



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:57 AM UTC

PDB ID : 4C0A / pdb_00004c0a
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 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

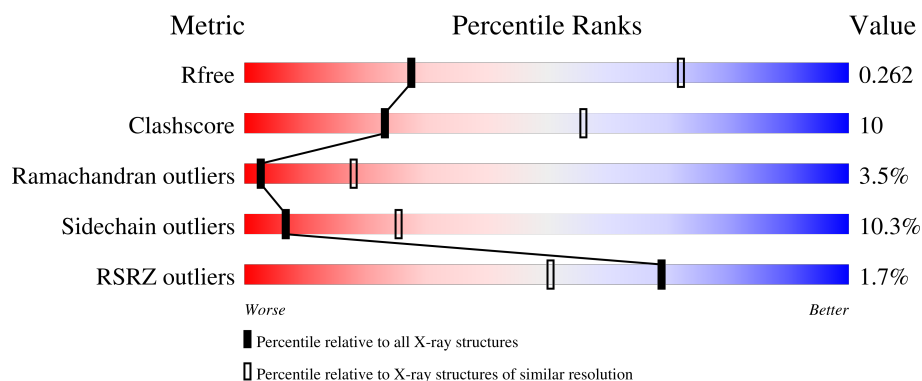
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 $\leq 5\%$. 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	 63% 24% 8%
1	B	383	 2% 62% 25% 5% 7%
1	E	383	 60% 26% 8%
1	F	383	 58% 29% 8%
2	C	164	 65% 26% 5%

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Mol	Chain	Length	Quality of chain
2	D	164	% 65% 27% 6% •
2	G	164	4% 68% 26% • •
2	H	164	11% 57% 32% 6% • •

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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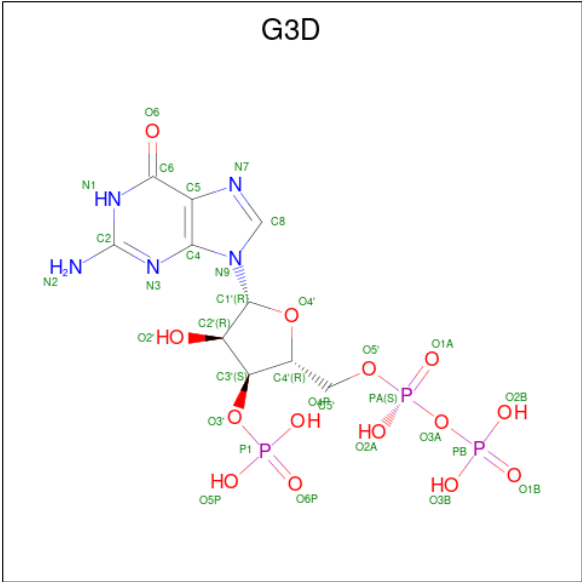
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Chain	Residue	Modelled	Actual	Comment	Reference
E	381	GLY	-	expression tag	UNP Q6DN90
E	382	ALA	-	expression tag	UNP Q6DN90
E	383	MET	-	expression tag	UNP Q6DN90
E	384	GLY	-	expression tag	UNP Q6DN90
E	385	SER	-	expression tag	UNP Q6DN90
E	386	GLY	-	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 (CCD ID: G3D) (formula: C₁₀H₁₆N₅O₁₄P₃).

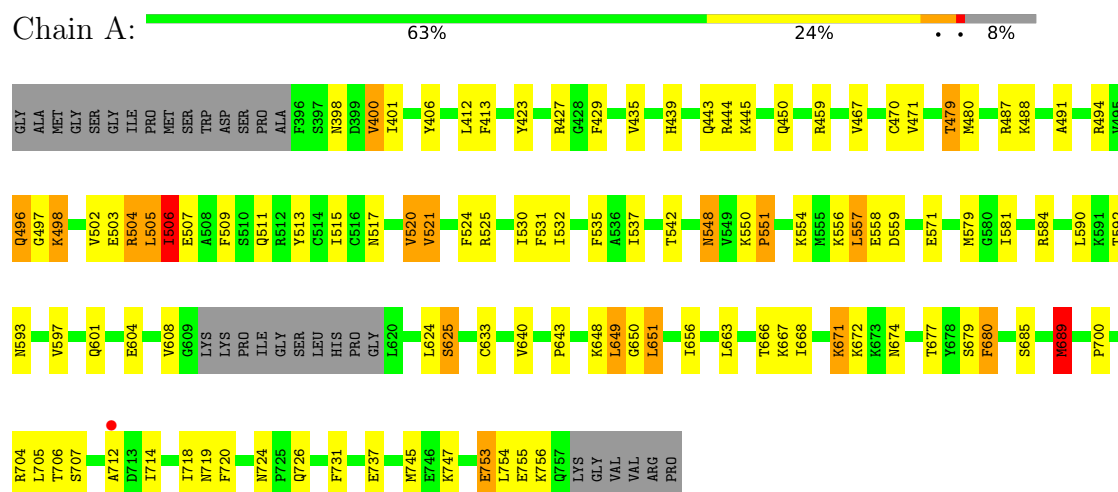


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	G	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	H	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

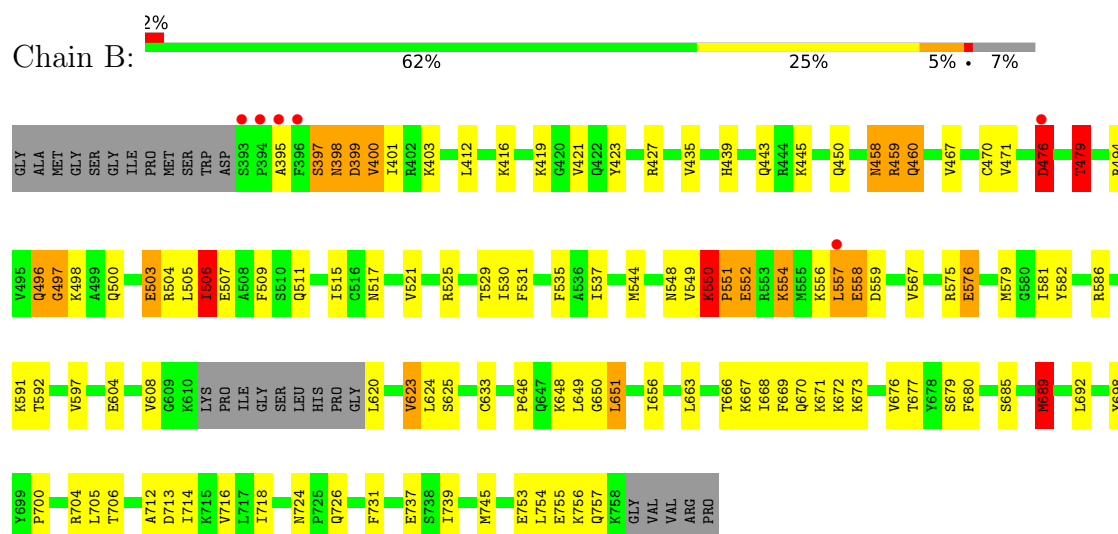
3 Residue-property plots

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 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

