



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2023 – 11:04 pm GMT

PDB ID : 8QW7
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

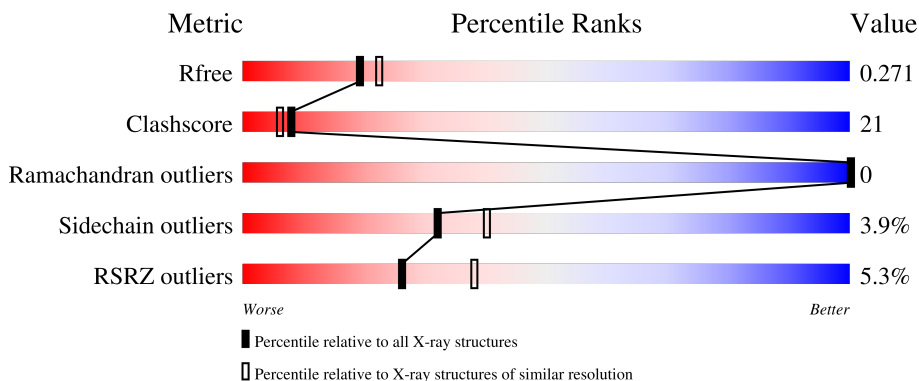
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



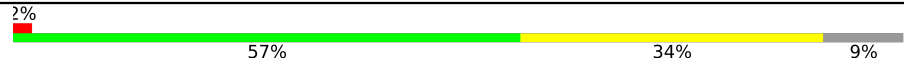

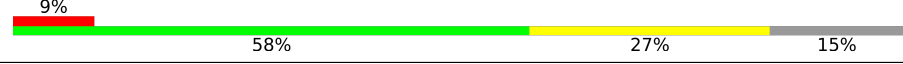
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	
1	H	104	
2	C	97	
2	G	97	
3	B	162	

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Mol	Chain	Length	Quality of chain
3	F	162	 <p>2% 57% 34% 9%</p>
4	A	170	 <p>8% 72% 25% ..</p>
4	E	170	 <p>9% 58% 27% 15%</p>

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	D	102	751	471	128	148	4	0	0	0
1	H	103	798	507	136	151	4	0	0	0

- Molecule 2 is a protein called Elongin-C.

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

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
			Total	C	N	O	S			
3	B	148	1187	755	218	212	2	0	0	0
3	F	148	1192	756	219	215	2	0	0	0

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

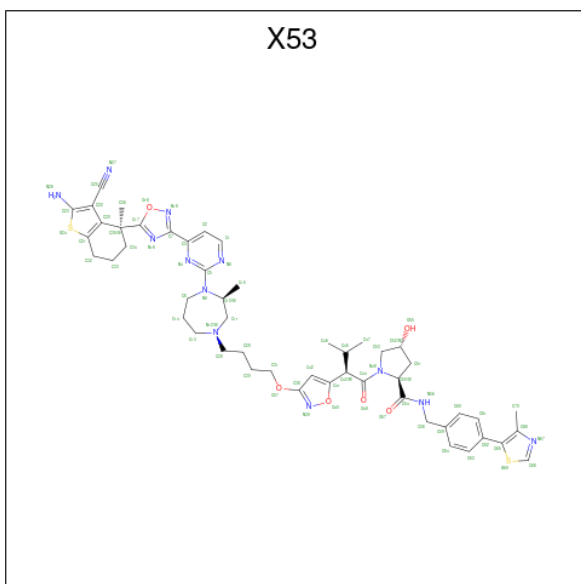
- Molecule 4 is a protein called GTPase KRas.

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

There are 6 discrepancies between the modelled and reference sequences:

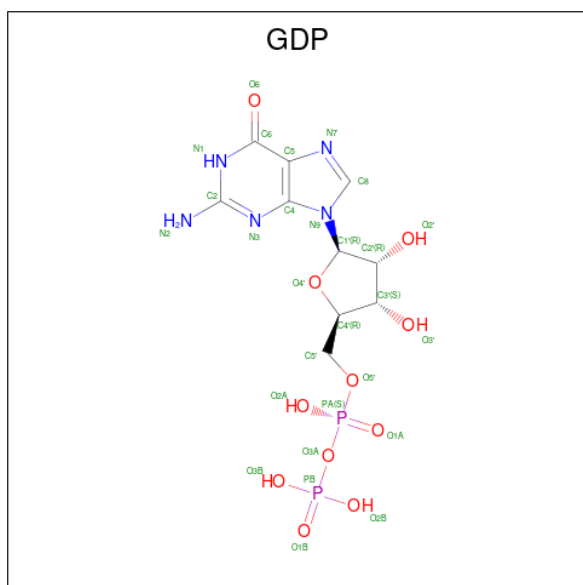
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P01116
A	12	VAL	GLY	engineered mutation	UNP P01116
A	118	SER	CYS	engineered mutation	UNP P01116
E	0	GLY	-	expression tag	UNP P01116
E	12	VAL	GLY	engineered mutation	UNP P01116
E	118	SER	CYS	engineered mutation	UNP P01116

- 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 (three-letter code: 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	0	0
			130	50	60	12	6	2		
5	F	1	Total	C	H	N	O	S	0	0
			130	50	60	12	6	2		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: 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	0	0
			28	10	5	11	2		
6	E	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 8 is water.

