HD23	2.18	0.44
1:B:123:GLU:O	1:B:124:ASP:C	2.61	0.44
2:D:96:LYS:O	2:D:99:PRO:HD2	2.17	0.44
2:D:29:PRO:HB2	2:D:34:PRO:HD2	2.00	0.44
1:B:188:LYS:HB3	1:B:188:LYS:HZ3	1.77	0.44
2:D:75:THR:HG22	2:D:76:ASP:N	2.32	0.43
1:A:43:LYS:O	1:A:46:SER:HB3	2.17	0.43
1:A:68:LEU:HB3	1:A:93:GLN:HG2	2.00	0.43
1:A:218:LYS:HD2	5:A:297:HOH:O	2.17	0.43
1:B:30:LEU:O	1:B:34:ILE:HG12	2.18	0.43
1:A:48:LEU:HD12	1:A:48:LEU:HA	1.81	0.43
1:A:152:GLY:C	1:A:154:ARG:H	2.25	0.43
1:B:117:LEU:O	1:B:117:LEU:HG	2.17	0.43
1:B:180:ARG:HA	1:B:183:VAL:CG1	2.49	0.43
1:B:198:MET:SD	5:B:251:HOH:O	2.62	0.43
1:A:96:LEU:O	1:A:97:CYS:C	2.62	0.43
1:A:129:VAL:O	1:A:133:GLU:HG3	2.19	0.43
2:D:40:TYR:CD1	2:D:40:TYR:N	2.87	0.43
1:A:58:LEU:HD21	1:A:103:LEU:CG	2.47	0.43
2:D:10:GLY:O	2:D:11:ASP:C	2.61	0.43
1:B:117:LEU:HD22	5:B:251:HOH:O	2.19	0.42
2:D:72:TYR:N	2:D:73:PRO:CD	2.81	0.42
1:A:80:PRO:HA	5:A:285:HOH:O	2.19	0.42
2:D:67:LEU:HA	2:D:70:LEU:HD12	2.02	0.42
1:B:49:GLN:O	1:B:51:GLY:N	2.53	0.42
1:B:123:GLU:O	1:B:126:LEU:N	2.52	0.42
1:B:149:LEU:C	1:B:149:LEU:HD23	2.44	0.42
1:A:213:PHE:CE2	1:B:216:ASN:ND2	2.86	0.42
1:B:37:LEU:HD23	5:B:274:HOH:O	2.20	0.42
2:D:11:ASP:O	2:D:14:VAL:HG22	2.19	0.42
1:B:185:ILE:O	1:B:189:PHE:HB2	2.20	0.42
1:A:145:ASP:O	1:A:149:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ARG:CD	1:B:42:ARG:C	2.93	0.42
1:B:176:TYR:CZ	1:B:180:ARG:NH2	2.88	0.42
2:D:128:LYS:HA	2:D:131:GLU:CB	2.49	0.42
2:D:46:VAL:O	2:D:49:LYS:HE3	2.19	0.42
1:B:93:GLN:CG	5:B:263:HOH:O	2.68	0.42
2:D:14:VAL:HG23	2:D:16:LYS:HG3	2.02	0.42
2:D:122:ASP:O	2:D:126:ILE:HB	2.20	0.42
2:D:140:PRO:O	2:D:141:GLN:C	2.63	0.42
1:A:68:LEU:HA	1:A:68:LEU:HD12	1.86	0.41
1:A:154:ARG:CD	1:A:155:ASP:N	2.83	0.41
2:D:12:GLY:O	2:D:13:ALA:CB	2.68	0.41
1:B:31:GLU:C	5:B:256:HOH:O	2.63	0.41
2:D:79:LEU:CD2	2:D:111:ILE:HB	2.50	0.41
1:B:176:TYR:OH	1:B:180:ARG:NH2	2.45	0.41
1:A:151:LEU:HD12	5:A:265:HOH:O	2.20	0.41
1:B:110:PHE:CD1	1:B:114:ILE:HD11	2.55	0.41
1:B:183:VAL:N	1:B:186:LYS:HB2	2.36	0.41
2:D:97:TRP:HA	2:D:97:TRP:CE3	2.56	0.41
1:A:30:LEU:HD11	1:A:183:VAL:HG23	2.03	0.40
2:D:117:LEU:HD11	2:D:120:ARG:NH1	2.35	0.40
1:A:195:ILE:HD13	1:B:81:GLU:HB2	2.03	0.40
1:B:123:GLU:OE1	1:B:123:GLU:HA	2.21	0.40
2:D:53:LEU:CD1	5:D:216:HOH:O	2.64	0.40
2:D:155:LEU:HD11	2:D:171:GLU:HG3	2.03	0.40
2:D:161:THR:C	2:D:163:ARG:H	2.30	0.40
1:B:182:ASP:C	1:B:186:LYS:HB2	2.47	0.40
1:B:202:LEU:HD12	1:B:202:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

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	181/224 (81%)	162 (90%)	18 (10%)	1 (1%)	21	44
1	B	174/224 (78%)	147 (84%)	19 (11%)	8 (5%)	2	4
2	D	175/192 (91%)	145 (83%)	24 (14%)	6 (3%)	3	7
All	All	530/640 (83%)	454 (86%)	61 (12%)	15 (3%)	4	9

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ASP
1	B	110	PHE
1	B	183	VAL
1	B	187	LEU
2	D	35	THR
2	D	107	ASN
2	D	124	ASP
1	B	32	LEU
1	B	174	ASP
2	D	30	GLY
1	B	29	GLU
1	B	150	SER
1	B	111	VAL
2	D	168	VAL
2	D	99	PRO

