



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2025 – 09:50 pm GMT

PDB ID : 9RKE / pdb_00009rke
Title : Crystal Structure of compound 1-mediated ternary complex of KRAS G12R
GCP with pVHL:ElonginC:ElonginB
Authors : Wijaya, A.J.; Karolak, N.K.; Ciulli, A.
Deposited on : 2025-06-13
Resolution : 2.83 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

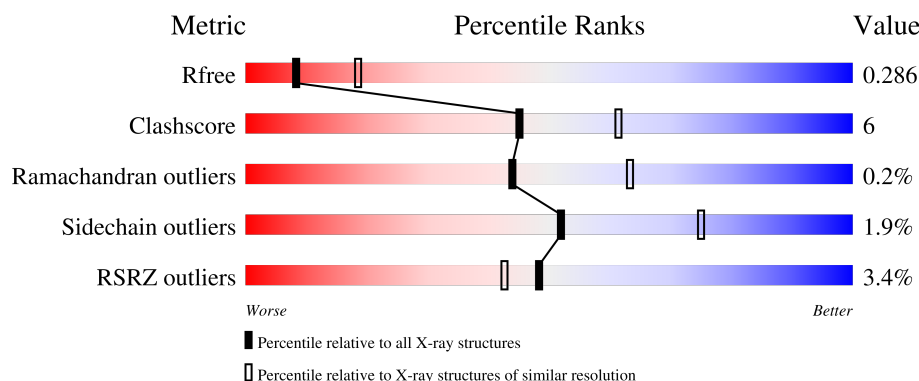
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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}	164625	1367 (2.86-2.82)
Clashscore	180529	1455 (2.86-2.82)
Ramachandran outliers	177936	1422 (2.86-2.82)
Sidechain outliers	177891	1423 (2.86-2.82)
RSRZ outliers	164620	1368 (2.86-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	104	 2% 88% 12%
1	E	104	 10% 81% 15%
2	B	97	 4% 79% 13% 7%
2	F	97	 4% 80% 8% 11%
3	C	162	 % 74% 17% 9%

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Mol	Chain	Length	Quality of chain
3	G	162	
4	D	170	
4	H	170	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	FLC	D	204	-	X	-	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7771 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			781	497	130	150	4			
1	E	100	Total	C	N	O	S	0	0	0
			672	423	113	131	5			

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	90	Total	C	N	O	S	0	0	0
			691	447	109	129	6			
2	F	86	Total	C	N	O	S	0	0	0
			631	408	102	115	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	initiating methionine	UNP Q15369
F	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	C	148	Total	C	N	O	S	0	1	0
			1161	740	209	210	2			
3	G	148	Total	C	N	O	S	0	0	0
			1123	718	203	200	2			

There are 4 discrepancies between the modelled and reference sequences:

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

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

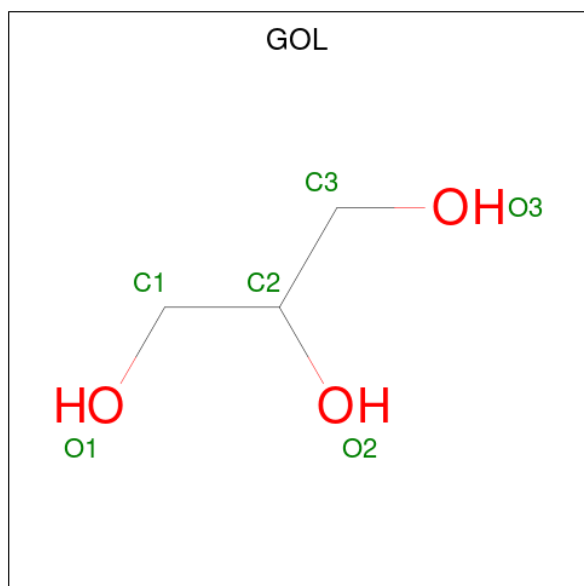
- Molecule 4 is a protein called Isoform 2B of GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	159	Total	C	N	O	S	0	0	0
			1234	775	220	232	7			
4	H	159	Total	C	N	O	S	0	0	0
			1234	775	220	232	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	GLY	-	expression tag	UNP P01116
D	12	ARG	GLY	engineered mutation	UNP P01116
H	0	GLY	-	expression tag	UNP P01116
H	12	ARG	GLY	engineered mutation	UNP P01116

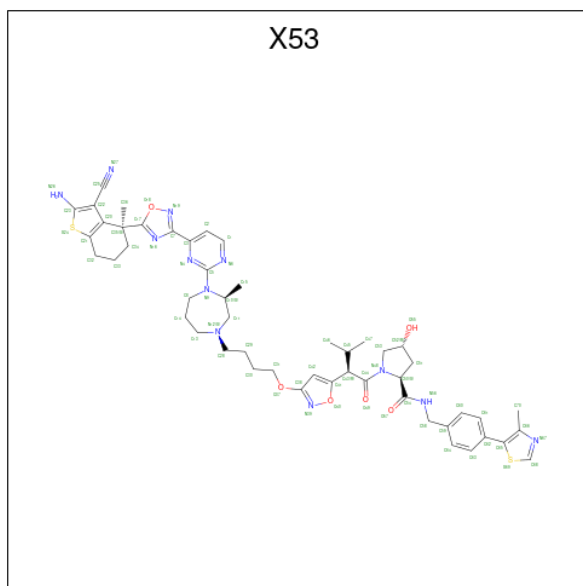
- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

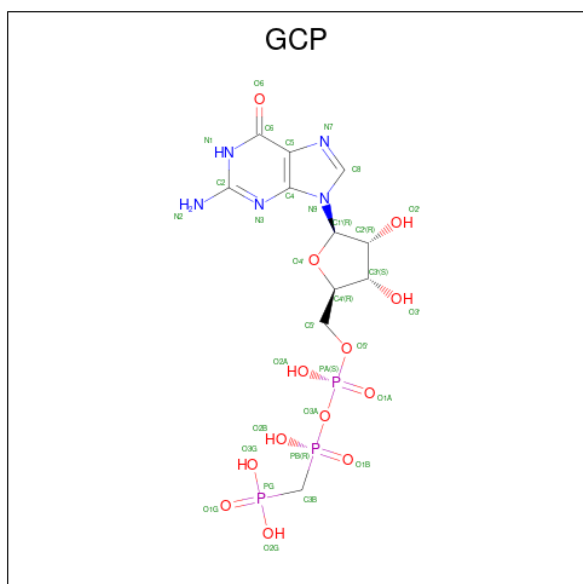
- Molecule 6 is (2S,4R)-1-[(2R)-2-[3-[4-[(3S)-4-[4-[5-[(4S)-2-azanyl-3-cyano-4-methyl-6,7-dihyd

ro-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: $C_{50}H_{60}N_{12}O_6S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	S	0	0
			70	50	12	6	2		
6	H	1	Total	C	N	O	S	0	0
			70	50	12	6	2		

