



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 11:01 PM BST

PDB ID : 5FBV
Title : PI4KB in complex with Rab11 and the MI364 Inhibitor
Authors : Chalupska, D.; Mejdrova, I.; Nencka, R.; Boura, E.
Deposited on : 2015-12-14
Resolution : 3.29 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

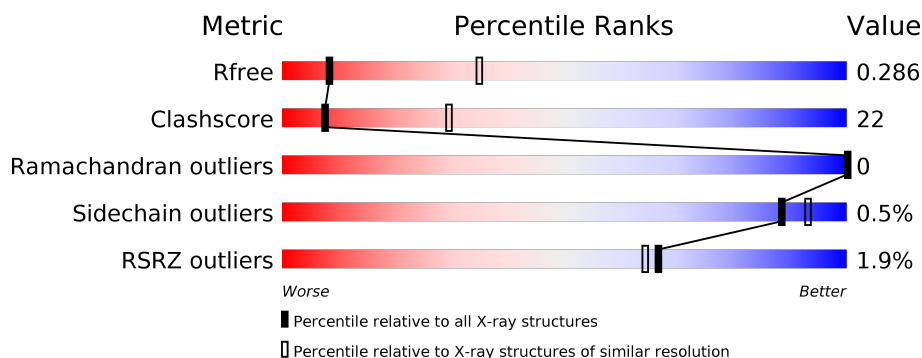
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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

Mol	Chain	Length	Quality of chain
1	A	572	<div> <div>2%</div> <div> <div></div> <div>53%</div> <div>28%</div> <div>19%</div> </div> </div>
2	B	221	<div> <div>%</div> <div> <div></div> <div>48%</div> <div>27%</div> <div>24%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5091 atoms, of which 14 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 Phosphatidylinositol 4-kinase beta,Phosphatidylinositol 4-kinase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3752	2410	648	670	24			

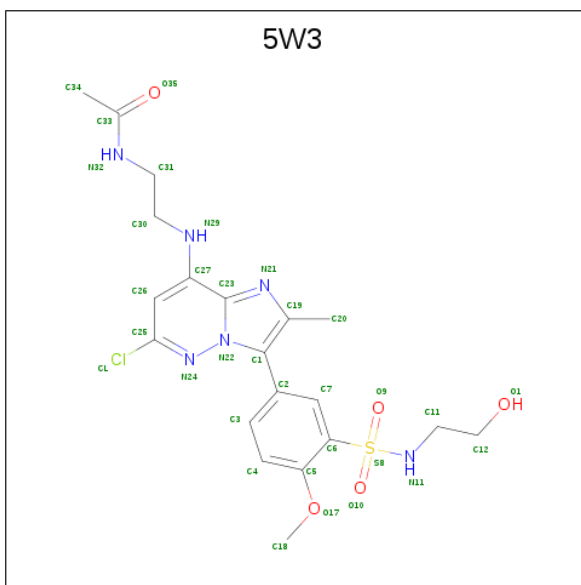
- Molecule 2 is a protein called Ras-related protein Rab-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	0	0
			1260	797	214	248	1			

There are 6 discrepancies between the modelled and reference sequences:

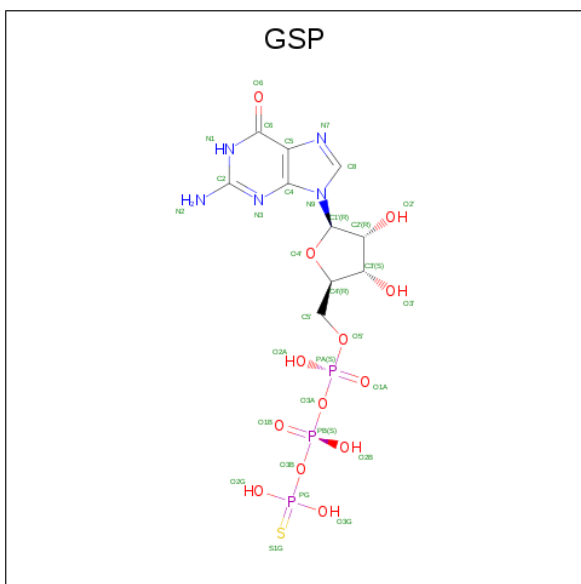
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P62491
B	-3	ALA	-	expression tag	UNP P62491
B	-2	MET	-	expression tag	UNP P62491
B	-1	GLY	-	expression tag	UNP P62491
B	0	SER	-	expression tag	UNP P62491
B	70	LEU	GLN	engineered mutation	UNP P62491