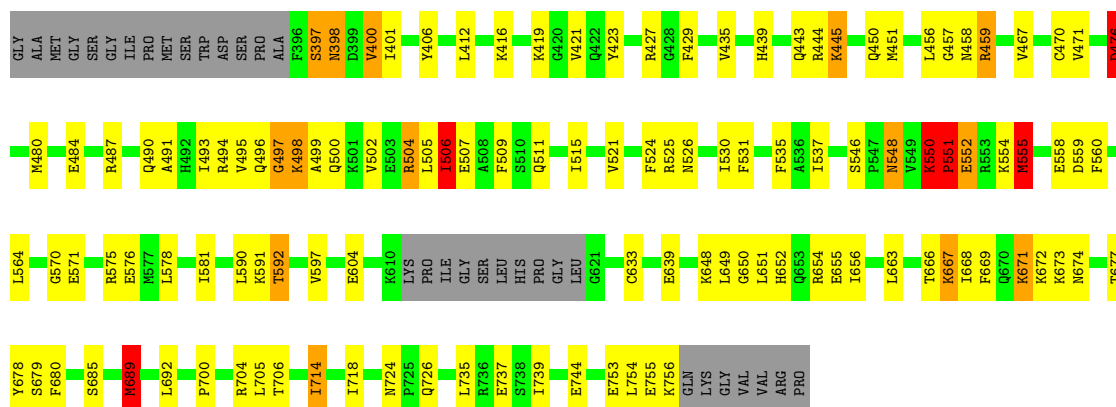


• Molecule 1: IQ MOTIF AND SEC7 DOMAIN-CONTAINING PROTEIN 1

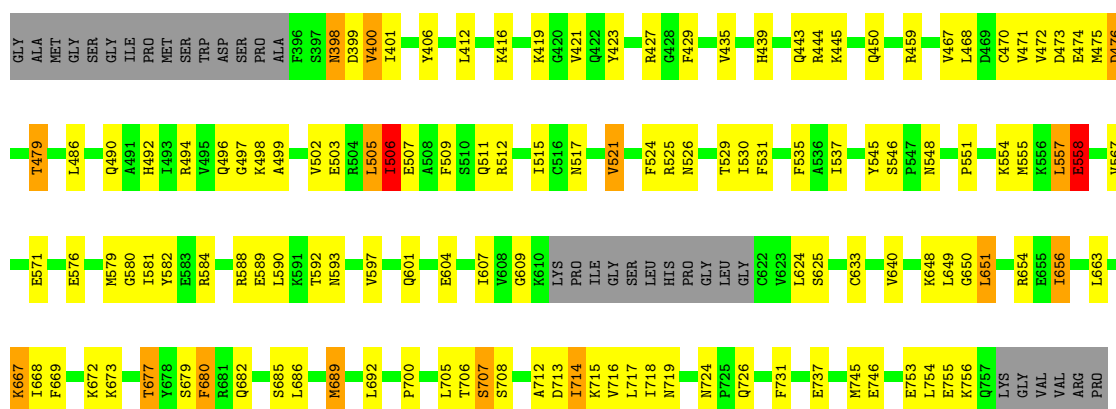


• Molecule 1: IQ MOTIF AND SEC7 DOMAIN-CONTAINING PROTEIN 1

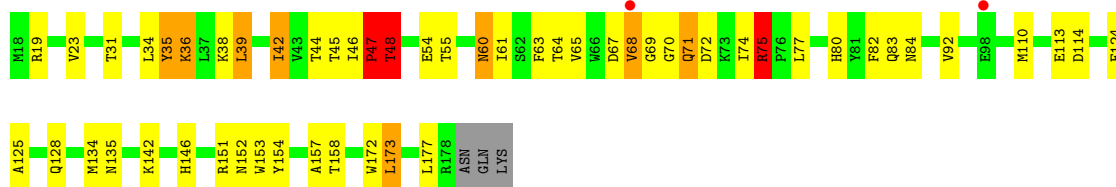




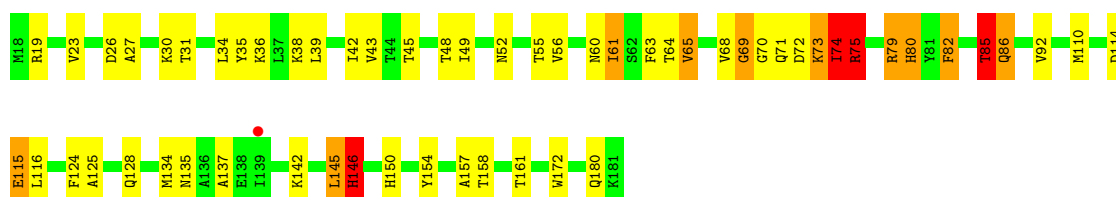
• Molecule 1: IQ MOTIF AND SEC7 DOMAIN-CONTAINING PROTEIN 1



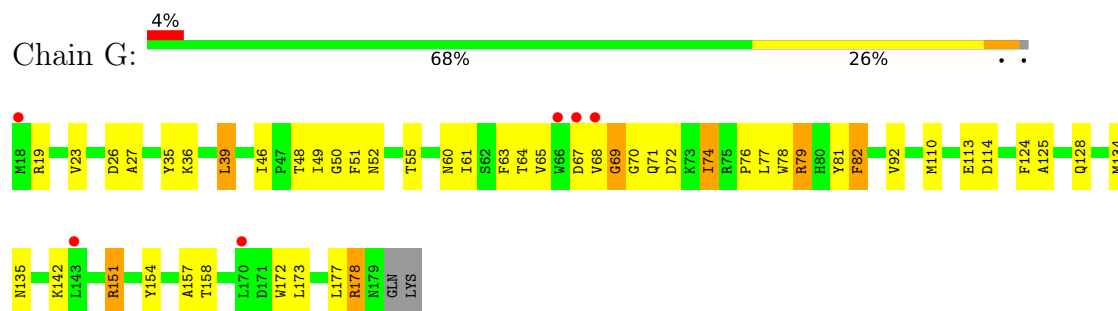
• Molecule 2: ADP-RIBOSYLATION FACTOR 1



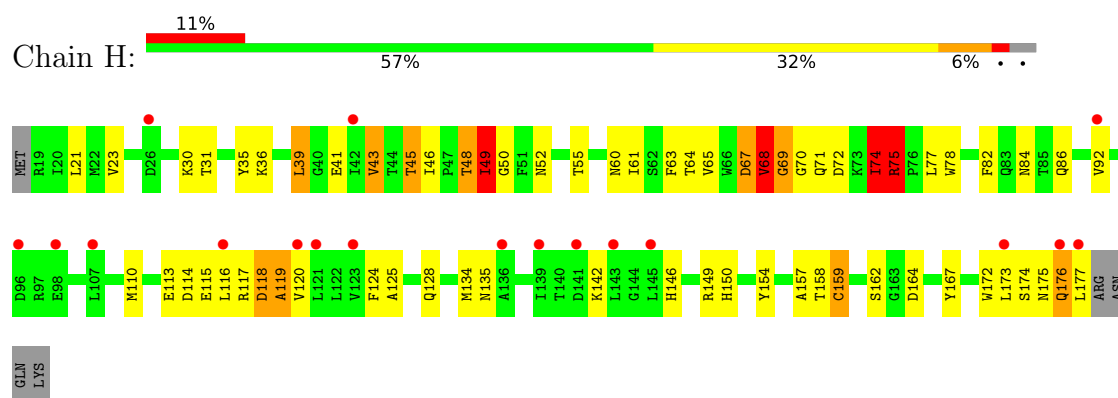
• Molecule 2: ADP-RIBOSYLATION FACTOR 1



- 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	90.98Å 65.78Å 196.86Å 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) 99.4 (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 3.32Å)	Xtrriage
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	Xtrriage
Anisotropy	0.565	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 91.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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	0.82	2/2950 (0.1%)	1.40	17/3962 (0.4%)
1	B	0.86	1/3002 (0.0%)	1.45	26/4030 (0.6%)
1	E	0.86	3/2946 (0.1%)	1.46	27/3955 (0.7%)
1	F	0.87	1/2936 (0.0%)	1.46	23/3944 (0.6%)
2	C	0.76	0/1316	1.36	6/1783 (0.3%)
2	D	0.84	0/1338	1.38	18/1813 (1.0%)
2	G	0.71	0/1321	1.27	7/1790 (0.4%)
2	H	0.71	0/1300	1.40	16/1762 (0.9%)
All	All	0.83	7/17109 (0.0%)	1.42	140/23039 (0.6%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	689	MET	SD-CE	-9.79	1.55	1.79
1	A	689	MET	SD-CE	-7.78	1.60	1.79
1	E	689	MET	SD-CE	-6.80	1.62	1.79
1	E	451	MET	SD-CE	-6.63	1.62	1.79
1	E	592	THR	CA-CB	5.23	1.62	1.53
1	F	476	ASP	CA-CB	5.11	1.57	1.53
1	A	608	VAL	CA-C	5.04	1.57	1.53