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

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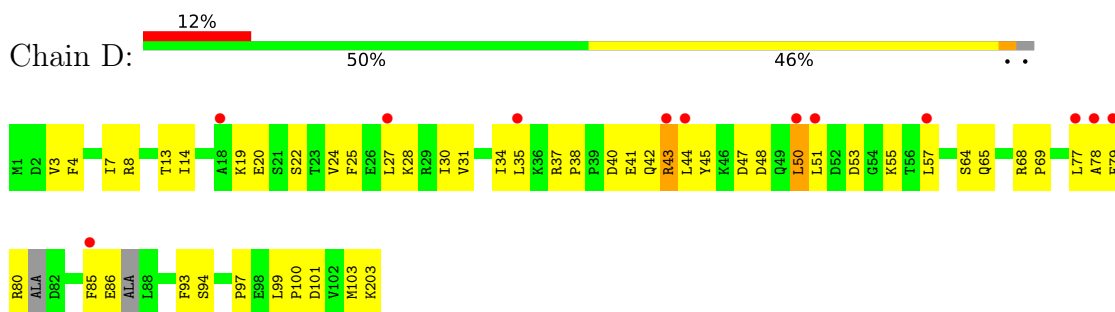
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	8	Total O 8 8	0	0
8	H	2	Total O 2 2	0	0
8	G	2	Total O 2 2	0	0
8	F	5	Total O 5 5	0	0
8	A	2	Total O 2 2	0	0
8	E	2	Total O 2 2	0	0

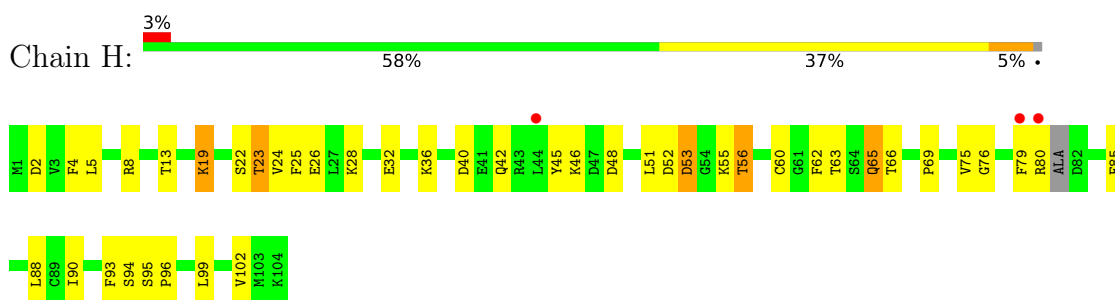
3 Residue-property plots i

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.

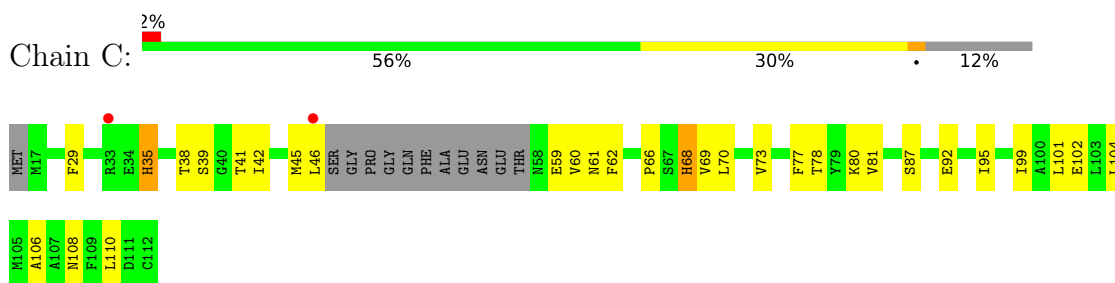
- Molecule 1: Elongin-B



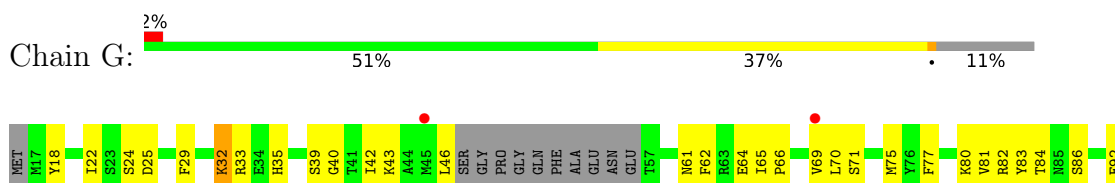
- Molecule 1: Elongin-B



- Molecule 2: Elongin-C



- Molecule 2: Elongin-C



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)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.246 , 0.273 0.244 , 0.271	Depositor DCC
R_{free} test set	2011 reflections (6.52%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtrriage
Anisotropy	0.080	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.62	0/763	0.79	0/1034
1	H	0.74	0/813	0.84	0/1098
2	C	0.70	0/664	0.79	0/901
2	G	0.81	0/696	0.77	0/940
3	B	0.86	0/1218	0.87	0/1667
3	F	0.80	0/1223	0.85	0/1673
4	A	0.64	0/1208	0.74	0/1644
4	E	0.66	0/986	0.77	0/1339
All	All	0.74	0/7571	0.81	0/10296

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	751	0	704	50	0
1	H	798	0	790	37	0
2	C	650	0	629	31	0
2	G	682	0	679	36	0
3	B	1187	0	1170	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1192	0	1171	52	0
4	A	1191	0	1070	37	0
4	E	978	0	780	43	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	313	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 21.

