



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:01 am BST

PDB ID : 4C0A
Title : Arf1(Delta1-17)in complex with BRAG2 Sec7-PH domain
Authors : Aizel, K.; Biou, V.; Navaza, J.; Duarte, L.; Campanacci, V.; Cherfils, J.; Zeghouf, M.
Deposited on : 2013-08-01
Resolution : 3.30 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) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

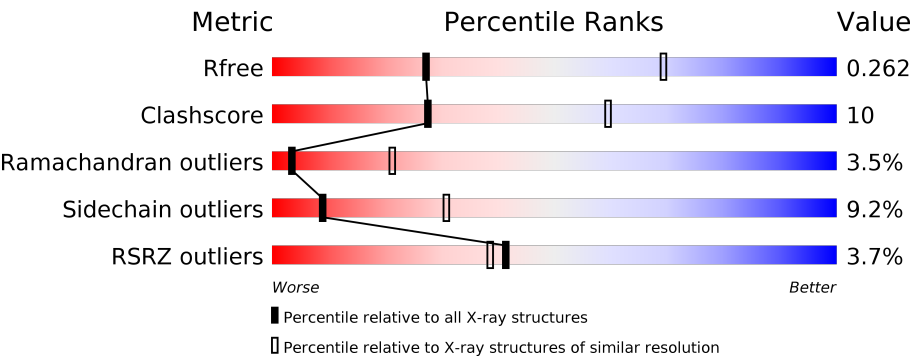
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	383	<div><div>3%</div><div><div></div><div>66%</div><div>23%</div><div>•</div><div>8%</div></div></div>
1	B	383	<div><div>2%</div><div><div></div><div>65%</div><div>24%</div><div>• •</div><div>7%</div></div></div>
1	E	383	<div><div></div><div><div></div><div>64%</div><div>24%</div><div>• •</div><div>8%</div></div></div>
1	F	383	<div><div></div><div><div></div><div>62%</div><div>26%</div><div>• •</div><div>8%</div></div></div>
2	C	164	<div><div></div><div><div></div><div>68%</div><div>23%</div><div>5%</div><div>• •</div></div></div>
2	D	164	<div><div>2%</div><div><div></div><div>68%</div><div>28%</div><div>• •</div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	164	<div><div></div><div>11%</div><div>71%</div><div>24%</div><div></div><div></div></div>
2	H	164	<div><div></div><div>20%</div><div>60%</div><div>31%</div><div>5%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16930 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 IQ MOTIF AND SEC7 DOMAIN-CONTAINING PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2897	1845	520	517	15			
1	B	357	Total	C	N	O	S	0	1	0
			2945	1875	531	524	15			
1	E	351	Total	C	N	O	S	0	0	0
			2893	1842	520	516	15			
1	F	351	Total	C	N	O	S	0	0	0
			2884	1834	519	516	15			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	GLY	-	expression tag	UNP Q6DN90
A	382	ALA	-	expression tag	UNP Q6DN90
A	383	MET	-	expression tag	UNP Q6DN90
A	384	GLY	-	expression tag	UNP Q6DN90
A	385	SER	-	expression tag	UNP Q6DN90
A	386	GLY	-	expression tag	UNP Q6DN90
A	387	ILE	-	expression tag	UNP Q6DN90
A	388	PRO	-	expression tag	UNP Q6DN90
A	389	MET	-	expression tag	UNP Q6DN90
A	498	LYS	GLU	engineered mutation	UNP Q6DN90
B	381	GLY	-	expression tag	UNP Q6DN90
B	382	ALA	-	expression tag	UNP Q6DN90
B	383	MET	-	expression tag	UNP Q6DN90
B	384	GLY	-	expression tag	UNP Q6DN90
B	385	SER	-	expression tag	UNP Q6DN90
B	386	GLY	-	expression tag	UNP Q6DN90
B	387	ILE	-	expression tag	UNP Q6DN90
B	388	PRO	-	expression tag	UNP Q6DN90
B	389	MET	-	expression tag	UNP Q6DN90
B	498	LYS	GLU	engineered mutation	UNP Q6DN90

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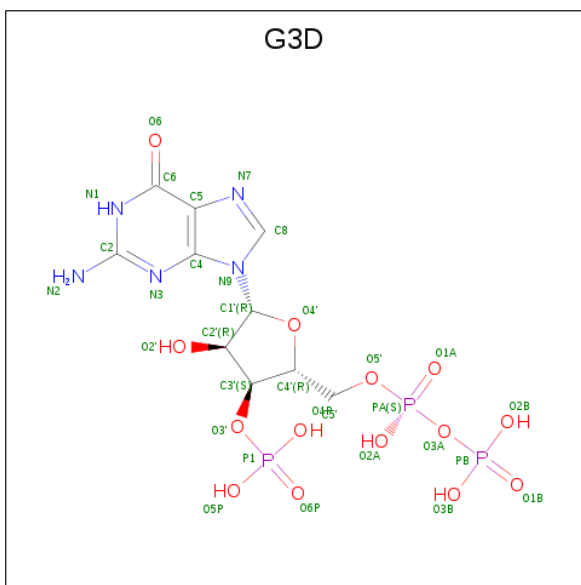
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Chain	Residue	Modelled	Actual	Comment	Reference
E	381	GLY	-	expression tag	UNP Q6DN90
E	382	ALA	-	expression tag	UNP Q6DN90
E	383	MET	-	expression tag	UNP Q6DN90
E	384	GLY	-	expression tag	UNP Q6DN90
E	385	SER	-	expression tag	UNP Q6DN90
E	386	GLY	-	expression tag	UNP Q6DN90
E	387	ILE	-	expression tag	UNP Q6DN90
E	388	PRO	-	expression tag	UNP Q6DN90
E	389	MET	-	expression tag	UNP Q6DN90
E	498	LYS	GLU	engineered mutation	UNP Q6DN90
F	381	GLY	-	expression tag	UNP Q6DN90
F	382	ALA	-	expression tag	UNP Q6DN90
F	383	MET	-	expression tag	UNP Q6DN90
F	384	GLY	-	expression tag	UNP Q6DN90
F	385	SER	-	expression tag	UNP Q6DN90
F	386	GLY	-	expression tag	UNP Q6DN90
F	387	ILE	-	expression tag	UNP Q6DN90
F	388	PRO	-	expression tag	UNP Q6DN90
F	389	MET	-	expression tag	UNP Q6DN90
F	498	LYS	GLU	engineered mutation	UNP Q6DN90

- Molecule 2 is a protein called ADP-RIBOSYLATION FACTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	161	Total	C	N	O	S	0	0	0
			1293	819	227	242	5			
2	D	164	Total	C	N	O	S	0	0	0
			1315	831	232	247	5			
2	G	162	Total	C	N	O	S	0	0	0
			1298	822	228	243	5			
2	H	159	Total	C	N	O	S	0	0	0
			1277	810	222	240	5			

- Molecule 3 is GUANOSINE-3'-MONOPHOSPHATE-5'-DIPHOSPHATE (three-letter code: G3D) (formula: C₁₀H₁₆N₅O₁₄P₃).

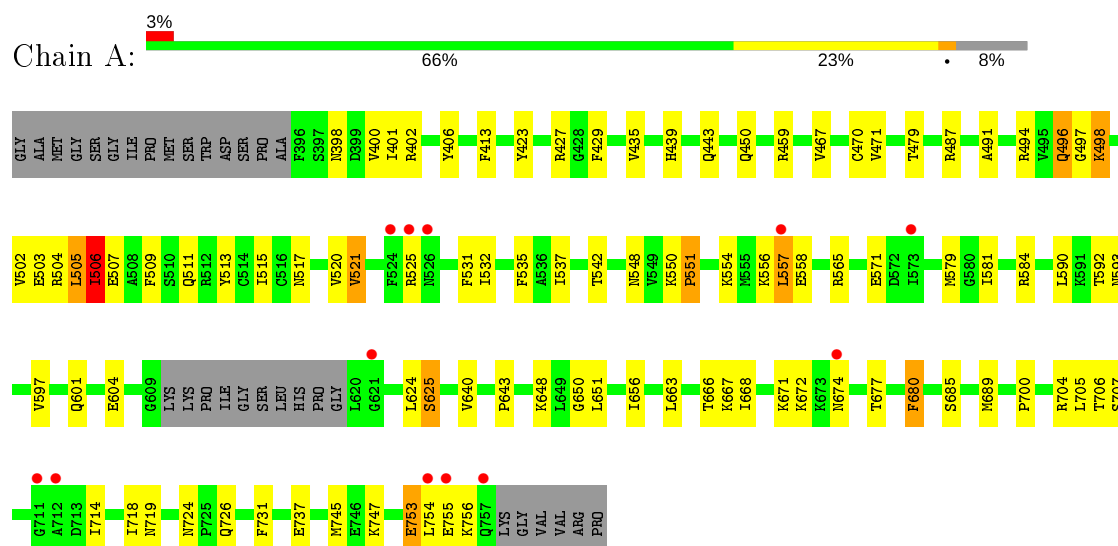


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total 32	C 10	N 5	O 14	P 3	0	0
3	D	1	Total 32	C 10	N 5	O 14	P 3	0	0
3	G	1	Total 32	C 10	N 5	O 14	P 3	0	0
3	H	1	Total 32	C 10	N 5	O 14	P 3	0	0

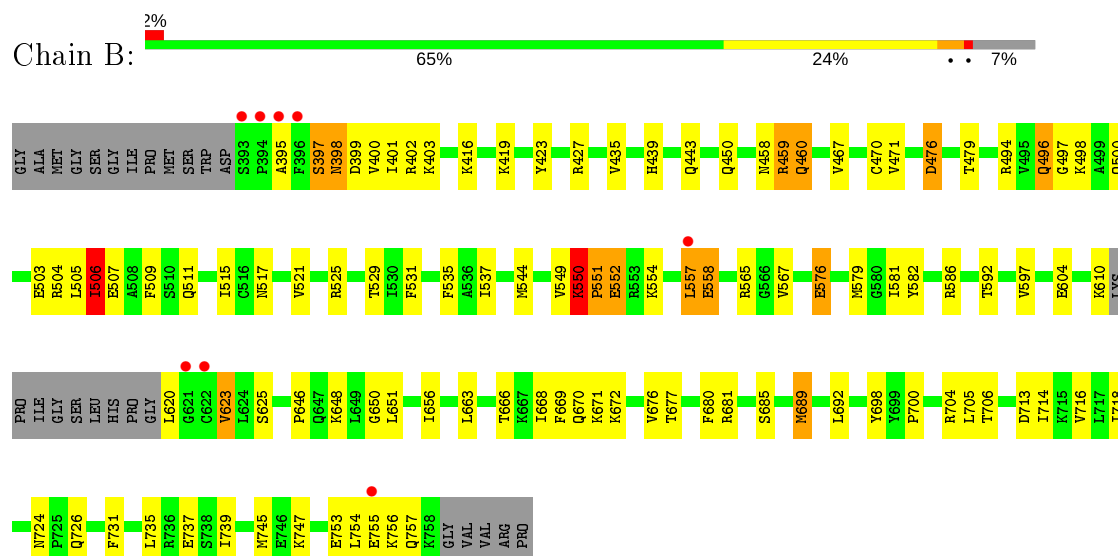
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: IQ MOTIF AND SEC7 DOMAIN-CONTAINING PROTEIN 1

