



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:31 AM UTC

PDB ID : 8QW7 / pdb_00008qw7
Title : Crystal Structure of compound 4 in complex with KRAS G12V C118S GDP and pVHL:ElonginC:ElonginB
Authors : Zollman, D.; Farnaby, W.; Ciulli, A.
Deposited on : 2023-10-18
Resolution : 2.36 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

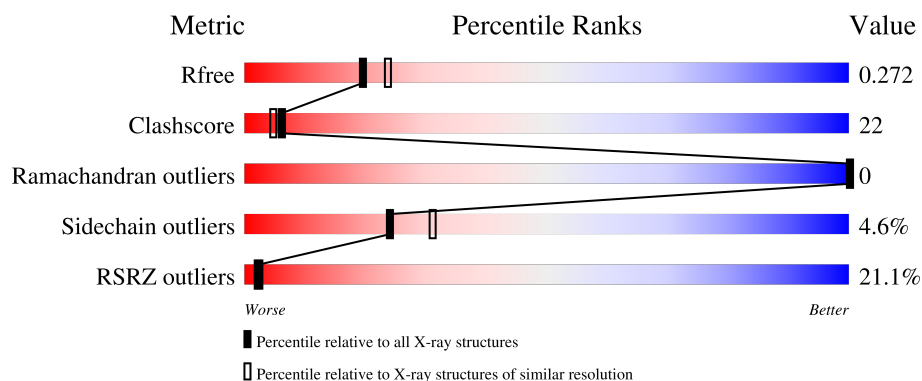
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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.



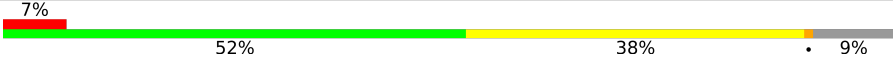
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	D	104	37% 43% 45% 10% .
1	H	104	10% 55% 38% 6% ..
2	C	97	15% 49% 35% . 12%
2	G	97	5% 44% 41% . 11%
3	B	162	7% 54% 31% 6% 9%

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Mol	Chain	Length	Quality of chain
3	F	162	
4	A	170	
4	E	170	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7770 atoms, of which 120 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 Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	102	Total	C	N	O	S	0	0	0
			751	471	128	148	4			
1	H	103	Total	C	N	O	S	0	0	0
			798	507	136	151	4			

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	85	Total	C	N	O	S	0	0	0
			650	423	103	119	5			
2	G	86	Total	C	N	O	S	0	0	0
			682	441	107	128	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	16	MET	-	initiating methionine	UNP Q15369
G	16	MET	-	initiating methionine	UNP Q15369

- Molecule 3 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	148	Total	C	N	O	S	0	0	0
			1187	755	218	212	2			
3	F	148	Total	C	N	O	S	0	0	0
			1192	756	219	215	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	52	GLY	-	expression tag	UNP P40337
B	53	SER	-	expression tag	UNP P40337

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Chain	Residue	Modelled	Actual	Comment	Reference
F	52	GLY	-	expression tag	UNP P40337
F	53	SER	-	expression tag	UNP P40337

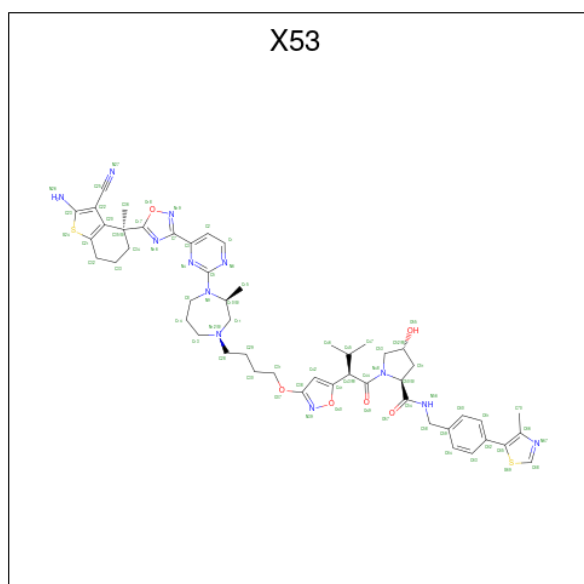
- Molecule 4 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	166	Total	C	N	O	S	0	0	0
			1191	747	206	233	5			
4	E	144	Total	C	N	O	S	0	0	0
			978	600	172	201	5			

There are 6 discrepancies between the modelled and reference sequences:

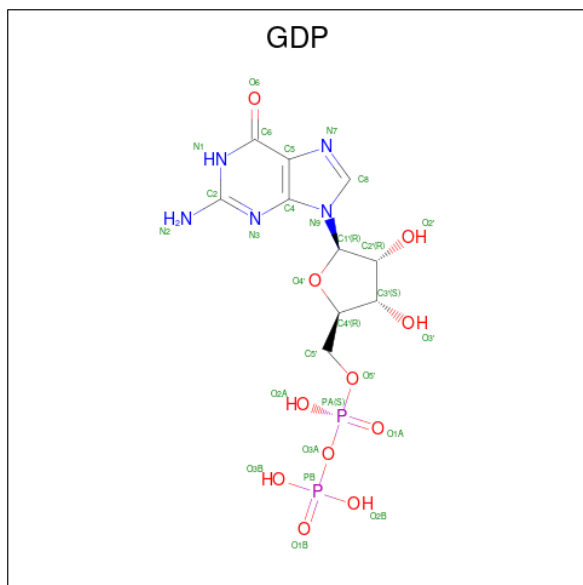
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P01116
A	12	VAL	GLY	engineered mutation	UNP P01116
A	118	SER	CYS	engineered mutation	UNP P01116
E	0	GLY	-	expression tag	UNP P01116
E	12	VAL	GLY	engineered mutation	UNP P01116
E	118	SER	CYS	engineered mutation	UNP P01116

- Molecule 5 is (2S,4R)-1-[(2R)-2-[3-[4-[(3S)-4-[4-[5-[(4S)-2-azanyl-3-cyano-4-methyl-6,7-dihydro-5H-1-benzothiophen-4-yl]-1,2,4-oxadiazol-3-yl]pyrimidin-2-yl]-3-methyl-1,4-diazepan-1-yl]butoxy]-1,2-oxazol-5-yl]-3-methyl-butanoyl]-N-[[4-(4-methyl-1,3-thiazol-5-yl)phenyl]methyl]-4-oxidanyl-pyrrolidine-2-carboxamide (CCD ID: X53) (formula: C₅₀H₆₀N₁₂O₆S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	S	
			130	50	60	12	6	2	0
5	F	1	Total	C	H	N	O	S	
			130	50	60	12	6	2	0

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P		
			28	10	5	11	2	0	0
6	E	1	Total	C	N	O	P		
			28	10	5	11	2	0	0

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg		
			1	1	0	0
7	E	1	Total	Mg		
			1	1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	2	Total	O		
			2	2	0	0

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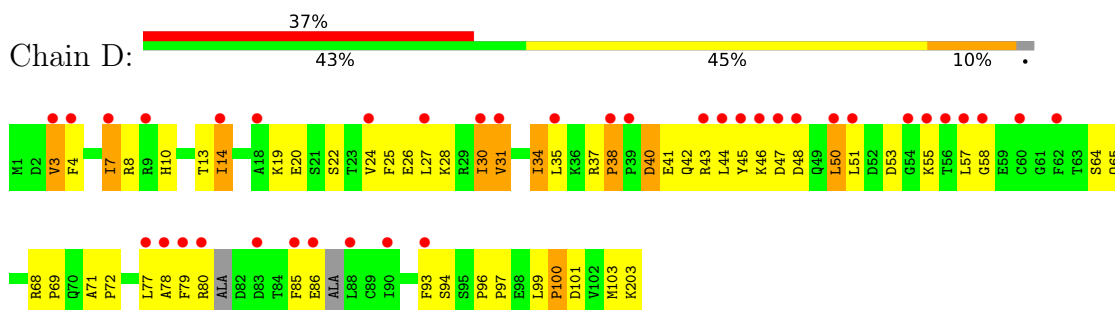
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	8	Total 8	O 8	0	0
8	H	2	Total 2	O 2	0	0
8	G	2	Total 2	O 2	0	0
8	F	5	Total 5	O 5	0	0
8	A	2	Total 2	O 2	0	0
8	E	2	Total 2	O 2	0	0

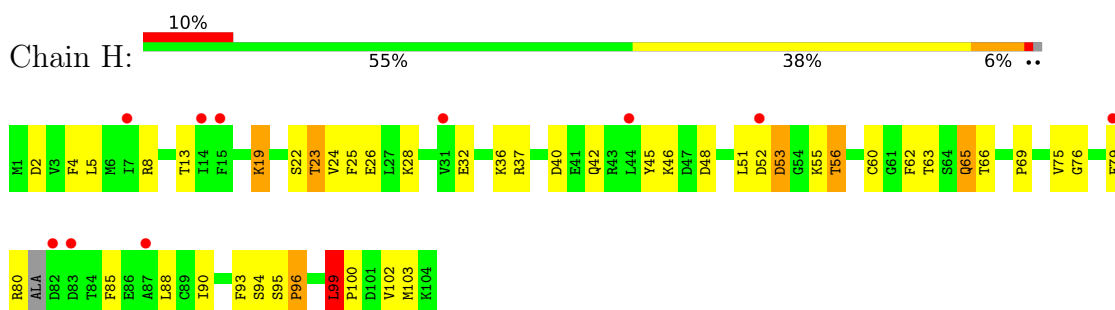
3 Residue-property plots [i](#)