All (313) 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	1.72	1.29
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
4:E:80:CYS:SG	4:E:111:MET:HE1	1.99	1.03
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:80:CYS:HG	4:E:111:MET:HE3	1.19	0.96
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
4:E:22:GLN:C	4:E:24:ILE:H	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:142:ILE:HD12	4:A:155:ALA:HA	1.89	0.55
4:E:164:ARG:O	4:E:165:LYS:C	2.43	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
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
4:E:68:ARG:HE	4:E:72:MET:HE2	1.72	0.55
1:H:4:PHE:CE2	1:H:69:PRO:HG3	2.42	0.54
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
2:C:99:ILE:HG12	2:C:99:ILE:O	2.08	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
2:G:22:ILE:HB	2:G:61:ASN:HA	1.90	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
4:E:119:ASP:CG	6:E:201:GDP:HN1	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:22:GLN:C	4:E:24:ILE:N	2.63	0.51
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
2:G:40:GLY:O	2:G:43:LYS:HG2	2.11	0.50
4:E:32:TYR:O	4:E:33:ASP:C	2.49	0.50
4:E:17:SER:OG	6:E:201:GDP:O2B	2.30	0.50
3:B:182:ARG:HA	3:B:185:TYR:CD2	2.47	0.49
4:E:96:TYR:C	4:E:100:ILE:HD12	2.30	0.49
2:G:98:GLU:H	2:G:98:GLU:CD	2.16	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: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:204:GLU:C	3:B:206:ILE:H	2.16	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
4:E:15:GLY:O	4:E:16:LYS:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:101:ASP:HA	1:D:203:LYS:HZ2	1.78	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
4:A:6:LEU:HD22	4:A:159:LEU:HD22	1.96	0.47
4:E:70:GLN:NE2	4:E:70:GLN:HA	2.27	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
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
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:A:20:THR:HG23	4:A:55:ILE:HG21	1.97	0.46
4:E:116:ASN:CG	4:E:117:LYS:N	2.69	0.46
3:F:112:TYR:HE2	5:F:401:X53:O49	1.98	0.46
4:E:73:ARG:O	4:E:74:THR:C	2.54	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:14:VAL:HG23	4:E:82:PHE:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:108:ASP:OD1	4:E:108:ASP:N	2.50	0.45
4:E:133:LEU:HD11	4:E:137:TYR:CZ	2.52	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
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
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
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
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
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
2:C:45:MET:HE1	2:C:60:VAL:HG13	2.00	0.43
4:A:88:LYS:O	4:A:89:SER:C	2.57	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
4:E:116:ASN:CG	4:E:117:LYS:H	2.23	0.42
3:B:82:ARG:NH1	3:B:82:ARG:HG3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:D:100:PRO:HG2	1:D:103:MET:HE2	2.03	0.40
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
4:E:9:VAL:O	4:E:9:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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%)	74 (96%)	3 (4%)	32	40
1	H	86/92 (94%)	79 (92%)	7 (8%)	11	11
2	C	69/86 (80%)	66 (96%)	3 (4%)	29	35
2	G	77/86 (90%)	76 (99%)	1 (1%)	69	80
3	B	132/148 (89%)	125 (95%)	7 (5%)	22	26
3	F	133/148 (90%)	129 (97%)	4 (3%)	41	50
4	A	111/150 (74%)	108 (97%)	3 (3%)	44	55
4	E	81/150 (54%)	79 (98%)	2 (2%)	47	58
All	All	766/952 (80%)	736 (96%)	30 (4%)	32	40

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	40	ASP
1	D	43	ARG
1	D	50	LEU
2	C	35	HIS
2	C	59	GLU
2	C	68	HIS
3	B	60	ARG
3	B	125	HIS
3	B	139	SER
3	B	140	LEU
3	B	170	VAL
3	B	179	ASP
3	B	183	SER
1	H	19	LYS
1	H	23	THR
1	H	40	ASP
1	H	48	ASP
1	H	53	ASP
1	H	56	THR

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Mol	Chain	Res	Type
1	H	65	GLN
2	G	32	LYS
3	F	116	LEU
3	F	139	SER
3	F	164	GLN
3	F	170	VAL
4	A	38	ASP
4	A	127	THR
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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	49	GLN
2	C	35	HIS
3	B	191	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 monosaccharides in this entry.

5.6 Ligand geometry

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
6	GDP	A	201	7	24,30,30	1.91	5 (20%)	30,47,47	1.86	9 (30%)
6	GDP	E	201	7	24,30,30	1.24	2 (8%)	30,47,47	1.64	9 (30%)
5	X53	B	401	-	61,78,78	4.04	18 (29%)	61,113,113	1.81	14 (22%)
5	X53	F	401	-	61,78,78	4.13	17 (27%)	61,113,113	1.81	13 (21%)

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
6	GDP	A	201	7	-	4/12/32/32	0/3/3/3
6	GDP	E	201	7	-	5/12/32/32	0/3/3/3
5	X53	B	401	-	-	5/37/92/92	0/9/9/9
5	X53	F	401	-	-	4/37/92/92	0/9/9/9