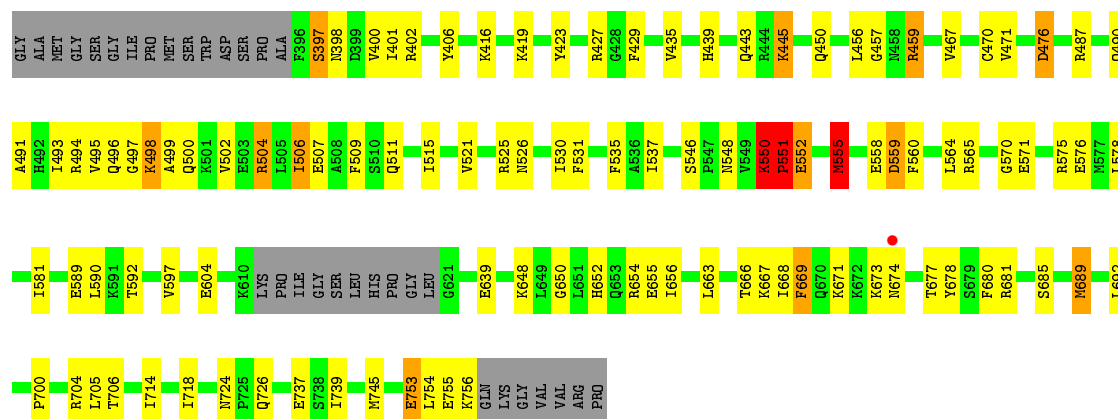


• Molecule 1: IQ MOTIF AND SEC7 DOMAIN-CONTAINING PROTEIN 1

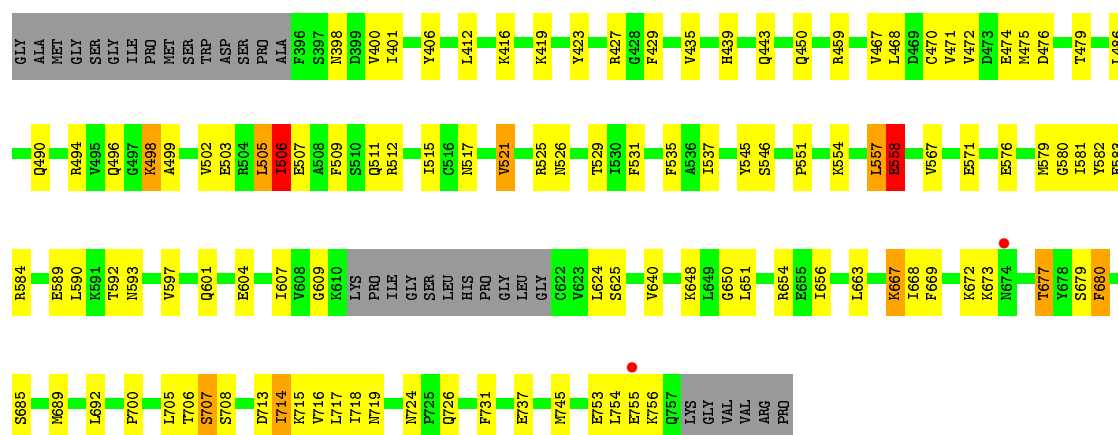


• Molecule 1: IQ MOTIF AND SEC7 DOMAIN-CONTAINING PROTEIN 1

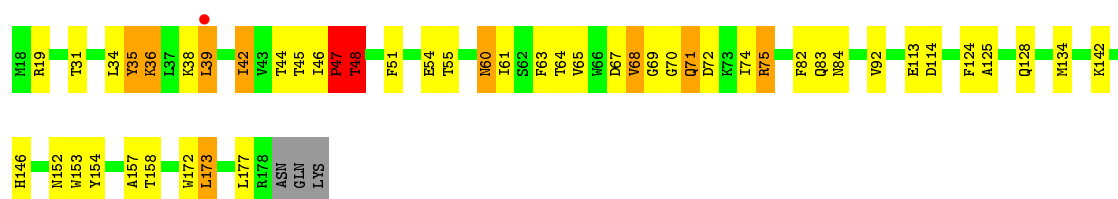




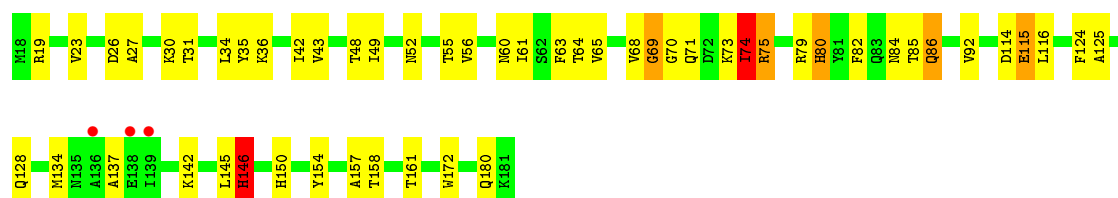
• Molecule 1: IQ MOTIF AND SEC7 DOMAIN-CONTAINING PROTEIN 1



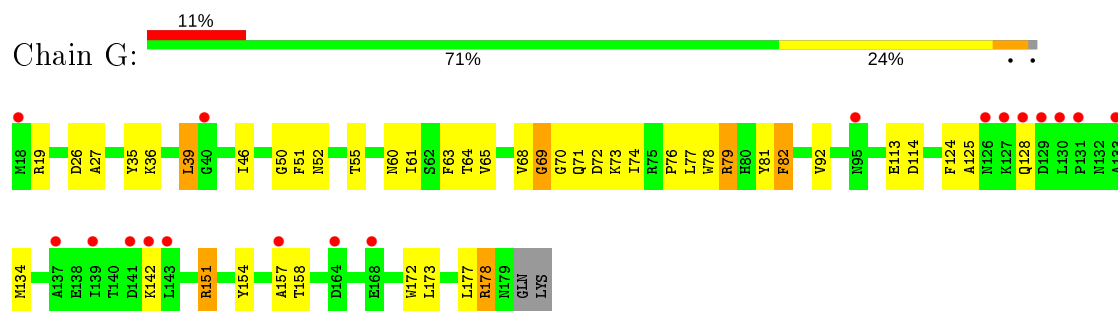
• Molecule 2: ADP-RIBOSYLATION FACTOR 1



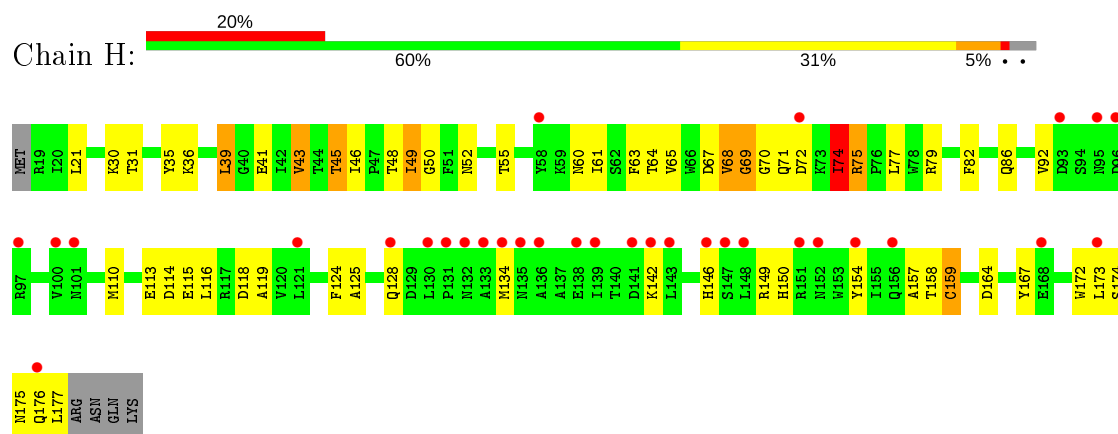
• Molecule 2: ADP-RIBOSYLATION FACTOR 1



- Molecule 2: ADP-RIBOSYLATION FACTOR 1



- Molecule 2: ADP-RIBOSYLATION FACTOR 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.98 Å 65.78 Å 196.86 Å 90.00° 96.13° 90.00°	Depositor
Resolution (Å)	42.84 – 3.30 42.84 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.84-3.30) 99.5 (42.84-3.30)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 3.32 Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.199 , 0.248 0.214 , 0.262	Depositor DCC
R_{free} test set	1757 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 82.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16930	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1182e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G3D

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	0.50	0/2950	0.78	4/3962 (0.1%)
1	B	0.54	0/3002	0.83	4/4030 (0.1%)
1	E	0.53	0/2946	0.82	3/3955 (0.1%)
1	F	0.54	0/2936	0.84	6/3944 (0.2%)
2	C	0.47	0/1316	0.81	2/1783 (0.1%)
2	D	0.51	0/1338	0.84	2/1813 (0.1%)
2	G	0.43	0/1321	0.74	0/1790
2	H	0.42	0/1300	0.80	0/1762
All	All	0.51	0/17109	0.81	21/23039 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	557	LEU	N-CA-C	-6.72	92.86	111.00
1	B	398	ASN	C-N-CA	6.20	137.20	121.70
1	A	506	ILE	N-CA-CB	6.10	124.82	110.80
1	F	474	GLU	C-N-CA	6.04	136.79	121.70
1	B	505	LEU	N-CA-C	-5.90	95.06	111.00
1	A	505	LEU	N-CA-C	-5.65	95.75	111.00
1	F	525	ARG	C-N-CA	5.55	135.57	121.70
2	C	60	ASN	CA-CB-CG	5.52	125.53	113.40
1	E	555	MET	N-CA-C	5.50	125.86	111.00
1	F	505	LEU	N-CA-C	-5.42	96.36	111.00
2	D	146	HIS	N-CA-CB	5.37	120.26	110.60
1	E	551	PRO	N-CA-C	5.32	125.94	112.10
2	D	86	GLN	N-CA-C	5.27	125.24	111.00
2	C	47	PRO	N-CA-C	5.27	125.80	112.10
1	E	397	SER	C-N-CA	5.26	134.85	121.70
1	B	557	LEU	N-CA-C	-5.21	96.92	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	506	ILE	N-CA-CB	5.18	122.71	110.80
1	A	525	ARG	C-N-CA	5.16	134.60	121.70
1	B	506	ILE	N-CA-CB	5.02	122.35	110.80
1	A	667	LYS	N-CA-C	-5.02	97.44	111.00
1	F	667	LYS	N-CA-C	-5.02	97.45	111.00

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	A	2897	0	2954	53	0
1	B	2945	0	3016	64	0
1	E	2893	0	2954	60	0
1	F	2884	0	2935	55	0
2	C	1293	0	1285	37	0
2	D	1315	0	1301	41	0
2	G	1298	0	1287	27	0
2	H	1277	0	1270	36	0
3	C	32	0	11	0	0
3	D	32	0	11	2	0
3	G	32	0	11	1	0
3	H	32	0	11	0	0
All	All	16930	0	17046	338	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 10.