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	60	ASN	CA-CB-CG	12.93	125.53	112.60
2	H	119	ALA	N-CA-C	12.74	123.14	108.49
1	E	555	MET	N-CA-C	12.29	125.86	111.11
1	B	505	LEU	N-CA-C	-11.99	95.06	110.53
1	F	557	LEU	N-CA-C	-11.77	92.86	110.28
1	B	398	ASN	CA-C-N	11.04	137.20	121.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	398	ASN	C-N-CA	11.04	137.20	121.42
1	F	505	LEU	N-CA-C	-10.51	96.36	110.55
1	A	505	LEU	N-CA-C	-9.95	95.75	110.48
1	E	505	LEU	N-CA-C	-9.45	98.34	110.53
2	H	117	ARG	CA-C-N	8.57	132.12	120.38
2	H	117	ARG	C-N-CA	8.57	132.12	120.38
1	F	667	LYS	N-CA-C	-8.43	97.45	110.17
1	B	667	LYS	N-CA-C	-8.40	98.08	110.52
1	B	591	LYS	N-CA-C	8.39	124.20	113.88
1	A	667	LYS	N-CA-C	-8.33	97.44	110.36
1	A	506	ILE	N-CA-CB	8.24	124.82	111.23
1	E	679	SER	N-CA-C	7.99	120.07	111.36
1	F	474	GLU	CA-C-N	7.99	136.79	121.54
1	F	474	GLU	C-N-CA	7.99	136.79	121.54
2	D	145	LEU	N-CA-C	-7.79	98.96	110.48
1	B	476	ASP	CA-CB-CG	7.62	120.22	112.60
2	H	135	ASN	CA-CB-CG	7.53	120.12	112.60
1	E	672	LYS	N-CA-C	7.37	121.18	110.42
2	G	135	ASN	CA-CB-CG	7.32	119.92	112.60
2	C	135	ASN	CA-CB-CG	7.31	119.91	112.60
1	B	608	VAL	N-CA-C	7.01	116.41	106.53
1	E	397	SER	CA-C-N	6.97	134.85	121.54
1	E	397	SER	C-N-CA	6.97	134.85	121.54
1	F	506	ILE	N-CA-CB	6.96	122.71	111.23
1	E	591	LYS	N-CA-C	6.88	122.57	114.04
1	E	476	ASP	CA-CB-CG	6.81	119.41	112.60
2	D	86	GLN	N-CA-C	6.78	125.24	110.80
2	D	73	LYS	CA-C-N	6.77	134.16	121.97
2	D	73	LYS	C-N-CA	6.77	134.16	121.97
1	B	506	ILE	N-CA-CB	6.74	122.35	111.23
2	D	135	ASN	CA-CB-CG	6.72	119.32	112.60
2	H	75	ARG	N-CA-C	6.69	122.45	108.39
1	F	476	ASP	CA-CB-CG	6.67	119.27	112.60
1	A	649	LEU	N-CA-C	6.65	119.13	111.02
1	E	548	ASN	CA-CB-CG	6.64	119.24	112.60
1	B	557	LEU	N-CA-C	-6.58	96.92	108.23
2	G	67	ASP	CA-C-N	6.56	129.89	122.48
2	G	67	ASP	C-N-CA	6.56	129.89	122.48
1	E	551	PRO	N-CA-C	6.54	125.94	112.47
2	C	75	ARG	N-CA-C	6.48	121.17	108.21
2	C	47	PRO	N-CA-C	6.47	125.80	112.47
1	B	458	ASN	N-CA-C	6.44	120.60	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	78	TRP	N-CA-C	-6.43	104.68	113.30
2	H	118	ASP	CA-CB-CG	6.43	119.03	112.60
1	F	398	ASN	CA-C-N	6.37	131.51	122.09
1	F	398	ASN	C-N-CA	6.37	131.51	122.09
1	E	506	ILE	N-CA-CB	6.35	121.71	111.23
1	E	672	LYS	CA-C-N	6.34	133.66	121.54
1	E	672	LYS	C-N-CA	6.34	133.66	121.54
1	A	679	SER	N-CA-C	6.32	118.98	111.71
2	D	39	LEU	N-CA-C	-6.28	103.14	113.50
1	B	554	LYS	N-CA-C	-6.27	100.61	109.96
1	E	524	PHE	N-CA-C	6.17	117.81	111.14
1	A	559	ASP	CA-CB-CG	6.17	118.77	112.60
1	B	548	ASN	CA-CB-CG	6.16	118.76	112.60
2	D	38	LYS	CA-C-N	6.11	129.57	120.17
2	D	38	LYS	C-N-CA	6.11	129.57	120.17
1	E	667	LYS	N-CA-C	-6.07	100.45	109.86
2	D	79	ARG	N-CA-C	-5.99	101.41	110.28
1	E	398	ASN	CA-C-N	5.97	130.76	121.26
1	E	398	ASN	C-N-CA	5.97	130.76	121.26
2	D	72	ASP	CA-C-N	5.96	132.92	121.54
2	D	72	ASP	C-N-CA	5.96	132.92	121.54
2	H	120	VAL	N-CA-C	5.87	118.39	109.12
2	D	85	THR	CA-C-N	5.84	132.69	121.54
2	D	85	THR	C-N-CA	5.84	132.69	121.54
2	D	146	HIS	N-CA-CB	5.78	120.26	110.49
1	A	548	ASN	CA-CB-CG	5.78	118.38	112.60
2	C	151	ARG	N-CA-C	5.73	118.74	109.40
2	H	68	VAL	N-CA-C	5.73	121.25	109.34
1	B	559	ASP	CA-CB-CG	5.70	118.30	112.60
2	G	74	ILE	CA-C-N	5.69	127.20	120.09
2	G	74	ILE	C-N-CA	5.69	127.20	120.09
2	H	48	THR	CA-C-N	5.67	132.17	121.97
2	H	48	THR	C-N-CA	5.67	132.17	121.97
1	E	671	LYS	CA-C-N	5.66	130.39	121.56
1	E	671	LYS	C-N-CA	5.66	130.39	121.56
1	F	525	ARG	CA-C-N	5.64	135.57	121.80
1	F	525	ARG	C-N-CA	5.64	135.57	121.80
1	E	714	ILE	N-CA-C	5.63	117.74	109.63
1	B	679	SER	N-CA-C	5.63	119.33	112.23
1	F	399	ASP	CA-CB-CG	5.62	118.22	112.60
2	D	65	VAL	N-CA-CB	5.62	117.78	111.21
1	A	671	LYS	CA-C-N	5.61	132.25	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	671	LYS	C-N-CA	5.61	132.25	121.54
1	E	744	GLU	CB-CG-CD	5.61	122.13	112.60
1	F	548	ASN	CA-CB-CG	5.60	118.20	112.60
1	E	444	ARG	N-CA-C	5.58	118.89	110.64
1	E	497	GLY	CA-C-N	5.44	128.83	121.05
1	E	497	GLY	C-N-CA	5.44	128.83	121.05
2	H	67	ASP	CA-CB-CG	5.44	118.04	112.60
1	F	633	CYS	N-CA-C	5.42	116.77	108.42
1	E	458	ASN	N-CA-C	5.41	117.88	111.33
2	H	176	GLN	N-CA-C	5.40	118.64	110.64
1	A	444	ARG	N-CA-C	5.40	118.63	110.64
1	F	712	ALA	CA-C-N	5.38	131.81	121.54
1	F	712	ALA	C-N-CA	5.38	131.81	121.54
1	B	712	ALA	CA-C-N	5.36	131.78	121.54
1	B	712	ALA	C-N-CA	5.36	131.78	121.54
1	F	497	GLY	CA-C-N	5.35	128.70	121.05
1	F	497	GLY	C-N-CA	5.35	128.70	121.05
2	H	74	ILE	CA-C-N	-5.34	116.59	123.16
2	H	74	ILE	C-N-CA	-5.34	116.59	123.16
1	B	673	LYS	CA-C-N	5.33	129.74	120.68
1	B	673	LYS	C-N-CA	5.33	129.74	120.68
1	F	746	GLU	CB-CG-CD	5.31	121.62	112.60
2	D	74	ILE	N-CA-C	5.29	120.34	109.34
1	F	444	ARG	N-CA-C	5.27	118.44	110.64
1	A	525	ARG	CA-C-N	5.25	134.60	121.80
1	A	525	ARG	C-N-CA	5.25	134.60	121.80
1	F	492	HIS	N-CA-C	5.24	119.39	112.89
2	G	48	THR	CB-CA-C	5.23	118.13	109.70
2	G	67	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	712	ALA	CA-C-N	5.17	128.19	120.90
1	A	712	ALA	C-N-CA	5.17	128.19	120.90
2	D	75	ARG	N-CA-C	5.16	118.54	108.21
2	H	84	ASN	CA-CB-CG	5.16	117.76	112.60
1	B	421	VAL	N-CA-CB	5.16	116.58	110.55
1	B	633	CYS	N-CA-C	5.14	116.34	108.42
1	F	524	PHE	N-CA-C	5.14	116.69	111.14
2	D	82	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	524	PHE	N-CA-C	5.12	116.55	111.07
1	F	421	VAL	N-CA-CB	5.12	116.54	110.55
1	B	399	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	720	PHE	CA-CB-CG	5.09	118.89	113.80
1	B	497	GLY	CA-C-N	5.07	128.31	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	497	GLY	C-N-CA	5.07	128.31	121.05
1	A	633	CYS	N-CA-C	5.04	116.18	108.42
2	C	135	ASN	N-CA-CB	-5.04	103.16	110.36
1	E	421	VAL	N-CA-CB	5.03	116.44	110.55
1	B	479	THR	CB-CA-C	5.02	119.65	111.26
1	E	633	CYS	N-CA-C	5.02	116.16	108.42
1	B	557	LEU	CA-C-N	5.01	131.12	121.54
1	B	557	LEU	C-N-CA	5.01	131.12	121.54