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

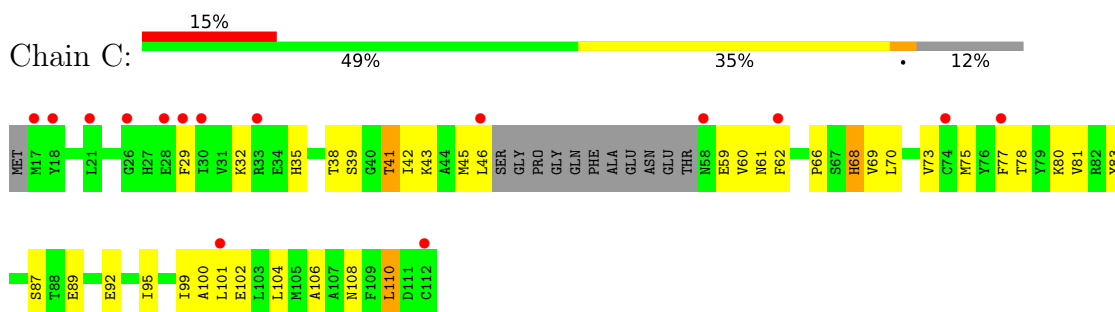
• Molecule 1: Elongin-B



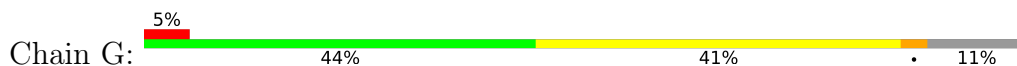
• Molecule 1: Elongin-B

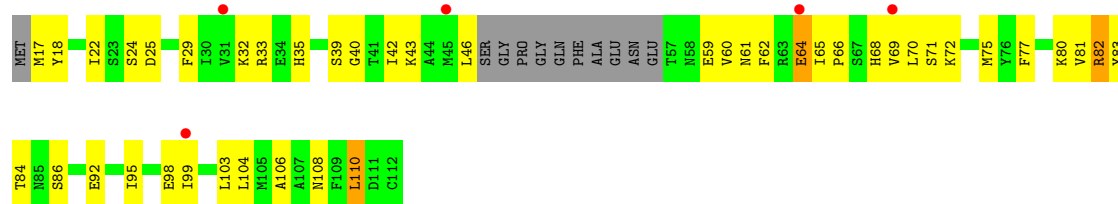


• Molecule 2: Elongin-C

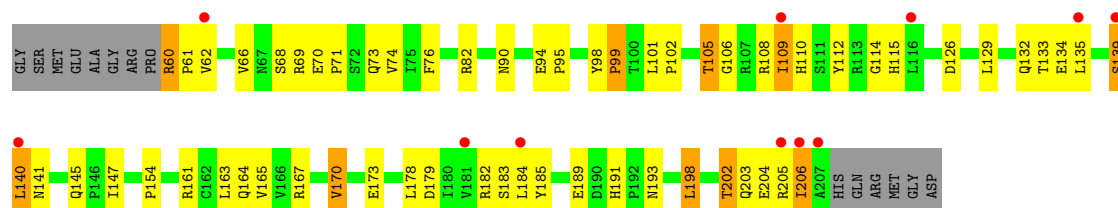


• Molecule 2: Elongin-C

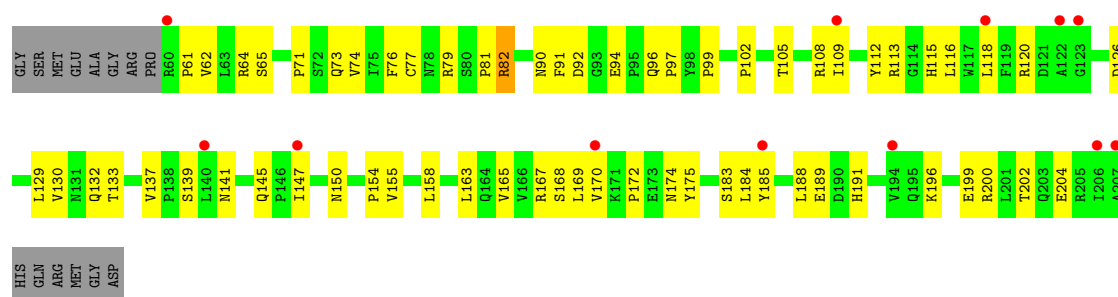




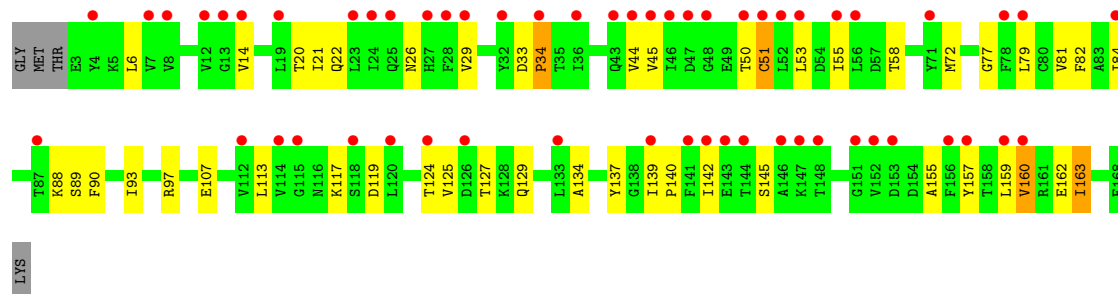
- Molecule 3: von Hippel-Lindau disease tumor suppressor



- Molecule 3: von Hippel-Lindau disease tumor suppressor

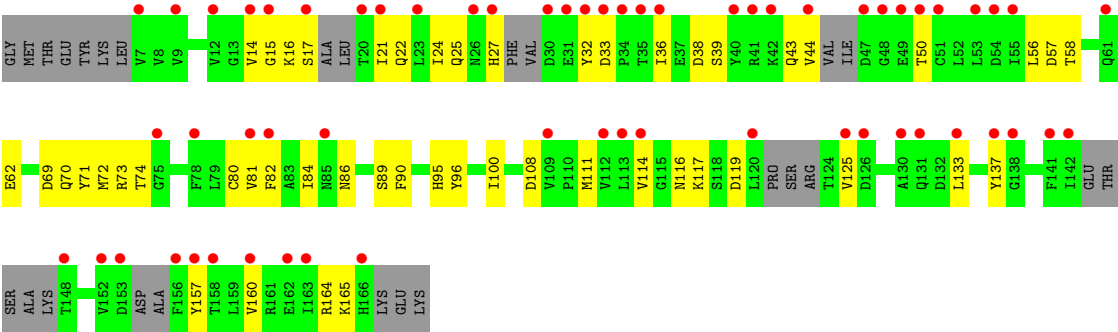


- Molecule 4: GTPase KRas



- Molecule 4: GTPase KRas





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.52Å 125.93Å 81.06Å 90.00° 111.61° 90.00°	Depositor
Resolution (Å)	67.42 – 2.36 67.42 – 2.36	Depositor EDS
% Data completeness (in resolution range)	55.6 (67.42-2.36) 55.6 (67.42-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.246 , 0.273 0.245 , 0.272	Depositor DCC
R_{free} test set	2012 reflections (3.63%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7770	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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: X53, MG, GDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	D	0.94	1/763 (0.1%)	1.28	10/1034 (1.0%)
1	H	1.04	2/813 (0.2%)	1.23	2/1098 (0.2%)
2	C	0.94	1/664 (0.2%)	1.14	7/901 (0.8%)
2	G	1.06	5/696 (0.7%)	1.13	2/940 (0.2%)
3	B	1.15	9/1218 (0.7%)	1.22	7/1667 (0.4%)
3	F	1.10	5/1223 (0.4%)	1.14	2/1673 (0.1%)
4	A	0.90	2/1208 (0.2%)	1.09	2/1644 (0.1%)
4	E	0.97	0/986	1.25	2/1339 (0.1%)
All	All	1.02	25/7571 (0.3%)	1.19	34/10296 (0.3%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	95	PRO	C-O	-8.80	1.13	1.23
3	F	81	PRO	C-O	-8.41	1.13	1.24
3	F	99	PRO	C-O	-7.97	1.13	1.23
3	B	99	PRO	C-O	-7.43	1.14	1.23
3	B	74	VAL	C-O	-7.37	1.16	1.24
3	F	97	PRO	C-O	-7.05	1.15	1.23
3	B	71	PRO	C-O	-6.36	1.15	1.23
4	A	34	PRO	C-O	-6.21	1.16	1.24
4	A	124	THR	CA-C	-6.21	1.47	1.52
2	G	60	VAL	C-O	-6.18	1.18	1.24
3	F	96	GLN	C-O	-6.02	1.16	1.24
1	D	14	ILE	C-O	-5.88	1.17	1.24
3	F	82	ARG	C-O	-5.86	1.16	1.23
2	G	82	ARG	C-O	-5.78	1.16	1.24
2	G	110	LEU	C-O	-5.71	1.16	1.24
2	G	99	ILE	C-O	-5.56	1.18	1.24
2	G	59	GLU	C-O	-5.54	1.17	1.24
1	H	99	LEU	C-O	-5.48	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	173	GLU	C-O	-5.45	1.17	1.24
3	B	98	TYR	C-O	-5.39	1.17	1.24
3	B	105	THR	C-O	-5.38	1.17	1.23
2	C	41	THR	C-O	-5.24	1.17	1.24
1	H	100	PRO	C-O	-5.19	1.17	1.23
3	B	106	GLY	C-O	-5.09	1.17	1.23
3	B	147	ILE	C-O	-5.04	1.18	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	10	HIS	CB-CA-C	-8.09	107.24	116.54
3	B	71	PRO	CB-CA-C	-8.05	101.34	111.56
4	A	107	GLU	N-CA-C	-7.37	103.24	112.90
4	A	51	CYS	N-CA-C	6.68	118.79	109.31
3	B	202	THR	CA-CB-OG1	-6.49	99.86	109.60
1	H	96	PRO	N-CA-C	6.46	118.58	110.70
1	H	37	ARG	CB-CA-C	6.14	116.71	109.47
1	D	100	PRO	CB-CA-C	-6.08	103.45	111.23
2	C	83	TYR	N-CA-C	6.07	120.30	113.02
3	B	205	ARG	N-CA-C	-6.04	106.27	113.21
1	D	96	PRO	N-CA-C	6.03	116.26	110.47
2	C	100	ALA	N-CA-C	6.03	117.54	110.97
2	C	41	THR	CB-CA-C	-5.92	99.30	110.67
1	D	40	ASP	N-CA-C	-5.76	106.15	112.72
4	E	69	ASP	CA-CB-CG	5.68	118.28	112.60
1	D	58	GLY	N-CA-C	5.63	119.03	112.50
3	F	126	ASP	CA-CB-CG	5.58	118.18	112.60
1	D	30	ILE	N-CA-C	-5.46	105.64	113.07
1	D	38	PRO	N-CA-C	5.43	116.39	110.58
3	B	139	SER	N-CA-C	-5.38	101.61	109.63
1	D	38	PRO	O-C-N	5.37	123.67	121.15
4	E	27	HIS	CA-CB-CG	5.36	119.16	113.80
2	C	89	GLU	CA-C-N	5.25	131.83	122.13
2	C	89	GLU	C-N-CA	5.25	131.83	122.13
2	G	64	GLU	N-CA-C	-5.24	107.91	114.56
2	G	68	HIS	CA-CB-CG	5.22	119.02	113.80
2	C	32	LYS	N-CA-C	5.17	116.96	110.24
3	B	109	ILE	N-CA-C	5.16	116.01	108.53
3	B	193	ASN	CA-C-N	-5.15	112.19	120.64
3	B	193	ASN	C-N-CA	-5.15	112.19	120.64
3	F	71	PRO	N-CA-C	5.13	119.14	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	43	LYS	N-CA-C	-5.09	106.75	113.12
1	D	46	LYS	N-CA-C	-5.07	102.14	109.59
1	D	31	VAL	N-CA-C	-5.06	105.96	113.39

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	D	751	0	704	52	0
1	H	798	0	790	38	0
2	C	650	0	629	33	0
2	G	682	0	679	40	0
3	B	1187	0	1170	51	0
3	F	1192	0	1171	55	0
4	A	1191	0	1070	40	0
4	E	978	0	780	46	0
5	B	70	60	0	5	0
5	F	70	60	0	5	0
6	A	28	0	12	4	0
6	E	28	0	12	5	0
7	A	1	0	0	0	0
7	E	1	0	0	0	0
8	A	2	0	0	0	0
8	B	8	0	0	1	0
8	C	2	0	0	0	0
8	E	2	0	0	0	0
8	F	5	0	0	0	0
8	G	2	0	0	0	0
8	H	2	0	0	0	0
All	All	7650	120	7017	328	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 22.