All (338) 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:C:152:ASN:OD1	2:D:137:ALA:HB2	1.53	1.09
2:G:151:ARG:HH11	2:G:151:ARG:HG3	1.21	1.03
1:F:580:GLY:O	1:F:584:ARG:HG2	1.61	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:THR:HG21	2:D:116:LEU:CD2	1.91	1.00
2:D:85:THR:HG21	2:D:116:LEU:HD23	1.47	0.96
2:D:30:LYS:HE3	2:D:69:GLY:HA3	1.55	0.88
2:D:71:GLN:HA	2:D:75:ARG:HG2	1.55	0.87
2:H:86:GLN:O	2:H:119:ALA:HB3	1.74	0.87
2:C:35:TYR:HA	2:C:38:LYS:HE3	1.57	0.86
2:H:159:CYS:SG	2:H:164:ASP:HB2	2.19	0.83
2:C:38:LYS:HD3	2:C:54:GLU:HG3	1.60	0.83
2:D:82:PHE:HB3	2:D:115:GLU:HB3	1.62	0.80
1:E:555:MET:O	1:E:559:ASP:HB2	1.80	0.80
2:G:151:ARG:NH1	2:G:151:ARG:HG3	1.91	0.80
1:F:706:THR:HG22	1:F:716:VAL:HA	1.71	0.73
1:F:467:VAL:O	1:F:471:VAL:HG23	1.89	0.73
1:B:467:VAL:O	1:B:471:VAL:HG23	1.89	0.73
1:F:557:LEU:O	1:F:558:GLU:HB3	1.90	0.72
2:C:68:VAL:HG12	2:C:69:GLY:H	1.53	0.72
1:B:557:LEU:HD21	1:B:579:MET:HG2	1.71	0.71
1:E:467:VAL:O	1:E:471:VAL:HG23	1.91	0.71
1:A:467:VAL:O	1:A:471:VAL:HG23	1.91	0.71
2:C:68:VAL:HG12	2:C:69:GLY:N	2.06	0.70
1:F:472:VAL:O	1:F:475:MET:HB3	1.91	0.70
2:D:31:THR:HG21	1:E:498:LYS:HA	1.74	0.69
1:A:551:PRO:HA	1:A:554:LYS:HG2	1.74	0.68
2:H:86:GLN:O	2:H:119:ALA:CB	2.41	0.68
2:C:173:LEU:HD23	2:C:177:LEU:CD2	2.23	0.68
1:E:445:LYS:HE3	1:E:445:LYS:H	1.57	0.68
2:D:74:ILE:O	2:D:75:ARG:NH1	2.27	0.66
1:E:506:ILE:HA	1:E:509:PHE:HB3	1.78	0.66
1:E:457:GLY:HA2	1:E:504:ARG:HG2	1.76	0.65
1:E:531:PHE:CZ	1:E:535:PHE:HE2	2.15	0.65
2:D:61:ILE:HG12	2:D:63:PHE:CE1	2.32	0.64
2:C:45:THR:HG22	1:F:601:GLN:HB3	1.79	0.64
1:B:479:THR:H	1:B:517:ASN:HD21	1.45	0.64
1:B:620:LEU:HD11	1:B:623:VAL:HA	1.79	0.64
2:C:48:THR:HG21	1:F:546:SER:HA	1.79	0.64
1:F:503:GLU:HA	1:F:535:PHE:CZ	2.33	0.64
1:A:556:LYS:HD3	1:A:558:GLU:H	1.63	0.64
1:A:439:HIS:O	1:A:443:GLN:HG2	1.97	0.64
1:F:503:GLU:HA	1:F:535:PHE:HZ	1.63	0.63
2:G:27:ALA:HA	3:G:401:G3D:H5'1	1.81	0.63
1:A:532:ILE:HG23	2:H:77:LEU:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:ARG:HH21	1:E:535:PHE:HB2	1.64	0.62
1:A:542:THR:HA	2:H:48:THR:HG21	1.80	0.62
1:E:439:HIS:O	1:E:443:GLN:HG2	1.99	0.62
1:F:439:HIS:O	1:F:443:GLN:HG2	1.98	0.62
1:A:502:VAL:O	1:A:505:LEU:O	2.17	0.62
1:A:531:PHE:CZ	1:A:535:PHE:HE2	2.18	0.62
2:D:52:ASN:HD21	1:E:497:GLY:HA2	1.66	0.61
1:F:531:PHE:CZ	1:F:535:PHE:HE2	2.19	0.61
1:B:724:ASN:HD22	1:B:726:GLN:HE21	1.46	0.60
2:H:21:LEU:HD22	2:H:68:VAL:HG21	1.84	0.60
1:B:531:PHE:CZ	1:B:535:PHE:HE2	2.19	0.60
2:G:134:MET:HE1	2:G:142:LYS:HG3	1.84	0.60
2:H:134:MET:HE1	2:H:142:LYS:HG3	1.84	0.60
2:D:134:MET:HE1	2:D:142:LYS:HG3	1.84	0.60
1:E:487:ARG:HG3	1:E:590:LEU:HD23	1.83	0.60
2:C:134:MET:HE1	2:C:142:LYS:HG3	1.84	0.60
1:B:671:LYS:HA	1:B:676:VAL:HG23	1.82	0.59
1:B:439:HIS:O	1:B:443:GLN:HG2	2.01	0.59
1:E:724:ASN:OD1	1:E:726:GLN:HB2	2.02	0.59
1:F:551:PRO:HA	1:F:554:LYS:HG2	1.83	0.59
2:D:79:ARG:O	2:D:80:HIS:CB	2.50	0.58
1:F:724:ASN:OD1	1:F:726:GLN:HB2	2.03	0.58
2:D:145:LEU:O	2:D:146:HIS:HB2	2.03	0.58
2:C:31:THR:HG21	1:F:498:LYS:HG3	1.85	0.58
2:C:38:LYS:CD	2:C:54:GLU:HG3	2.32	0.58
2:C:152:ASN:CG	2:D:137:ALA:HB2	2.23	0.58
2:G:151:ARG:CG	2:G:151:ARG:HH11	2.06	0.58
2:D:124:PHE:CD1	2:D:158:THR:HG21	2.39	0.57
2:H:124:PHE:CD1	2:H:158:THR:HG21	2.39	0.57
2:C:124:PHE:CD1	2:C:158:THR:HG21	2.39	0.57
2:G:124:PHE:CD1	2:G:158:THR:HG21	2.39	0.57
1:B:669:PHE:HD1	1:B:670:GLN:HG3	1.69	0.57
1:E:537:ILE:HG12	1:E:581:ILE:CG2	2.35	0.57
1:E:666:THR:HG22	1:E:680:PHE:HA	1.86	0.57
2:D:85:THR:CG2	2:D:116:LEU:HD23	2.29	0.57
2:D:75:ARG:HH21	1:E:535:PHE:CB	2.18	0.57
1:A:503:GLU:HA	1:A:535:PHE:HZ	1.68	0.56
1:B:551:PRO:HA	1:B:554:LYS:HG3	1.87	0.56
1:B:549:VAL:HB	1:B:554:LYS:HE2	1.86	0.56
2:C:31:THR:HG22	2:C:67:ASP:OD2	2.04	0.56
1:A:724:ASN:OD1	1:A:726:GLN:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:82:PHE:CD2	2:G:113:GLU:HG2	2.41	0.56
2:C:134:MET:CE	2:C:142:LYS:HG3	2.36	0.56
2:G:134:MET:CE	2:G:142:LYS:HG3	2.36	0.56
1:A:666:THR:HG22	1:A:680:PHE:HA	1.87	0.56
2:C:153:TRP:CZ2	2:D:146:HIS:CG	2.94	0.56
1:B:666:THR:HG22	1:B:680:PHE:HA	1.88	0.55
2:H:134:MET:CE	2:H:142:LYS:HG3	2.36	0.55
2:D:134:MET:CE	2:D:142:LYS:HG3	2.37	0.55
1:B:550:LYS:O	1:B:552:GLU:N	2.32	0.55
2:D:68:VAL:C	2:D:70:GLY:H	2.10	0.55
2:C:146:HIS:CD2	2:D:146:HIS:O	2.60	0.55
2:C:173:LEU:HD23	2:C:177:LEU:HD23	1.88	0.55
1:A:581:ILE:HD13	1:A:584:ARG:HH21	1.71	0.55
1:B:458:ASN:O	1:B:460:GLN:N	2.32	0.55
1:B:398:ASN:HB3	1:B:403:LYS:HE2	1.89	0.55
1:B:497:GLY:HA2	2:G:52:ASN:HD21	1.71	0.55
1:A:557:LEU:HD11	1:A:579:MET:HG2	1.89	0.55
1:B:557:LEU:HD11	1:B:579:MET:HA	1.89	0.55
1:E:656:ILE:HG23	1:E:663:LEU:HD11	1.88	0.55
1:F:502:VAL:O	1:F:505:LEU:O	2.25	0.54
2:C:35:TYR:CA	2:C:38:LYS:HE3	2.34	0.54
2:D:61:ILE:HG12	2:D:63:PHE:HE1	1.72	0.54
1:E:552:GLU:CD	1:E:552:GLU:H	2.10	0.54
1:F:557:LEU:HD21	1:F:579:MET:HG2	1.90	0.54
1:F:656:ILE:HG23	1:F:663:LEU:HD11	1.89	0.54
1:A:491:ALA:HA	1:A:592:THR:HA	1.90	0.54
1:B:656:ILE:HG23	1:B:663:LEU:HD11	1.90	0.54
1:A:656:ILE:HG23	1:A:663:LEU:HD11	1.89	0.53
2:C:38:LYS:HD3	2:C:54:GLU:CG	2.37	0.53
1:E:570:GLY:HA2	2:G:60:ASN:HB2	1.89	0.53
1:F:537:ILE:HG12	1:F:581:ILE:CG2	2.38	0.53
2:H:159:CYS:HG	2:H:164:ASP:HB2	1.71	0.53
1:E:570:GLY:HA2	2:G:60:ASN:CB	2.39	0.53
2:H:110:MET:O	2:H:116:LEU:HD11	2.09	0.53
1:B:500:GLN:HG3	2:G:26:ASP:HB3	1.91	0.53
2:C:71:GLN:HA	2:C:75:ARG:HB2	1.89	0.53
2:C:46:ILE:O	2:C:47:PRO:O	2.26	0.53
1:A:400:VAL:HG13	1:A:401:ILE:HD12	1.92	0.52
1:B:689:MET:HE3	1:B:705:LEU:HD22	1.92	0.52
2:H:67:ASP:O	2:H:69:GLY:N	2.43	0.52
1:E:560:PHE:O	1:E:564:LEU:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:450:GLN:HA	1:F:494:ARG:HB3	1.92	0.52
1:A:496:GLN:HB2	2:H:50:GLY:H	1.75	0.52
2:H:173:LEU:C	2:H:175:ASN:H	2.14	0.52
1:E:704:ARG:HG2	1:E:706:THR:HG23	1.92	0.52
1:E:476:ASP:N	1:E:476:ASP:OD1	2.42	0.52
1:F:531:PHE:CZ	1:F:535:PHE:CE2	2.97	0.52
1:B:689:MET:HG2	1:B:739:ILE:HD11	1.90	0.51
1:F:406:TYR:HB2	1:F:429:PHE:CE1	2.45	0.51
1:B:395:ALA:HB3	1:B:399:ASP:HB2	1.91	0.51
1:B:459:ARG:HE	1:B:500:GLN:HB3	1.76	0.51
1:E:400:VAL:HG13	1:E:401:ILE:HD12	1.93	0.51
1:B:400:VAL:HG13	1:B:401:ILE:HD12	1.93	0.51
2:H:68:VAL:O	2:H:70:GLY:N	2.44	0.51
1:A:689:MET:HE3	1:A:705:LEU:HD22	1.93	0.51
1:B:576:GLU:HA	1:B:579:MET:HE2	1.92	0.51
2:H:113:GLU:HB3	2:H:116:LEU:HG	1.93	0.50
1:F:400:VAL:HG13	1:F:401:ILE:HD12	1.94	0.50
2:D:154:TYR:HB2	2:D:172:TRP:CE2	2.46	0.50
2:H:154:TYR:HB2	2:H:172:TRP:CE2	2.46	0.50
1:B:706:THR:HG22	1:B:716:VAL:HG22	1.93	0.49
1:A:406:TYR:HB2	1:A:429:PHE:CE1	2.47	0.49
1:A:704:ARG:HG2	1:A:706:THR:HG23	1.94	0.49
1:B:450:GLN:HA	1:B:494:ARG:HB3	1.94	0.49
1:E:531:PHE:CZ	1:E:535:PHE:CE2	3.00	0.49
1:F:592:THR:HG22	1:F:593:ASN:H	1.77	0.49
2:H:82:PHE:HB3	2:H:115:GLU:HB3	1.94	0.49
2:H:173:LEU:O	2:H:175:ASN:N	2.44	0.49
2:C:154:TYR:HB2	2:C:172:TRP:CE2	2.47	0.49
1:B:531:PHE:CZ	1:B:535:PHE:CE2	3.00	0.49
1:B:544:MET:HE1	1:B:586:ARG:HA	1.95	0.49
2:G:154:TYR:HB2	2:G:172:TRP:CE2	2.47	0.48
1:A:435:VAL:HG12	1:A:470:CYS:SG	2.53	0.48
2:D:68:VAL:O	2:D:70:GLY:N	2.45	0.48
1:E:511:GLN:O	1:E:515:ILE:HG12	2.13	0.48
1:A:537:ILE:HG12	1:A:581:ILE:CG2	2.42	0.48
2:D:128:GLN:HG3	2:D:157:ALA:HB1	1.95	0.48
1:A:548:ASN:HB3	2:H:55:THR:HG23	1.94	0.48
1:E:450:GLN:HA	1:E:494:ARG:HB3	1.96	0.48
1:B:506:ILE:HA	1:B:509:PHE:HB3	1.94	0.48
2:C:38:LYS:CE	2:C:54:GLU:HG3	2.44	0.48
1:A:502:VAL:HG12	1:A:535:PHE:HE1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:564:LEU:HD13	1:E:578:LEU:HD22	1.96	0.48
1:A:531:PHE:CZ	1:A:535:PHE:CE2	3.00	0.48
1:F:753:GLU:HA	1:F:756:LYS:HD2	1.96	0.48
1:F:506:ILE:HA	1:F:509:PHE:HB3	1.95	0.48
2:G:68:VAL:HG12	2:G:69:GLY:N	2.29	0.48
1:B:753:GLU:HA	1:B:756:LYS:HD2	1.96	0.48