- Molecule 3 is {N}-[2-[6-chloranyl-3-[3-(2-hydroxyethylsulfamoyl)-4-methoxy-phenyl]-2-methyl-imidazo[1,2-b]pyridazin-8-yl]amino]ethyl]ethanamide (three-letter code: 5W3) (formula: C₂₀H₂₅ClN₆O₅S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			33	20	1	6	5	1		

- Molecule 4 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	P	S	0	0
			46	10	14	5	13	3	1		

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.

- Chain A: ■ 29% ■ 53% ■ 19%

L737	L652	K563	L354	LYS	L236	S128
M744	F653	K564	P355	VAL		W129
Q749	V654		F359	GLU		F134
E752	C657	D567	D568	ASN	T240	
I753	Y660	L569	H561	GLU	S242	F139
M754	C661	Q571	V364	ASP		D140
Q756	L662	R572	H568	GLU		I141
	V663	L573	T369	LEU		S142
		L574		LEU		M143
	L667	A575	K379	SER	ALA	Y149
	Q668	F576		THR	HIS	
F763	V669	Q577	L383	GLU	ARG	M162
	K670	V578	E387	SER	LYS	R163
T768	D671	L579	V388	ILE	ARG	L164
I769	K672	K580	L389	ASN	GLU	F165
	H673	W586	E390	SER	LEU	V172
F776	M674	L593	C392	SER	PRO	
M780	L679	K599	N393	SER	LEU	L176
	H684	I600	F394	THR	PRO	P177
L785	H687	L601	D395	ALA	ALA	Q178
S798	I688	V602	T396	PRO	PRO	L179
S799	D689	I603	R402	THR	ASP	M181
			I403	GLY	GLY	M182
	F692	G608	R311	LEU	LEU	M186
	L693	M609	E312	SER	SER	
	L694	ARG	F313	PRO	PRO	K195
	S695	P612	L317	LYS	LYS	P196
	S696	V613	ASP	ARG	ARG	R201
	S697	V614	PRO	THR	THR	
	PRO	N615	N318	HIS	HIS	Q204
	ASN	A616	L324	GLN	GLN	S205
	GLY	V617	ASP	ARG	ARG	I206
	LEU	S618	PRO	SER	SER	H207
	PHE	I619	ALA	LYS	LYS	F208
	GLU		V531	SER	SER	S209
	THR	V622	A532	ASP	ASP	
	SER	K623	L533	THR	THR	C212
	SER	L628	K534	ALA	ALA	A213
	F708		W537	SER	SER	L214
	K709	L630		ILE	ILE	L216
	V715	L631	K540	SER	SER	
	M718	D632	I544	SER	SER	S221
	L721	Y633	S548	ASN	ASN	ASP
	F726	E637	P549	LEU	LEU	HIS
		S640	Y550	LYS	LYS	I15
	Y729	T643	N555	ARG	ARG	SER
		F646	W556	THR	THR	GLN
	L732	I647	R557	ALA	ALA	ARG
		S648	L558	SER	SER	HIS
			V559	ASN	ASN	SER
				PRO	PRO	P352