- Molecule 7 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

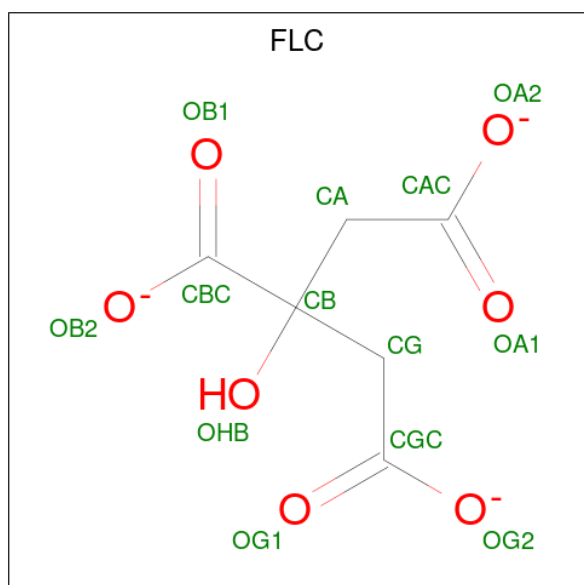


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
7	H	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	Mg	0	0
			1	1		
8	H	1	Total	Mg	0	0
			1	1		

- Molecule 9 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			13	6	7		
9	F	1	Total	C	O	0	0
			13	6	7		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	O	0	0
			1	1		

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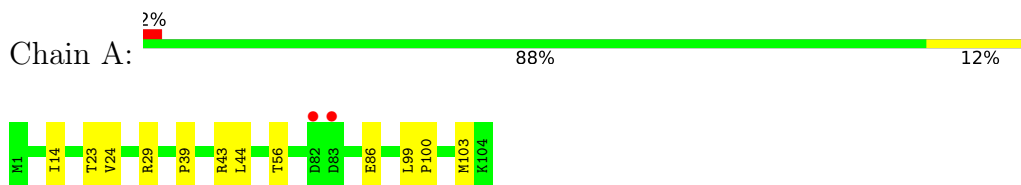
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	1	Total 1	O 1	0	0
10	F	1	Total 1	O 1	0	0
10	G	1	Total 1	O 1	0	0
10	H	2	Total 2	O 2	0	0

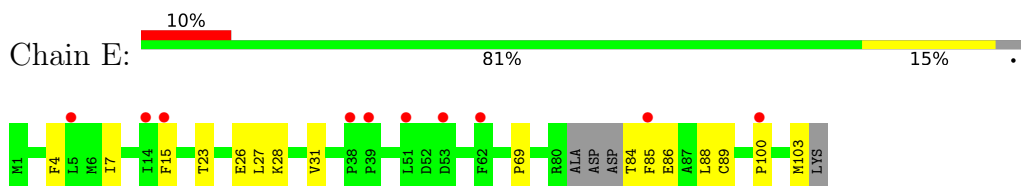
3 Residue-property plots [i](#)

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.

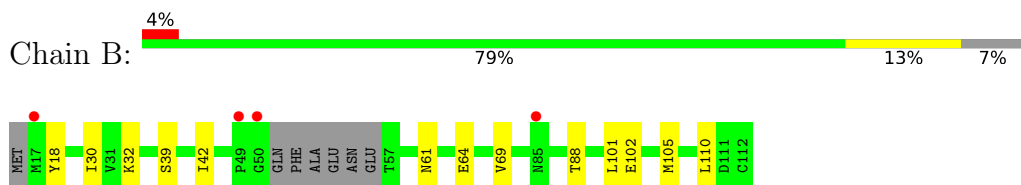
- Molecule 1: Elongin-B



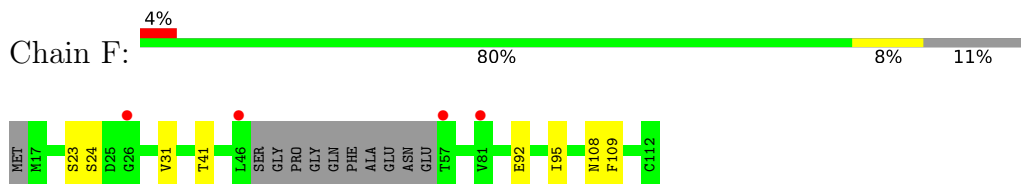
- Molecule 1: Elongin-B



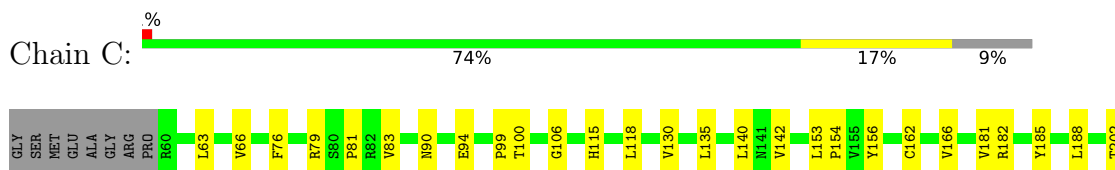
- Molecule 2: Elongin-C

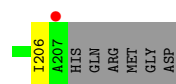


- Molecule 2: Elongin-C

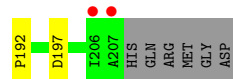
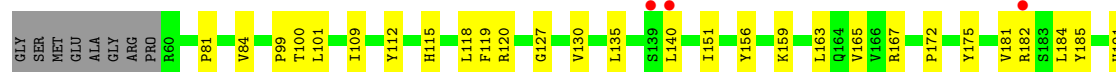


- Molecule 3: von Hippel-Lindau disease tumor suppressor

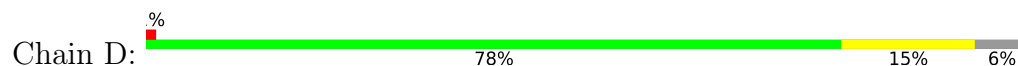




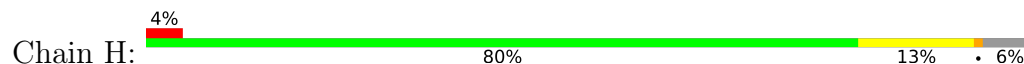
- Molecule 3: von Hippel-Lindau disease tumor suppressor



- Molecule 4: Isoform 2B of GTPase KRas



- Molecule 4: Isoform 2B of GTPase KRas



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.93Å 101.93Å 275.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	91.89 – 2.83 91.89 – 2.83	Depositor EDS
% Data completeness (in resolution range)	99.5 (91.89-2.83) 98.1 (91.89-2.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.234 , 0.286 0.235 , 0.286	Depositor DCC
R_{free} test set	2014 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	75.5	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 80.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.056 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7771	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: MG, FLC, X53, GCP, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.10	0/797	0.30	0/1082
1	E	0.12	0/685	0.35	0/939
2	B	0.10	0/706	0.28	0/956
2	F	0.10	0/645	0.29	0/877
3	C	0.13	0/1192	0.34	0/1636
3	G	0.14	0/1154	0.32	0/1588
4	D	0.11	0/1252	0.27	0/1688
4	H	0.11	0/1252	0.28	0/1688
All	All	0.12	0/7683	0.30	0/10454

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	A	781	0	752	7	0
1	E	672	0	559	8	0
2	B	691	0	675	11	0
2	F	631	0	579	6	0
3	C	1161	0	1112	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1123	0	1050	20	0
4	D	1234	0	1208	16	0
4	H	1234	0	1208	11	0
5	B	6	0	8	1	0
6	D	70	0	0	2	0
6	H	70	0	0	1	0
7	D	32	0	14	2	0
7	H	32	0	14	1	0
8	D	1	0	0	0	0
8	H	1	0	0	0	0
9	D	13	0	5	0	0
9	F	13	0	5	1	0
10	A	1	0	0	0	0
10	D	1	0	0	0	0
10	F	1	0	0	0	0
10	G	1	0	0	0	0
10	H	2	0	0	0	0
All	All	7771	0	7189	87	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 6.