1:B:689:MET:HE2	1:B:735:LEU:HD11	1.96	0.47
1:E:435:VAL:HG12	1:E:470:CYS:SG	2.54	0.47
1:E:490:GLN:HE22	1:E:592:THR:H	1.61	0.47
1:B:503:GLU:HA	1:B:535:PHE:HZ	1.78	0.47
2:D:55:THR:HG22	2:D:64:THR:OG1	2.15	0.47
1:E:654:ARG:HH12	1:E:667:LYS:HE3	1.79	0.47
1:F:435:VAL:HG12	1:F:470:CYS:SG	2.53	0.47
2:H:128:GLN:HG3	2:H:157:ALA:HB1	1.96	0.47
1:F:529:THR:HG23	1:F:567:VAL:HG12	1.96	0.47
2:G:82:PHE:HD2	2:G:113:GLU:HG2	1.77	0.47
1:A:753:GLU:HA	1:A:756:LYS:HD2	1.97	0.47
2:C:128:GLN:HG3	2:C:157:ALA:HB1	1.96	0.47
1:B:435:VAL:HG12	1:B:470:CYS:SG	2.54	0.47
1:E:459:ARG:HB3	1:E:504:ARG:HD3	1.97	0.47
2:D:26:ASP:HB3	1:E:500:GLN:HE21	1.79	0.47
1:E:406:TYR:HB2	1:E:429:PHE:CE1	2.50	0.47
2:D:48:THR:HG21	1:E:546:SER:HA	1.96	0.47
1:F:511:GLN:O	1:F:515:ILE:HG12	2.14	0.47
2:G:55:THR:HG22	2:G:64:THR:OG1	2.13	0.47
1:B:476:ASP:N	1:B:476:ASP:OD1	2.48	0.47
2:D:26:ASP:HB3	1:E:500:GLN:NE2	2.30	0.47
1:B:459:ARG:HB3	1:B:504:ARG:HD3	1.97	0.47
1:B:479:THR:O	1:B:479:THR:CG2	2.63	0.47
1:B:704:ARG:HG2	1:B:706:THR:HG23	1.97	0.47
2:G:61:ILE:HG12	2:G:63:PHE:CE1	2.50	0.47
2:H:61:ILE:HG12	2:H:63:PHE:CE1	2.49	0.47
2:C:45:THR:C	2:C:47:PRO:HD2	2.36	0.46
1:B:507:GLU:O	1:B:511:GLN:HG3	2.16	0.46
1:E:753:GLU:HA	1:E:756:LYS:HD2	1.98	0.46
2:C:19:ARG:NH1	2:C:84:ASN:HB2	2.31	0.46
2:C:61:ILE:HG12	2:C:63:PHE:CE1	2.51	0.46
1:F:486:LEU:O	1:F:490:GLN:HG3	2.15	0.46
1:A:487:ARG:HG3	1:A:590:LEU:HD23	1.97	0.46
2:G:76:PRO:HA	2:G:79:ARG:HH21	1.81	0.46
1:E:689:MET:HE3	1:E:705:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:55:THR:HG22	2:H:64:THR:OG1	2.16	0.46
2:D:79:ARG:O	2:D:80:HIS:HB3	2.15	0.45
2:G:128:GLN:HG3	2:G:157:ALA:HB1	1.97	0.45
1:B:706:THR:HG22	1:B:716:VAL:HA	1.98	0.45
1:F:592:THR:HG22	1:F:593:ASN:N	2.32	0.45
1:B:648:LYS:NZ	1:B:650:GLY:H	2.14	0.45
2:C:46:ILE:N	2:C:47:PRO:HD2	2.32	0.45
2:D:23:VAL:CG1	2:D:68:VAL:HB	2.47	0.45
1:F:607:ILE:CG2	1:F:680:PHE:HB2	2.47	0.45
2:G:76:PRO:HA	2:G:79:ARG:HE	1.81	0.45
1:B:689:MET:HG2	1:B:739:ILE:CD1	2.47	0.45
1:A:511:GLN:O	1:A:515:ILE:HG12	2.17	0.45
1:B:557:LEU:O	1:B:558:GLU:HB2	2.16	0.45
1:A:507:GLU:O	1:A:511:GLN:HG3	2.17	0.44
1:A:513:TYR:HE1	1:A:520:VAL:HG21	1.82	0.44
1:F:545:TYR:CD2	1:F:589:GLU:HG3	2.52	0.44
1:F:648:LYS:NZ	1:F:650:GLY:H	2.15	0.44
1:A:648:LYS:NZ	1:A:650:GLY:H	2.16	0.44
1:E:537:ILE:HG12	1:E:581:ILE:HG21	1.98	0.44
1:A:592:THR:OG1	2:H:49:ILE:HD11	2.17	0.44
1:A:531:PHE:HE2	2:H:75:ARG:HH22	1.64	0.44
1:B:656:ILE:HG21	1:B:731:PHE:CE1	2.52	0.44
1:A:592:THR:HG22	1:A:593:ASN:H	1.83	0.44
1:A:705:LEU:HD12	1:A:718:ILE:CG2	2.48	0.44
1:B:479:THR:N	1:B:517:ASN:HD21	2.13	0.44
1:A:479:THR:H	1:A:517:ASN:HD21	1.64	0.44
1:E:648:LYS:NZ	1:E:650:GLY:H	2.16	0.44
1:F:537:ILE:HG12	1:F:581:ILE:HG21	1.99	0.44
1:F:708:SER:HA	1:F:714:ILE:H	1.82	0.43
1:B:511:GLN:O	1:B:515:ILE:HG12	2.18	0.43
1:F:507:GLU:O	1:F:511:GLN:HG3	2.18	0.43
2:H:69:GLY:C	2:H:71:GLN:H	2.22	0.43
1:E:491:ALA:HA	1:E:592:THR:HA	2.01	0.43
1:A:656:ILE:HG21	1:A:731:PHE:CE1	2.53	0.43
1:B:496:GLN:HB2	2:G:50:GLY:H	1.84	0.43
2:C:34:LEU:HG	2:C:38:LYS:HE2	1.98	0.43
1:E:416:LYS:HD3	1:E:419:LYS:HD2	1.99	0.43
1:A:498:LYS:HG2	2:H:31:THR:HG21	2.00	0.43
2:D:161:THR:HG22	3:D:401:G3D:C6	2.49	0.43
1:E:669:PHE:HB3	1:E:677:THR:OG1	2.18	0.43
2:H:30:LYS:NZ	2:H:69:GLY:HA3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:GLN:HA	1:A:494:ARG:HB3	1.99	0.43
1:A:506:ILE:HA	1:A:509:PHE:HB3	2.01	0.43
2:C:55:THR:HG22	2:C:64:THR:OG1	2.18	0.43
2:C:68:VAL:CG1	2:C:69:GLY:N	2.76	0.43
1:F:705:LEU:HD12	1:F:718:ILE:CG2	2.48	0.43
1:B:423:TYR:OH	1:B:427:ARG:NH1	2.52	0.43
1:F:669:PHE:HB3	1:F:677:THR:OG1	2.19	0.43
1:B:537:ILE:HG12	1:B:581:ILE:CG2	2.49	0.42
2:C:48:THR:HG21	1:F:546:SER:CA	2.47	0.42
2:D:19:ARG:O	2:D:85:THR:O	2.37	0.42
2:D:27:ALA:HA	3:D:401:G3D:H5'1	2.00	0.42
2:D:70:GLY:CA	1:E:499:ALA:HB1	2.49	0.42
1:E:531:PHE:CE1	1:E:535:PHE:HE2	2.37	0.42
1:E:689:MET:HG2	1:E:739:ILE:HD11	2.02	0.42
1:A:601:GLN:HE22	2:H:46:ILE:HG23	1.84	0.42
2:D:92:VAL:HG13	2:D:125:ALA:HA	2.01	0.42
1:F:503:GLU:CA	1:F:535:PHE:HZ	2.28	0.42
2:G:76:PRO:O	2:G:79:ARG:HB2	2.20	0.42
1:A:498:LYS:HA	2:H:31:THR:HG21	2.02	0.42
1:E:656:ILE:CG2	1:E:663:LEU:HD11	2.49	0.42
1:F:656:ILE:HG21	1:F:731:PHE:CE1	2.55	0.42
1:B:557:LEU:HB2	1:B:582:TYR:CD2	2.55	0.42
1:E:531:PHE:CE1	1:E:535:PHE:CE2	3.08	0.42
1:E:525:ARG:HD3	2:H:167:TYR:CD2	2.55	0.42
2:H:39:LEU:HA	2:H:39:LEU:HD12	1.99	0.42
2:H:74:ILE:H	2:H:74:ILE:HG13	1.58	0.42
2:C:82:PHE:CD2	2:C:113:GLU:HG2	2.54	0.42
1:E:423:TYR:OH	1:E:427:ARG:NH1	2.53	0.42
1:F:423:TYR:OH	1:F:427:ARG:NH1	2.53	0.42
1:F:707:SER:HB2	1:F:717:LEU:HD21	2.01	0.42
1:A:413:PHE:C	1:A:413:PHE:CD1	2.94	0.42
1:A:648:LYS:HB3	1:A:651:LEU:HD13	2.02	0.42
1:E:550:LYS:HA	1:E:551:PRO:HD2	1.78	0.42
1:A:643:PRO:HG2	1:A:704:ARG:HH21	1.84	0.42
1:B:576:GLU:HA	1:B:579:MET:CE	2.49	0.41
1:B:648:LYS:HB3	1:B:651:LEU:HD13	2.01	0.41
1:B:689:MET:HE2	1:B:739:ILE:HD11	2.02	0.41
1:A:497:GLY:HA2	2:H:52:ASN:HD21	1.85	0.41
1:B:479:THR:H	1:B:517:ASN:ND2	2.13	0.41
1:B:529:THR:HG23	1:B:567:VAL:HG12	2.02	0.41
2:C:36:LYS:O	2:C:39:LEU:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:92:VAL:HG13	2:C:125:ALA:HA	2.01	0.41
1:E:639:GLU:HB3	1:E:652:HIS:HB3	2.01	0.41
1:F:479:THR:H	1:F:517:ASN:HD21	1.68	0.41
1:F:490:GLN:O	1:F:592:THR:HA	2.21	0.41
1:F:589:GLU:HG2	1:F:590:LEU:N	2.35	0.41
1:F:654:ARG:HH22	1:F:667:LYS:NZ	2.18	0.41
2:G:77:LEU:O	2:G:78:TRP:HB2	2.20	0.41
2:H:92:VAL:HG13	2:H:125:ALA:HA	2.03	0.41
1:A:656:ILE:CG2	1:A:663:LEU:HD11	2.50	0.41
1:B:503:GLU:HA	1:B:535:PHE:CZ	2.55	0.41
1:E:655:GLU:HG2	1:E:678:TYR:HE1	1.85	0.41
1:F:640:VAL:O	1:F:719:ASN:HB2	2.20	0.41
2:H:68:VAL:C	2:H:70:GLY:H	2.23	0.41
1:A:423:TYR:OH	1:A:427:ARG:NH1	2.54	0.41
1:F:416:LYS:HD3	1:F:419:LYS:HD2	2.01	0.41
2:G:177:LEU:O	2:G:178:ARG:C	2.59	0.41
2:C:70:GLY:HA2	1:F:499:ALA:HB1	2.03	0.41
1:E:459:ARG:NH1	1:E:500:GLN:O	2.53	0.41
1:E:705:LEU:HD12	1:E:718:ILE:CG2	2.51	0.41
1:F:557:LEU:HD13	1:F:582:TYR:CG	2.56	0.41
1:A:503:GLU:HA	1:A:535:PHE:CZ	2.52	0.41
1:E:495:VAL:HG12	1:E:502:VAL:HG13	2.02	0.41
1:E:459:ARG:HB3	1:E:504:ARG:CD	2.51	0.41
1:A:517:ASN:O	1:A:521:VAL:HG13	2.20	0.41
1:A:537:ILE:HG12	1:A:581:ILE:HG21	2.03	0.41
1:B:397:SER:OG	1:B:398:ASN:N	2.52	0.41
1:B:416:LYS:HD3	1:B:419:LYS:HD2	2.02	0.41
1:F:468:LEU:O	1:F:472:VAL:HG22	2.21	0.41
1:F:648:LYS:HB3	1:F:651:LEU:HD13	2.02	0.41
2:G:19:ARG:NH1	2:G:81:TYR:HA	2.35	0.41
1:B:544:MET:CE	1:B:586:ARG:HA	2.51	0.41
1:A:640:VAL:O	1:A:719:ASN:HB2	2.21	0.40
1:B:506:ILE:HD11	1:B:535:PHE:CD2	2.56	0.40
2:D:64:THR:HG23	1:E:548:ASN:HB3	2.03	0.40
1:E:656:ILE:HG23	1:E:663:LEU:CD1	2.50	0.40
1:F:656:ILE:HG23	1:F:663:LEU:CD1	2.51	0.40
1:B:535:PHE:CG	2:G:74:ILE:HD13	2.57	0.40
1:F:517:ASN:O	1:F:521:VAL:HG13	2.21	0.40
1:A:459:ARG:HA	1:A:504:ARG:HD3	2.03	0.40
1:B:646:PRO:HB3	1:B:698:TYR:CD1	2.56	0.40
2:G:92:VAL:HG13	2:G:125:ALA:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:VAL:HG13	2:D:68:VAL:HB	2.03	0.40
1:E:589:GLU:HG2	1:E:590:LEU:N	2.37	0.40
1:B:557:LEU:HD12	1:B:582:TYR:CD2	2.57	0.40
1:B:705:LEU:HD12	1:B:718:ILE:CG2	2.51	0.40
2:D:145:LEU:O	2:D:146:HIS:CB	2.67	0.40
2:D:74:ILE:C	2:D:75:ARG:HD2	2.41	0.40
1:E:745:MET:HE3	1:E:745:MET:HB2	1.88	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	348/383 (91%)	320 (92%)	18 (5%)	10 (3%)	4	24
1	B	354/383 (92%)	322 (91%)	21 (6%)	11 (3%)	4	23
1	E	347/383 (91%)	316 (91%)	21 (6%)	10 (3%)	4	24
1	F	347/383 (91%)	320 (92%)	18 (5%)	9 (3%)	5	27
2	C	159/164 (97%)	145 (91%)	6 (4%)	8 (5%)	2	14
2	D	162/164 (99%)	146 (90%)	6 (4%)	10 (6%)	1	10
2	G	160/164 (98%)	147 (92%)	8 (5%)	5 (3%)	4	23
2	H	157/164 (96%)	136 (87%)	13 (8%)	8 (5%)	2	13
All	All	2034/2188 (93%)	1852 (91%)	111 (6%)	71 (4%)	3	21