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	401	X53	C32-C21	-17.53	1.37	1.50
5	B	401	X53	C32-C21	-17.24	1.38	1.50
5	F	401	X53	C62-C65	-15.16	1.33	1.48
5	B	401	X53	C62-C65	-14.99	1.33	1.48
5	F	401	X53	C23-S24	-12.37	1.53	1.72
5	B	401	X53	C23-S24	-11.87	1.53	1.72
5	F	401	X53	C21-S24	-8.17	1.58	1.74
5	B	401	X53	C21-S24	-8.01	1.59	1.74
5	F	401	X53	C50-C54	-6.46	1.37	1.52
5	B	401	X53	C50-C54	-6.00	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	401	X53	C58-C59	-5.54	1.39	1.51
5	F	401	X53	C3-C7	-5.53	1.32	1.48
5	B	401	X53	C3-C7	-5.46	1.32	1.48
5	B	401	X53	C58-C59	-5.43	1.39	1.51
5	B	401	X53	C35-C20	-5.40	1.40	1.53
5	F	401	X53	C35-C20	-5.28	1.41	1.53
5	B	401	X53	C42-C41	-5.21	1.32	1.39
5	F	401	X53	C42-C41	-5.20	1.32	1.39
5	B	401	X53	C42-C38	-5.12	1.31	1.39
6	A	201	GDP	C6-N1	-4.89	1.30	1.37
5	F	401	X53	C42-C38	-4.74	1.31	1.39
5	B	401	X53	C22-C20	-4.57	1.34	1.41
5	F	401	X53	C22-C20	-4.36	1.34	1.41
5	F	401	X53	C22-C25	-4.02	1.36	1.44
5	F	401	X53	C25-N27	-4.00	1.05	1.14
5	F	401	X53	C35-C17	-3.42	1.37	1.55
5	B	401	X53	C35-C17	-3.31	1.38	1.55
6	A	201	GDP	C2-N1	-3.24	1.29	1.37
6	A	201	GDP	PB-O2B	-3.13	1.42	1.54
6	E	201	GDP	C6-N1	-3.10	1.33	1.37
6	A	201	GDP	C2'-C1'	-3.03	1.49	1.53
6	A	201	GDP	PB-O3B	-2.95	1.43	1.54
5	B	401	X53	C25-N27	-2.84	1.08	1.14
5	B	401	X53	C7-N16	-2.73	1.32	1.35
6	E	201	GDP	C2'-C1'	-2.65	1.49	1.53
5	B	401	X53	C34-C35	-2.63	1.50	1.55
5	F	401	X53	C7-N16	-2.53	1.32	1.35
5	F	401	X53	C34-C35	-2.46	1.50	1.55
5	B	401	X53	C22-C25	-2.44	1.39	1.44
5	B	401	X53	C1-N6	2.15	1.39	1.34
5	B	401	X53	C34-C33	-2.04	1.47	1.52
5	F	401	X53	C34-C33	-2.01	1.47	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	X53	N6-C5-N4	-5.95	120.06	126.00
5	F	401	X53	N6-C5-N4	-5.50	120.50	126.00
5	B	401	X53	C1-N6-C5	5.26	120.89	115.08
5	F	401	X53	C1-N6-C5	4.98	120.58	115.08
5	F	401	X53	C2-C1-N6	-4.29	118.63	123.96
5	B	401	X53	C2-C1-N6	-4.28	118.64	123.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	201	GDP	C5-C6-N1	3.94	120.90	113.95
6	A	201	GDP	PA-O3A-PB	-3.66	120.27	132.83
6	A	201	GDP	O2B-PB-O3A	-3.56	92.69	104.64
6	E	201	GDP	O3'-C3'-C2'	3.20	122.17	111.82
6	E	201	GDP	PA-O3A-PB	-3.19	121.89	132.83
5	B	401	X53	C34-C35-C20	3.13	113.35	105.65
5	F	401	X53	C34-C35-C20	3.12	113.32	105.65
5	F	401	X53	C31-O37-C38	-3.05	112.78	117.59
6	A	201	GDP	O6-C6-N1	-3.05	117.04	120.65
5	F	401	X53	C53-N48-C50	-3.04	107.31	111.70
5	F	401	X53	C33-C32-C21	-2.99	108.61	113.53
5	B	401	X53	C51-C50-C54	-2.93	105.47	111.32
5	F	401	X53	C7-C3-N4	2.93	120.38	117.28
6	E	201	GDP	C8-N7-C5	2.86	108.43	102.99
5	B	401	X53	C7-C3-N4	2.78	120.22	117.28
5	B	401	X53	C33-C32-C21	-2.75	109.01	113.53
5	F	401	X53	C51-C50-C54	-2.75	105.84	111.32
6	A	201	GDP	O2B-PB-O1B	2.67	121.12	110.68
5	F	401	X53	C7-N16-C17	2.65	105.13	101.38
5	B	401	X53	C20-C22-C25	-2.51	123.30	126.02
5	B	401	X53	C14-C8-N9	-2.49	107.85	113.91
5	F	401	X53	C14-C8-N9	-2.48	107.88	113.91
5	B	401	X53	C52-C53-N48	2.42	105.65	103.08
6	A	201	GDP	C8-N7-C5	2.42	107.59	102.99
5	B	401	X53	C7-N16-C17	2.40	104.78	101.38
6	A	201	GDP	O3'-C3'-C4'	-2.36	104.22	111.05
6	A	201	GDP	C3'-C2'-C1'	2.34	104.50	100.98
5	F	401	X53	C13-C14-C8	-2.32	108.80	114.17
6	A	201	GDP	C2-N1-C6	-2.28	120.90	125.10
6	E	201	GDP	O2'-C2'-C3'	2.26	119.12	111.82
6	E	201	GDP	O3B-PB-O3A	-2.24	97.12	104.64
6	E	201	GDP	O3A-PB-O1B	-2.23	98.80	111.19
6	E	201	GDP	C3'-C2'-C1'	2.22	104.32	100.98
5	B	401	X53	C53-N48-C50	-2.22	108.50	111.70
6	E	201	GDP	O2A-PA-O1A	2.21	123.18	112.24
6	E	201	GDP	O2B-PB-O3A	2.15	111.84	104.64
5	B	401	X53	C31-O37-C38	-2.10	114.28	117.59
5	B	401	X53	C13-C14-C8	-2.05	109.42	114.17
5	F	401	X53	C51-C50-N48	2.01	105.76	103.10

There are no chirality outliers.