All (87) 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)
1:A:100:PRO:HD2	1:A:103:MET:HE2	1.66	0.76
3:G:167:ARG:HH12	3:G:191:HIS:HA	1.53	0.72
4:H:142:ILE:HD13	4:H:155:ALA:HA	1.72	0.71
1:E:100:PRO:HD2	1:E:103:MET:HE2	1.74	0.68
4:D:142:ILE:HD13	4:D:155:ALA:HA	1.74	0.68
1:A:29:ARG:HH11	1:A:39:PRO:HG2	1.60	0.67
1:A:14:ILE:HG12	2:B:30:ILE:HB	1.77	0.65
4:D:22:GLN:NE2	4:D:146:ALA:O	2.28	0.63
3:G:167:ARG:NH1	3:G:191:HIS:HA	2.13	0.63
3:G:163:LEU:HB3	3:G:167:ARG:HE	1.63	0.63
2:B:105:MET:HE1	3:C:181:VAL:HG23	1.82	0.62
4:D:13:GLY:H	7:D:202:GCP:H3B1	1.65	0.61
3:G:163:LEU:HD13	3:G:167:ARG:HH21	1.66	0.61
3:G:127:GLY:O	3:G:156:TYR:OH	2.21	0.59
1:A:99:LEU:H	1:A:99:LEU:HD23	1.68	0.58
3:C:63:LEU:HD22	3:C:202:THR:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:99:PRO:HG3	4:H:105:ASP:HA	1.86	0.58
4:H:63:GLU:HB3	4:H:68:ARG:HH11	1.68	0.58
1:E:23:THR:HG23	1:E:26:GLU:H	1.69	0.58
4:H:84:ILE:HD11	4:H:118:CYS:HA	1.86	0.58
4:D:84:ILE:HD11	4:D:118:CYS:HA	1.86	0.58
2:B:88:THR:HG22	5:B:201:GOL:H11	1.86	0.56
2:B:42:ILE:HD11	2:B:110:LEU:HD22	1.87	0.56
3:G:167:ARG:NH1	3:G:192:PRO:HD3	2.21	0.56
1:E:84:THR:OG1	1:E:85:PHE:N	2.39	0.56
4:D:73:ARG:NH1	4:D:103:VAL:O	2.39	0.55
3:C:166:VAL:HG23	3:C:188:LEU:HD21	1.89	0.54
4:H:13:GLY:H	7:H:202:GCP:H3B1	1.72	0.54
3:C:99:PRO:HG3	4:D:105:ASP:HA	1.91	0.52
3:G:182:ARG:HA	3:G:185:TYR:CD2	2.45	0.52
1:E:15:PHE:HB2	2:F:31:VAL:HG12	1.92	0.51
3:G:118:LEU:HB3	3:G:135:LEU:HD23	1.92	0.51
1:A:23:THR:HA	1:A:56:THR:HA	1.91	0.51
3:C:81:PRO:HD2	3:C:153:LEU:HG	1.93	0.51
2:F:95:ILE:HB	3:G:165:VAL:HG21	1.92	0.51
4:D:22:GLN:HG3	4:D:149:ARG:HD2	1.91	0.51
3:C:118:LEU:HB3	3:C:135:LEU:HD23	1.93	0.51
1:E:4:PHE:CE1	1:E:69:PRO:HG3	2.46	0.51
4:D:63:GLU:HB3	4:D:68:ARG:HH11	1.76	0.50
4:D:47:ASP:OD1	4:D:161:ARG:NH2	2.42	0.49
1:A:24:VAL:HG13	1:A:44:LEU:HD12	1.95	0.49
2:B:69:VAL:HG21	2:B:102:GLU:HB3	1.95	0.49
4:D:8:VAL:HG12	4:D:16:LYS:HG2	1.95	0.49
4:H:86:ASN:HD22	4:H:89:SER:HB3	1.79	0.47
2:F:92:GLU:HB2	3:G:81:PRO:HG3	1.95	0.47
4:D:86:ASN:HD22	4:D:89:SER:HB3	1.79	0.47
4:H:73:ARG:NH1	4:H:103:VAL:O	2.49	0.46
3:C:115:HIS:ND1	6:D:201:X53:O55	2.47	0.46
1:E:27:LEU:O	1:E:31:VAL:HG13	2.15	0.46
4:D:22:GLN:O	4:D:149:ARG:NH1	2.45	0.46
3:G:112:TYR:HB2	3:G:115:HIS:NE2	2.29	0.46
3:C:106:GLY:H	9:F:201:FLC:HG1	1.81	0.46
2:B:39:SER:OG	2:B:42:ILE:HD13	2.16	0.46
4:H:8:VAL:HG12	4:H:16:LYS:HG2	1.97	0.46
2:B:18:TYR:CE2	2:B:32:LYS:HG2	2.51	0.45
3:G:119:PHE:O	3:G:120:ARG:HD3	2.16	0.45
4:H:45:VAL:HG22	4:H:50:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:101:LEU:HD11	6:H:201:X53:C68	2.47	0.45
3:C:182:ARG:HA	3:C:185:TYR:CD2	2.52	0.44
1:A:43:ARG:NH2	1:A:86:GLU:O	2.51	0.44
3:C:140:LEU:HD23	3:C:140:LEU:HA	1.82	0.44
3:C:162:CYS:O	3:C:166:VAL:HG22	2.17	0.44
4:D:12:ARG:NH2	7:D:202:GCP:O1G	2.40	0.43
2:F:41:THR:HG21	2:F:109:PHE:O	2.18	0.43
3:G:181:VAL:HG22	3:G:184:LEU:HG	2.01	0.43
3:C:90:ASN:OD1	3:C:94:GLU:N	2.48	0.43
4:D:82:PHE:HB3	4:D:93:ILE:HD11	2.01	0.42
3:C:79:ARG:HA	3:C:79:ARG:HD2	1.86	0.42
2:F:108:ASN:HA	3:G:159:LYS:HD2	2.01	0.42
3:C:154:PRO:HD2	3:C:156:TYR:CZ	2.54	0.42
4:D:102:ARG:HD3	6:D:201:X53:O57	2.19	0.42
3:C:166:VAL:CG2	3:C:188:LEU:HD21	2.49	0.42
2:F:23:SER:OG	2:F:24:SER:N	2.51	0.42
2:B:105:MET:HE3	2:B:105:MET:HB3	1.88	0.42
3:G:84:VAL:HG21	3:G:151:ILE:HG21	2.02	0.41
2:B:64:GLU:N	2:B:64:GLU:OE1	2.54	0.41
4:H:22:GLN:CD	4:H:149:ARG:HG2	2.44	0.41
3:C:76:PHE:O	3:C:106:GLY:HA2	2.21	0.41
4:D:77:GLY:HA3	4:D:163:ILE:HD11	2.01	0.41
1:E:86:GLU:HG3	1:E:88:LEU:H	1.85	0.41
3:G:140:LEU:HA	3:G:140:LEU:HD23	1.86	0.41
2:B:32:LYS:HE2	2:B:32:LYS:HB3	1.75	0.40
1:E:28:LYS:O	1:E:31:VAL:HG22	2.20	0.40
3:G:172:PRO:HA	3:G:175:TYR:CZ	2.57	0.40
2:B:101:LEU:HD13	2:B:101:LEU:HA	1.90	0.40
3:G:120:ARG:HH22	3:G:197:ASP:CG	2.29	0.40
4:H:47:ASP:OD1	4:H:161:ARG:NH2	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
1	E	96/104 (92%)	89 (93%)	6 (6%)	1 (1%)	13	25
2	B	86/97 (89%)	86 (100%)	0	0	100	100
2	F	82/97 (84%)	79 (96%)	3 (4%)	0	100	100
3	C	147/162 (91%)	138 (94%)	8 (5%)	1 (1%)	19	36
3	G	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
4	D	155/170 (91%)	149 (96%)	6 (4%)	0	100	100
4	H	155/170 (91%)	150 (97%)	5 (3%)	0	100	100
All	All	969/1066 (91%)	929 (96%)	38 (4%)	2 (0%)	44	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	89	CYS
3	C	206	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	81/92 (88%)	81 (100%)	0	100	100
1	E	55/92 (60%)	54 (98%)	1 (2%)	54	76
2	B	75/86 (87%)	74 (99%)	1 (1%)	65	83
2	F	62/86 (72%)	62 (100%)	0	100	100
3	C	125/148 (84%)	120 (96%)	5 (4%)	27	51
3	G	115/148 (78%)	112 (97%)	3 (3%)	41	67
4	D	129/150 (86%)	128 (99%)	1 (1%)	79	90
4	H	129/150 (86%)	125 (97%)	4 (3%)	35	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	771/952 (81%)	756 (98%)	15 (2%)	52 75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	61	ASN
3	C	66	VAL
3	C	83	VAL
3	C	100	THR
3	C	130	VAL
3	C	142	VAL
4	D	109	VAL
1	E	7	ILE
3	G	100	THR
3	G	109	ILE
3	G	130	VAL
4	H	27	HIS
4	H	29	VAL
4	H	109	VAL
4	H	149	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	X53	D	201	-	61,78,78	0.90	4 (6%)	61,113,113	0.84	3 (4%)
6	X53	H	201	-	61,78,78	0.89	4 (6%)	61,113,113	0.84	3 (4%)
7	GCP	H	202	8	27,34,34	1.19	3 (11%)	34,54,54	2.10	8 (23%)
7	GCP	D	202	8	27,34,34	1.20	3 (11%)	34,54,54	2.09	8 (23%)
5	GOL	B	201	-	5,5,5	0.95	0	5,5,5	0.92	0
9	FLC	D	204	-	12,12,12	1.87	6 (50%)	17,17,17	2.53	6 (35%)
9	FLC	F	201	-	12,12,12	1.87	6 (50%)	17,17,17	2.53	6 (35%)