All (328) 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)
4:E:80:CYS:SG	4:E:111:MET:HE3	1.59	1.41
4:E:80:CYS:SG	4:E:111:MET:CE	2.23	1.26
3:B:102:PRO:O	3:B:105:THR:HG22	1.51	1.11
6:A:201:GDP:H5'	6:A:201:GDP:H8	1.22	1.02
1:H:23:THR:HG22	1:H:26:GLU:HG3	1.45	0.98
4:E:96:TYR:O	4:E:100:ILE:HD12	1.66	0.96
3:B:102:PRO:HD2	3:B:105:THR:HG21	1.48	0.96
4:E:14:VAL:HG21	4:E:81:VAL:HG12	1.47	0.94
4:E:80:CYS:HG	4:E:111:MET:HE3	1.17	0.92
6:A:201:GDP:H5'	6:A:201:GDP:C8	2.06	0.91
1:H:23:THR:HG22	1:H:26:GLU:H	1.34	0.90
3:F:109:ILE:HG23	5:F:401:X53:C61	2.00	0.90
4:E:80:CYS:SG	4:E:111:MET:HE1	2.14	0.86
1:D:68:ARG:HD2	1:D:69:PRO:HD3	1.59	0.84
3:B:109:ILE:HG23	5:B:401:X53:C61	2.09	0.82
4:A:77:GLY:HA3	4:A:163:ILE:HD11	1.62	0.82
3:F:109:ILE:CG2	5:F:401:X53:C61	2.58	0.82
1:D:31:VAL:HG12	1:D:35:LEU:HB2	1.62	0.81
2:G:64:GLU:HG2	2:G:65:ILE:HG13	1.63	0.81
3:F:112:TYR:HB2	3:F:115:HIS:CE1	2.16	0.79
1:D:27:LEU:HA	1:D:30:ILE:HG12	1.65	0.78
2:C:87:SER:HA	3:B:132:GLN:HG3	1.65	0.77
1:D:42:GLN:HG2	1:D:79:PHE:HE1	1.49	0.77
3:F:167:ARG:HD3	3:F:191:HIS:CD2	2.20	0.75
1:D:68:ARG:HD2	1:D:69:PRO:CD	2.17	0.75
3:B:102:PRO:CD	3:B:105:THR:HG21	2.16	0.74
1:D:99:LEU:HD12	1:D:100:PRO:HD2	1.70	0.73
1:D:38:PRO:HG2	1:D:41:GLU:HB2	1.70	0.72
4:E:16:LYS:N	6:E:201:GDP:O1B	2.23	0.71
4:A:82:PHE:HE2	4:A:125:VAL:HG21	1.56	0.71
1:H:24:VAL:CG2	1:H:53:ASP:HA	2.20	0.70
4:A:58:THR:CG2	4:A:72:MET:HE1	2.21	0.70
2:C:101:LEU:HD21	3:B:178:LEU:HD22	1.73	0.70
1:D:8:ARG:HD2	1:D:13:THR:HG22	1.72	0.70
2:G:72:LYS:HD2	2:G:75:MET:HE2	1.73	0.70
4:E:14:VAL:CG2	4:E:81:VAL:HG12	2.20	0.70
1:D:43:ARG:HB3	1:D:45:TYR:HE1	1.56	0.69
2:G:80:LYS:O	2:G:84:THR:HG23	1.92	0.69
1:D:71:ALA:HA	2:C:75:MET:HE3	1.75	0.68
3:F:62:VAL:HG12	3:F:202:THR:HG23	1.75	0.68
1:D:43:ARG:HB2	1:D:78:ALA:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:119:ASP:OD1	4:A:145:SER:HB2	1.94	0.67
1:D:80:ARG:HA	1:D:85:PHE:HA	1.75	0.67
1:D:42:GLN:HG2	1:D:79:PHE:CE1	2.30	0.66
1:H:102:VAL:HG21	3:F:174:ASN:HB3	1.77	0.66
4:A:157:TYR:O	4:A:160:VAL:HG22	1.95	0.66
3:F:90:ASN:HD21	3:F:94:GLU:HB2	1.61	0.66
3:B:60:ARG:HD3	3:B:61:PRO:HD2	1.79	0.65
3:B:102:PRO:O	3:B:105:THR:CG2	2.38	0.65
1:H:23:THR:HG23	1:H:25:PHE:H	1.61	0.65
1:H:63:THR:HG22	1:H:66:THR:HG23	1.77	0.65
4:A:58:THR:HG21	4:A:72:MET:HE1	1.78	0.65
1:H:63:THR:HG23	1:H:65:GLN:H	1.60	0.65
3:F:65:SER:HB3	3:F:115:HIS:CD2	2.31	0.65
3:F:61:PRO:HG2	3:F:92:ASP:O	1.96	0.64
4:A:33:ASP:OD1	4:A:34:PRO:HD2	1.98	0.64
4:A:33:ASP:OD1	4:A:34:PRO:CD	2.45	0.64
3:F:64:ARG:HD2	3:F:91:PHE:O	1.97	0.64
3:B:112:TYR:HB2	3:B:115:HIS:CE1	2.33	0.64
1:D:38:PRO:HG2	1:D:41:GLU:CB	2.28	0.63
2:G:65:ILE:HG23	2:G:69:VAL:HG13	1.79	0.63
2:G:106:ALA:O	2:G:110:LEU:HD12	1.98	0.63
4:A:160:VAL:HA	4:A:163:ILE:HG13	1.80	0.62
4:E:14:VAL:HG21	4:E:81:VAL:CG1	2.24	0.62
4:E:22:GLN:C	4:E:24:ILE:H	2.07	0.61
3:B:66:VAL:HG22	3:B:114:GLY:HA3	1.82	0.61
3:F:62:VAL:CG1	3:F:202:THR:HG23	2.30	0.61
2:G:39:SER:HB3	2:G:42:ILE:HB	1.83	0.60
1:D:43:ARG:HB3	1:D:45:TYR:CE1	2.37	0.60
2:C:39:SER:HB3	2:C:42:ILE:HB	1.83	0.60
4:A:22:GLN:O	4:A:26:ASN:HA	2.00	0.60
4:A:113:LEU:H	4:A:139:ILE:HD12	1.66	0.60
4:E:164:ARG:O	4:E:165:LYS:C	2.43	0.60
1:D:3:VAL:HG23	1:D:20:GLU:HG2	1.83	0.60
1:D:8:ARG:HD2	1:D:13:THR:CG2	2.32	0.59
4:A:82:PHE:CE2	4:A:125:VAL:HG21	2.37	0.59
3:B:145:GLN:HG2	3:F:133:THR:HG21	1.84	0.59
4:A:45:VAL:HA	4:A:50:THR:HA	1.85	0.59
3:F:172:PRO:HA	3:F:175:TYR:CE2	2.38	0.59
3:B:198:LEU:O	3:B:202:THR:HG23	2.03	0.58
3:F:102:PRO:O	3:F:105:THR:HG23	2.04	0.58
2:G:66:PRO:HG2	2:G:69:VAL:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:29:PHE:CD1	2:C:70:LEU:HD23	2.38	0.58
1:H:8:ARG:HB2	1:H:90:ILE:HD13	1.86	0.58
3:F:167:ARG:HD3	3:F:191:HIS:HD2	1.67	0.58
3:F:65:SER:HB3	3:F:115:HIS:HD2	1.68	0.58
3:B:108:ARG:HD3	3:F:132:GLN:OE1	2.04	0.57
4:E:119:ASP:CG	6:E:201:GDP:HN1	2.11	0.57
3:B:60:ARG:HD3	3:B:61:PRO:CD	2.33	0.57
1:H:23:THR:CG2	1:H:26:GLU:HG3	2.28	0.57
3:F:90:ASN:ND2	3:F:94:GLU:O	2.37	0.57
3:F:76:PHE:CD2	3:F:109:ILE:HG13	2.40	0.57
1:H:46:LYS:HG3	1:H:62:PHE:CZ	2.40	0.57
3:B:76:PHE:CD2	3:B:109:ILE:HG13	2.40	0.57
1:H:23:THR:CG2	1:H:26:GLU:H	2.12	0.57
4:E:56:LEU:HD11	4:E:71:TYR:CZ	2.40	0.57
2:C:77:PHE:O	2:C:81:VAL:HG23	2.06	0.56
3:B:203:GLN:O	3:B:206:ILE:HG23	2.06	0.56
1:H:63:THR:HG23	1:H:65:GLN:HG3	1.87	0.56
4:E:84:ILE:HG13	4:E:116:ASN:O	2.04	0.56
4:E:157:TYR:HA	4:E:160:VAL:HG22	1.88	0.56
2:C:68:HIS:CE1	2:C:69:VAL:HG23	2.41	0.56
4:E:32:TYR:HE1	4:E:36:ILE:CB	2.19	0.56
1:D:103:MET:HG2	3:B:170:VAL:HG12	1.88	0.55
1:H:23:THR:HG23	1:H:25:PHE:N	2.21	0.55
4:E:22:GLN:C	4:E:24:ILE:N	2.63	0.55
4:A:142:ILE:HD12	4:A:155:ALA:HA	1.89	0.55
4:A:77:GLY:HA3	4:A:159:LEU:HD21	1.88	0.55
2:C:38:THR:HG23	2:C:80:LYS:HD3	1.87	0.55
1:H:42:GLN:HG2	1:H:79:PHE:CE1	2.42	0.55
1:D:103:MET:HG2	3:B:170:VAL:CG1	2.36	0.55
2:C:42:ILE:O	2:C:42:ILE:HG22	2.06	0.55
2:C:46:LEU:HD11	2:C:60:VAL:CG2	2.37	0.55
3:F:204:GLU:O	3:F:204:GLU:HG2	2.07	0.55
1:D:3:VAL:CG2	1:D:20:GLU:HG2	2.36	0.55
4:E:32:TYR:O	4:E:33:ASP:C	2.49	0.55
1:D:99:LEU:HD12	1:D:100:PRO:CD	2.36	0.55
1:H:13:THR:HB	2:G:29:PHE:HD1	1.72	0.55
2:G:29:PHE:HD2	2:G:70:LEU:HD23	1.72	0.55
2:G:92:GLU:OE2	3:F:82:ARG:NH2	2.28	0.55
2:G:95:ILE:HB	3:F:165:VAL:HG21	1.89	0.55
4:A:79:LEU:HD13	4:A:159:LEU:HD12	1.89	0.55
1:H:4:PHE:CE2	1:H:69:PRO:HG3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:119:ASP:OD1	4:E:119:ASP:N	2.40	0.54
2:G:33:ARG:NH2	2:G:46:LEU:HB3	2.23	0.54
4:E:96:TYR:C	4:E:100:ILE:HD12	2.30	0.54
2:G:98:GLU:H	2:G:98:GLU:CD	2.16	0.54
2:C:104:LEU:HG	3:B:184:LEU:HD13	1.89	0.54
4:A:84:ILE:HA	4:A:125:VAL:HG22	1.90	0.54
1:D:19:LYS:O	1:D:57:LEU:HD12	2.07	0.54
4:A:84:ILE:HA	4:A:125:VAL:CG2	2.38	0.53
1:D:100:PRO:HD2	1:D:103:MET:HE3	1.90	0.53
3:B:204:GLU:C	3:B:206:ILE:H	2.16	0.53
2:G:22:ILE:HB	2:G:61:ASN:HA	1.90	0.53
4:E:15:GLY:O	4:E:16:LYS:C	2.51	0.53
2:C:99:ILE:HG12	2:C:99:ILE:O	2.08	0.53
3:B:90:ASN:HD21	3:B:94:GLU:HB2	1.73	0.53
3:B:167:ARG:HD3	3:B:191:HIS:CD2	2.44	0.53
3:B:68:SER:O	3:B:70:GLU:HG3	2.09	0.53
3:B:167:ARG:HD3	3:B:191:HIS:HD2	1.74	0.53
4:A:134:ALA:HB1	4:A:139:ILE:HG13	1.91	0.53
1:D:25:PHE:CB	1:D:53:ASP:HB3	2.39	0.53
3:B:66:VAL:CG2	3:B:114:GLY:HA3	2.38	0.53
4:A:14:VAL:HG11	4:A:81:VAL:HG23	1.91	0.53
6:A:201:GDP:C8	6:A:201:GDP:C5'	2.85	0.53
1:D:24:VAL:HG23	1:D:55:LYS:O	2.09	0.53
1:D:65:GLN:OE1	1:D:65:GLN:N	2.39	0.53
2:G:95:ILE:HD12	2:G:103:LEU:HD23	1.91	0.53
3:F:64:ARG:HB3	3:F:64:ARG:NH1	2.23	0.52
3:B:185:TYR:O	3:B:189:GLU:HG2	2.08	0.52
2:C:106:ALA:O	2:C:110:LEU:HD12	2.10	0.52
3:F:196:LYS:O	3:F:199:GLU:HG2	2.10	0.52
4:A:82:PHE:CE2	4:A:90:PHE:CD1	2.97	0.52
1:D:64:SER:O	1:D:68:ARG:HG2	2.09	0.52
3:B:140:LEU:HD23	3:B:141:ASN:H	1.75	0.52
1:H:24:VAL:HG23	1:H:53:ASP:HA	1.90	0.51
2:G:83:TYR:O	2:G:86:SER:HB3	2.10	0.51
1:H:63:THR:HG22	1:H:66:THR:CG2	2.40	0.51
4:A:97:ARG:HD3	4:A:137:TYR:CD2	2.44	0.51
4:E:81:VAL:HG22	4:E:114:VAL:HB	1.93	0.51
1:D:44:LEU:HD23	1:D:77:LEU:HD13	1.92	0.51
4:A:82:PHE:CE2	4:A:90:PHE:HD1	2.28	0.51
4:E:15:GLY:HA2	6:E:201:GDP:O1A	2.11	0.51
4:E:116:ASN:CG	4:E:117:LYS:N	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:ARG:NH1	1:D:93:PHE:CZ	2.79	0.51
2:G:108:ASN:ND2	3:F:184:LEU:HD21	2.25	0.51
4:E:73:ARG:O	4:E:74:THR:C	2.54	0.51
2:G:40:GLY:O	2:G:43:LYS:HG2	2.11	0.50
4:E:14:VAL:HG23	4:E:82:PHE:C	2.36	0.50
3:B:182:ARG:HA	3:B:185:TYR:CD2	2.47	0.49
4:A:21:ILE:HD12	4:A:29:VAL:HG11	1.93	0.49
1:H:42:GLN:HG2	1:H:79:PHE:HE1	1.77	0.49
3:F:163:LEU:O	3:F:167:ARG:HG3	2.12	0.49