All (18) torsion outliers are listed below:

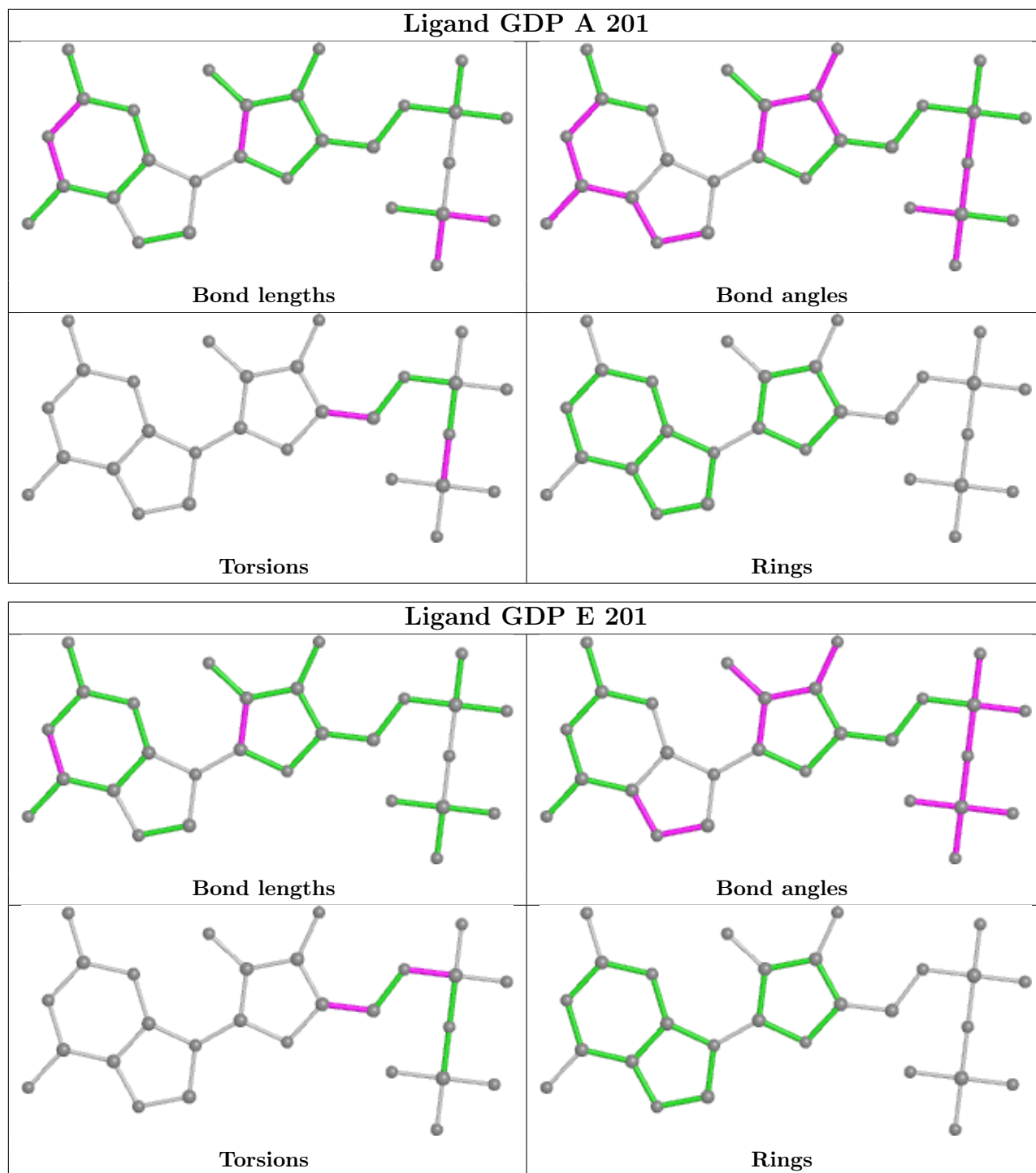
Mol	Chain	Res	Type	Atoms
5	B	401	X53	C44-C43-C45-C47
5	F	401	X53	C45-C43-C44-N48
5	F	401	X53	C45-C43-C44-O49
6	E	201	GDP	C5'-O5'-PA-O1A
6	E	201	GDP	C5'-O5'-PA-O2A
6	E	201	GDP	O4'-C4'-C5'-O5'
6	E	201	GDP	C3'-C4'-C5'-O5'
5	F	401	X53	N12-C28-C29-C30
5	B	401	X53	N12-C28-C29-C30
5	B	401	X53	C28-C29-C30-C31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