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	X53	D	201	-	-	1/37/92/92	0/9/9/9
6	X53	H	201	-	-	1/37/92/92	0/9/9/9
7	GCP	H	202	8	-	3/15/38/38	0/3/3/3
7	GCP	D	202	8	-	1/15/38/38	0/3/3/3
5	GOL	B	201	-	-	2/4/4/4	-
9	FLC	D	204	-	-	7/16/16/16	-
9	FLC	F	201	-	-	3/16/16/16	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	201	X53	C42-C41	-4.02	1.34	1.39
6	D	201	X53	C42-C41	-3.95	1.34	1.39
6	D	201	X53	C5-N9	3.41	1.42	1.36
6	H	201	X53	C11-N12	3.27	1.49	1.46
7	H	202	GCP	C6-N1	3.16	1.38	1.33
7	D	202	GCP	C6-N1	3.15	1.38	1.33
7	D	202	GCP	PB-O3A	3.07	1.61	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	201	X53	C11-N12	2.97	1.49	1.46
7	H	202	GCP	PB-O3A	2.92	1.61	1.58
6	H	201	X53	C5-N9	2.86	1.41	1.36
9	D	204	FLC	OB1-CBC	2.81	1.31	1.22
9	F	201	FLC	OB1-CBC	2.80	1.31	1.22
9	F	201	FLC	OA1-CAC	2.76	1.31	1.22
9	D	204	FLC	OG1-CGC	2.75	1.31	1.22
9	F	201	FLC	OG1-CGC	2.75	1.31	1.22
9	D	204	FLC	OA1-CAC	2.73	1.31	1.22
9	F	201	FLC	OG2-CGC	-2.65	1.21	1.30
9	D	204	FLC	OG2-CGC	-2.65	1.21	1.30
9	D	204	FLC	OA2-CAC	-2.64	1.21	1.30
9	F	201	FLC	OA2-CAC	-2.62	1.21	1.30
7	D	202	GCP	PB-O2B	-2.60	1.50	1.56
7	H	202	GCP	PB-O2B	-2.59	1.50	1.56
6	D	201	X53	C7-N16	2.34	1.38	1.35
6	H	201	X53	C7-N16	2.29	1.38	1.35
9	D	204	FLC	OB2-CBC	-2.23	1.22	1.30
9	F	201	FLC	OB2-CBC	-2.20	1.22	1.30