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	2897	0	2954	54	0
1	B	2945	0	3016	63	0
1	E	2893	0	2954	61	0
1	F	2884	0	2935	58	0
2	C	1293	0	1285	39	0
2	D	1315	0	1301	43	0
2	G	1298	0	1287	28	0
2	H	1277	0	1270	39	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	349	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 (349) 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:HG3	2:G:151:ARG:HH11	1.21	1.03
1:F:580:GLY:O	1:F:584:ARG:HG2	1.61	1.01
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
1:B:575:ARG:HG2	1:B:579:MET:HE2	1.60	0.82
1:B:576:GLU:HA	1:B:579:MET:HE3	1.62	0.81
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:HG3	2:G:151:ARG:NH1	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
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
1:F:557:LEU:O	1:F:558:GLU:HB3	1.90	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
1:B:544:MET:HE1	1:B:586:ARG:HA	1.77	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:23:VAL:HG21	2:G:110:MET:HE2	1.80	0.63
2:C:152:ASN:CG	2:D:137:ALA:HB2	2.23	0.62
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:D:68:VAL:C	2:D:70:GLY:H	2.10	0.60
1:E:487:ARG:HG3	1:E:590:LEU:HD23	1.83	0.60
1:E:552:GLU:H	1:E:552:GLU:CD	2.10	0.60
1:B:671:LYS:HA	1:B:676:VAL:HG23	1.82	0.59
2:C:134:MET:HE1	2:C:142:LYS:HG3	1.83	0.59
2:D:134:MET:HE1	2:D:142:LYS:HG3	1.84	0.59
1:B:439:HIS:O	1:B:443:GLN:HG2	2.01	0.59
2:G:134:MET:HE1	2:G:142:LYS:HG3	1.83	0.59
2:H:134:MET:HE1	2:H:142:LYS:HG3	1.84	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:C:31:THR:HG21	1:F:498:LYS:HG3	1.85	0.58
2:D:145:LEU:O	2:D:146:HIS:HB2	2.03	0.58
2:D:23:VAL:HG21	2:D:110:MET:HE2	1.85	0.58
2:C:38:LYS:CD	2:C:54:GLU:HG3	2.32	0.58
2:C:23:VAL:HG21	2:C:110:MET:HE2	1.84	0.58
2:G:151:ARG:HH11	2:G:151:ARG:CG	2.06	0.58
2:H:23:VAL:HG21	2:H:110:MET:HE2	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:686:LEU:HD23	1:F:689:MET:HE3	1.85	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
2:H:173:LEU:C	2:H:175:ASN:H	2.14	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
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: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:B:689:MET:HE3	1:B:705:LEU:HD22	1.88	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: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:E:555:MET:HE2	1:E:560:PHE:HA	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:159:CYS:HG	2:H:162:SER:HG	1.54	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
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
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
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
2:C:45:THR:C	2:C:47:PRO:HD2	2.36	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
2:H:113:GLU:HB3	2:H:116:LEU:HG	1.93	0.50
1:A:689:MET:HE3	1:A:705:LEU:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:548:ASN:HB3	2:H:55:THR:HG23	1.94	0.48
2:D:128:GLN:HG3	2:D:157:ALA:HB1	1.95	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
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: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
1:B:476:ASP:N	1:B:476:ASP:OD1	2.48	0.47
2:D:26:ASP:HB3	1:E:500:GLN:HE21	1.79	0.47
2:D:26:ASP:HB3	1:E:500:GLN:NE2	2.30	0.47
2:D:48:THR:HG21	1:E:546:SER:HA	1.96	0.47
1:E:406:TYR:HB2	1:E:429:PHE:CE1	2.50	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:459:ARG:HB3	1:B:504:ARG:HD3	1.97	0.47
2:H:69:GLY:C	2:H:71:GLN:H	2.22	0.47
1:B:479:THR:CG2	1:B:479:THR:O	2.63	0.47
1:B:704:ARG:HG2	1:B:706:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:413:PHE:CD1	1:A:413:PHE:C	2.94	0.46
1:E:480:MET:HE2	1:E:484:GLU:HB3	1.96	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
1:B:689:MET:HE2	1:B:739:ILE:HD11	1.97	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:E:689:MET:HE3	1:E:705:LEU:HD22	1.96	0.46
1:F:486:LEU:O	1:F:490:GLN:HG3	2.15	0.46
2:G:177:LEU:O	2:G:178:ARG:C	2.59	0.46
2:H:68:VAL:C	2:H:70:GLY:H	2.23	0.46
1:A:487:ARG:HG3	1:A:590:LEU:HD23	1.97	0.46
1:B:544:MET:HE2	1:B:544:MET:HB3	1.73	0.46
2:G:76:PRO:HA	2:G:79:ARG:HH21	1.81	0.46
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
2:D:74:ILE:C	2:D:75:ARG:HD2	2.41	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
2:D:68:VAL:C	2:D:70:GLY:N	2.75	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:592:THR:OG1	2:H:49:ILE:HD11	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:A:480:MET:HE1	1:A:488:LYS:HD2	2.01	0.42
1:A:601:GLN:HE22	2:H:46:ILE:HG23	1.84	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
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
2:C:80:HIS:CG	1:F:555:MET:HE3	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:525:ARG:HD3	2:H:167:TYR:CD2	2.55	0.42
1:E:531:PHE:CE1	1:E:535:PHE:CE2	3.08	0.42
2:H:39:LEU:HD12	2:H:39:LEU:HA	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: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:A:497:GLY:HA2	2:H:52:ASN:HD21	1.85	0.41
1:B:648:LYS:HB3	1:B:651:LEU:HD13	2.01	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
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
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
1:F:473:ASP:C	1:F:475:MET:H	2.29	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
2:H:173:LEU:C	2:H:175:ASN:N	2.79	0.41
1:A:503:GLU:HA	1:A:535:PHE:CZ	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:459:ARG:HB3	1:E:504:ARG:CD	2.51	0.41
1:E:495:VAL:HG12	1:E:502:VAL:HG13	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: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:E:689:MET:HE2	1:E:735:LEU:HD11	2.03	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
2:D:23:VAL:HG13	2:D:68:VAL:HB	2.03	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

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%)	3	21
1	B	354/383 (92%)	322 (91%)	21 (6%)	11 (3%)	3	20
1	E	347/383 (91%)	316 (91%)	21 (6%)	10 (3%)	3	21
1	F	347/383 (91%)	320 (92%)	18 (5%)	9 (3%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	159/164 (97%)	145 (91%)	6 (4%)	8 (5%)	1	11
2	D	162/164 (99%)	146 (90%)	6 (4%)	10 (6%)	1	9
2	G	160/164 (98%)	147 (92%)	8 (5%)	5 (3%)	3	20
2	H	157/164 (96%)	136 (87%)	13 (8%)	8 (5%)	1	11
All	All	2034/2188 (93%)	1852 (91%)	111 (6%)	71 (4%)	3	18

All (71) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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
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%)	292 (90%)	31 (10%)	8	29
1	B	329/347 (95%)	296 (90%)	33 (10%)	7	27
1	E	323/347 (93%)	290 (90%)	33 (10%)	7	26
1	F	321/347 (92%)	285 (89%)	36 (11%)	6	22
2	C	138/142 (97%)	126 (91%)	12 (9%)	9	32
2	D	140/142 (99%)	126 (90%)	14 (10%)	7	27
2	G	138/142 (97%)	125 (91%)	13 (9%)	8	30
2	H	137/142 (96%)	118 (86%)	19 (14%)	3	15
All	All	1849/1956 (94%)	1658 (90%)	191 (10%)	7	25

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	398	ASN
1	A	400	VAL
1	A	412	LEU
1	A	445	LYS
1	A	479	THR
1	A	496	GLN
1	A	498	LYS
1	A	504	ARG
1	A	506	ILE
1	A	520	VAL
1	A	521	VAL
1	A	530	ILE
1	A	557	LEU
1	A	571	GLU
1	A	597	VAL
1	A	604	GLU
1	A	624	LEU
1	A	625	SER
1	A	649	LEU

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Mol	Chain	Res	Type
1	A	651	LEU
1	A	668	ILE
1	A	677	THR
1	A	685	SER
1	A	689	MET
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	400	VAL
1	B	412	LEU
1	B	445	LYS
1	B	460	GLN
1	B	476	ASP
1	B	479	THR
1	B	496	GLN
1	B	498	LYS
1	B	503	GLU
1	B	506	ILE
1	B	521	VAL
1	B	525	ARG
1	B	530	ILE
1	B	550	LYS
1	B	552	GLU
1	B	556	LYS
1	B	576	GLU
1	B	597	VAL
1	B	604	GLU
1	B	624	LEU
1	B	649	LEU
1	B	651	LEU
1	B	668	ILE
1	B	672	LYS
1	B	677	THR
1	B	685	SER
1	B	689	MET
1	B	692	LEU
1	B	737	GLU
1	B	745	MET