- Chain B:
-
- 48% 27% 24%
- GLY ALA MET GLY SER MET GLY THR ARG ASP ASP GLU Y8 D9 Y10 L11 F12 K13 V14 V15 L16 L17 S20 G21 V22 G23 K24 S25 L28 S29 R30 F31 T32 L38 T43 V46 A49 T50 R51 Q54 V55 K58 T59 I60 I64 W65 D66 G69 L70
- ARG TYR R74 A75 I76 T77 S78 A79 Y80 Y81 R82 A87 L88 L89 D82 I93 A94 V102 W105 L109 V118 I119 M120 L121 K125 L128 F129 H130 L131 R140 A141 F142 G147 L148 V161 F165 Q166 T167 I172 I175 Q178 LYS GLN MET

ASP	ARG	GLU	ASN	ASP	MET	SER	PRO	SER	ASN	ASN	VAL	VAL	PRO	ILE	HIS	VAL	PRO	PRO	THR	THR	GLU	ASN	LYS	PRO	LYS	VAL	GLN	CYS	CYS	GLN	ASN	ILE
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.54Å 102.78Å 186.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.97 – 3.29 46.97 – 3.29	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.97-3.29) 86.8 (46.97-3.29)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.29 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.237 , 0.281 0.241 , 0.286	Depositor DCC
R_{free} test set	738 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	82.7	Xtriage
Anisotropy	0.839	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5091	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: 5W3, GSP

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	0.63	1/3829 (0.0%)	0.80	2/5169 (0.0%)
2	B	0.54	0/1278	0.71	0/1737
All	All	0.61	1/5107 (0.0%)	0.78	2/6906 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	PRO	N-CD	-7.27	1.37	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	PRO	N-CA-CB	-7.89	93.83	103.30
1	A	349	PRO	N-CD-CG	-6.14	93.99	103.20