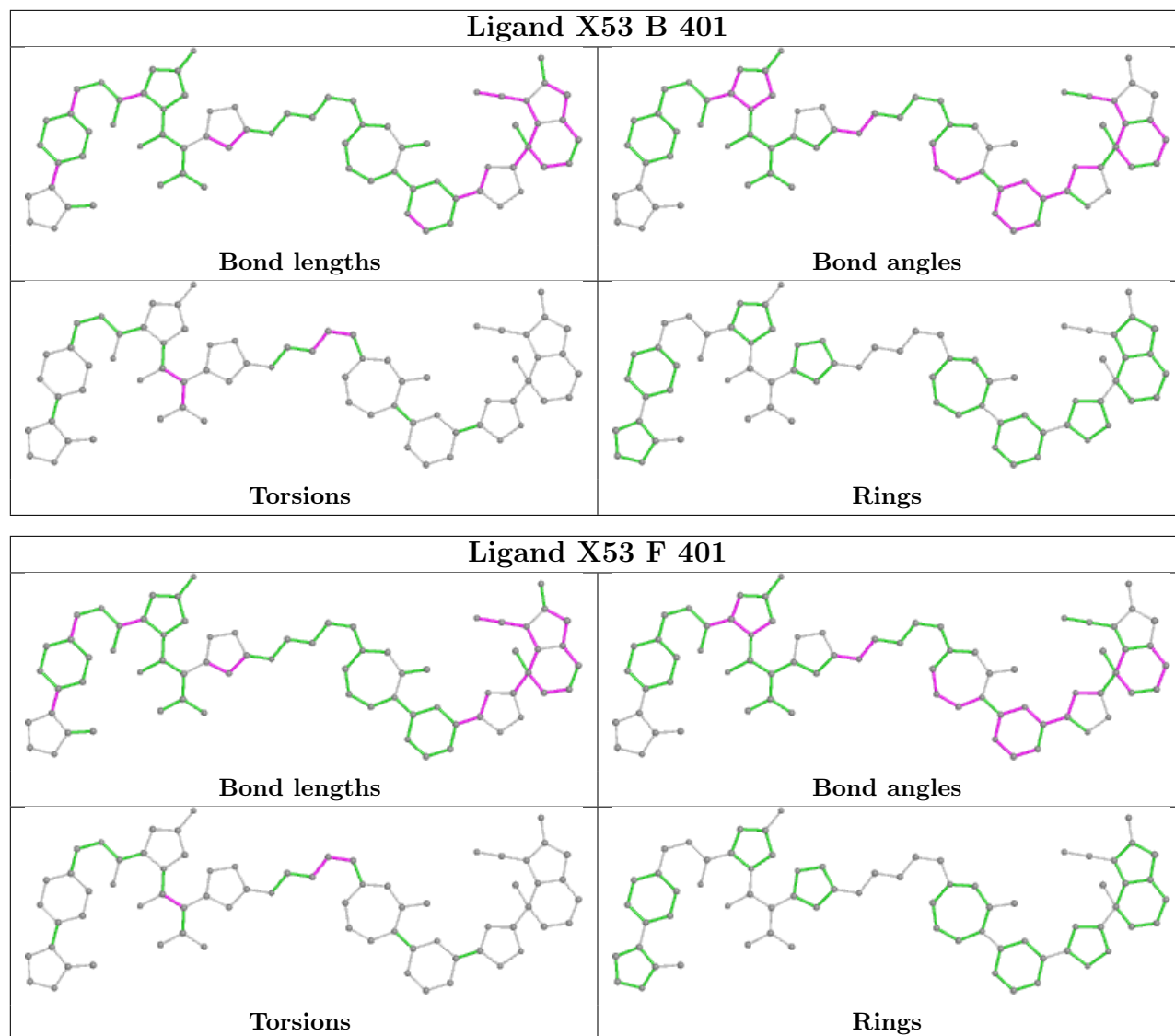
There are no ring outliers.

4 monomers are involved in 19 short contacts:

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





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%)	0.75	12 (11%) 4 7	47, 82, 103, 113	0
1	H	103/104 (99%)	0.37	3 (2%) 51 62	34, 55, 69, 86	0
2	C	85/97 (87%)	0.33	2 (2%) 59 68	35, 57, 71, 74	0
2	G	86/97 (88%)	0.38	2 (2%) 60 70	29, 49, 62, 69	0
3	B	148/162 (91%)	0.25	1 (0%) 87 92	23, 39, 62, 89	0
3	F	148/162 (91%)	0.35	4 (2%) 54 64	25, 45, 67, 78	0
4	A	166/170 (97%)	0.45	13 (7%) 13 19	39, 78, 91, 105	0
4	E	144/170 (84%)	0.58	15 (10%) 6 10	44, 81, 97, 100	0
All	All	982/1066 (92%)	0.43	52 (5%) 26 38	23, 58, 94, 113	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	79	PHE	4.7
4	E	152	VAL	4.5
1	D	50	LEU	4.4
1	D	77	LEU	4.4
4	A	46	ILE	4.4
4	E	53	LEU	4.3
1	D	35	LEU	4.2
1	D	43	ARG	4.1
1	D	78	ALA	4.0
4	E	142	ILE	3.9
4	E	21	ILE	3.7
4	E	113	LEU	3.6
1	D	51	LEU	3.5
1	D	44	LEU	3.4
4	A	159	LEU	3.4
1	D	57	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
4	A	152	VAL	3.2
4	A	53	LEU	3.2
4	E	34	PRO	3.1
4	A	112	VAL	3.0
1	H	79	PHE	3.0
4	E	41	ARG	3.0
4	A	51	CYS	3.0
4	E	32	TYR	2.9
4	E	14	VAL	2.9
4	A	19	LEU	2.8
4	A	141	PHE	2.8
2	C	33	ARG	2.8
2	G	69	VAL	2.7
4	E	48	GLY	2.7
3	B	184	LEU	2.7
4	A	36	ILE	2.7
1	D	18	ALA	2.6
4	E	158	THR	2.5
1	H	80	ARG	2.4
1	H	44	LEU	2.4
4	E	117	LYS	2.4
1	D	85	PHE	2.4
1	D	27	LEU	2.3
4	E	75	GLY	2.3
3	F	109	ILE	2.2
4	A	146	ALA	2.2
4	E	20	THR	2.2
4	A	23	LEU	2.2
2	G	45	MET	2.1
3	F	185	TYR	2.1
4	A	50	THR	2.1
3	F	207	ALA	2.1
4	E	141	PHE	2.1
4	A	55	ILE	2.1
2	C	46	LEU	2.0
3	F	60	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