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	672	LYS
1	B	459	ARG
1	B	625	SER

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Mol	Chain	Res	Type
1	B	713	ASP
2	C	39	LEU
2	C	47	PRO
2	C	71	GLN
2	D	42	ILE
2	D	43	VAL
2	D	74	ILE
2	D	80	HIS
2	D	86	GLN
1	E	398	ASN
1	E	526	ASN
1	E	671	LYS
1	F	558	GLU
1	F	625	SER
1	F	673	LYS
1	F	713	ASP
2	G	70	GLY
2	G	178	ARG
2	H	43	VAL
2	H	45	THR
2	H	68	VAL
2	H	69	GLY
1	A	625	SER
1	B	397	SER
1	B	558	GLU
2	C	44	THR
2	C	68	VAL
2	C	72	ASP
2	D	69	GLY
2	D	146	HIS
2	D	150	HIS
1	E	550	LYS
1	E	673	LYS
1	F	609	GLY
1	F	680	PHE
2	G	39	LEU
2	G	82	PHE
2	H	72	ASP
2	H	174	SER
1	A	714	ILE
2	D	73	LYS
1	E	459	ARG

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Mol	Chain	Res	Type
1	E	551	PRO
1	E	674	ASN
2	G	69	GLY
1	A	506	ILE
1	A	550	LYS
1	A	671	LYS
1	A	674	ASN
1	A	680	PHE
1	B	714	ILE
2	D	49	ILE
1	E	397	SER
1	F	714	ILE
1	B	592	THR
2	H	49	ILE
1	A	700	PRO
1	B	700	PRO
2	C	48	THR
1	E	700	PRO
1	F	700	PRO
1	A	551	PRO
1	B	550	LYS
1	B	623	VAL
2	C	42	ILE
1	F	526	ASN
1	B	551	PRO
2	H	74	ILE

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	323/347 (93%)	300 (93%)	23 (7%)	14	42
1	B	329/347 (95%)	301 (92%)	28 (8%)	10	35
1	E	323/347 (93%)	289 (90%)	34 (10%)	7	25
1	F	321/347 (92%)	292 (91%)	29 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	138/142 (97%)	126 (91%)	12 (9%)	10	34
2	D	140/142 (99%)	128 (91%)	12 (9%)	10	35
2	G	138/142 (97%)	125 (91%)	13 (9%)	8	30
2	H	137/142 (96%)	118 (86%)	19 (14%)	3	16
All	All	1849/1956 (94%)	1679 (91%)	170 (9%)	9	31

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	398	ASN
1	A	402	ARG
1	A	496	GLN
1	A	498	LYS
1	A	506	ILE
1	A	521	VAL
1	A	557	LEU
1	A	565	ARG
1	A	571	GLU
1	A	597	VAL
1	A	604	GLU
1	A	624	LEU
1	A	625	SER
1	A	668	ILE
1	A	677	THR
1	A	685	SER
1	A	707	SER
1	A	737	GLU
1	A	745	MET
1	A	747	LYS
1	A	753	GLU
1	A	754	LEU
1	A	755	GLU
1	B	402	ARG
1	B	460	GLN
1	B	476	ASP
1	B	496	GLN
1	B	498	LYS
1	B	506	ILE
1	B	521	VAL
1	B	525	ARG
1	B	550	LYS

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Mol	Chain	Res	Type
1	B	552	GLU
1	B	565	ARG
1	B	576	GLU
1	B	597	VAL
1	B	604	GLU
1	B	610	LYS
1	B	668	ILE
1	B	672	LYS
1	B	677	THR
1	B	681	ARG
1	B	685	SER
1	B	689	MET
1	B	692	LEU
1	B	737	GLU
1	B	745	MET
1	B	747	LYS
1	B	754	LEU
1	B	755	GLU
1	B	757	GLN
2	C	35	TYR
2	C	36	LYS
2	C	42	ILE
2	C	48	THR
2	C	51	PHE
2	C	60	ASN
2	C	65	VAL
2	C	74	ILE
2	C	75	ARG
2	C	83	GLN
2	C	114	ASP
2	C	173	LEU
2	D	34	LEU
2	D	35	TYR
2	D	36	LYS
2	D	56	VAL
2	D	60	ASN
2	D	65	VAL
2	D	74	ILE
2	D	75	ARG
2	D	84	ASN
2	D	114	ASP
2	D	115	GLU

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Mol	Chain	Res	Type
2	D	180	GLN
1	E	402	ARG
1	E	445	LYS
1	E	456	LEU
1	E	476	ASP
1	E	493	ILE
1	E	496	GLN
1	E	498	LYS
1	E	504	ARG
1	E	506	ILE
1	E	507	GLU
1	E	521	VAL
1	E	530	ILE
1	E	550	LYS
1	E	552	GLU
1	E	555	MET
1	E	558	GLU
1	E	559	ASP
1	E	565	ARG
1	E	571	GLU
1	E	575	ARG
1	E	576	GLU
1	E	597	VAL
1	E	604	GLU
1	E	668	ILE
1	E	669	PHE
1	E	681	ARG
1	E	685	SER
1	E	689	MET
1	E	692	LEU
1	E	714	ILE
1	E	737	GLU
1	E	753	GLU
1	E	754	LEU
1	E	755	GLU
1	F	398	ASN
1	F	412	LEU
1	F	459	ARG
1	F	476	ASP
1	F	496	GLN
1	F	498	LYS
1	F	506	ILE

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Mol	Chain	Res	Type
1	F	512	ARG
1	F	521	VAL
1	F	558	GLU
1	F	571	GLU
1	F	576	GLU
1	F	583	GLU
1	F	597	VAL
1	F	604	GLU
1	F	624	LEU
1	F	668	ILE
1	F	672	LYS
1	F	677	THR
1	F	679	SER
1	F	685	SER
1	F	689	MET
1	F	692	LEU
1	F	707	SER
1	F	715	LYS
1	F	737	GLU
1	F	745	MET
1	F	754	LEU
1	F	755	GLU
2	G	35	TYR
2	G	36	LYS
2	G	39	LEU
2	G	46	ILE
2	G	51	PHE
2	G	65	VAL
2	G	71	GLN
2	G	72	ASP
2	G	73	LYS
2	G	79	ARG
2	G	114	ASP
2	G	151	ARG
2	G	173	LEU
2	H	35	TYR
2	H	36	LYS
2	H	39	LEU
2	H	41	GLU
2	H	43	VAL
2	H	45	THR
2	H	60	ASN

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Mol	Chain	Res	Type
2	H	65	VAL
2	H	74	ILE
2	H	75	ARG
2	H	79	ARG
2	H	114	ASP
2	H	118	ASP
2	H	146	HIS
2	H	149	ARG
2	H	150	HIS
2	H	159	CYS
2	H	176	GLN
2	H	177	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	496	GLN
1	A	517	ASN
1	A	548	ASN
1	A	743	GLN
1	B	458	ASN
1	B	517	ASN
1	B	726	GLN
1	B	743	GLN
2	C	52	ASN
2	C	83	GLN
2	C	146	HIS
2	C	176	GLN
2	D	52	ASN
2	D	150	HIS
2	D	156	GLN
2	D	176	GLN
1	E	490	GLN
1	E	496	GLN
1	E	500	GLN
1	E	517	ASN
1	E	526	ASN
1	E	548	ASN
1	E	670	GLN
1	E	743	GLN
1	F	517	ASN
1	F	526	ASN