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Mol	Chain	Res	Type
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	60	ASN
2	C	65	VAL
2	C	74	ILE
2	C	75	ARG
2	C	77	LEU
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	45	THR
2	D	56	VAL
2	D	60	ASN
2	D	61	ILE
2	D	65	VAL
2	D	74	ILE
2	D	75	ARG
2	D	85	THR
2	D	114	ASP
2	D	115	GLU
2	D	180	GLN
1	E	400	VAL
1	E	412	LEU
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

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Mol	Chain	Res	Type
1	E	550	LYS
1	E	552	GLU
1	E	554	LYS
1	E	555	MET
1	E	558	GLU
1	E	571	GLU
1	E	575	ARG
1	E	576	GLU
1	E	597	VAL
1	E	604	GLU
1	E	649	LEU
1	E	651	LEU
1	E	668	ILE
1	E	685	SER
1	E	689	MET
1	E	692	LEU
1	E	714	ILE
1	E	737	GLU
1	E	754	LEU
1	E	755	GLU
1	F	398	ASN
1	F	400	VAL
1	F	412	LEU
1	F	445	LYS
1	F	459	ARG
1	F	476	ASP
1	F	479	THR
1	F	496	GLN
1	F	506	ILE
1	F	512	ARG
1	F	521	VAL
1	F	530	ILE
1	F	558	GLU
1	F	571	GLU
1	F	576	GLU
1	F	588	ARG
1	F	597	VAL
1	F	604	GLU
1	F	624	LEU
1	F	649	LEU
1	F	651	LEU
1	F	656	ILE

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Mol	Chain	Res	Type
1	F	668	ILE
1	F	672	LYS
1	F	677	THR
1	F	679	SER
1	F	682	GLN
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	49	ILE
2	G	51	PHE
2	G	65	VAL
2	G	71	GLN
2	G	72	ASP
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	49	ILE
2	H	60	ASN
2	H	65	VAL
2	H	74	ILE
2	H	75	ARG
2	H	114	ASP
2	H	118	ASP
2	H	146	HIS
2	H	149	ARG

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Mol	Chain	Res	Type
2	H	150	HIS
2	H	159	CYS
2	H	176	GLN
2	H	177	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	500	GLN
1	A	517	ASN
1	A	523	GLN
1	A	548	ASN
1	A	599	GLN
1	A	653	GLN
1	A	690	GLN
1	A	743	GLN
1	B	398	ASN
1	B	500	GLN
1	B	517	ASN
1	B	523	GLN
1	B	548	ASN
1	B	599	GLN
1	B	653	GLN
1	B	726	GLN
2	C	52	ASN
2	C	60	ASN
2	C	80	HIS
2	C	128	GLN
2	C	146	HIS
2	C	150	HIS
2	C	176	GLN
2	D	52	ASN
2	D	128	GLN
2	D	150	HIS
2	D	176	GLN
1	E	398	ASN
1	E	458	ASN
1	E	490	GLN
1	E	496	GLN
1	E	500	GLN
1	E	517	ASN
1	E	523	GLN

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Mol	Chain	Res	Type
1	E	526	ASN
1	E	548	ASN
1	E	599	GLN
1	E	653	GLN
1	E	743	GLN
1	F	517	ASN
1	F	523	GLN
1	F	526	ASN
1	F	599	GLN
1	F	652	HIS
1	F	653	GLN
1	F	690	GLN
1	F	697	GLN
2	G	52	ASN
2	G	128	GLN
2	G	146	HIS
2	G	176	GLN
2	H	52	ASN
2	H	128	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 ⓘ

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	H	401	-	33,34,34	1.07	1 (3%)	52,54,54	1.22	5 (9%)
3	G3D	C	401	-	33,34,34	1.50	1 (3%)	52,54,54	1.23	6 (11%)
3	G3D	G	401	-	33,34,34	1.27	1 (3%)	52,54,54	1.30	8 (15%)
3	G3D	D	401	-	33,34,34	1.01	2 (6%)	52,54,54	1.04	3 (5%)

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	H	401	-	-	4/21/37/37	0/3/3/3
3	G3D	C	401	-	-	6/21/37/37	0/3/3/3
3	G3D	G	401	-	-	5/21/37/37	0/3/3/3
3	G3D	D	401	-	-	3/21/37/37	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	G3D	PA-O3A	-7.88	1.51	1.59
3	G	401	G3D	PA-O3A	-6.47	1.52	1.59
3	H	401	G3D	PA-O3A	-4.74	1.54	1.59
3	D	401	G3D	PA-O3A	-4.50	1.54	1.59
3	D	401	G3D	P1-O6P	2.10	1.57	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	C	401	G3D	P1-O3'-C3'	3.47	132.70	123.43
3	G	401	G3D	P1-O3'-C3'	3.46	132.68	123.43
3	H	401	G3D	P1-O3'-C3'	3.33	132.34	123.43
3	G	401	G3D	O3A-PA-O1A	-2.85	102.12	110.70
3	C	401	G3D	O3A-PA-O1A	-2.79	102.31	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	401	G3D	O3A-PA-O1A	-2.66	102.70	110.70
3	G	401	G3D	O3B-PB-O3A	-2.56	96.07	104.64
3	D	401	G3D	O4P-P1-O3'	2.49	115.56	105.85
3	G	401	G3D	O3'-P1-O6P	-2.36	100.92	109.33
3	H	401	G3D	O3A-PB-O1B	-2.36	98.63	111.04
3	D	401	G3D	O3A-PB-O1B	-2.32	98.81	111.04
3	G	401	G3D	O2A-PA-O5'	2.23	117.67	107.57
3	G	401	G3D	O3B-PB-O2B	2.14	115.82	107.80
3	C	401	G3D	O3B-PB-O3A	-2.14	97.47	104.64
3	C	401	G3D	O2A-PA-O5'	2.10	117.11	107.57
3	G	401	G3D	O5'-PA-O1A	-2.09	100.66	108.94
3	C	401	G3D	O3B-PB-O2B	2.08	115.59	107.80
3	H	401	G3D	O4P-P1-O3'	2.07	113.92	105.85

There are no chirality outliers.

All (18) torsion outliers are listed below:

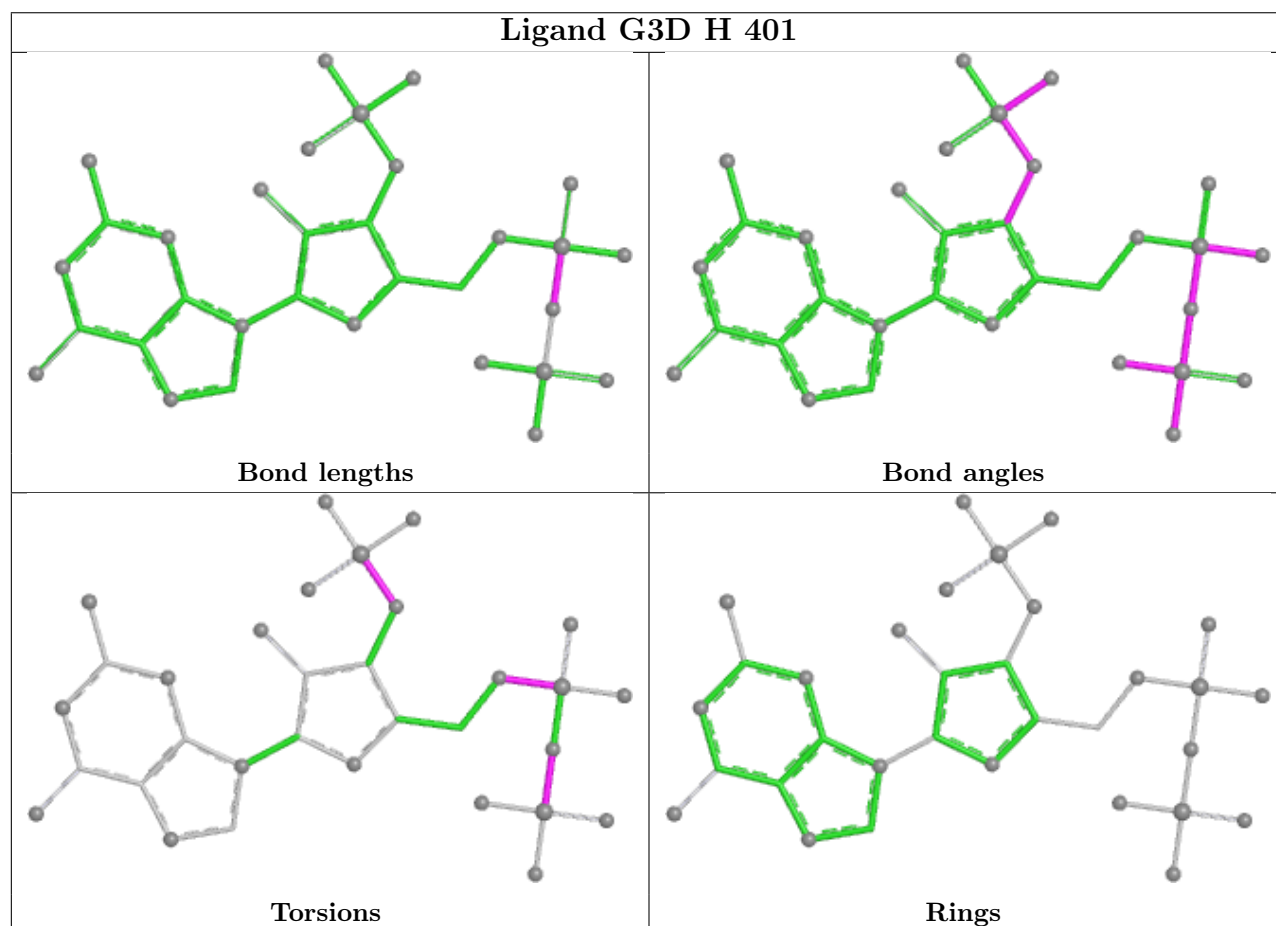
Mol	Chain	Res	Type	Atoms
3	C	401	G3D	C5'-O5'-PA-O1A
3	H	401	G3D	PA-O3A-PB-O3B
3	H	401	G3D	C5'-O5'-PA-O1A
3	G	401	G3D	O4'-C4'-C5'-O5'
3	C	401	G3D	C5'-O5'-PA-O3A
3	C	401	G3D	C5'-O5'-PA-O2A
3	H	401	G3D	C5'-O5'-PA-O2A
3	C	401	G3D	PB-O3A-PA-O2A
3	D	401	G3D	PB-O3A-PA-O2A
3	G	401	G3D	C3'-C4'-C5'-O5'
3	C	401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