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	159/193 (82%)	144 (91%)	15 (9%)	8	21
1	B	155/193 (80%)	141 (91%)	14 (9%)	9	23
2	D	153/168 (91%)	147 (96%)	6 (4%)	28	57
All	All	467/554 (84%)	432 (92%)	35 (8%)	12	31

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	48	LEU
1	A	75	LEU
1	A	81	GLU
1	A	88	TYR
1	A	92	THR
1	A	93	GLN
1	A	119	THR
1	A	121	THR
1	A	137	LEU
1	A	146	LEU
1	A	154	ARG
1	A	179	LEU
1	A	193	ASN
1	A	195	ILE
1	B	31	GLU
1	B	45	GLU
1	B	75	LEU
1	B	81	GLU
1	B	96	LEU
1	B	137	LEU
1	B	138	GLU
1	B	142	TYR
1	B	177	GLU
1	B	186	LYS
1	B	193	ASN
1	B	202	LEU
1	B	203	LEU
1	B	222	GLN
2	D	11	ASP
2	D	67	LEU
2	D	107	ASN
2	D	123	LYS
2	D	129	LEU
2	D	153	LYS

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	33	GLN
1	A	63	GLN
1	A	83	GLN
1	A	93	GLN

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Mol	Chain	Res	Type
1	A	99	ASN
1	A	131	GLN
1	A	199	HIS
1	A	206	HIS
1	A	207	ASN
1	A	219	GLN
1	B	33	GLN
1	B	65	GLN
1	B	83	GLN
1	B	93	GLN
1	B	115	ASN
1	B	206	HIS
2	D	43	ASN
2	D	74	GLN
2	D	107	ASN

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 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
4	GDP	D	200	3	29,30,30	0.79	0	45,47,47	1.59	8 (17%)

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	GDP	D	200	3	-	2/16/32/32	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	200	GDP	C5-C4-N3	-4.57	121.12	128.39
4	D	200	GDP	C2-N3-C4	4.45	119.97	112.30
4	D	200	GDP	N9-C8-N7	-2.96	107.91	113.40
4	D	200	GDP	N9-C4-N3	2.77	131.50	125.95
4	D	200	GDP	C2-N1-C6	-2.76	120.11	125.11
4	D	200	GDP	C8-N7-C5	2.61	108.91	104.26
4	D	200	GDP	O6-C6-C5	-2.34	120.36	126.53
4	D	200	GDP	C5-C6-N1	2.24	118.95	113.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	200	GDP	PA-O3A-PB-O2B
4	D	200	GDP	PA-O3A-PB-O1B

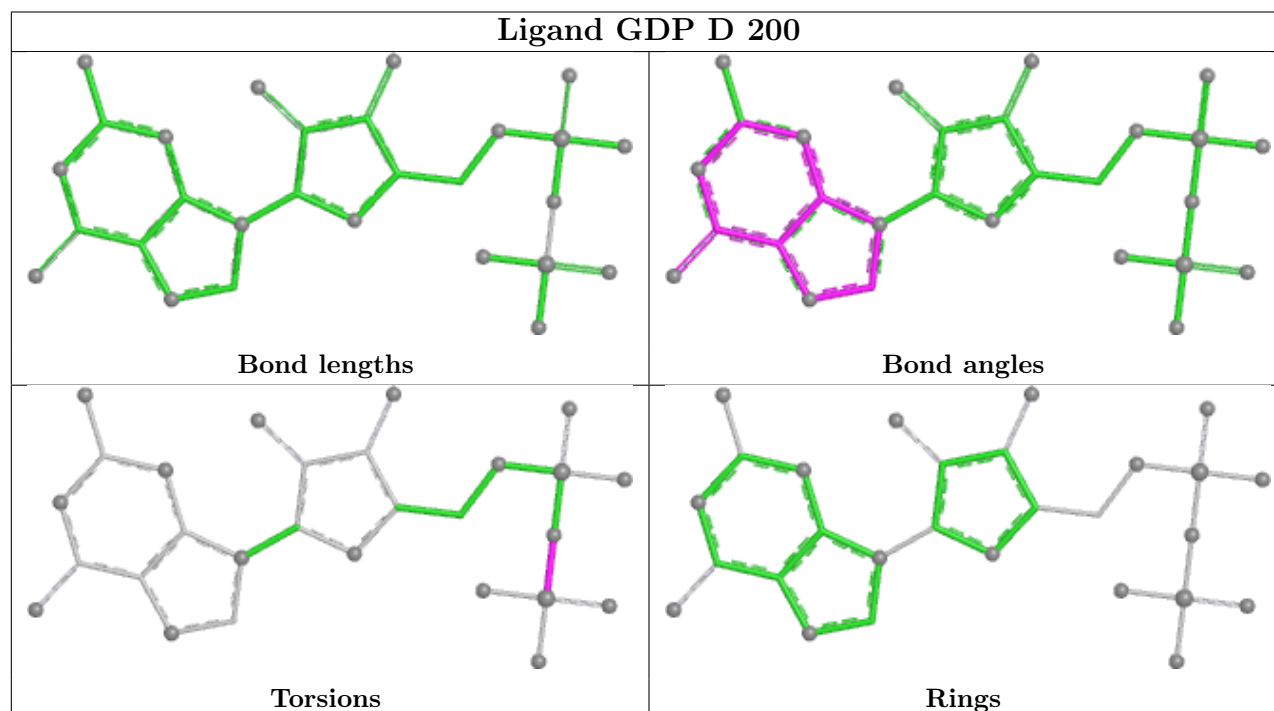
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	200	GDP	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.