1:D:22:SER:O	1:D:57:LEU:HG	2.13	0.49
2:G:29:PHE:CD2	2:G:70:LEU:HD23	2.46	0.49
2:G:92:GLU:CD	3:F:82:ARG:HH21	2.19	0.49
2:C:61:ASN:OD1	2:C:61:ASN:N	2.42	0.49
2:G:71:SER:O	2:G:75:MET:HG3	2.13	0.49
2:C:66:PRO:HB2	2:C:68:HIS:ND1	2.28	0.48
1:H:52:ASP:HB2	1:H:55:LYS:HE2	1.94	0.48
1:D:37:ARG:HG3	1:D:79:PHE:CZ	2.47	0.48
3:B:90:ASN:OD1	3:B:94:GLU:N	2.37	0.48
1:H:51:LEU:HD22	1:H:60:CYS:SG	2.53	0.48
4:A:77:GLY:CA	4:A:163:ILE:HD11	2.40	0.48
3:B:73:GLN:NE2	8:B:501:HOH:O	2.41	0.48
4:A:53:LEU:N	4:A:53:LEU:HD12	2.29	0.48
3:B:129:LEU:HG	3:B:154:PRO:HB3	1.95	0.48
1:H:63:THR:CG2	1:H:65:GLN:HG3	2.43	0.48
2:G:65:ILE:CG2	2:G:69:VAL:HG13	2.43	0.48
2:C:95:ILE:HB	3:B:165:VAL:HG21	1.95	0.48
3:B:109:ILE:CG2	5:B:401:X53:C61	2.88	0.48
3:B:145:GLN:HE22	3:F:137:VAL:HG23	1.79	0.48
1:H:28:LYS:HD2	1:H:42:GLN:HB2	1.95	0.48
2:C:60:VAL:HG12	2:C:62:PHE:CE1	2.49	0.48
3:F:130:VAL:HA	3:F:150:ASN:O	2.14	0.48
1:D:37:ARG:NH1	1:D:41:GLU:OE1	2.47	0.48
3:F:108:ARG:HE	3:F:108:ARG:HB3	1.55	0.48
3:F:185:TYR:O	3:F:189:GLU:HG2	2.14	0.48
4:A:140:PRO:CD	4:A:162:GLU:OE2	2.62	0.47
2:C:87:SER:HA	3:B:132:GLN:CG	2.39	0.47
3:B:126:ASP:OD2	3:B:164:GLN:HG2	2.14	0.47
4:A:88:LYS:O	4:A:89:SER:C	2.57	0.47
2:C:70:LEU:HA	2:C:73:VAL:HB	1.96	0.47
1:D:79:PHE:O	1:D:86:GLU:HG2	2.15	0.47
2:G:104:LEU:HG	3:F:184:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:6:LEU:HD22	4:A:159:LEU:HD22	1.96	0.47
4:E:116:ASN:CG	4:E:117:LYS:H	2.23	0.47
1:H:63:THR:CG2	1:H:66:THR:HG23	2.45	0.47
3:F:64:ARG:HB3	3:F:64:ARG:HH11	1.79	0.47
3:F:141:ASN:OD1	3:F:147:ILE:HG12	2.15	0.47
4:E:70:GLN:NE2	4:E:70:GLN:HA	2.27	0.47
1:D:44:LEU:CD2	1:D:77:LEU:HD13	2.45	0.47
1:H:32:GLU:O	1:H:36:LYS:HA	2.15	0.47
4:E:58:THR:HG22	4:E:72:MET:HE1	1.97	0.47
3:F:64:ARG:HG2	3:F:65:SER:O	2.15	0.46
1:D:27:LEU:HA	1:D:30:ILE:CG1	2.43	0.46
2:G:80:LYS:HA	3:F:155:VAL:HG11	1.96	0.46
3:B:134:GLU:O	3:B:135:LEU:HD23	2.16	0.46
3:F:73:GLN:HB3	3:F:108:ARG:HH21	1.80	0.46
3:F:102:PRO:HD2	3:F:105:THR:HG21	1.98	0.46
4:E:17:SER:OG	4:E:57:ASP:OD2	2.33	0.46
4:A:20:THR:HG23	4:A:55:ILE:HG21	1.97	0.46
3:F:112:TYR:HE2	5:F:401:X53:O49	1.98	0.46
2:C:38:THR:CG2	2:C:80:LYS:HD3	2.46	0.46
1:H:80:ARG:HB2	1:H:85:PHE:CE1	2.51	0.46
1:D:101:ASP:HA	1:D:203:LYS:NZ	2.31	0.46
2:G:82:ARG:HD2	2:G:82:ARG:O	2.16	0.46
4:E:58:THR:CG2	4:E:72:MET:HE1	2.46	0.46
1:H:22:SER:O	1:H:56:THR:HA	2.16	0.45
2:G:35:HIS:CE1	2:G:81:VAL:HG11	2.51	0.45
1:D:97:PRO:HD2	2:C:102:GLU:OE2	2.15	0.45
2:G:24:SER:HB3	2:G:66:PRO:HA	1.98	0.45
3:F:130:VAL:HG13	3:F:130:VAL:O	2.16	0.45
1:D:35:LEU:HD23	1:D:35:LEU:HA	1.54	0.45
4:A:14:VAL:HG21	4:A:82:PHE:HA	1.98	0.45
4:A:90:PHE:O	4:A:93:ILE:HB	2.16	0.45
1:D:7:ILE:O	1:D:7:ILE:HG22	2.16	0.45
2:C:35:HIS:HD2	2:C:78:THR:HG22	1.82	0.45
4:E:22:GLN:O	4:E:24:ILE:N	2.50	0.45
4:E:133:LEU:HD11	4:E:137:TYR:CZ	2.52	0.45
1:D:25:PHE:O	1:D:26:GLU:C	2.59	0.45
3:B:73:GLN:NE2	3:B:110:HIS:HB2	2.32	0.45
1:H:94:SER:OG	2:G:25:ASP:OD2	2.34	0.45
3:F:129:LEU:HG	3:F:154:PRO:HB3	1.98	0.45
4:E:86:ASN:HB3	4:E:89:SER:HB3	1.97	0.45
1:H:103:MET:HE3	3:F:169:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:117:LYS:HG2	6:A:201:GDP:C6	2.51	0.45
1:D:44:LEU:O	1:D:50:LEU:HD23	2.17	0.44
2:C:106:ALA:O	2:C:110:LEU:HB2	2.18	0.44
4:E:17:SER:OG	6:E:201:GDP:O2B	2.30	0.44
1:H:45:TYR:CD1	1:H:88:LEU:HD22	2.53	0.44
1:D:42:GLN:O	1:D:43:ARG:NE	2.50	0.44
3:B:69:ARG:HG2	5:B:401:X53:C31	2.47	0.44
2:G:72:LYS:CD	2:G:75:MET:HE2	2.45	0.44
3:B:101:LEU:HB3	3:B:105:THR:HG23	1.98	0.44
3:B:161:ARG:O	3:B:164:GLN:HB2	2.18	0.44
3:B:163:LEU:O	3:B:167:ARG:HG3	2.18	0.44
1:H:99:LEU:HD12	2:G:98:GLU:HA	2.00	0.44
5:F:401:X53:C3	4:E:96:TYR:HE1	2.31	0.44
1:D:94:SER:O	2:C:68:HIS:HB3	2.18	0.44
4:A:113:LEU:HB2	4:A:139:ILE:CD1	2.48	0.44
4:E:44:VAL:C	4:E:50:THR:HA	2.43	0.44
1:D:50:LEU:CD2	1:D:51:LEU:H	2.31	0.43
1:H:63:THR:HG22	1:H:66:THR:OG1	2.18	0.43
4:E:108:ASP:OD1	4:E:108:ASP:N	2.50	0.43
1:D:68:ARG:HD2	1:D:69:PRO:HD2	1.98	0.43
4:E:90:PHE:HB2	4:E:125:VAL:HG11	2.01	0.43
2:G:18:TYR:CE2	2:G:32:LYS:HG2	2.54	0.43
3:F:112:TYR:HB2	3:F:115:HIS:ND1	2.33	0.43
4:A:58:THR:HG22	4:A:72:MET:HE1	1.97	0.43
2:C:45:MET:HE1	2:C:60:VAL:HG13	2.00	0.43
3:B:204:GLU:C	3:B:206:ILE:N	2.77	0.43
4:A:90:PHE:HB2	4:A:125:VAL:HG11	2.01	0.43
1:H:13:THR:HB	2:G:29:PHE:CD1	2.51	0.43
2:C:68:HIS:NE2	2:C:102:GLU:OE2	2.51	0.42
3:F:168:SER:C	3:F:169:LEU:HD23	2.45	0.42
3:B:82:ARG:NH1	3:B:82:ARG:HG3	2.34	0.42
3:B:133:THR:HG21	3:F:145:GLN:HG2	2.01	0.42
2:G:103:LEU:HD11	3:F:158:LEU:HD21	2.02	0.42
2:G:104:LEU:HD12	2:G:104:LEU:O	2.19	0.42
1:D:19:LYS:O	1:D:22:SER:N	2.51	0.42
3:F:113:ARG:HE	3:F:113:ARG:HB2	1.51	0.42
3:B:60:ARG:HA	3:B:61:PRO:HD3	1.94	0.42
4:E:116:ASN:O	4:E:117:LYS:HB2	2.20	0.42
5:B:401:X53:C42	5:B:401:X53:C47	2.97	0.42
4:E:14:VAL:HG11	4:E:81:VAL:HG12	2.01	0.42
1:H:76:GLY:HA2	1:H:90:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:35:HIS:CD2	2:C:78:THR:HG22	2.55	0.41
2:C:41:THR:O	2:C:41:THR:HG22	2.16	0.41
3:F:172:PRO:HA	3:F:175:TYR:CD2	2.55	0.41
3:F:200:ARG:HE	3:F:200:ARG:HB3	1.59	0.41
2:C:45:MET:HE1	2:C:60:VAL:CG1	2.51	0.41
3:B:108:ARG:HE	3:B:108:ARG:HB3	1.73	0.41
4:E:38:ASP:OD1	4:E:39:SER:N	2.47	0.41
1:D:31:VAL:CG1	1:D:35:LEU:HB2	2.42	0.41
1:D:47:ASP:HB3	1:D:48:ASP:H	1.72	0.41
3:B:99:PRO:HB2	5:B:401:X53:C68	2.51	0.41
4:E:17:SER:CB	6:E:201:GDP:O2B	2.69	0.41
2:C:92:GLU:OE2	3:B:82:ARG:NE	2.35	0.41
1:D:14:ILE:HG12	1:D:34:ILE:CD1	2.51	0.41
1:D:25:PHE:O	1:D:28:LYS:N	2.53	0.41
2:G:17:MET:HE2	2:G:17:MET:HB2	1.79	0.41
3:F:118:LEU:CD1	3:F:120:ARG:HD3	2.51	0.41
3:F:118:LEU:HD13	3:F:120:ARG:HD3	2.01	0.41
4:A:33:ASP:HA	4:A:34:PRO:HD3	1.87	0.41
1:D:4:PHE:CE1	1:D:69:PRO:HG3	2.55	0.41
2:G:33:ARG:HH22	2:G:46:LEU:HB3	1.86	0.41
2:C:42:ILE:O	2:C:42:ILE:CG2	2.68	0.41
3:F:74:VAL:HG22	3:F:147:ILE:HB	2.03	0.41
3:F:77:CYS:SG	3:F:79:ARG:HD3	2.61	0.41
3:F:184:LEU:HD23	3:F:184:LEU:HA	1.84	0.41
5:F:401:X53:C15	4:E:95:HIS:CD2	3.03	0.41
4:A:93:ILE:HD13	4:A:93:ILE:HA	1.91	0.41
1:H:95:SER:HA	1:H:96:PRO:HD2	1.91	0.41
4:A:44:VAL:O	4:A:51:CYS:N	2.53	0.41
1:H:93:PHE:CE1	2:G:29:PHE:CE1	3.09	0.40
2:G:62:PHE:HB3	2:G:64:GLU:OE2	2.20	0.40
1:D:72:PRO:HD2	2:C:75:MET:HE3	2.04	0.40
2:G:77:PHE:O	2:G:81:VAL:HG23	2.20	0.40
4:A:84:ILE:O	4:A:84:ILE:HD12	2.22	0.40
4:E:21:ILE:O	4:E:25:GLN:N	2.54	0.40
2:C:108:ASN:HB2	3:B:184:LEU:HD21	2.03	0.40
2:G:64:GLU:N	2:G:64:GLU:OE1	2.54	0.40
1:H:5:LEU:HD22	1:H:75:VAL:CG2	2.52	0.40
3:F:167:ARG:NE	3:F:188:LEU:O	2.40	0.40
3:B:102:PRO:N	3:B:105:THR:HG21	2.36	0.40
1:H:2:ASP:OD1	1:H:19:LYS:HE3	2.21	0.40
4:E:111:MET:HE2	4:E:111:MET:HB3	1.79	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	D	96/104 (92%)	85 (88%)	11 (12%)	0	100	100
1	H	99/104 (95%)	91 (92%)	8 (8%)	0	100	100
2	C	81/97 (84%)	76 (94%)	5 (6%)	0	100	100
2	G	82/97 (84%)	77 (94%)	5 (6%)	0	100	100
3	B	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
3	F	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
4	A	164/170 (96%)	152 (93%)	12 (7%)	0	100	100
4	E	130/170 (76%)	121 (93%)	9 (7%)	0	100	100
All	All	944/1066 (89%)	882 (93%)	62 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	D	77/92 (84%)	72 (94%)	5 (6%)	15	18
1	H	86/92 (94%)	78 (91%)	8 (9%)	8	8
2	C	69/86 (80%)	66 (96%)	3 (4%)	26	34
2	G	77/86 (90%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	132/148 (89%)	123 (93%)	9 (7%)	14	16
3	F	133/148 (90%)	129 (97%)	4 (3%)	36	48
4	A	111/150 (74%)	107 (96%)	4 (4%)	31	41
4	E	81/150 (54%)	79 (98%)	2 (2%)	42	55
All	All	766/952 (80%)	731 (95%)	35 (5%)	24	31