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Mol	Chain	Res	Type
1	F	743	GLN
2	G	52	ASN
2	G	146	HIS
2	G	176	GLN
2	H	52	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	G3D	D	401	-	28,34,34	1.19	3 (10%)	37,54,54	2.80	8 (21%)
3	G3D	C	401	-	28,34,34	1.02	1 (3%)	37,54,54	2.90	10 (27%)
3	G3D	H	401	-	28,34,34	1.11	2 (7%)	37,54,54	2.89	8 (21%)
3	G3D	G	401	-	28,34,34	1.03	1 (3%)	37,54,54	2.96	12 (32%)

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	G3D	D	401	-	-	3/17/37/37	0/3/3/3
3	G3D	C	401	-	-	6/17/37/37	0/3/3/3
3	G3D	H	401	-	-	4/17/37/37	0/3/3/3
3	G3D	G	401	-	-	5/17/37/37	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	G3D	C6-N1	3.41	1.39	1.33
3	G	401	G3D	C6-N1	3.36	1.38	1.33
3	C	401	G3D	C6-N1	3.29	1.38	1.33
3	H	401	G3D	C6-N1	3.25	1.38	1.33
3	D	401	G3D	C6-C5	3.19	1.46	1.41
3	H	401	G3D	C6-C5	2.15	1.45	1.41
3	D	401	G3D	P1-O6P	2.00	1.57	1.50

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	401	G3D	PA-O3A-PB	11.78	173.24	132.83
3	C	401	G3D	PA-O3A-PB	11.70	172.97	132.83
3	H	401	G3D	PA-O3A-PB	11.51	172.31	132.83
3	D	401	G3D	PA-O3A-PB	10.82	169.96	132.83
3	D	401	G3D	C5-C6-N1	-8.52	111.78	123.43
3	H	401	G3D	C5-C6-N1	-8.13	112.31	123.43
3	G	401	G3D	C5-C6-N1	-8.11	112.34	123.43
3	C	401	G3D	C5-C6-N1	-8.07	112.40	123.43
3	D	401	G3D	C6-N1-C2	5.94	125.37	115.93
3	G	401	G3D	C6-N1-C2	5.83	125.19	115.93
3	H	401	G3D	C6-N1-C2	5.82	125.17	115.93
3	C	401	G3D	C6-N1-C2	5.77	125.10	115.93
3	H	401	G3D	O2B-PB-O3A	4.71	120.43	104.64
3	C	401	G3D	O2B-PB-O3A	4.52	119.80	104.64
3	G	401	G3D	O2B-PB-O3A	4.52	119.78	104.64
3	D	401	G3D	O2B-PB-O3A	3.81	117.43	104.64
3	D	401	G3D	C6-C5-C4	-3.08	117.86	120.80
3	H	401	G3D	C6-C5-C4	-3.07	117.86	120.80
3	G	401	G3D	N3-C2-N1	-2.89	123.37	127.22
3	C	401	G3D	N3-C2-N1	-2.88	123.39	127.22
3	G	401	G3D	C6-C5-C4	-2.80	118.13	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	401	G3D	N3-C2-N1	-2.80	123.49	127.22
3	C	401	G3D	C6-C5-C4	-2.76	118.17	120.80
3	D	401	G3D	N3-C2-N1	-2.72	123.60	127.22
3	G	401	G3D	O3B-PB-O3A	-2.56	96.07	104.64
3	C	401	G3D	C2-N3-C4	-2.29	112.74	115.36
3	H	401	G3D	O3A-PB-O1B	-2.26	98.63	111.19
3	D	401	G3D	O3A-PB-O1B	-2.23	98.81	111.19
3	G	401	G3D	C2-N3-C4	-2.22	112.83	115.36
3	G	401	G3D	O3'-P1-O6P	-2.19	100.92	109.39
3	G	401	G3D	O5'-PA-O1A	-2.15	100.66	109.07
3	G	401	G3D	O3B-PB-O2B	2.14	115.82	107.64
3	G	401	G3D	O2A-PA-O5'	2.14	117.67	107.75
3	D	401	G3D	O4P-P1-O3'	2.14	115.56	105.99
3	C	401	G3D	O3B-PB-O3A	-2.14	97.47	104.64
3	C	401	G3D	O3B-PB-O2B	2.08	115.59	107.64
3	H	401	G3D	C2-N3-C4	-2.03	113.03	115.36
3	C	401	G3D	O2A-PA-O5'	2.02	117.11	107.75

There are no chirality outliers.

All (18) torsion outliers are listed below:

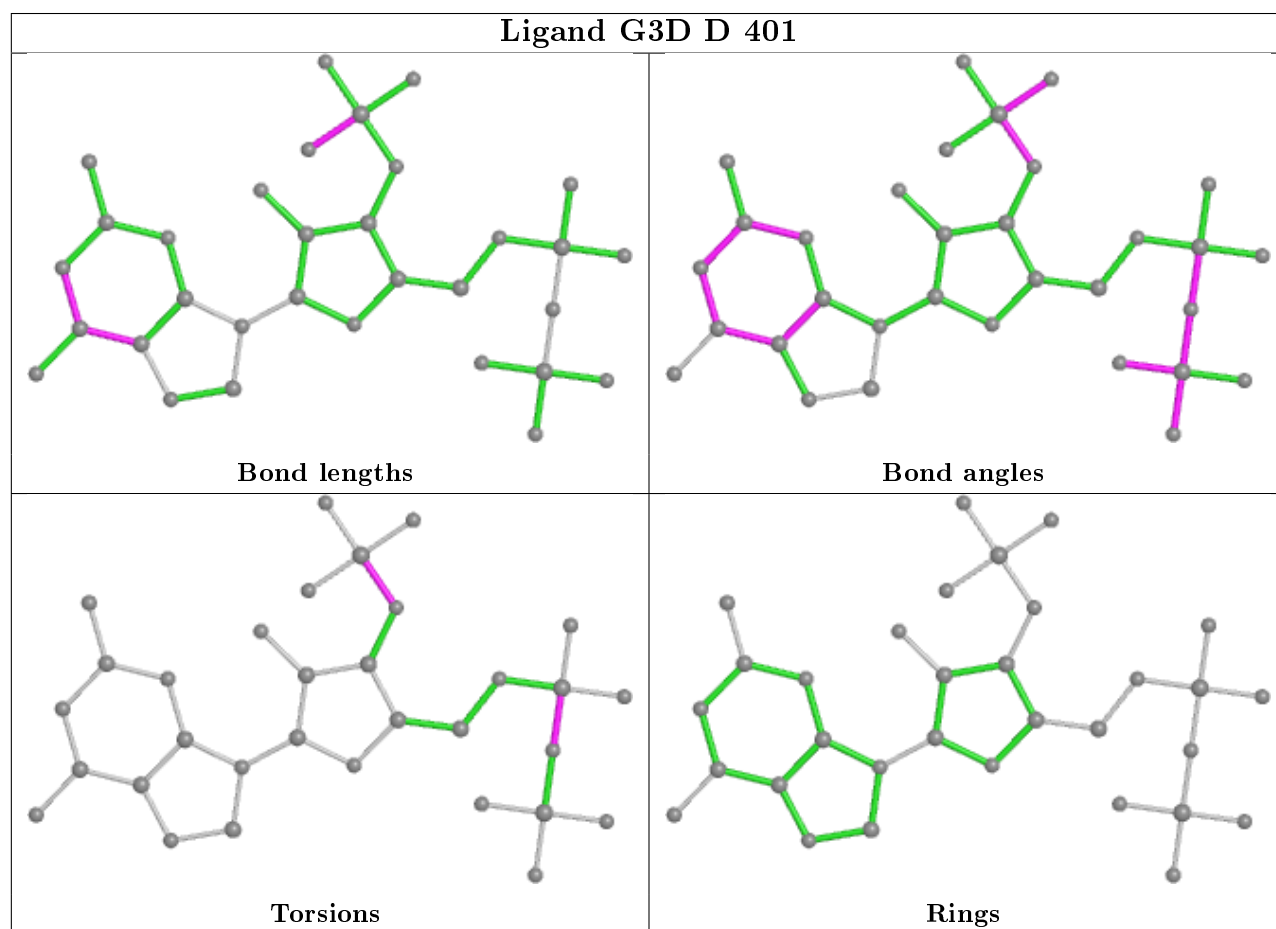
Mol	Chain	Res	Type	Atoms
3	D	401	G3D	C3'-O3'-P1-O5P
3	C	401	G3D	C5'-O5'-PA-O1A
3	C	401	G3D	C3'-O3'-P1-O5P
3	H	401	G3D	PA-O3A-PB-O3B
3	H	401	G3D	C5'-O5'-PA-O1A
3	C	401	G3D	C5'-O5'-PA-O3A
3	H	401	G3D	C3'-O3'-P1-O5P
3	C	401	G3D	C5'-O5'-PA-O2A
3	H	401	G3D	C5'-O5'-PA-O2A
3	G	401	G3D	C3'-C4'-C5'-O5'
3	G	401	G3D	O4'-C4'-C5'-O5'
3	C	401	G3D	C4'-C5'-O5'-PA
3	D	401	G3D	PB-O3A-PA-O2A
3	C	401	G3D	PB-O3A-PA-O2A
3	D	401	G3D	PB-O3A-PA-O1A
3	G	401	G3D	PA-O3A-PB-O1B
3	G	401	G3D	PA-O3A-PB-O2B
3	G	401	G3D	PA-O3A-PB-O3B

There are no ring outliers.