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	202	GCP	C5-C6-N1	-8.34	112.02	123.43
7	D	202	GCP	C5-C6-N1	-8.33	112.04	123.43
9	D	204	FLC	OB1-CBC-CB	-6.46	113.10	122.25
9	F	201	FLC	OB1-CBC-CB	-6.42	113.16	122.25
7	H	202	GCP	C2-N1-C6	5.82	125.18	115.93
7	D	202	GCP	C2-N1-C6	5.81	125.17	115.93
9	F	201	FLC	OB2-CBC-CB	5.62	122.81	113.05
9	D	204	FLC	OB2-CBC-CB	5.56	122.70	113.05
6	D	201	X53	C33-C32-C21	-3.45	107.87	113.53
6	H	201	X53	C33-C32-C21	-3.32	108.08	113.53
9	D	204	FLC	OA1-CAC-CA	-3.27	113.40	122.94
9	F	201	FLC	OA1-CAC-CA	-3.22	113.52	122.94
6	H	201	X53	C34-C35-C20	3.21	113.55	105.65
9	D	204	FLC	OG1-CGC-CG	-3.18	113.65	122.94
9	F	201	FLC	OG1-CGC-CG	-3.17	113.68	122.94
6	D	201	X53	C34-C35-C20	3.12	113.31	105.65
7	H	202	GCP	N3-C2-N1	-2.81	123.48	127.22
7	D	202	GCP	N3-C2-N1	-2.80	123.48	127.22
9	F	201	FLC	OA2-CAC-CA	2.73	123.11	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	204	FLC	OA2-CAC-CA	2.71	123.06	114.35
9	F	201	FLC	OG2-CGC-CG	2.70	123.03	114.35
9	D	204	FLC	OG2-CGC-CG	2.69	123.00	114.35
7	D	202	GCP	O1G-PG-C3B	-2.61	105.61	111.24
7	H	202	GCP	O1G-PG-C3B	-2.47	105.92	111.24
7	H	202	GCP	C4-C5-C6	-2.43	118.47	120.80
7	H	202	GCP	C2-N3-C4	-2.42	112.59	115.36
7	D	202	GCP	C2-N3-C4	-2.42	112.59	115.36
7	H	202	GCP	PB-O3A-PA	2.40	140.19	132.56
7	D	202	GCP	C4-C5-C6	-2.39	118.51	120.80
7	H	202	GCP	O2B-PB-O1B	2.36	117.96	110.07
7	D	202	GCP	O2B-PB-O1B	2.26	117.61	110.07
6	H	201	X53	C31-O37-C38	-2.26	114.03	117.59
7	D	202	GCP	PB-O3A-PA	2.14	139.36	132.56
6	D	201	X53	C14-C13-N12	-2.10	111.37	115.35

There are no chirality outliers.

All (18) torsion outliers are listed below:

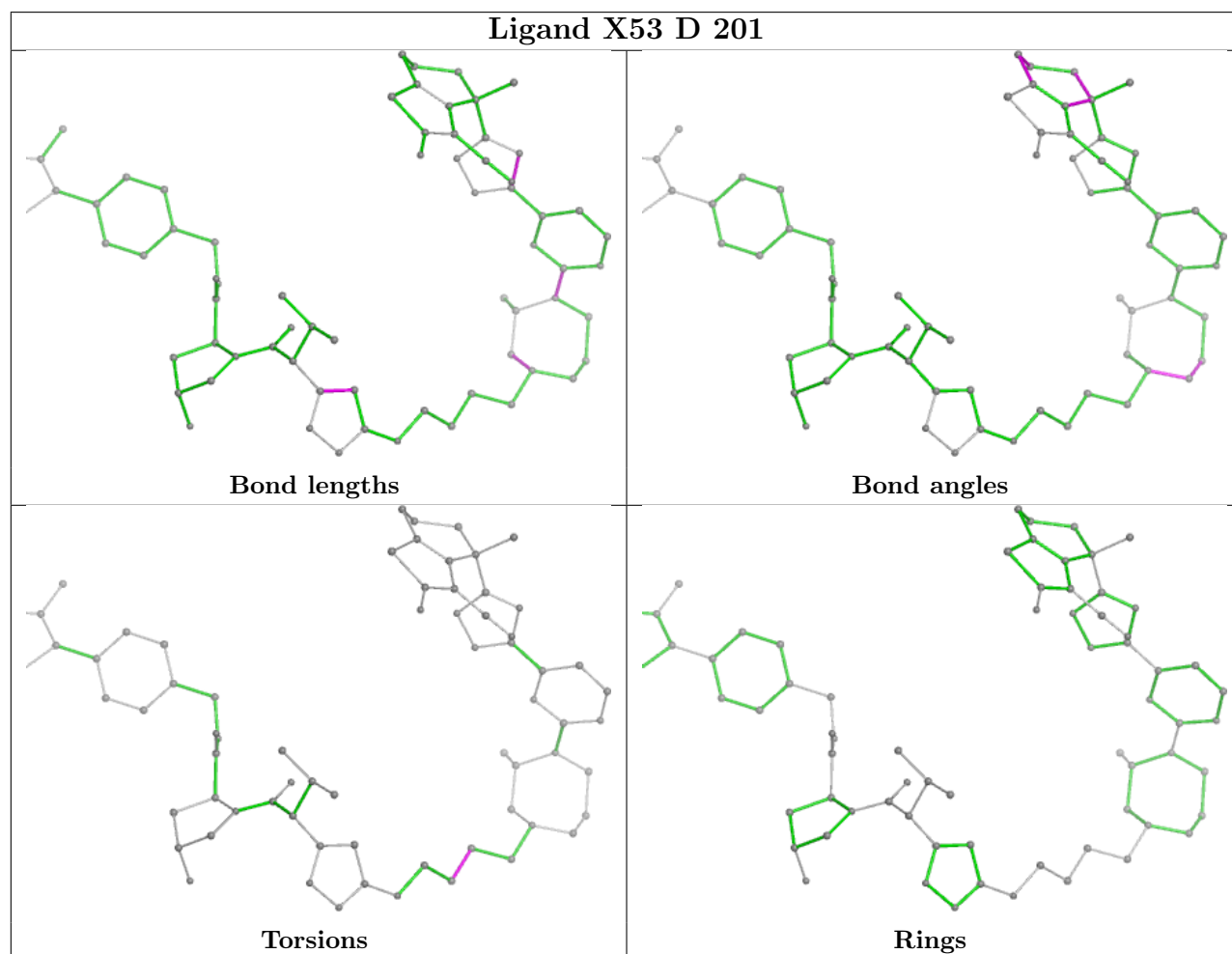
Mol	Chain	Res	Type	Atoms
7	D	202	GCP	PG-C3B-PB-O1B
7	H	202	GCP	PG-C3B-PB-O1B
7	H	202	GCP	PG-C3B-PB-O3A
9	D	204	FLC	CA-CB-CBC-OB1
9	D	204	FLC	CA-CB-CBC-OB2
9	D	204	FLC	OHB-CB-CBC-OB1
9	D	204	FLC	OHB-CB-CBC-OB2
5	B	201	GOL	C1-C2-C3-O3
5	B	201	GOL	O2-C2-C3-O3
9	D	204	FLC	CAC-CA-CB-CBC
9	D	204	FLC	CAC-CA-CB-CG
9	D	204	FLC	CAC-CA-CB-OHB
9	F	201	FLC	OHB-CB-CG-CGC
6	H	201	X53	C28-C29-C30-C31
7	H	202	GCP	PB-C3B-PG-O1G
9	F	201	FLC	CAC-CA-CB-CBC
9	F	201	FLC	CAC-CA-CB-CG
6	D	201	X53	C28-C29-C30-C31

There are no ring outliers.