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

Mol	Chain	Res	Type
1	D	3	VAL
1	D	7	ILE
1	D	34	ILE
1	D	40	ASP
1	D	50	LEU
2	C	59	GLU
2	C	68	HIS
2	C	110	LEU
3	B	60	ARG
3	B	62	VAL
3	B	139	SER
3	B	140	LEU
3	B	170	VAL
3	B	179	ASP
3	B	183	SER
3	B	198	LEU
3	B	206	ILE
1	H	19	LYS
1	H	23	THR
1	H	40	ASP
1	H	48	ASP
1	H	53	ASP
1	H	56	THR
1	H	65	GLN
1	H	99	LEU
3	F	116	LEU
3	F	139	SER
3	F	170	VAL
3	F	183	SER
4	A	127	THR
4	A	129	GLN
4	A	160	VAL

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Mol	Chain	Res	Type
4	A	163	ILE
4	E	43	GLN
4	E	62	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	49	GLN
2	C	35	HIS
2	C	108	ASN
3	B	191	HIS
1	H	49	GLN
4	A	94	HIS
4	A	95	HIS
4	E	25	GLN
4	E	43	GLN
4	E	70	GLN
4	E	94	HIS
4	E	95	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	X53	B	401	-	75,78,78	3.17	25 (33%)	91,113,113	3.40	31 (34%)
5	X53	F	401	-	75,78,78	3.31	25 (33%)	91,113,113	3.44	33 (36%)
6	GDP	A	201	7	29,30,30	2.10	8 (27%)	45,47,47	2.23	12 (26%)
6	GDP	E	201	7	29,30,30	1.43	4 (13%)	45,47,47	1.86	15 (33%)

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
5	X53	B	401	-	-	9/48/92/92	0/9/9/9
5	X53	F	401	-	-	8/48/92/92	0/9/9/9
6	GDP	A	201	7	-	3/16/32/32	0/3/3/3
6	GDP	E	201	7	-	5/16/32/32	0/3/3/3

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	401	X53	C23-S24	-12.10	1.53	1.73
5	B	401	X53	C23-S24	-11.65	1.53	1.73
5	F	401	X53	C3-C7	-9.27	1.32	1.47
5	B	401	X53	C3-C7	-9.15	1.32	1.47
5	F	401	X53	C21-S24	-7.49	1.58	1.74
5	B	401	X53	C21-S24	-7.35	1.59	1.74
5	F	401	X53	C35-C17	-7.17	1.37	1.51
5	F	401	X53	C62-C65	-7.11	1.33	1.48
5	B	401	X53	C62-C65	-7.03	1.33	1.48
5	B	401	X53	C35-C17	-6.90	1.38	1.51
5	F	401	X53	C32-C21	-6.81	1.37	1.50
5	B	401	X53	C32-C21	-6.69	1.38	1.50
5	F	401	X53	C65-S69	-6.56	1.56	1.73
5	F	401	X53	C50-C54	-6.51	1.37	1.52
5	B	401	X53	C50-C54	-6.04	1.38	1.52
5	B	401	X53	C35-C20	-5.92	1.40	1.52
5	F	401	X53	C35-C20	-5.79	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	401	X53	C68-S69	-5.59	1.62	1.72
5	B	401	X53	O18-N19	-5.47	1.32	1.42
5	F	401	X53	C58-C59	-5.44	1.39	1.51
5	F	401	X53	C25-N27	-5.42	1.05	1.14
5	B	401	X53	C68-S69	-5.40	1.62	1.72
5	B	401	X53	C58-C59	-5.33	1.39	1.51
6	A	201	GDP	PA-O3A	-5.28	1.53	1.59
5	F	401	X53	C22-C23	-5.11	1.32	1.39
5	B	401	X53	C65-S69	-5.07	1.60	1.73
5	B	401	X53	C22-C23	-4.75	1.32	1.39
6	A	201	GDP	C6-N1	-4.42	1.30	1.38
5	F	401	X53	O40-N39	-4.25	1.34	1.42
5	F	401	X53	O18-N19	-4.22	1.34	1.42
5	B	401	X53	C25-N27	-3.88	1.08	1.14
5	B	401	X53	C42-C38	-3.84	1.31	1.41
5	F	401	X53	C42-C38	-3.60	1.31	1.41
5	F	401	X53	C17-N16	3.56	1.32	1.28
5	B	401	X53	C17-N16	3.38	1.32	1.28
6	A	201	GDP	C2-N1	-3.26	1.29	1.37
6	A	201	GDP	C5-N7	-3.24	1.32	1.39
6	A	201	GDP	PB-O2B	-3.23	1.42	1.54
6	E	201	GDP	C4-N9	-3.15	1.30	1.38
5	F	401	X53	C66-N67	-3.09	1.33	1.38
6	A	201	GDP	PB-O3B	-3.04	1.43	1.54
5	F	401	X53	C25-C22	-3.02	1.36	1.43
5	B	401	X53	C66-N67	-3.00	1.33	1.38
6	E	201	GDP	C6-N1	-2.99	1.33	1.38
5	B	401	X53	C34-C35	-2.85	1.50	1.55
5	B	401	X53	C22-C20	-2.81	1.34	1.41
6	A	201	GDP	C4-N9	-2.78	1.31	1.38
5	B	401	X53	O40-N39	-2.74	1.37	1.42
6	E	201	GDP	C5-N7	-2.71	1.33	1.39
6	E	201	GDP	C5-C4	2.69	1.46	1.38
5	F	401	X53	C22-C20	-2.69	1.34	1.41
5	F	401	X53	C34-C35	-2.64	1.50	1.55
6	A	201	GDP	C8-N9	-2.39	1.32	1.37
5	F	401	X53	C11-C10	-2.37	1.48	1.52
5	B	401	X53	C7-N16	-2.36	1.32	1.37
5	F	401	X53	C7-N16	-2.24	1.32	1.37
5	B	401	X53	C1-N6	2.17	1.39	1.34
5	B	401	X53	C34-C33	-2.14	1.47	1.52
5	F	401	X53	C34-C33	-2.10	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	401	X53	C11-C10	-2.10	1.48	1.52
5	F	401	X53	O18-C17	-2.05	1.31	1.33
5	B	401	X53	C43-C44	2.01	1.54	1.52