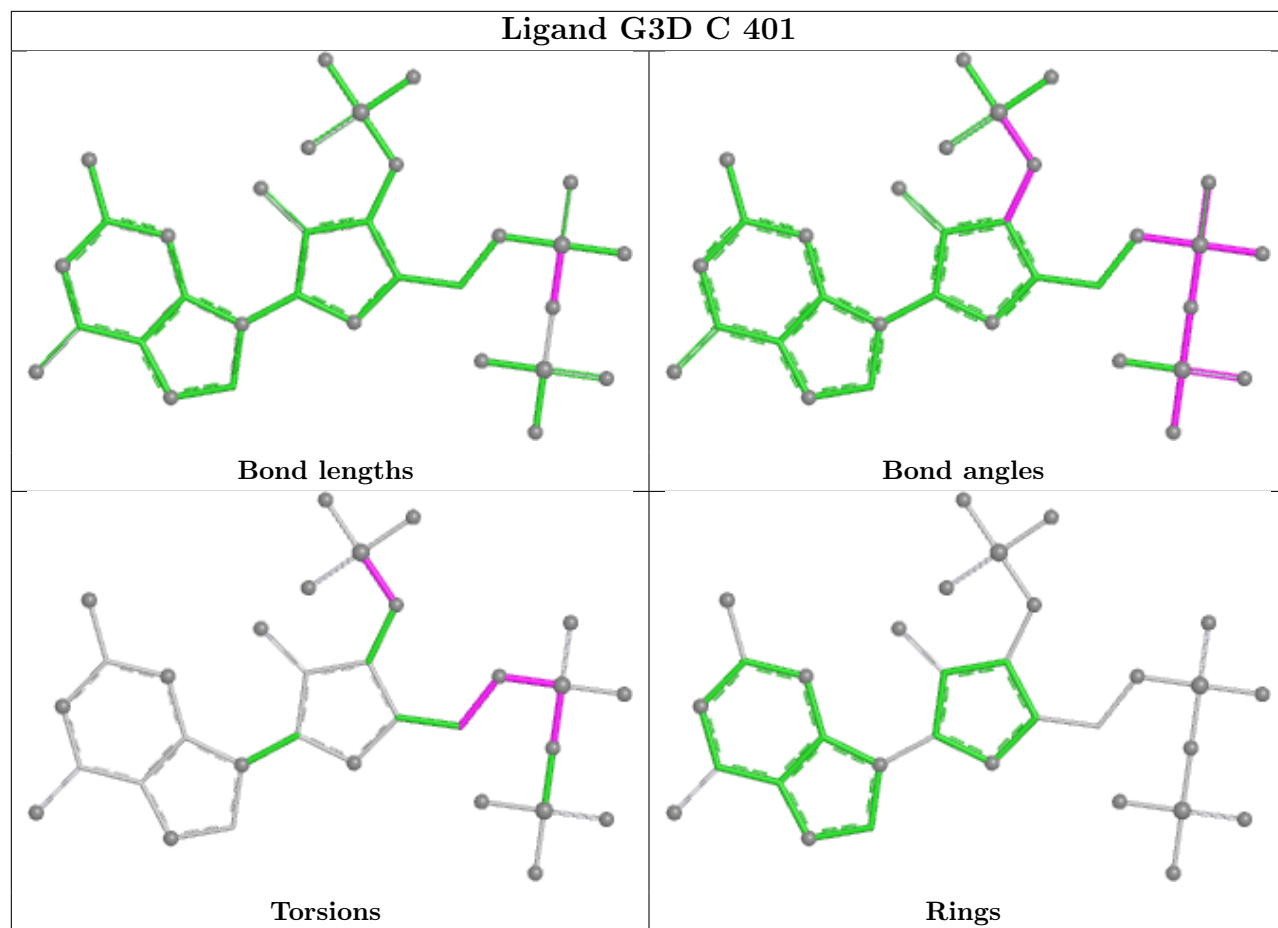
There are no ring outliers.

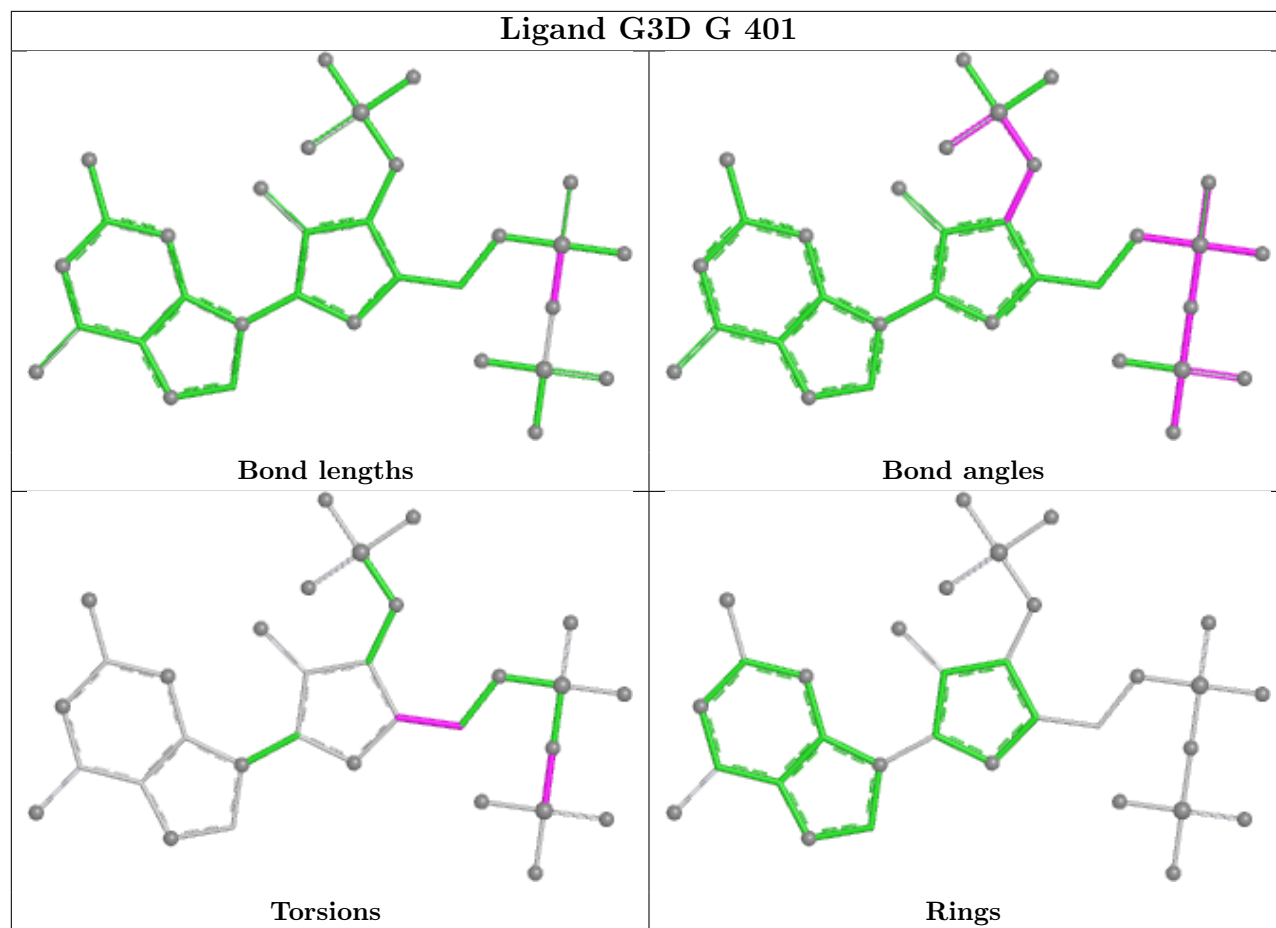
2 monomers are involved in 3 short contacts:

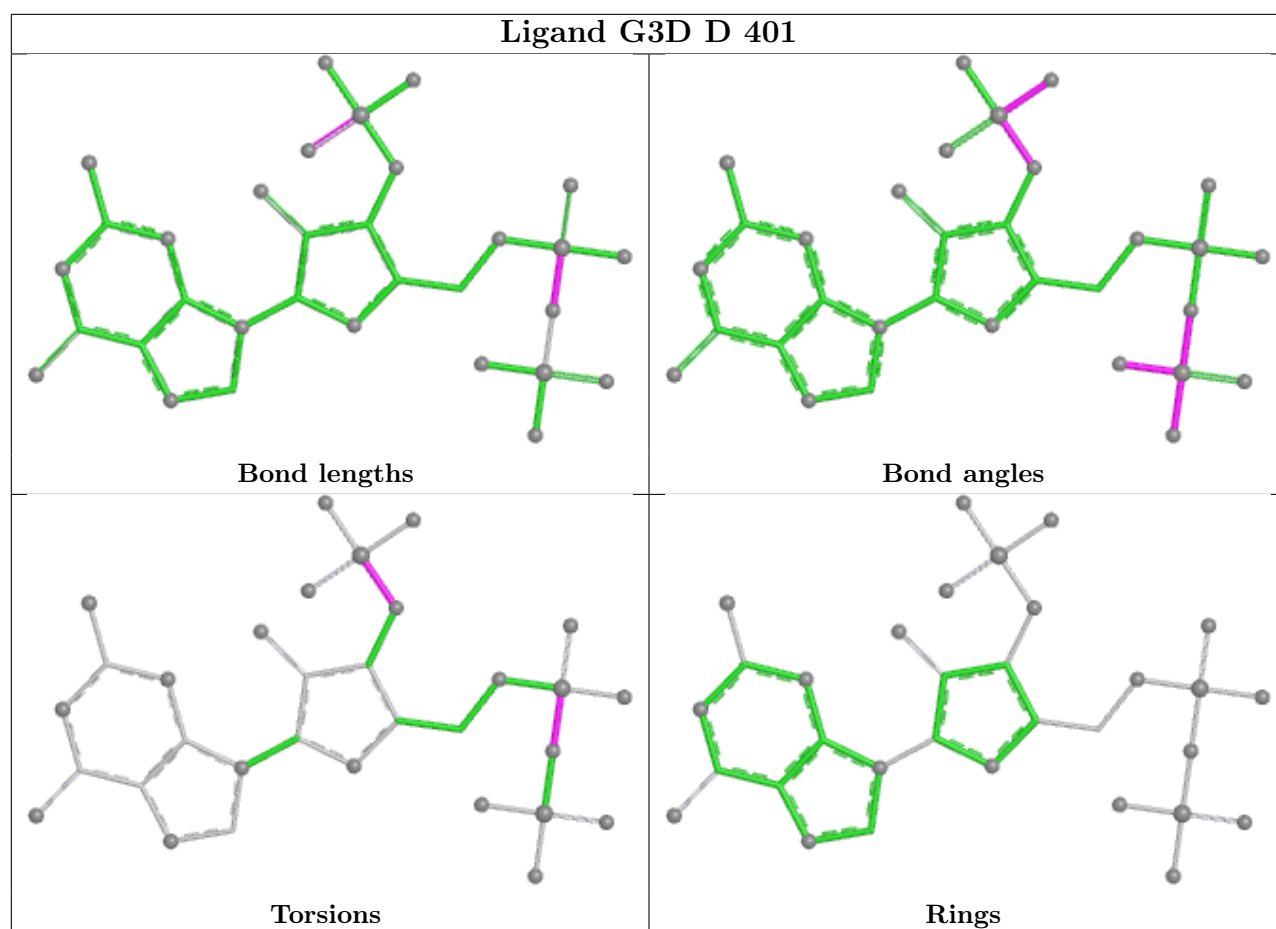
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	401	G3D	1	0
3	D	401	G3D	2	0

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 ⓘ

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%)	-0.18	1 (0%) 90 82	25, 59, 103, 132	0
1	B	357/383 (93%)	-0.14	6 (1%) 69 50	9, 52, 104, 126	1 (0%)
1	E	351/383 (91%)	-0.19	0 100 100	27, 53, 94, 134	0
1	F	351/383 (91%)	-0.17	0 100 100	25, 52, 92, 120	0
2	C	161/164 (98%)	0.15	2 (1%) 76 58	34, 70, 114, 141	0
2	D	164/164 (100%)	0.16	1 (0%) 85 73	31, 65, 102, 127	0
2	G	162/164 (98%)	0.52	6 (3%) 45 31	54, 100, 139, 155	0
2	H	159/164 (96%)	1.05	18 (11%) 10 8	69, 135, 196, 215	0
All	All	2057/2188 (94%)	0.03	34 (1%) 69 50	9, 61, 132, 215	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	143	LEU	4.7
2	H	139	ILE	4.5
2	H	107	LEU	3.7
2	H	136	ALA	3.6
1	B	557	LEU	3.5
2	H	173	LEU	3.5
2	H	121	LEU	3.4
2	G	68	VAL	3.1
1	B	393	SER	3.1
2	H	177	LEU	3.0
2	G	67	ASP	3.0
2	H	145	LEU	2.9
1	A	712	ALA	2.8
1	B	395	ALA	2.7
2	D	139	ILE	2.5
2	H	42	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	26	ASP	2.4
2	H	92	VAL	2.4
1	B	396	PHE	2.4
2	H	141	ASP	2.3
2	H	120	VAL	2.3
2	G	170	LEU	2.3
2	C	68	VAL	2.2
2	G	18	MET	2.2
2	H	96	ASP	2.2
2	G	143	LEU	2.2
2	H	116	LEU	2.1
1	B	476	ASP	2.1
2	G	66	TRP	2.1
2	H	176	GLN	2.1
2	H	98	GLU	2.1
2	H	123	VAL	2.0
1	B	394	PRO	2.0
2	C	98	GLU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

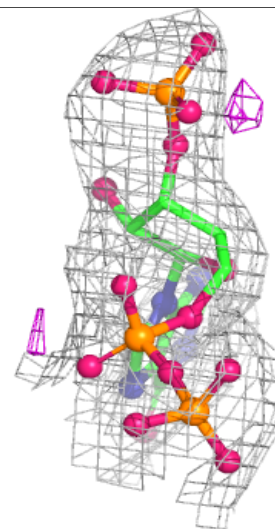
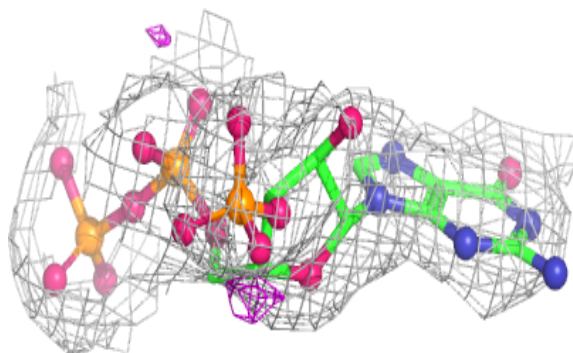
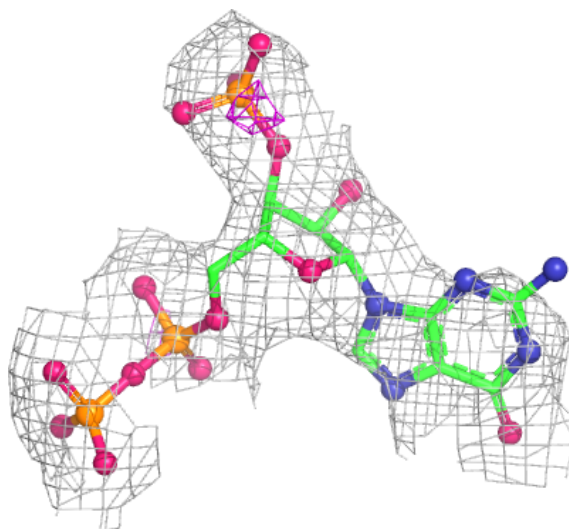
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	G3D	H	401	32/32	0.83	0.10	97,113,124,129	0
3	G3D	G	401	32/32	0.94	0.07	66,89,99,105	0
3	G3D	C	401	32/32	0.95	0.07	42,69,88,93	0
3	G3D	D	401	32/32	0.95	0.06	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.