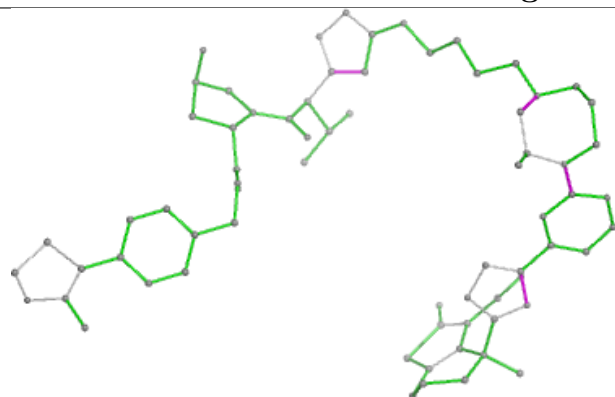
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	201	X53	2	0
6	H	201	X53	1	0
7	H	202	GCP	1	0
7	D	202	GCP	2	0
5	B	201	GOL	1	0
9	F	201	FLC	1	0

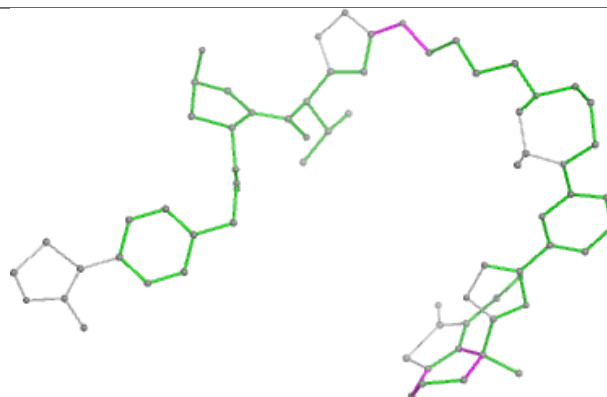
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