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	401	X53	C68-S69-C65	16.50	97.60	88.96
5	B	401	X53	C68-S69-C65	15.08	96.86	88.96
5	F	401	X53	C21-S24-C23	11.00	98.84	91.55
5	B	401	X53	C21-S24-C23	10.48	98.50	91.55
5	F	401	X53	S69-C68-N67	-10.24	107.28	116.08
5	B	401	X53	S69-C68-N67	-9.89	107.58	116.08
5	B	401	X53	C3-N4-C5	7.49	121.48	115.85
5	B	401	X53	O18-C17-N16	-7.39	110.50	115.25
5	F	401	X53	C3-N4-C5	7.19	121.25	115.85
5	F	401	X53	C20-C21-S24	-7.04	108.25	113.42
5	F	401	X53	O18-C17-N16	-6.99	110.76	115.25
5	B	401	X53	C20-C21-S24	-6.83	108.40	113.42
6	A	201	GDP	C5-C4-N3	-6.81	117.56	128.39
6	A	201	GDP	C2-N3-C4	6.07	122.76	112.30
5	B	401	X53	N6-C5-N4	-5.96	120.06	126.12
5	B	401	X53	C1-N6-C5	5.87	120.89	115.13
5	B	401	X53	O40-C41-C43	5.67	124.52	117.31
5	F	401	X53	C1-N6-C5	5.56	120.58	115.13
5	F	401	X53	N6-C5-N4	-5.52	120.50	126.12
5	B	401	X53	O18-N19-C7	5.43	106.46	103.28
5	F	401	X53	O40-C41-C43	5.25	123.99	117.31
5	F	401	X53	N16-C7-N19	-5.09	110.76	114.47
6	A	201	GDP	N9-C4-N3	5.08	136.12	125.95
5	B	401	X53	C17-O18-N19	4.94	107.39	105.34
5	B	401	X53	N16-C7-N19	-4.94	110.87	114.47
5	F	401	X53	C21-C20-C22	-4.76	109.61	111.77
5	F	401	X53	C17-O18-N19	4.73	107.31	105.34
5	F	401	X53	O18-N19-C7	4.71	106.04	103.28
6	E	201	GDP	C5-C4-N3	-4.58	121.10	128.39
5	B	401	X53	C43-C41-C42	-4.49	125.83	134.74
5	B	401	X53	C62-C65-S69	4.46	127.05	118.77
5	F	401	X53	C2-C1-N6	-4.36	118.63	123.97
5	B	401	X53	C2-C1-N6	-4.35	118.64	123.97
5	F	401	X53	C43-C41-C42	-4.24	126.34	134.74
5	B	401	X53	C32-C21-S24	4.15	129.01	121.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	X53	C62-C65-C66	-4.11	125.24	130.81
5	F	401	X53	C32-C21-S24	4.04	128.78	121.01
5	B	401	X53	C21-C20-C22	-4.03	109.94	111.77
6	A	201	GDP	C6-C5-N7	3.94	137.46	130.29
6	E	201	GDP	C6-C5-N7	3.73	137.08	130.29
5	F	401	X53	C42-C38-N39	-3.73	109.93	113.57
5	F	401	X53	C17-N16-C7	3.73	105.13	101.53
6	A	201	GDP	O2B-PB-O3A	-3.56	92.69	104.64
5	B	401	X53	N4-C5-N9	3.56	120.93	116.96
5	F	401	X53	N4-C5-N9	3.53	120.90	116.96
5	F	401	X53	C62-C65-S69	3.47	125.22	118.77
5	B	401	X53	C42-C38-N39	-3.46	110.19	113.57
5	F	401	X53	C53-N48-C50	-3.41	107.31	111.83
6	E	201	GDP	C2-N3-C4	3.41	118.17	112.30
5	B	401	X53	C17-N16-C7	3.36	104.78	101.53
6	E	201	GDP	N9-C4-N3	3.25	132.45	125.95
6	E	201	GDP	O3'-C3'-C2'	3.23	122.17	111.82
6	E	201	GDP	C4-C5-N7	-3.20	105.61	110.67
5	B	401	X53	C66-C65-S69	-3.17	107.70	109.64
5	B	401	X53	C51-C50-C54	-3.07	105.47	111.36
6	A	201	GDP	C5-C6-N1	3.01	120.90	113.25
5	F	401	X53	C62-C65-C66	-2.98	126.77	130.81
5	F	401	X53	C1-C2-C3	2.97	118.85	117.02
5	F	401	X53	C51-C50-C54	-2.88	105.84	111.36
6	E	201	GDP	C4'-O4'-C1'	-2.84	103.20	109.47
5	B	401	X53	C52-C53-N48	2.75	105.65	103.00
5	B	401	X53	C14-C8-N9	-2.74	107.85	113.84
5	F	401	X53	C14-C8-N9	-2.73	107.88	113.84
5	F	401	X53	C66-C65-S69	-2.68	108.00	109.64
6	A	201	GDP	O2B-PB-O1B	2.64	121.12	110.83
5	B	401	X53	C1-C2-C3	2.61	118.62	117.02
5	B	401	X53	C53-N48-C50	-2.52	108.50	111.83
5	F	401	X53	C34-C33-C32	-2.49	105.80	111.28
6	A	201	GDP	C4-C5-N7	-2.48	106.74	110.67
5	B	401	X53	C34-C33-C32	-2.43	105.94	111.28
6	A	201	GDP	O3'-C3'-C4'	-2.39	104.22	111.08
5	B	401	X53	C68-N67-C66	2.35	113.36	110.71
5	F	401	X53	C2-C3-N4	-2.35	120.18	122.92
6	E	201	GDP	C8-N7-C5	2.34	108.43	104.26
6	E	201	GDP	O3A-PB-O1B	-2.33	98.80	111.04
6	A	201	GDP	C2-N1-C6	-2.32	120.90	125.11
6	E	201	GDP	O2A-PA-O1A	2.31	123.18	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	201	GDP	O2'-C2'-C3'	2.28	119.12	111.82
6	E	201	GDP	C8-N9-C4	2.27	110.29	106.03
6	E	201	GDP	N9-C8-N7	-2.25	109.23	113.40
6	E	201	GDP	O3B-PB-O3A	-2.24	97.12	104.64
5	B	401	X53	C2-C3-N4	-2.23	120.31	122.92
6	A	201	GDP	O4'-C1'-N9	-2.22	103.32	108.36
5	F	401	X53	C13-C14-C8	-2.21	108.80	113.99
5	F	401	X53	C7-C3-N4	2.21	120.38	116.58
5	F	401	X53	C31-O37-C38	-2.18	112.78	117.09
5	F	401	X53	C51-C50-N48	2.18	105.76	103.17
6	E	201	GDP	O2B-PB-O3A	2.15	111.84	104.64
5	B	401	X53	C7-C3-N4	2.11	120.22	116.58
6	A	201	GDP	C6-C5-C4	-2.02	115.79	118.83
5	F	401	X53	O40-N39-C38	2.00	106.04	104.58

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	401	X53	C44-C43-C45-C47
5	F	401	X53	N16-C17-C35-C34
5	F	401	X53	O40-C41-C43-C44
5	F	401	X53	C45-C43-C44-N48
5	F	401	X53	C45-C43-C44-O49
6	E	201	GDP	C5'-O5'-PA-O3A
6	E	201	GDP	C5'-O5'-PA-O1A
6	E	201	GDP	C5'-O5'-PA-O2A
6	E	201	GDP	O4'-C4'-C5'-O5'
6	E	201	GDP	C3'-C4'-C5'-O5'
5	F	401	X53	N12-C28-C29-C30
5	B	401	X53	N12-C28-C29-C30
5	B	401	X53	C28-C29-C30-C31
5	F	401	X53	C28-C29-C30-C31
6	A	201	GDP	PA-O3A-PB-O1B
6	A	201	GDP	PA-O3A-PB-O2B
5	B	401	X53	C45-C43-C44-O49
5	B	401	X53	C45-C43-C44-N48
5	B	401	X53	O40-C41-C43-C44
5	F	401	X53	O40-C41-C43-C45
5	B	401	X53	C44-C43-C45-C46
6	A	201	GDP	PA-O3A-PB-O3B
5	B	401	X53	N16-C17-C35-C34

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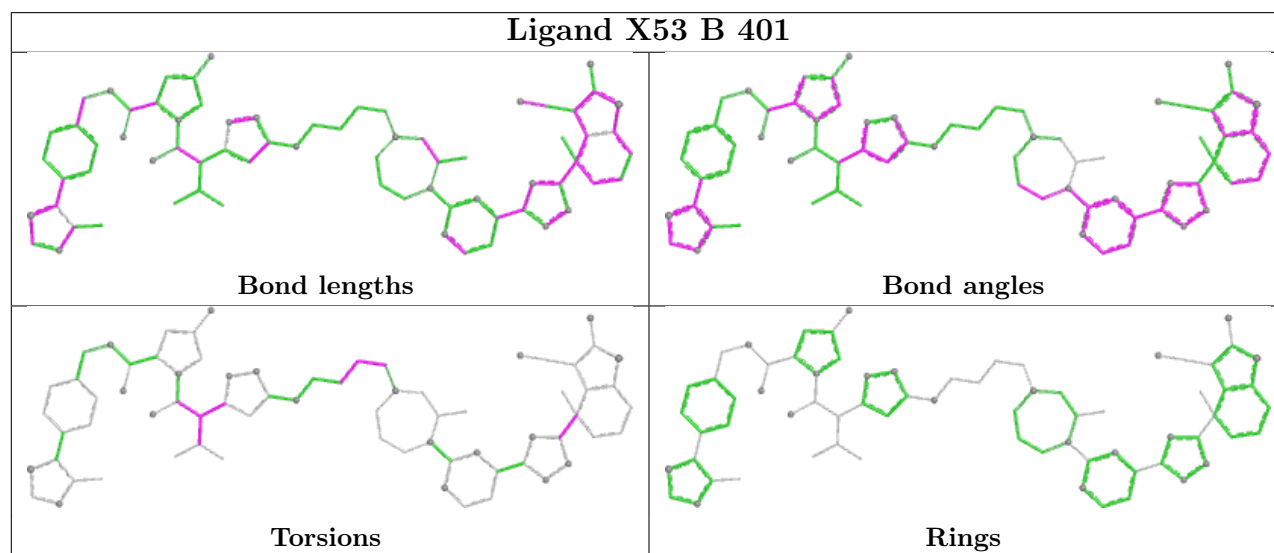
Mol	Chain	Res	Type	Atoms
5	B	401	X53	O18-C17-C35-C34
5	F	401	X53	N4-C3-C7-N19

There are no ring outliers.