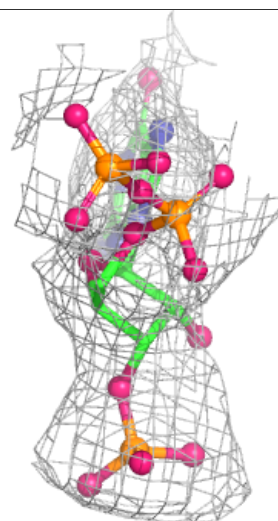
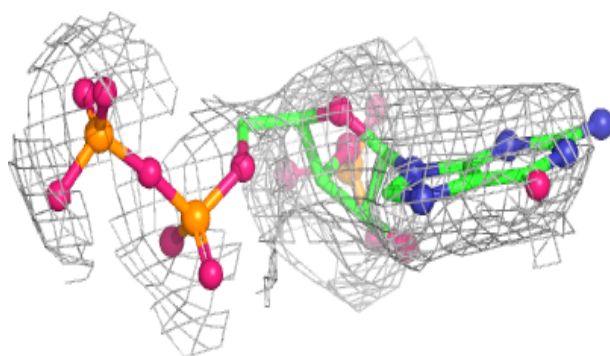
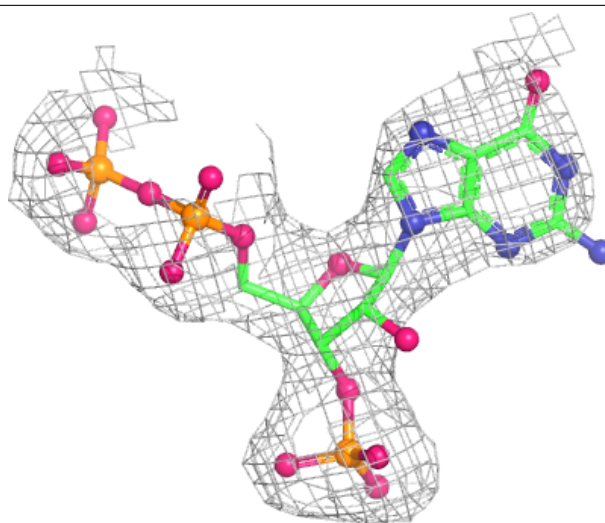
Electron density around G3D H 401:

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



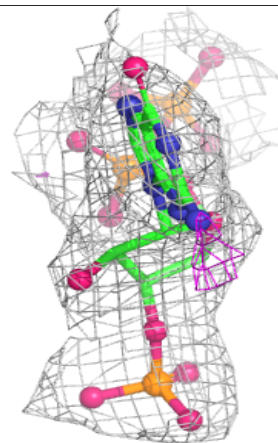
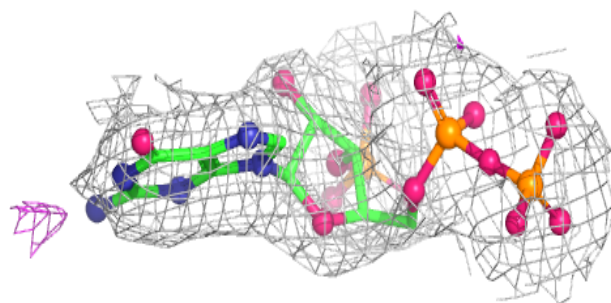
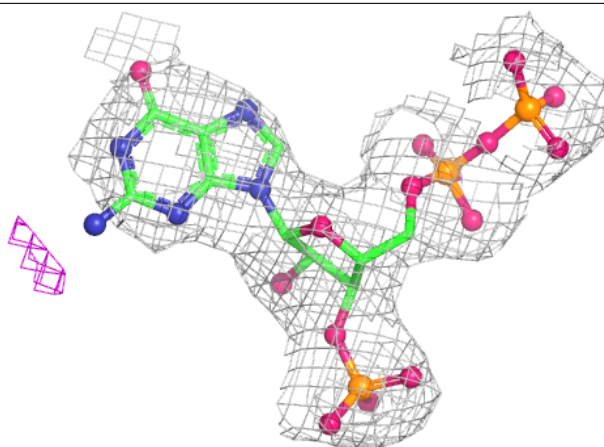
Electron density around G3D G 401:

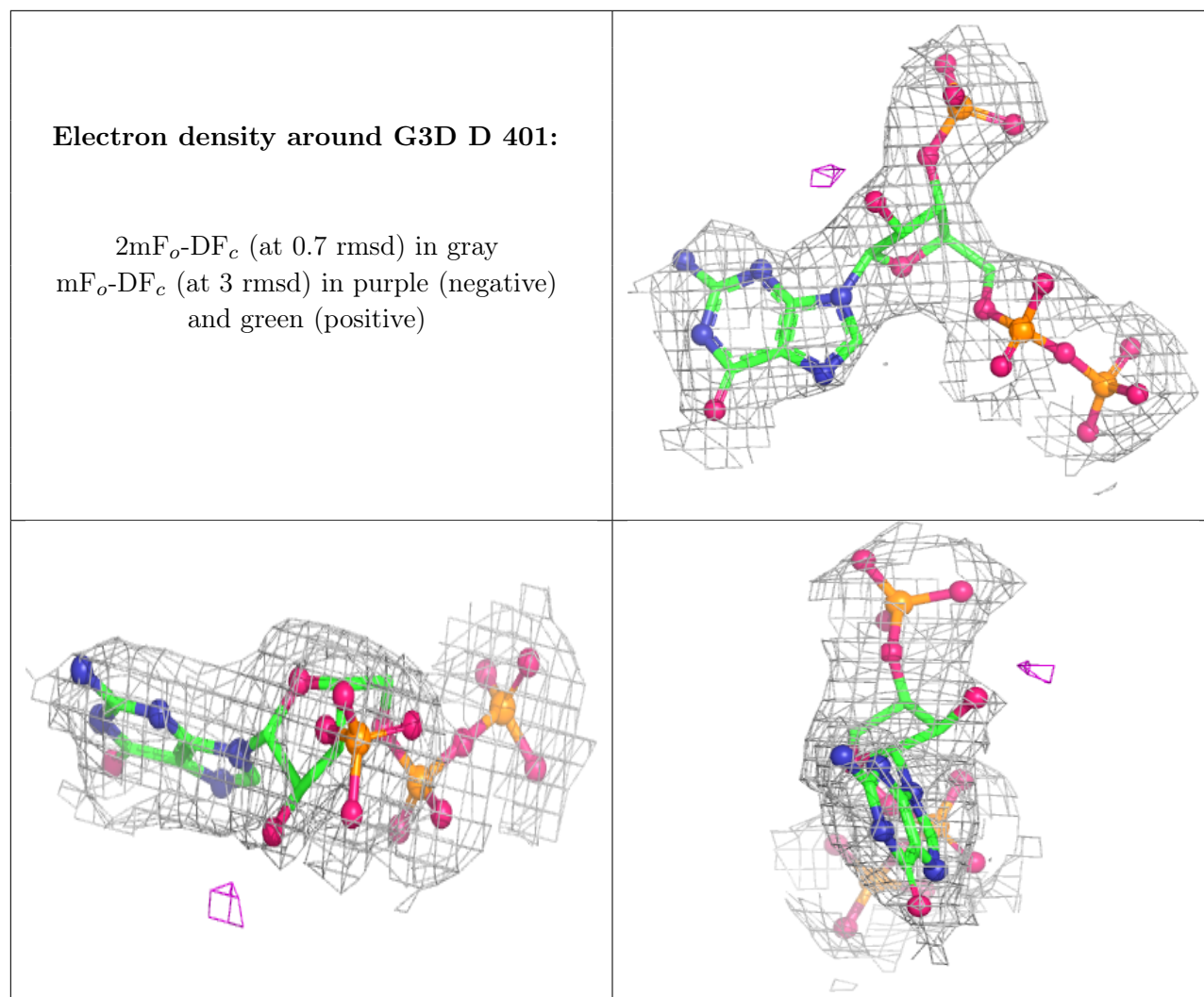
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.