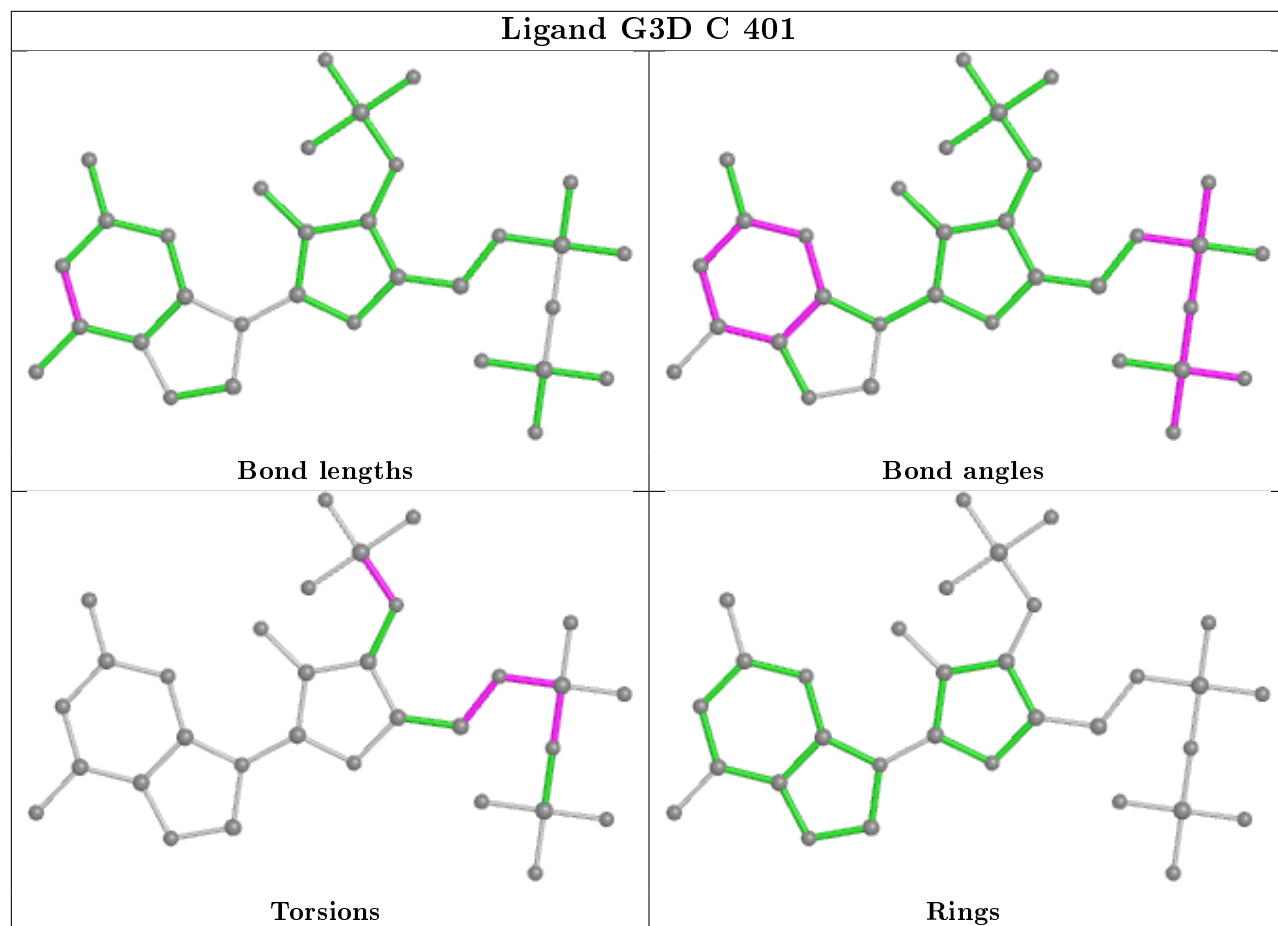
2 monomers are involved in 3 short contacts:

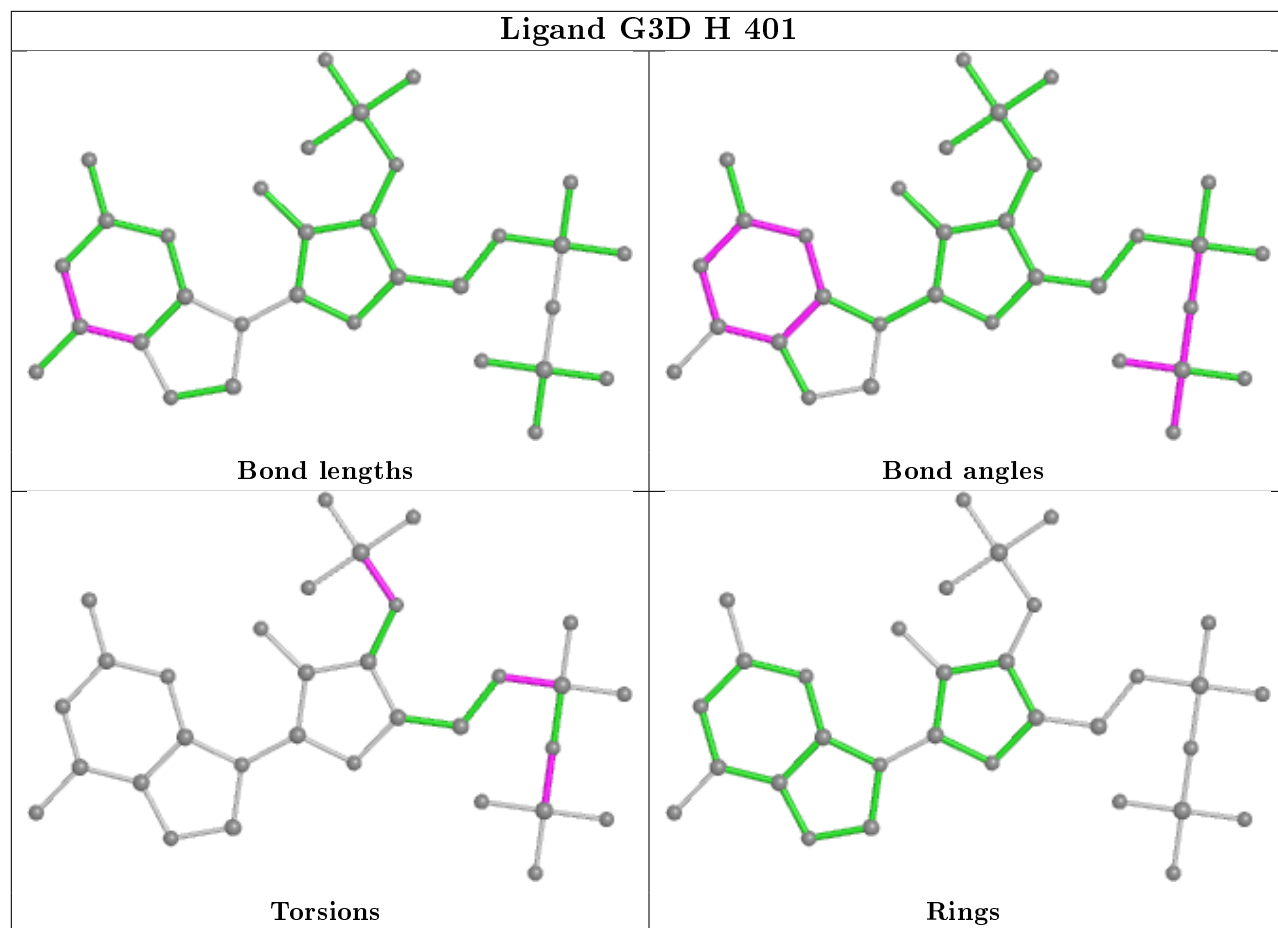
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	G3D	2	0
3	G	401	G3D	1	0

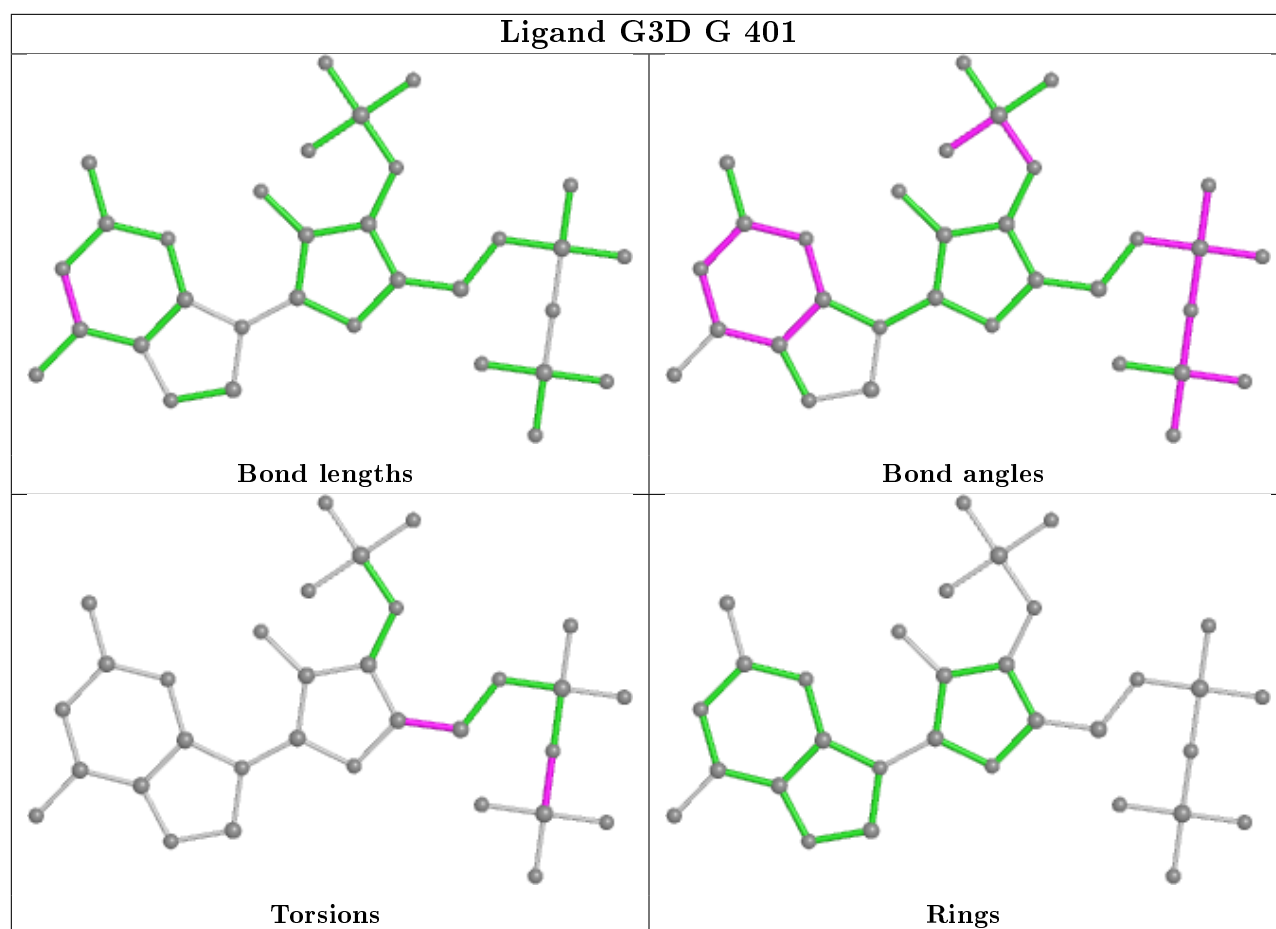
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand G3D C 401







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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	352/383 (91%)	0.03	12 (3%) 45 43	25, 59, 103, 132	0
1	B	357/383 (93%)	-0.05	8 (2%) 62 60	16, 52, 104, 126	0
1	E	351/383 (91%)	-0.09	1 (0%) 94 94	27, 53, 94, 134	0
1	F	351/383 (91%)	-0.10	2 (0%) 89 90	25, 52, 92, 120	0
2	C	161/164 (98%)	0.04	1 (0%) 89 90	34, 70, 114, 141	0
2	D	164/164 (100%)	0.07	3 (1%) 68 67	31, 65, 102, 127	0
2	G	162/164 (98%)	0.66	18 (11%) 5 5	54, 100, 139, 155	0
2	H	159/164 (96%)	1.09	32 (20%) 1 1	69, 135, 196, 215	0
All	All	2057/2188 (94%)	0.11	77 (3%) 41 38	16, 61, 132, 215	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	139	ILE	6.2
2	H	141	ASP	5.6
2	H	143	LEU	5.2
2	H	173	LEU	4.8
2	H	136	ALA	4.8
2	G	129	ASP	4.5
1	A	674	ASN	4.2
2	G	40	GLY	4.2
2	H	130	LEU	4.0
2	G	157	ALA	4.0
1	B	393	SER	3.9
2	H	146	HIS	3.9
2	G	128	GLN	3.7
2	G	130	LEU	3.7
2	G	139	ILE	3.7
2	G	18	MET	3.6