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	3752	0	3802	157	0
2	B	1260	0	1214	67	0
3	A	33	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	32	14	11	6	0
All	All	5077	14	5027	222	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 (222) 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:348:LEU:HB2	1:A:402:ARG:NH1	1.29	1.39
1:A:348:LEU:CB	1:A:402:ARG:NH1	2.14	1.11
1:A:139:PHE:HA	1:A:143:MET:HE2	1.36	1.02
1:A:310:GLU:HA	1:A:352:VAL:HG12	1.51	0.91
1:A:348:LEU:HB2	1:A:402:ARG:HH12	1.09	0.88
1:A:643:THR:HG23	1:A:646:PHE:H	1.39	0.87
1:A:355:PRO:HG2	1:A:601:LEU:HD22	1.58	0.85
1:A:329:THR:HG23	1:A:332:GLN:H	1.47	0.80
1:A:348:LEU:HB2	1:A:402:ARG:HH11	1.43	0.80
1:A:310:GLU:OE1	1:A:352:VAL:HB	1.83	0.79
1:A:617:VAL:HG23	1:A:622:VAL:HG23	1.62	0.79
2:B:23:GLY:N	4:B:301:GSP:O2B	2.13	0.78
1:A:345:ASN:HB3	1:A:348:LEU:HD13	1.65	0.78
2:B:17:ILE:HD13	2:B:109:LEU:HD11	1.65	0.77
1:A:310:GLU:CA	1:A:352:VAL:HG12	2.15	0.77
1:A:348:LEU:CB	1:A:402:ARG:HH11	1.93	0.77
2:B:32:THR:HG21	2:B:49:ALA:HB1	1.66	0.76
1:A:403:ILE:HG22	1:A:549:PRO:HB3	1.65	0.76
1:A:348:LEU:HD23	1:A:550:TYR:OH	1.86	0.75
1:A:633:TYR:CZ	1:A:637:GLU:HG3	2.22	0.74
1:A:652:ASN:HB3	1:A:684:HIS:CD2	2.24	0.73
1:A:310:GLU:HA	1:A:352:VAL:CG1	2.18	0.73
2:B:89:LEU:HD11	2:B:105:TRP:HB3	1.70	0.72
1:A:348:LEU:HB3	1:A:349:PRO:HD3	1.73	0.71
1:A:310:GLU:OE1	1:A:352:VAL:CB	2.39	0.70
2:B:88:LEU:HD23	2:B:120:MET:HB3	1.74	0.70
1:A:617:VAL:HG23	1:A:622:VAL:CG2	2.21	0.70
2:B:55:VAL:HG22	2:B:60:ILE:HD13	1.74	0.70
1:A:206:ILE:HD11	1:A:394:PHE:CE2	2.27	0.69
1:A:564:LYS:HE3	1:A:567:ASP:HB2	1.76	0.68
1:A:579:LEU:HD21	1:A:663:VAL:HG11	1.77	0.67
1:A:640:SER:O	1:A:643:THR:HG22	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LEU:HD22	1:A:603:ILE:HA	1.77	0.67
1:A:695:SER:OG	1:A:768:THR:HG22	1.96	0.66
1:A:324:LEU:O	1:A:333:LYS:HE3	1.96	0.66
2:B:28:LEU:HD22	2:B:66:ASP:HB2	1.77	0.65
1:A:355:PRO:HG2	1:A:601:LEU:CD2	2.25	0.65
2:B:89:LEU:HD21	2:B:102:VAL:HG13	1.77	0.65
1:A:672:ARG:NH2	1:A:689:ASP:O	2.29	0.65
2:B:125:LYS:HG2	4:B:301:GSP:C6	2.32	0.65
1:A:242:SER:O	1:A:306:ARG:HD3	1.97	0.64
1:A:344:LEU:O	1:A:346:HIS:O	2.17	0.63
2:B:14:VAL:HB	2:B:64:ILE:HD13	1.81	0.62
1:A:673:HIS:HA	1:A:709:LYS:HE3	1.80	0.62
1:A:564:LYS:NZ	3:A:801:5W3:O10	2.24	0.62
1:A:149:TYR:HA	1:A:182:MET:HE3	1.82	0.61
1:A:593:LEU:CD2	1:A:732:LEU:HB3	2.31	0.61
1:A:537:TRP:HB2	1:A:614:VAL:HB	1.83	0.60
1:A:612:PRO:HA	3:A:801:5W3:C20	2.31	0.60
1:A:780:MET:SD	1:A:785:LEU:HD23	2.41	0.60
1:A:149:TYR:HA	1:A:182:MET:CE	2.30	0.60
2:B:12:PHE:CD2	2:B:60:ILE:HG21	2.37	0.60
2:B:23:GLY:HA2	4:B:301:GSP:O1A	2.02	0.60
1:A:345:ASN:HB3	1:A:348:LEU:CD1	2.32	0.60