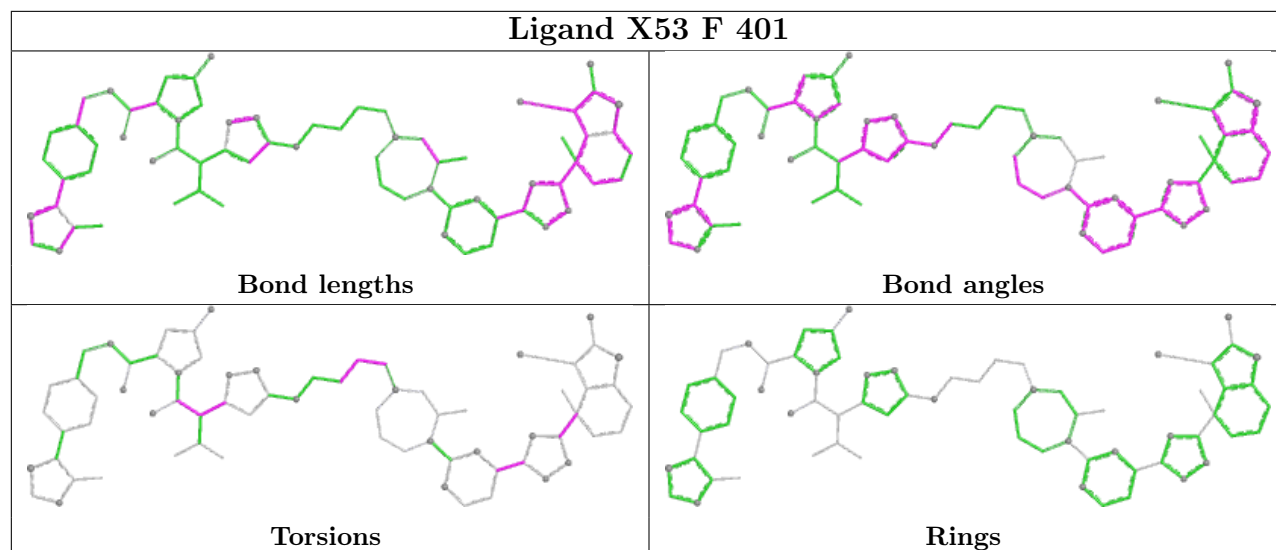
4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	401	X53	5	0
5	F	401	X53	5	0
6	A	201	GDP	4	0
6	E	201	GDP	5	0

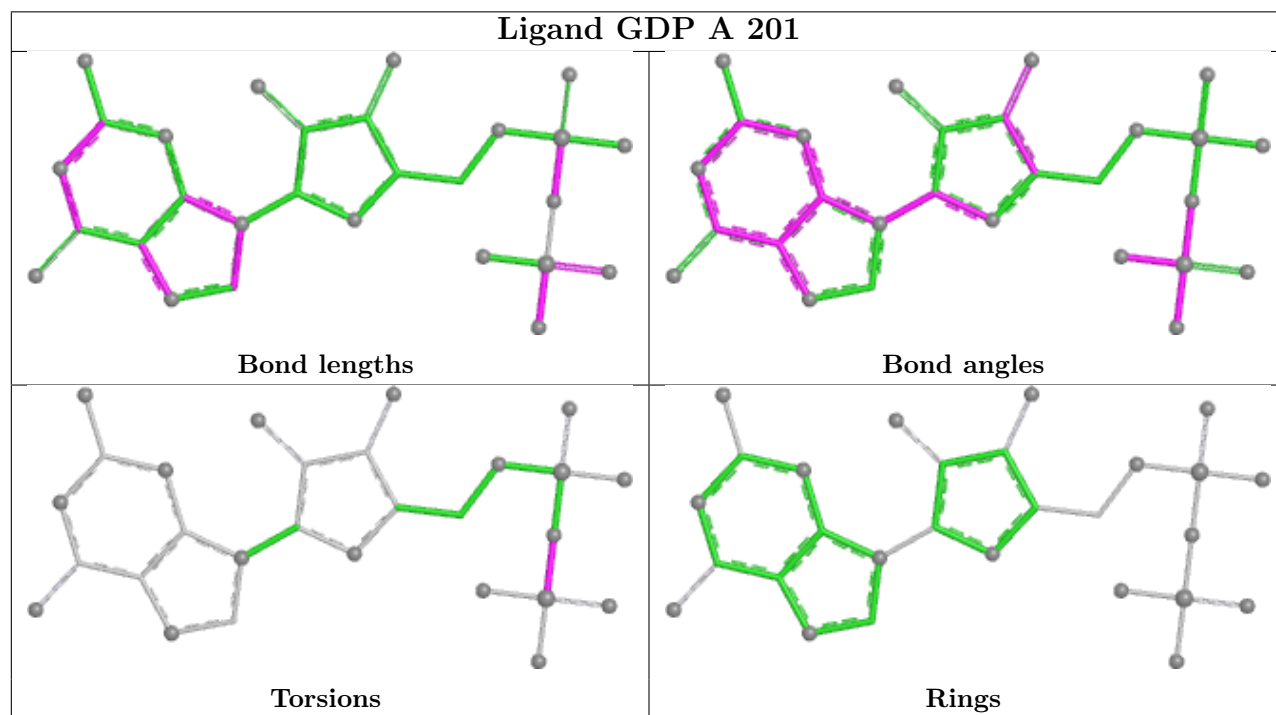
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

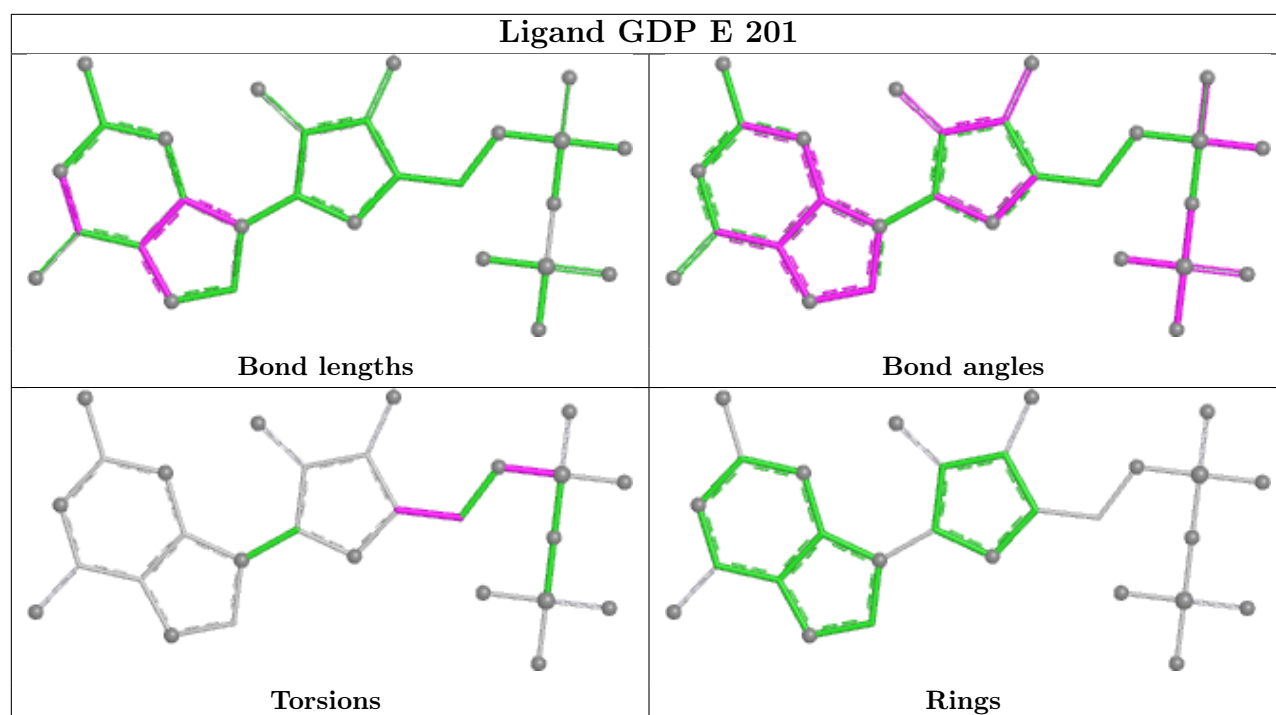


Ligand X53 F 401



Ligand GDP A 201





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	D	102/104 (98%)	1.84	38 (37%) 1 0	47, 82, 103, 113	0
1	H	103/104 (99%)	0.87	10 (9%) 13 15	34, 55, 69, 86	0
2	C	85/97 (87%)	1.20	15 (17%) 4 4	35, 57, 71, 74	0
2	G	86/97 (88%)	0.95	5 (5%) 29 33	29, 49, 62, 69	0
3	B	148/162 (91%)	0.58	11 (7%) 20 23	23, 39, 62, 89	0
3	F	148/162 (91%)	0.80	12 (8%) 18 20	25, 45, 67, 78	0
4	A	166/170 (97%)	1.67	56 (33%) 1 0	39, 78, 91, 105	0
4	E	144/170 (84%)	1.82	60 (41%) 0 0	44, 81, 97, 100	0
All	All	982/1066 (92%)	1.23	207 (21%) 2 2	23, 58, 94, 113	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	77	LEU	6.2
4	E	152	VAL	5.9
4	A	19	LEU	5.3
1	D	35	LEU	4.9
4	E	41	ARG	4.9
1	D	79	PHE	4.7
4	E	126	ASP	4.6
4	E	141	PHE	4.6
4	E	158	THR	4.4
4	E	142	ILE	4.4
4	A	53	LEU	4.4
1	D	50	LEU	4.3
4	A	44	VAL	4.1
4	A	126	ASP	4.0
4	A	32	TYR	4.0
4	E	34	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
4	A	152	VAL	3.9
1	D	51	LEU	3.9
3	B	207	ALA	3.9
4	A	141	PHE	3.9
4	E	156	PHE	3.9
4	A	51	CYS	3.7
1	D	31	VAL	3.7
1	D	60	CYS	3.6
4	A	4	TYR	3.6
1	H	79	PHE	3.6
4	A	46	ILE	3.6
4	A	45	VAL	3.5
4	A	159	LEU	3.5
4	E	53	LEU	3.5
4	A	112	VAL	3.5
4	A	23	LEU	3.5
4	A	52	LEU	3.5
4	E	153	ASP	3.5
4	E	113	LEU	3.5
4	A	146	ALA	3.4
3	F	206	ILE	3.4
4	A	156	PHE	3.4
4	E	160	VAL	3.4
1	H	82	ASP	3.4
3	F	207	ALA	3.3
4	A	115	GLY	3.3
4	E	7	VAL	3.3
1	D	43	ARG	3.3
4	A	28	PHE	3.3
4	A	143	GLU	3.3
3	B	140	LEU	3.2
4	E	42	LYS	3.2
4	E	20	THR	3.2
1	D	44	LEU	3.2
4	E	75	GLY	3.1
4	A	47	ASP	3.1
4	E	32	TYR	3.1
4	A	142	ILE	3.1
1	D	78	ALA	3.1
3	B	184	LEU	3.1
1	D	93	PHE	3.0
2	C	33	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	58	GLY	3.0
2	C	58	ASN	3.0
1	D	39	PRO	3.0
1	D	27	LEU	3.0
1	D	62	PHE	2.9
4	E	82	PHE	2.9
1	H	31	VAL	2.9
4	A	29	VAL	2.9
3	F	109	ILE	2.9
2	C	101	LEU	2.9
1	D	85	PHE	2.9
4	A	147	LYS	2.9
2	C	112	CYS	2.9
4	A	55	ILE	2.9
2	C	62	PHE	2.9
4	E	125	VAL	2.9
1	D	14	ILE	2.9
4	A	36	ILE	2.9
1	D	57	LEU	2.8
4	A	12	VAL	2.8
4	E	26	ASN	2.8
4	A	78	PHE	2.8
4	A	114	VAL	2.8
4	A	118	SER	2.8
2	G	69	VAL	2.8
4	A	144	THR	2.8
2	C	74	CYS	2.8
3	B	109	ILE	2.7
3	B	135	LEU	2.7
4	E	157	TYR	2.7
4	E	21	ILE	2.7
2	C	46	LEU	2.7
4	E	50	THR	2.7
1	D	88	LEU	2.7
1	H	52	ASP	2.7
2	C	18	TYR	2.6
4	E	137	TYR	2.6
4	E	30	ASP	2.6
4	E	33	ASP	2.6
4	E	114	VAL	2.6
3	F	123	GLY	2.6
3	B	116	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
4	E	120	LEU	2.6
4	E	78	PHE	2.6
4	A	84	ILE	2.6
3	B	181	VAL	2.6
3	F	170	VAL	2.6
3	F	185	TYR	2.6
4	A	148	THR	2.6
4	E	163	ILE	2.6
3	B	205	ARG	2.6
2	G	45	MET	2.6
4	E	17	SER	2.6
4	A	27	HIS	2.6
4	A	160	VAL	2.5
1	D	45	TYR	2.5
2	G	64	GLU	2.5
4	E	40	TYR	2.5
1	H	44	LEU	2.5
3	F	140	LEU	2.5
1	D	56	THR	2.5
1	D	83	ASP	2.5
4	A	43	GLN	2.5
4	E	148	THR	2.4
1	D	4	PHE	2.4
4	E	14	VAL	2.4
4	A	151	GLY	2.4
4	E	47	ASP	2.4
1	D	24	VAL	2.4
1	H	14	ILE	2.4
4	E	54	ASP	2.4
1	D	3	VAL	2.4
4	A	7	VAL	2.4
4	E	109	VAL	2.4
1	D	86	GLU	2.4
1	D	48	ASP	2.3
1	D	38	PRO	2.3
1	D	54	GLY	2.3
4	A	48	GLY	2.3
4	A	50	THR	2.3
4	A	87	THR	2.3
4	E	36	ILE	2.3
4	E	12	VAL	2.3
4	A	56	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
4	E	23	LEU	2.3
4	E	51	CYS	2.3
4	E	133	LEU	2.3
4	E	166	HIS	2.3
4	A	139	ILE	2.3
3	B	62	VAL	2.3
4	E	44	VAL	2.3
4	E	48	GLY	2.3
4	E	27	HIS	2.3
2	C	29	PHE	2.2
4	A	8	VAL	2.3
4	E	9	VAL	2.3
4	E	81	VAL	2.3
4	E	31	GLU	2.2
4	E	35	THR	2.2
4	E	49	GLU	2.2
1	D	30	ILE	2.2
3	B	206	ILE	2.2
2	C	21	LEU	2.2
4	A	120	LEU	2.2
1	D	55	LYS	2.2
1	H	87	ALA	2.2
1	D	7	ILE	2.2
2	C	30	ILE	2.2
1	D	9	ARG	2.2
4	E	85	ASN	2.2
4	A	34	PRO	2.2
4	A	25	GLN	2.2
4	A	133	LEU	2.2
4	E	55	ILE	2.2
4	E	112	VAL	2.2
4	E	131	GLN	2.2
4	A	157	TYR	2.1
1	D	90	ILE	2.1
1	D	47	ASP	2.1
2	G	31	VAL	2.1
3	F	194	VAL	2.1
4	A	14	VAL	2.1
4	E	162	GLU	2.1
3	F	122	ALA	2.1
4	E	130	ALA	2.1
1	D	80	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
4	A	71	TYR	2.1
1	D	46	LYS	2.1
4	A	24	ILE	2.1
2	C	26	GLY	2.1
1	H	7	ILE	2.1
4	A	153	ASP	2.1
1	D	18	ALA	2.1
2	C	17	MET	2.1
3	F	118	LEU	2.1
1	H	83	ASP	2.1
3	F	147	ILE	2.1
1	H	15	PHE	2.1
4	A	13	GLY	2.1
4	E	138	GLY	2.1
3	B	139	SER	2.0
4	A	124	THR	2.0
2	C	28	GLU	2.0
4	E	15	GLY	2.0
2	C	77	PHE	2.0
4	E	61	GLN	2.0
4	A	79	LEU	2.0
2	G	99	ILE	2.0
3	F	60	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