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Mol	Chain	Res	Type	RSRZ
2	H	147	SER	3.5
2	H	131	PRO	3.5
2	G	131	PRO	3.5
1	B	755	GLU	3.3
1	B	557	LEU	3.3
1	B	395	ALA	3.3
1	F	755	GLU	3.3
2	G	127	LYS	3.3
1	B	396	PHE	3.2
2	C	39	LEU	3.1
2	G	133	ALA	3.0
2	G	164	ASP	3.0
2	H	128	GLN	3.0
2	H	96	ASP	2.9
1	B	394	PRO	2.9
1	F	674	ASN	2.9
1	A	621	GLY	2.9
2	H	121	LEU	2.9
2	D	139	ILE	2.9
2	H	138	GLU	2.7
2	H	58	TYR	2.7
1	B	622	CYS	2.7
2	H	154	TYR	2.7
2	H	132	ASN	2.6
1	B	621	GLY	2.6
2	G	137	ALA	2.6
2	G	141	ASP	2.6
2	G	142	LYS	2.6
2	H	133	ALA	2.5
2	H	168	GLU	2.5
2	H	100	VAL	2.5
1	A	524	PHE	2.5
2	H	101	ASN	2.5
2	H	93	ASP	2.5
2	G	95	ASN	2.5
1	A	526	ASN	2.5
1	E	674	ASN	2.4
2	H	95	ASN	2.4
2	H	156	GLN	2.4
1	A	711	GLY	2.4
2	H	134	MET	2.4
1	A	525	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	G	143	LEU	2.4
1	A	557	LEU	2.3
2	H	151	ARG	2.3
1	A	755	GLU	2.3
2	H	135	ASN	2.2
2	H	142	LYS	2.2
2	H	72	ASP	2.2
2	H	148	LEU	2.2
1	A	757	GLN	2.2
1	A	573	ILE	2.1
1	A	754	LEU	2.1
2	D	136	ALA	2.1
2	D	138	GLU	2.1
2	H	152	ASN	2.1
2	G	168	GLU	2.1
2	G	126	ASN	2.0
1	A	712	ALA	2.0
2	H	176	GLN	2.0
2	H	97	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

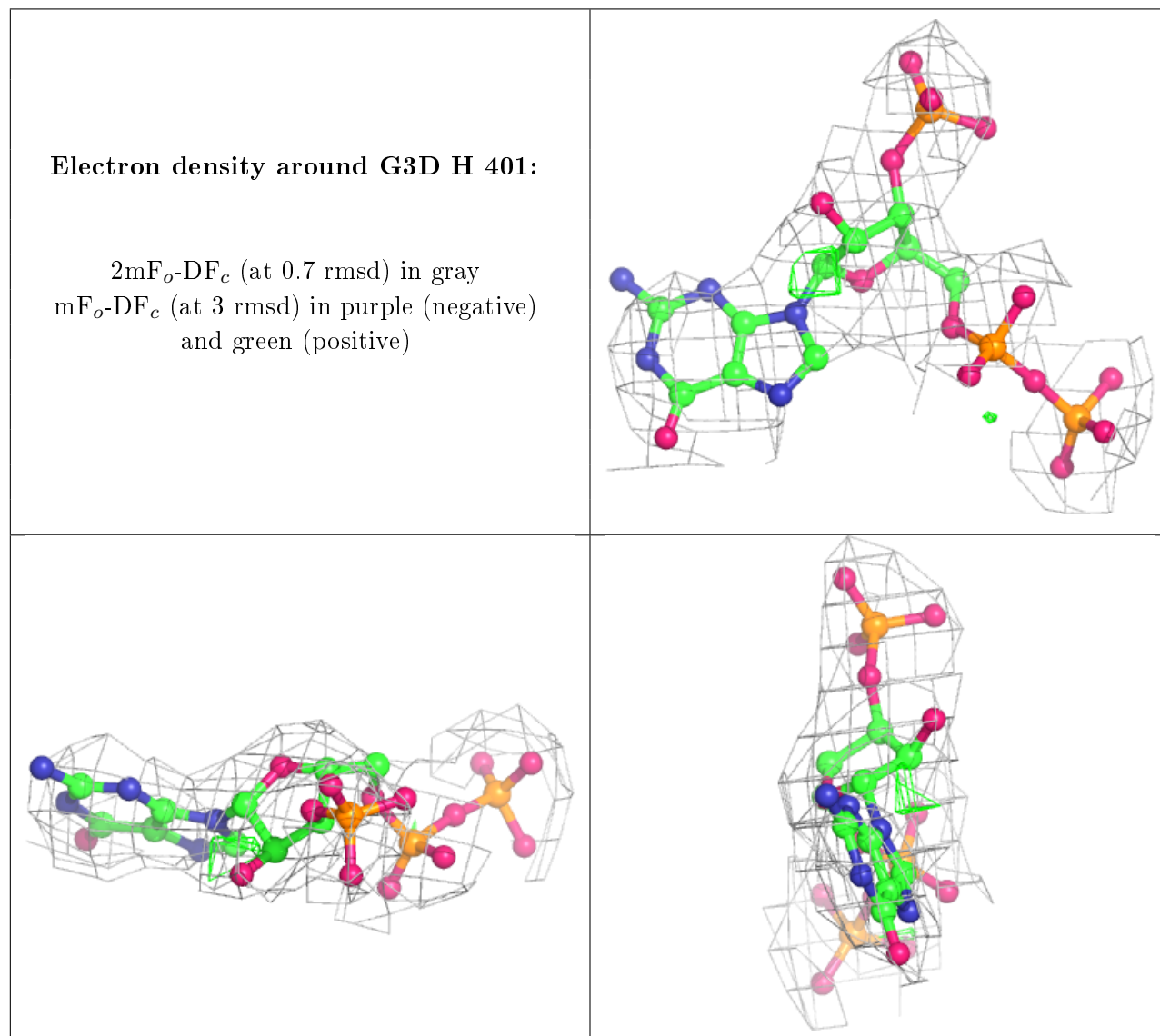
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

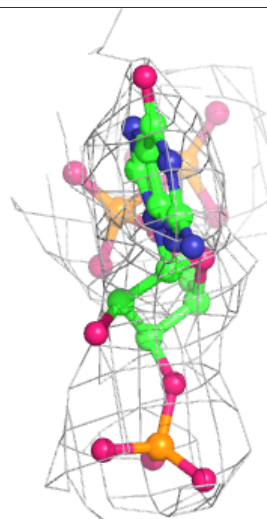
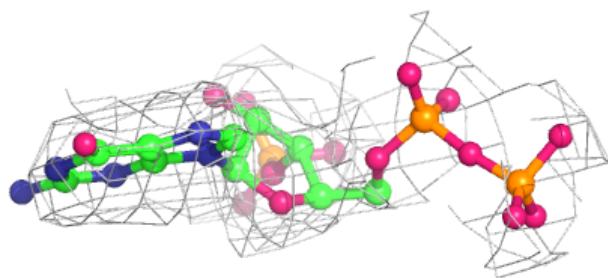
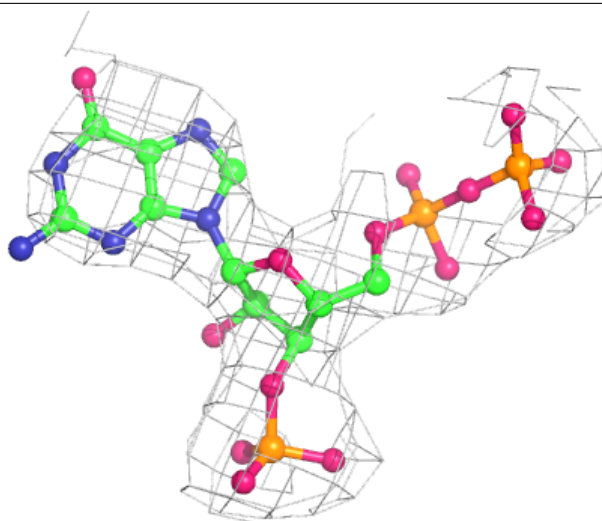
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	G3D	H	401	32/32	0.83	0.23	97,113,124,129	0
3	G3D	G	401	32/32	0.87	0.23	66,89,99,105	0
3	G3D	C	401	32/32	0.92	0.19	42,69,88,93	0
3	G3D	D	401	32/32	0.95	0.17	47,53,83,91	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



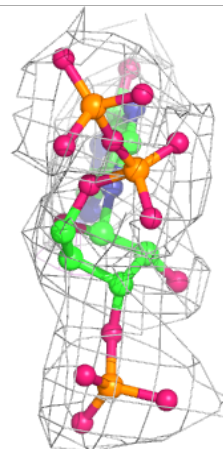
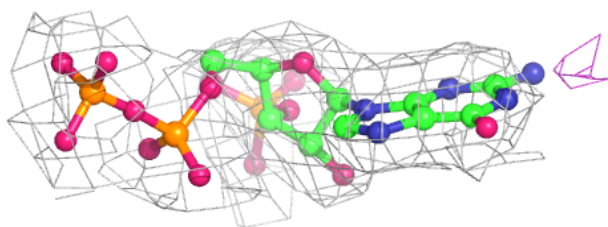
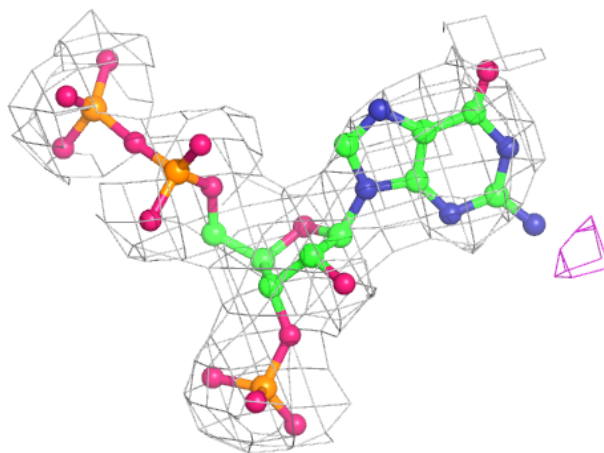
Electron density around G3D G 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



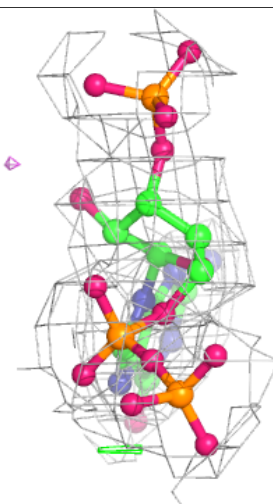
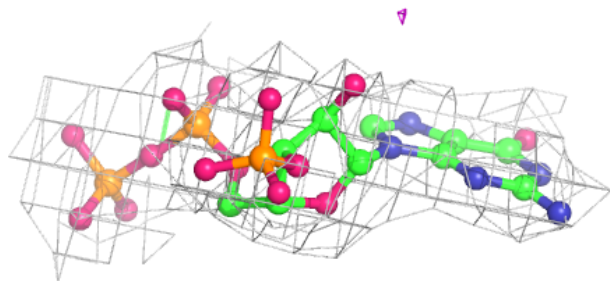
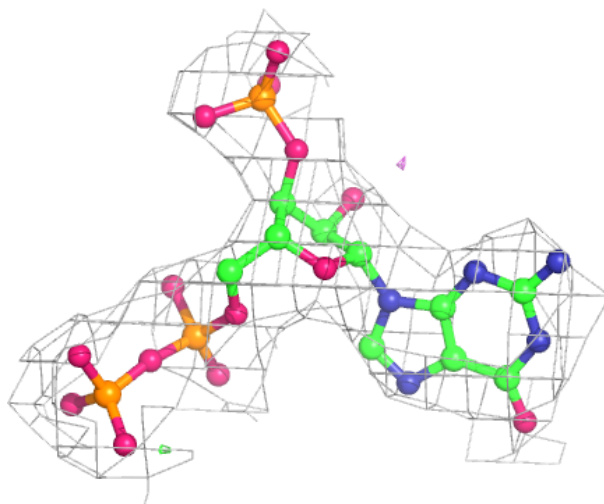
Electron density around G3D C 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around G3D D 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.