1:A:564:LYS:HE3	1:A:567:ASP:CB	2.31	0.60
2:B:31:PHE:O	2:B:51:ARG:NH1	2.31	0.60
1:A:348:LEU:CD2	1:A:550:TYR:OH	2.48	0.59
2:B:28:LEU:HD13	2:B:64:ILE:HG21	1.85	0.59
1:A:178:GLN:HA	1:A:754:MET:HE2	1.84	0.59
1:A:313:PHE:HB2	1:A:352:VAL:HG11	1.84	0.59
1:A:749:GLN:O	1:A:753:ILE:HG13	2.03	0.59
1:A:329:THR:HG22	1:A:332:GLN:HB2	1.84	0.58
1:A:571:GLN:OE1	1:A:761:PRO:HG2	2.03	0.58
1:A:628:LEU:HD22	1:A:632:ASP:HB3	1.86	0.58
2:B:9:ASP:HB2	2:B:59:THR:O	2.04	0.57
1:A:208:PHE:CE1	1:A:212:CYS:SG	2.97	0.57
2:B:11:LEU:O	2:B:11:LEU:HD23	2.05	0.57
2:B:55:VAL:HG22	2:B:60:ILE:CD1	2.34	0.57
1:A:654:VAL:HG13	1:A:729:TYR:HB2	1.86	0.57
2:B:89:LEU:CD2	2:B:102:VAL:HG13	2.35	0.56
1:A:310:GLU:OE1	1:A:352:VAL:CA	2.53	0.56
1:A:752:GLU:HA	1:A:769:ILE:HD11	1.87	0.56
2:B:76:ILE:H	2:B:76:ILE:HD12	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASN:O	1:A:348:LEU:HA	2.05	0.56
2:B:31:PHE:CB	2:B:165:PHE:CE1	2.89	0.56
2:B:17:ILE:CD1	2:B:109:LEU:HD11	2.36	0.56
1:A:329:THR:HG22	1:A:332:GLN:CG	2.36	0.55
2:B:172:ILE:O	2:B:175:ILE:HG12	2.06	0.55
1:A:345:ASN:O	1:A:348:LEU:CA	2.55	0.55
1:A:586:TRP:CE2	1:A:593:LEU:HD12	2.42	0.55
1:A:726:PHE:O	1:A:729:TYR:HB3	2.07	0.54
1:A:537:TRP:N	1:A:615:ASN:OD1	2.39	0.54
1:A:633:TYR:CE2	1:A:637:GLU:HG3	2.42	0.54
1:A:345:ASN:O	1:A:348:LEU:HB2	2.08	0.53
1:A:540:LYS:O	1:A:544:ILE:HG13	2.08	0.53
2:B:30:ARG:HG3	2:B:161:VAL:HG11	1.89	0.53
1:A:393:ASN:HB3	1:A:396:THR:HG22	1.90	0.53
1:A:342:SER:HA	1:A:345:ASN:HD21	1.72	0.53
1:A:318:MET:HE1	1:A:563:VAL:HG13	1.91	0.53
1:A:342:SER:HA	1:A:345:ASN:ND2	2.23	0.53
1:A:310:GLU:OE1	1:A:352:VAL:HA	2.08	0.53
2:B:119:ILE:HB	2:B:148:LEU:HD23	1.90	0.53
2:B:120:MET:HE1	2:B:167:THR:HB	1.91	0.53
1:A:348:LEU:HB3	1:A:402:ARG:HH11	1.72	0.52
2:B:14:VAL:HB	2:B:64:ILE:CD1	2.39	0.52
1:A:134:PHE:O	1:A:163:ARG:NH1	2.43	0.52
2:B:16:LEU:CD2	2:B:88:LEU:HB2	2.40	0.52
1:A:176:LEU:N	1:A:177:PRO:CD	2.72	0.52
1:A:763:PHE:HA	1:A:768:THR:HG21	1.92	0.52
1:A:533:LEU:HG	1:A:534:LYS:H	1.75	0.52
2:B:89:LEU:CD1	2:B:105:TRP:HB3	2.40	0.52
1:A:348:LEU:HG	1:A:364:VAL:O	2.10	0.51
2:B:17:ILE:HD11	2:B:89:LEU:HD12	1.91	0.51
2:B:89:LEU:HD11	2:B:105:TRP:CB	2.38	0.51
1:A:599:LYS:O	1:A:600:ILE:HD13	2.10	0.51
1:A:351:ARG:O	1:A:351:ARG:HG2	2.11	0.51
1:A:206:ILE:HD11	1:A:394:PHE:HE2	1.72	0.50
1:A:129:TRP:N	1:A:129:TRP:CD1	2.79	0.50
1:A:573:LEU:O	1:A:576:PHE:HB3	2.11	0.50
1:A:752:GLU:HA	1:A:769:ILE:CD1	2.41	0.50
2:B:17:ILE:HG13	2:B:89:LEU:HA	1.93	0.50
1:A:324:LEU:HD23	1:A:336:ARG:HD2	1.93	0.50
1:A:139:PHE:HA	1:A:143:MET:CE	2.27	0.50
1:A:568:ASP:C	1:A:569:LEU:HD23	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:ASP:O	2:B:10:TYR:HD2	1.94	0.49
1:A:329:THR:CG2	1:A:332:GLN:H	2.22	0.49