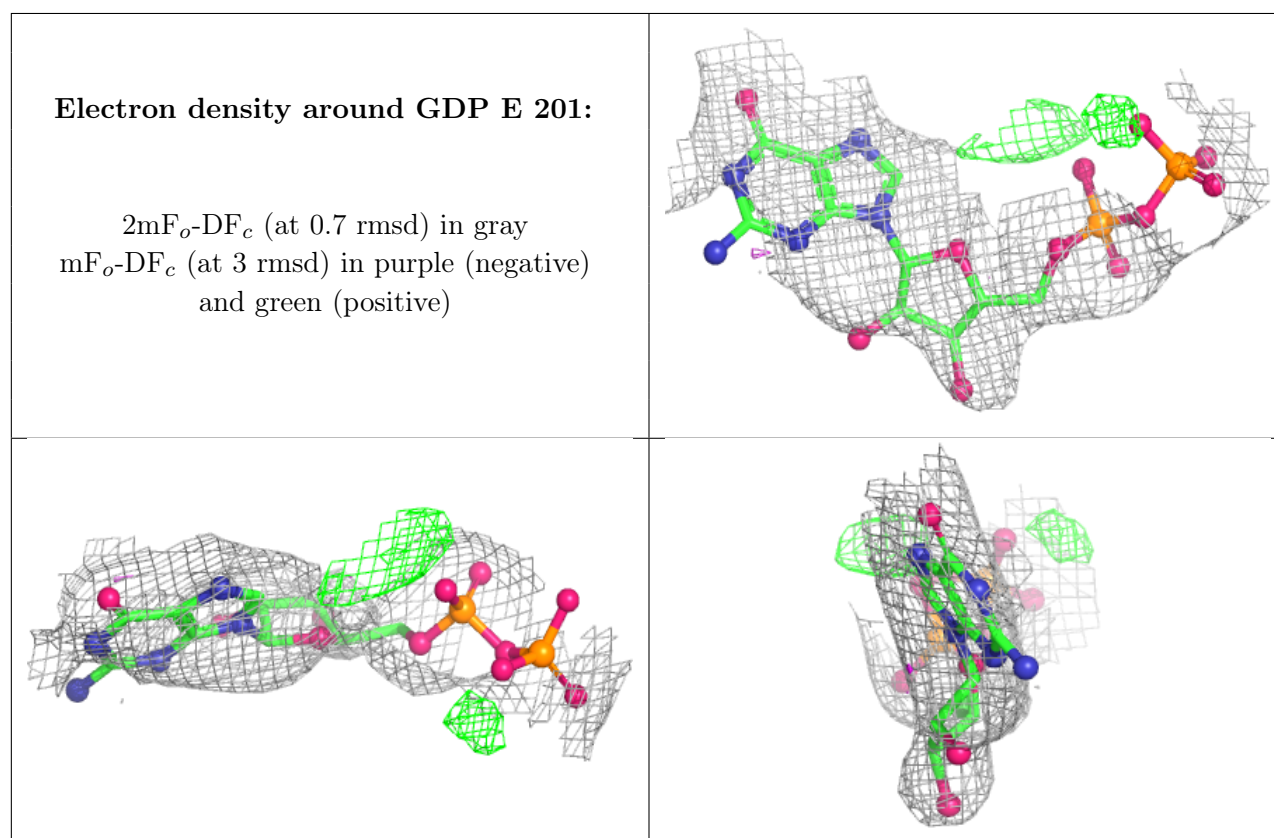
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

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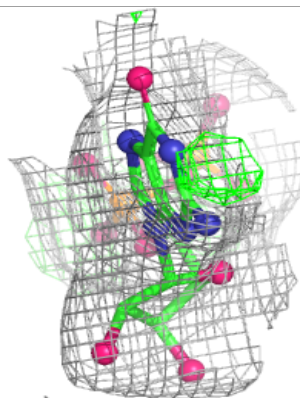
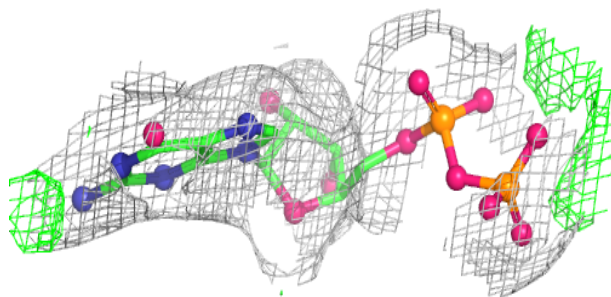
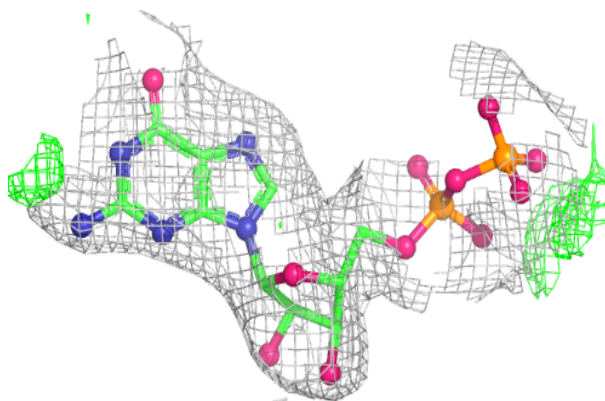
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GDP	E	201	28/28	0.69	0.14	91,105,112,114	0
6	GDP	A	201	28/28	0.84	0.12	71,84,88,93	0
7	MG	E	202	1/1	0.90	0.10	88,88,88,88	0
7	MG	A	202	1/1	0.91	0.26	55,55,55,55	0
5	X53	B	401	70/70	0.92	0.10	28,47,69,75	0
5	X53	F	401	70/70	0.92	0.10	33,54,83,91	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.

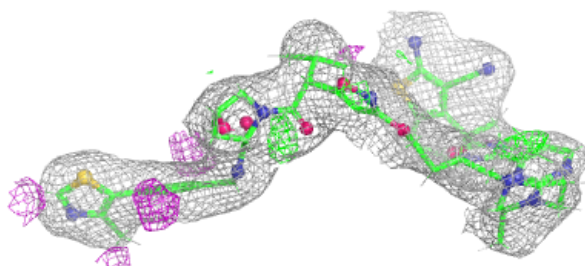
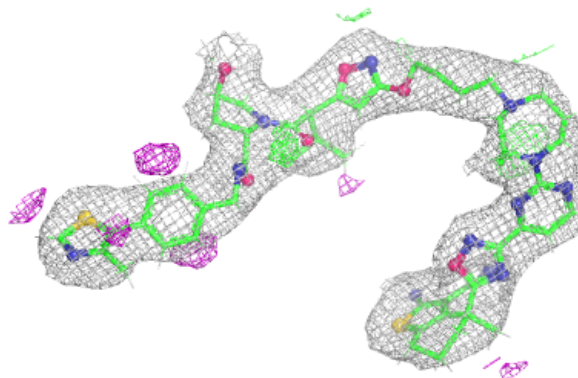


Electron density around GDP A 201:

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

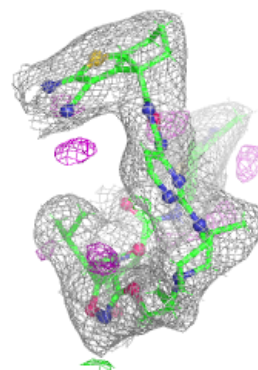
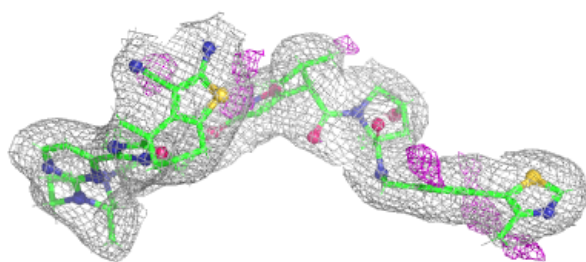
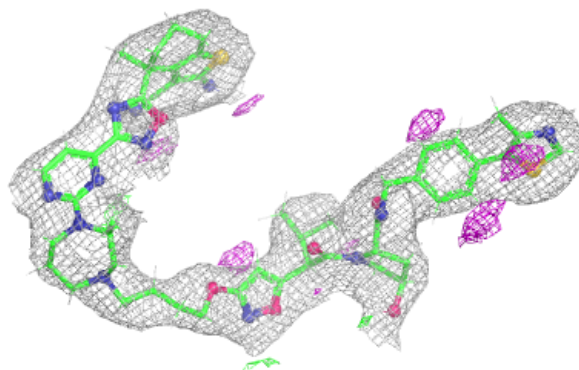
**Electron density around X53 B 401:**

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



Electron density around X53 F 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 [i](#)

There are no such residues in this entry.