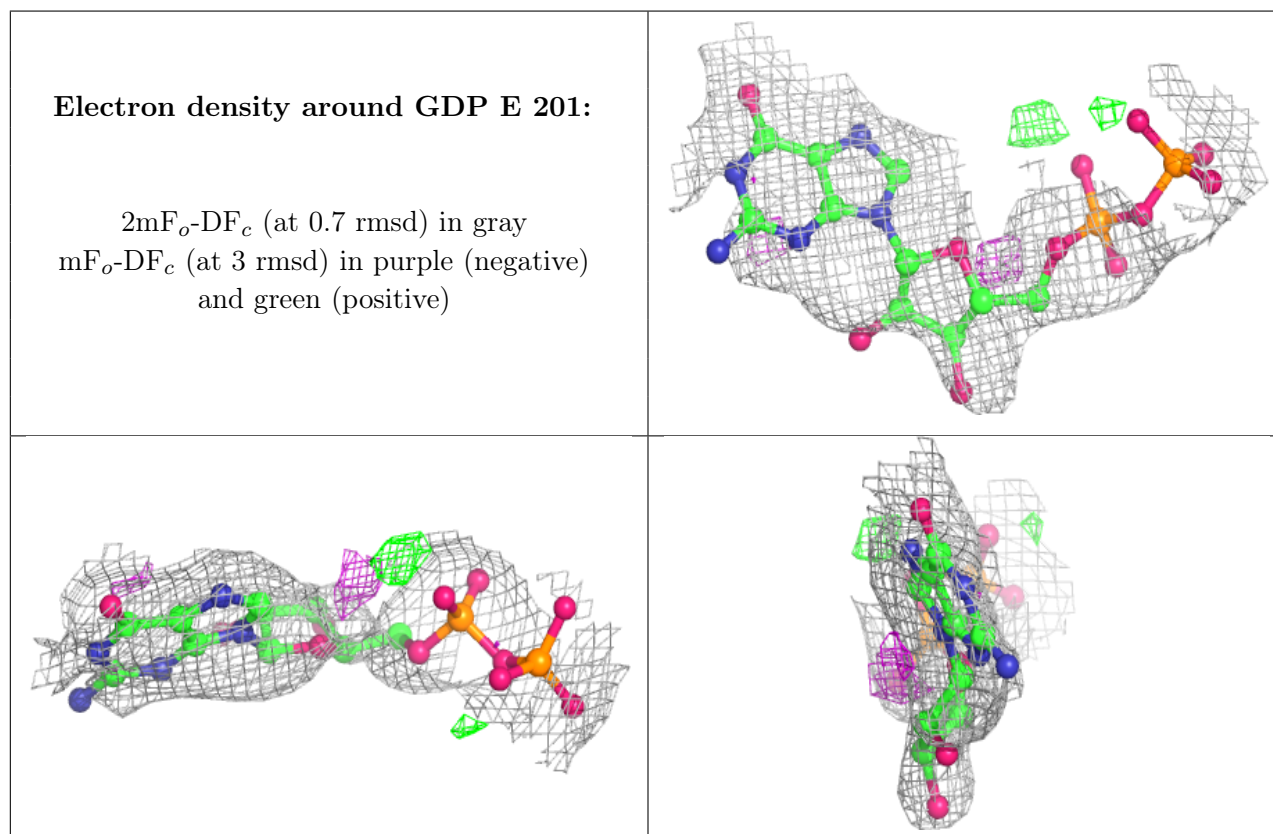
There are no monosaccharides in this entry.

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.

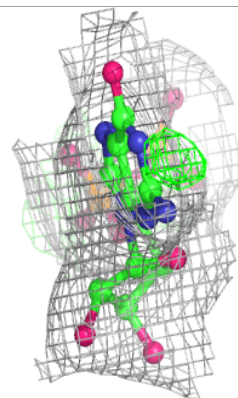
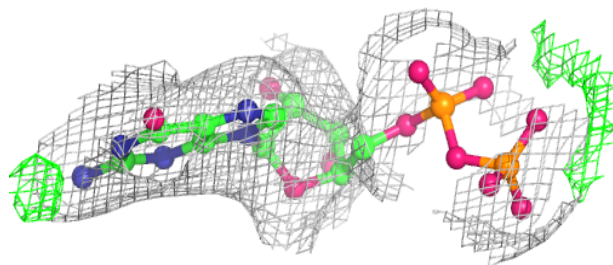
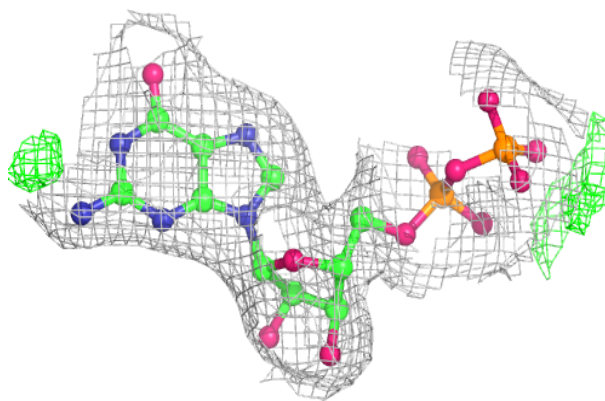
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GDP	E	201	28/28	0.76	0.21	91,105,112,114	0
6	GDP	A	201	28/28	0.91	0.13	71,84,88,93	0
5	X53	F	401	70/70	0.94	0.15	33,54,83,91	0
7	MG	E	202	1/1	0.94	0.06	88,88,88,88	0
5	X53	B	401	70/70	0.95	0.15	28,47,69,75	0
7	MG	A	202	1/1	0.98	0.28	55,55,55,55	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.