1:A:564:LYS:HD3	1:A:569:LEU:HD21	1.94	0.49
2:B:102:VAL:HG11	2:B:121:LEU:HD11	1.95	0.49
1:A:329:THR:CG2	1:A:332:GLN:HG3	2.42	0.49
2:B:93:ILE:C	2:B:93:ILE:HD12	2.32	0.49
1:A:165:PHE:CZ	2:B:130:HIS:HB3	2.48	0.48
1:A:619:ILE:HB	1:A:674:ASN:HB3	1.94	0.48
2:B:140:ARG:HB2	2:B:140:ARG:NH1	2.28	0.48
1:A:340:GLU:HG3	1:A:343:LEU:HD12	1.96	0.48
1:A:657:CYS:HB3	1:A:729:TYR:HE1	1.79	0.48
1:A:662:LEU:HD22	1:A:737:LEU:HD13	1.95	0.48
2:B:16:LEU:HD23	2:B:88:LEU:HB2	1.95	0.48
1:A:141:ILE:HG12	1:A:172:VAL:HA	1.95	0.48
1:A:329:THR:HG22	1:A:332:GLN:CB	2.42	0.48
1:A:715:VAL:HG11	1:A:721:LEU:HD23	1.95	0.48
1:A:195:LYS:N	1:A:196:PRO:CD	2.77	0.48
1:A:236:LEU:O	1:A:240:ILE:HG13	2.14	0.48
1:A:341:LEU:O	1:A:344:LEU:HB2	2.13	0.47
1:A:533:LEU:HG	1:A:534:LYS:N	2.29	0.47
2:B:46:VAL:HG11	2:B:65:TRP:HE3	1.79	0.47
1:A:139:PHE:HD1	1:A:143:MET:CE	2.26	0.47
2:B:15:VAL:HG23	2:B:87:ALA:CB	2.44	0.47
2:B:128:LEU:HD21	4:B:301:GSP:N2	2.29	0.47
1:A:389:LEU:HD22	1:A:555:ASN:HB3	1.97	0.47
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.63	0.47
1:A:348:LEU:HD23	1:A:402:ARG:HG3	1.95	0.47
2:B:119:ILE:CG2	2:B:148:LEU:HD22	2.44	0.47
2:B:175:ILE:O	2:B:175:ILE:HG22	2.15	0.47
2:B:79:ALA:O	2:B:82:ARG:HG2	2.14	0.47
1:A:670:LYS:HB2	1:A:692:PHE:HB3	1.97	0.46
1:A:317:LEU:HA	1:A:317:LEU:HD23	1.66	0.46
1:A:359:PHE:CZ	1:A:559:LEU:HD21	2.50	0.46
1:A:162:ASN:OD1	2:B:130:HIS:HB2	2.15	0.46
1:A:744:MET:HG3	1:A:776:PHE:CD2	2.51	0.46
2:B:78:SER:HA	2:B:81:TYR:CE2	2.51	0.46
1:A:603:ILE:HD11	1:A:609:MET:HG3	1.97	0.46
1:A:654:VAL:HG22	1:A:718:MET:HG2	1.96	0.46
1:A:695:SER:HB2	1:A:762:CYS:O	2.15	0.46
1:A:201:ARG:HD2	1:A:204:GLN:NE2	2.31	0.46
1:A:603:ILE:HD12	1:A:608:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ALA:N	1:A:309:PRO:CD	2.79	0.46
1:A:313:PHE:CB	1:A:352:VAL:HG11	2.46	0.46
1:A:388:VAL:HG22	1:A:557:ARG:O	2.16	0.46
1:A:619:ILE:O	1:A:623:LYS:HG3	2.16	0.45
1:A:318:MET:CE	1:A:563:VAL:HG13	2.46	0.45
1:A:345:ASN:ND2	1:A:345:ASN:H	2.13	0.45
1:A:354:LEU:H	1:A:361:HIS:CE1	2.34	0.45
1:A:206:ILE:HB	1:A:307:LEU:HD21	1.98	0.45
3:A:801:5W3:N24	3:A:801:5W3:C7	2.79	0.45
1:A:139:PHE:HD1	1:A:143:MET:HE3	1.81	0.45
1:A:657:CYS:HB3	1:A:729:TYR:CE1	2.51	0.44
1:A:196:PRO:HG2	2:B:131:LEU:HD22	1.98	0.44
1:A:182:MET:HA	1:A:186:MET:HG3	1.99	0.44
2:B:25:SER:OG	2:B:43:THR:OG1	2.35	0.44
2:B:109:LEU:HD12	2:B:109:LEU:N	2.32	0.44
1:A:241:LEU:HD22	1:A:311:ARG:HD2	1.98	0.44
1:A:345:ASN:O	1:A:348:LEU:CB	2.66	0.44
2:B:38:LEU:HA	4:B:301:GSP:O2'	2.18	0.44
1:A:593:LEU:HD21	1:A:732:LEU:O	2.17	0.44
1:A:756:GLN:HA	1:A:756:GLN:HE21	1.83	0.43
2:B:46:VAL:HG21	2:B:80:TYR:CD2	2.54	0.43
2:B:11:LEU:C	2:B:11:LEU:HD23	2.39	0.43