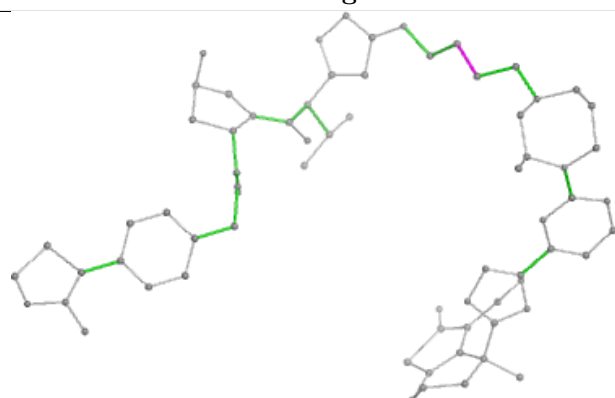
Ligand X53 H 201



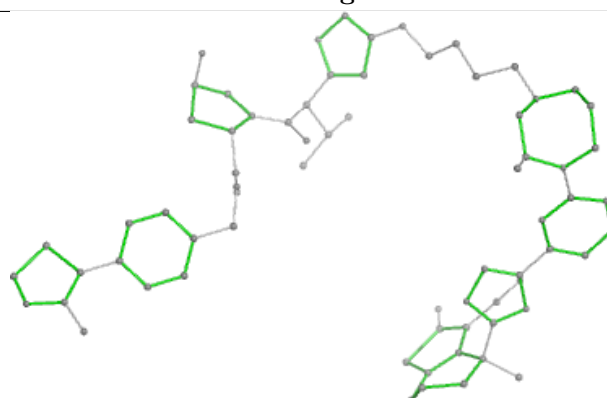
Bond lengths



Bond angles

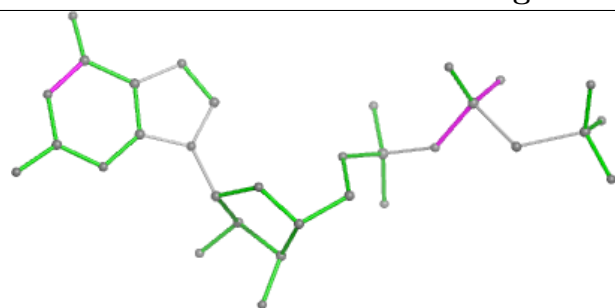


Torsions

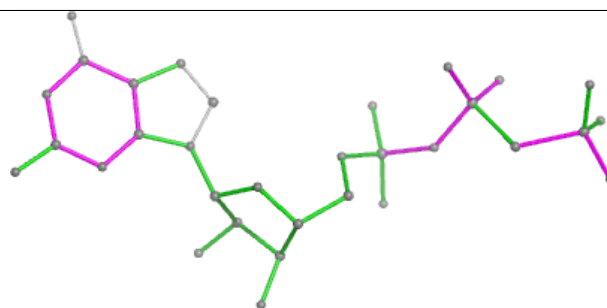


Rings

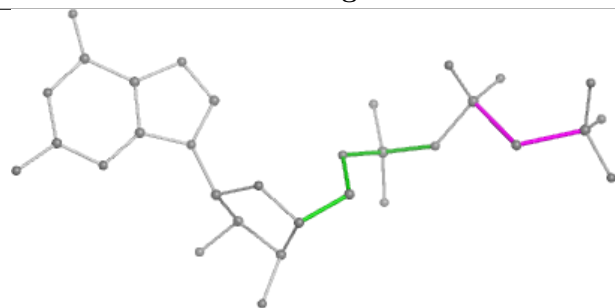
Ligand GCP H 202



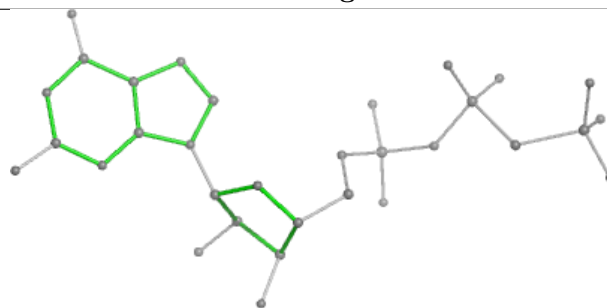
Bond lengths



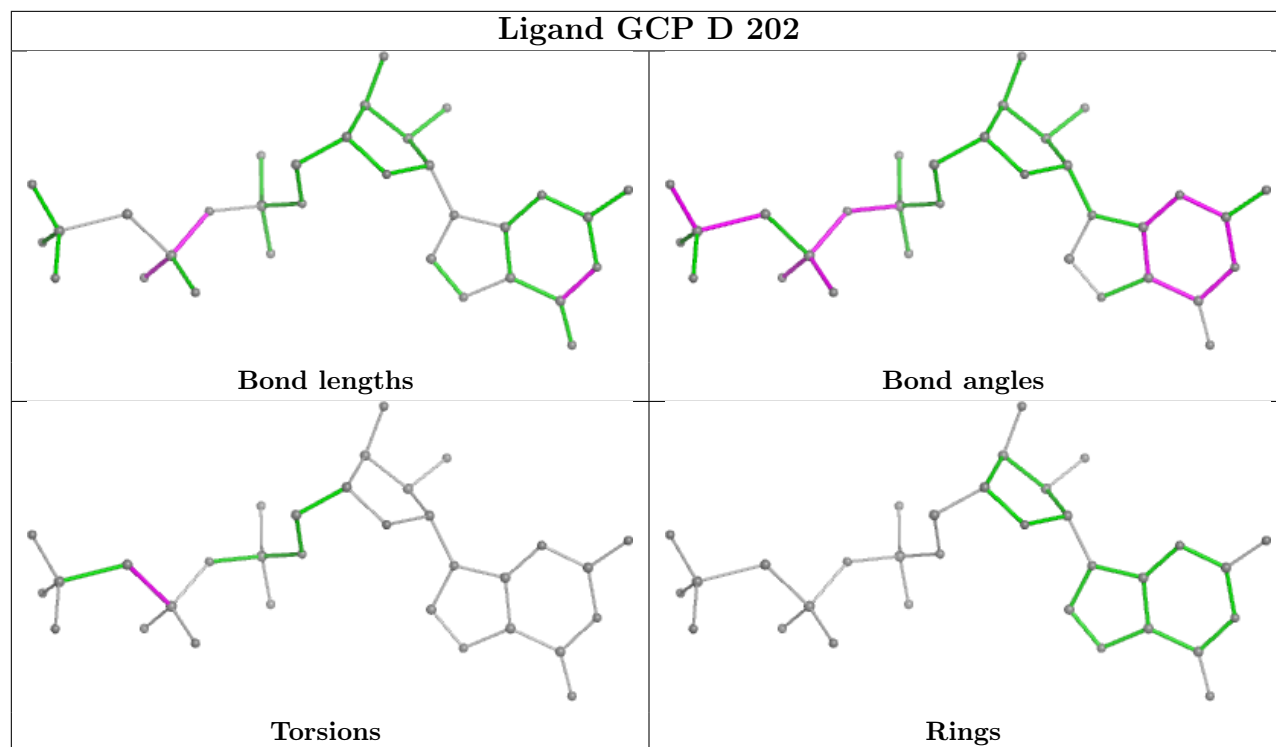
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	104/104 (100%)	-0.26	2 (1%) 66 62	64, 91, 123, 157	0
1	E	100/104 (96%)	0.64	10 (10%) 14 13	90, 134, 166, 181	0
2	B	90/97 (92%)	0.10	4 (4%) 39 34	55, 77, 114, 134	0
2	F	86/97 (88%)	0.12	4 (4%) 37 32	71, 96, 124, 150	0
3	C	148/162 (91%)	-0.23	1 (0%) 84 83	29, 69, 118, 141	1 (0%)
3	G	148/162 (91%)	-0.05	5 (3%) 48 42	48, 78, 124, 144	0
4	D	159/170 (93%)	-0.13	2 (1%) 74 71	56, 81, 117, 127	0
4	H	159/170 (93%)	0.23	6 (3%) 44 38	60, 85, 129, 176	0
All	All	994/1066 (93%)	0.03	34 (3%) 48 42	29, 87, 137, 181	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	207	ALA	4.2
1	E	14	ILE	3.4
2	B	50	GLY	3.2
1	E	39	PRO	3.0
4	H	40	TYR	2.9
3	C	207	ALA	2.9
1	E	38	PRO	2.8
3	G	139	SER	2.7
1	E	53	ASP	2.6
4	H	57	ASP	2.6
4	H	132	ASP	2.6
4	H	39	SER	2.6
4	D	29	VAL	2.5
1	E	100	PRO	2.5
1	E	5	LEU	2.5
2	F	57	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	46	LEU	2.4
4	H	27	HIS	2.4
1	E	62	PHE	2.4
1	E	85	PHE	2.4
2	B	49	PRO	2.3
3	G	182	ARG	2.3
1	A	82	ASP	2.2
2	F	26	GLY	2.2
3	G	140	LEU	2.2
2	F	81	VAL	2.2
1	E	15	PHE	2.1
1	A	83	ASP	2.1
2	B	17	MET	2.1
4	H	122	SER	2.1
3	G	206	ILE	2.1
4	D	118	CYS	2.1
2	B	85	ASN	2.1
1	E	51	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

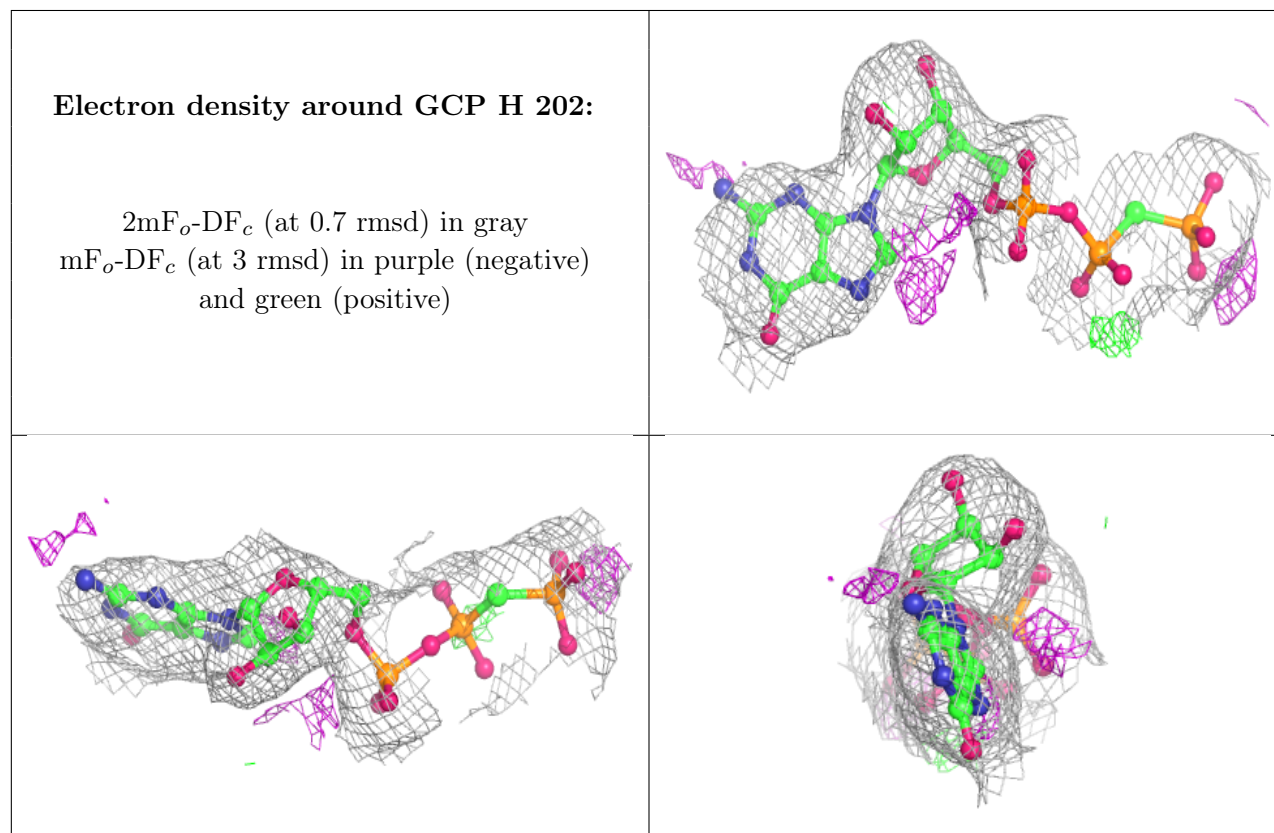
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	B	201	6/6	0.82	0.18	104,106,117,126	0
9	FLC	D	204	13/13	0.82	0.16	74,85,102,115	0
9	FLC	F	201	13/13	0.84	0.09	78,97,117,126	0
8	MG	H	203	1/1	0.90	0.07	106,106,106,106	0
7	GCP	H	202	32/32	0.94	0.08	64,80,93,116	0