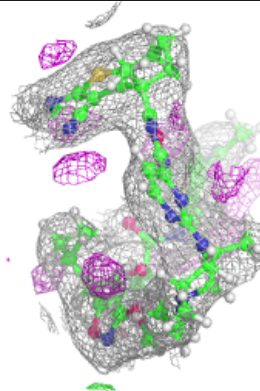
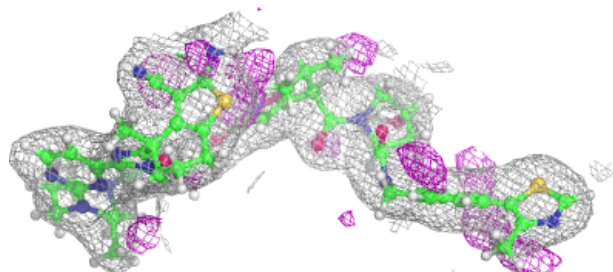
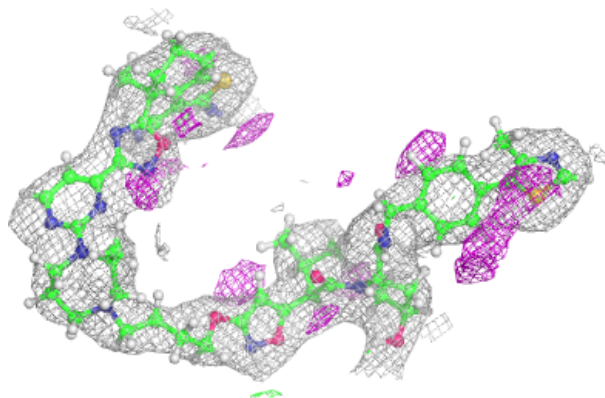


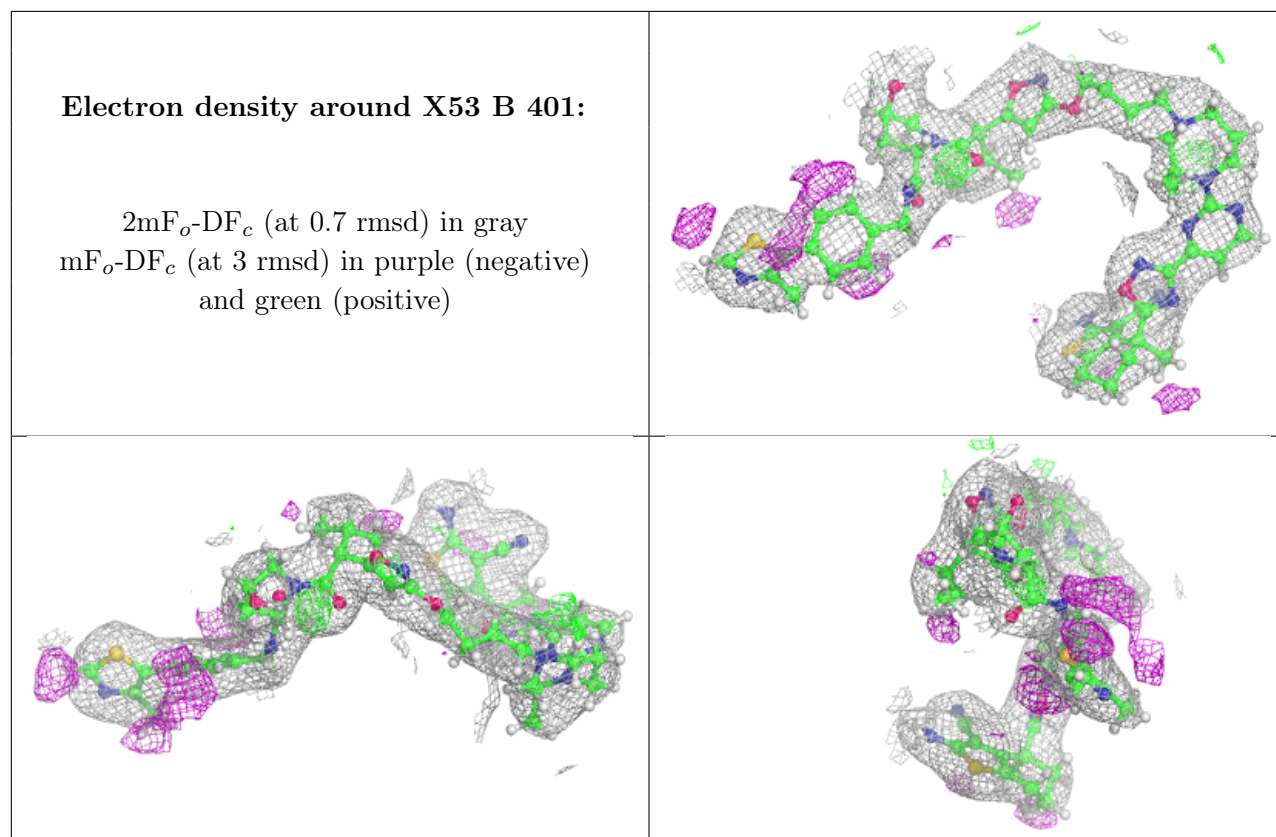
Electron density around GDP A 201:

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

**Electron density around X53 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.