2:B:125:LYS:HG2	4:B:301:GSP:C5	2.54	0.43
1:A:368:HIS:CE1	1:A:369:THR:HG23	2.53	0.43
1:A:669:VAL:HA	1:A:693:ILE:HG22	2.01	0.43
2:B:22:VAL:HA	2:B:92:ASP:HB2	2.00	0.43
2:B:89:LEU:C	2:B:89:LEU:HD23	2.39	0.43
1:A:737:LEU:HD12	1:A:737:LEU:HA	1.90	0.43
2:B:119:ILE:HG21	2:B:148:LEU:HD22	2.00	0.43
2:B:109:LEU:HD12	2:B:109:LEU:H	1.84	0.42
2:B:46:VAL:HA	2:B:66:ASP:O	2.19	0.42
1:A:206:ILE:HD11	1:A:394:PHE:CD2	2.54	0.42
1:A:177:PRO:HG2	1:A:577:GLN:OE1	2.19	0.42
2:B:20:SER:OG	2:B:69:GLY:HA3	2.18	0.42
2:B:118:VAL:HG21	2:B:172:ILE:HD13	2.01	0.42
2:B:15:VAL:HG23	2:B:87:ALA:HB1	2.01	0.42
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.71	0.42
1:A:149:TYR:HA	1:A:182:MET:HE1	2.01	0.42
1:A:667:LEU:HD23	1:A:667:LEU:HA	1.82	0.42
2:B:28:LEU:HD13	2:B:64:ILE:CG2	2.49	0.42
1:A:195:LYS:HB3	1:A:196:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:GLN:HA	2:B:58:LYS:O	2.19	0.42
1:A:387:GLU:OE1	1:A:548:SER:OG	2.26	0.42
1:A:354:LEU:HA	1:A:355:PRO:HD2	1.86	0.41
2:B:78:SER:HA	2:B:81:TYR:CD2	2.55	0.41
1:A:310:GLU:N	1:A:352:VAL:HG12	2.34	0.41
1:A:679:LEU:HD12	1:A:684:HIS:O	2.20	0.41
1:A:176:LEU:O	1:A:180:LEU:HG	2.21	0.41
1:A:342:SER:C	1:A:345:ASN:HD22	2.23	0.41
1:A:660:TYR:HB3	1:A:687:HIS:CD2	2.56	0.41
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.76	0.41
1:A:355:PRO:CG	1:A:601:LEU:CD2	2.97	0.41
1:A:306:ARG:HA	1:A:351:ARG:HH22	1.55	0.41
1:A:580:LYS:HA	1:A:580:LYS:HD2	1.82	0.41
2:B:120:MET:HE3	2:B:120:MET:HB2	1.83	0.41
1:A:206:ILE:O	1:A:209:SER:HB2	2.21	0.41
1:A:798:ARG:O	1:A:799:SER:CB	2.69	0.41
1:A:575:ALA:O	1:A:579:LEU:HG	2.21	0.41
1:A:593:LEU:HD23	1:A:732:LEU:HB3	2.01	0.41
2:B:118:VAL:CG2	2:B:172:ILE:HD13	2.51	0.41
1:A:379:LYS:HE2	1:A:379:LYS:HB2	1.75	0.40
1:A:177:PRO:C	1:A:754:MET:HE1	2.41	0.40
2:B:93:ILE:HD12	2:B:94:ALA:N	2.36	0.40
1:A:744:MET:O	1:A:744:MET:HG2	2.20	0.40
2:B:25:SER:HA	2:B:66:ASP:OD2	2.22	0.40
1:A:178:GLN:N	1:A:178:GLN:OE1	2.55	0.40
1:A:593:LEU:HD21	1:A:732:LEU:HB3	2.01	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	455/572 (80%)	440 (97%)	15 (3%)	0	100	100
2	B	163/221 (74%)	152 (93%)	11 (7%)	0	100	100
All	All	618/793 (78%)	592 (96%)	26 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	417/517 (81%)	414 (99%)	3 (1%)	84	90
2	B	129/191 (68%)	129 (100%)	0	100	100
All	All	546/708 (77%)	543 (100%)	3 (0%)	88	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	351	ARG
1	A	391	CYS
1	A	648	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	ASN
1	A	749	GLN
2	B	112	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GSP	B	301	-	26,34,34	4.17	13 (50%)	28,54,54	2.81	11 (39%)
3	5W3	A	801	-	31,35,35	2.91	8 (25%)	37,50,50	3.33	20 (54%)