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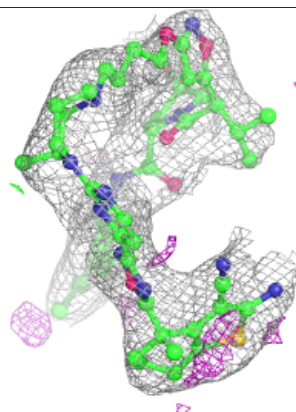
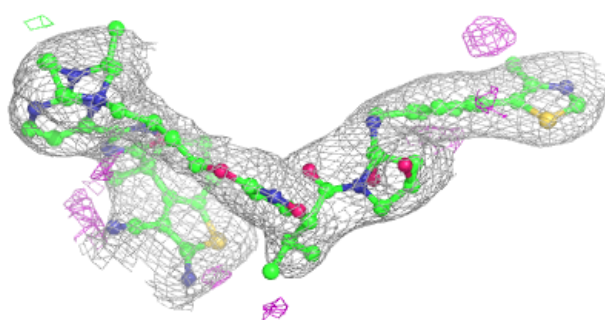
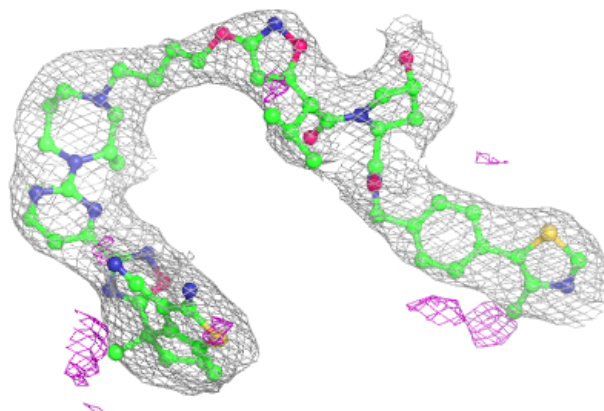
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	X53	H	201	70/70	0.94	0.10	49,67,86,95	0
8	MG	D	203	1/1	0.95	0.10	82,82,82,82	0
7	GCP	D	202	32/32	0.96	0.08	58,76,103,111	0
6	X53	D	201	70/70	0.96	0.08	42,58,74,81	0

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.

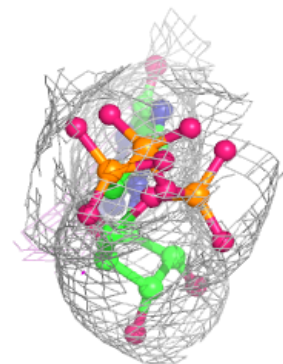
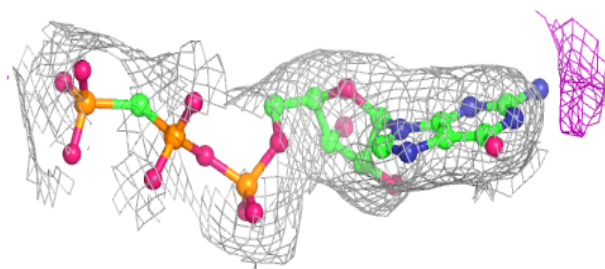
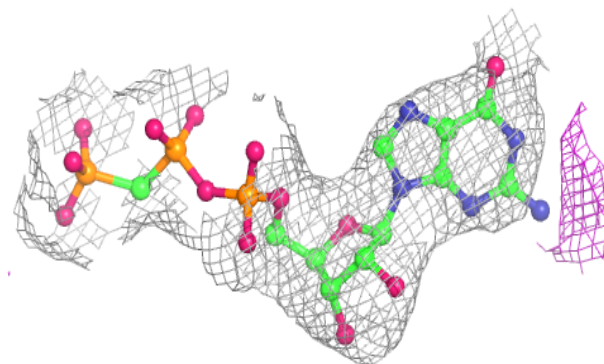


Electron density around X53 H 201:

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

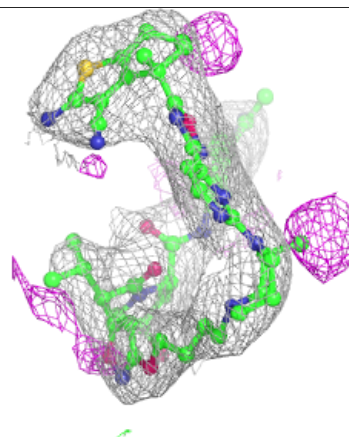
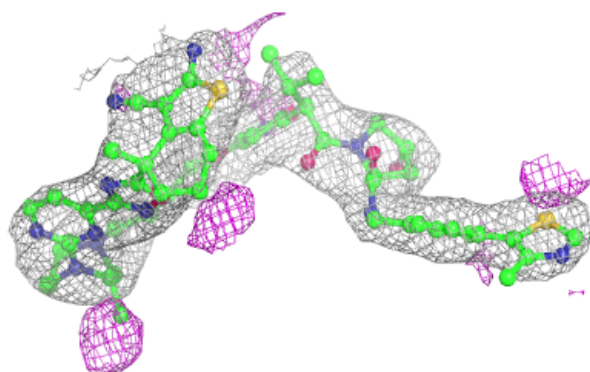
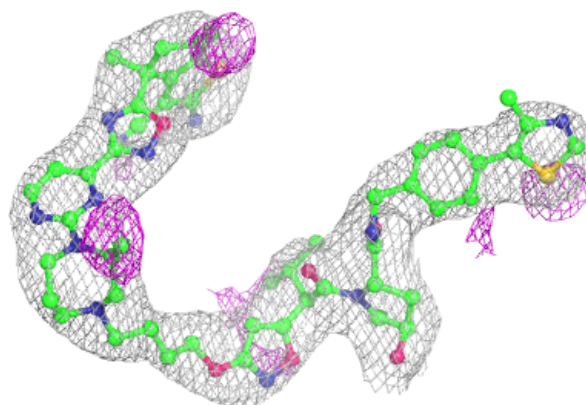
**Electron density around GCP D 202:**

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



Electron density around X53 D 201:

$2mF_o-DF_c$ (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.