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
4	GSP	B	301	-	-	3/17/38/38	0/3/3/3
3	5W3	A	801	-	-	7/24/24/24	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	5W3	C6-S8	-10.22	1.62	1.77
4	B	301	GSP	C2'-C3'	-10.15	1.25	1.53
4	B	301	GSP	O4'-C1'	8.43	1.52	1.41
3	A	801	5W3	C1-C19	7.67	1.50	1.37
4	B	301	GSP	C4-N3	6.94	1.46	1.35
4	B	301	GSP	O4'-C4'	-6.74	1.29	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	GSP	C6-C5	6.61	1.52	1.41
4	B	301	GSP	C3'-C4'	5.47	1.67	1.53
3	A	801	5W3	C27-C23	5.00	1.51	1.42
4	B	301	GSP	C2-N2	4.87	1.43	1.33
3	A	801	5W3	C23-N21	4.62	1.37	1.33
4	B	301	GSP	C6-N1	4.44	1.40	1.33
4	B	301	GSP	C2-N1	4.30	1.43	1.35
3	A	801	5W3	C25-CL	4.14	1.83	1.74
4	B	301	GSP	O2'-C2'	3.59	1.51	1.43
3	A	801	5W3	C25-N24	3.03	1.35	1.31
4	B	301	GSP	C2-N3	2.98	1.48	1.34
4	B	301	GSP	C2'-C1'	2.92	1.58	1.53
4	B	301	GSP	PG-S1G	2.14	1.95	1.90
3	A	801	5W3	C26-C25	2.13	1.41	1.38
3	A	801	5W3	C26-C27	2.07	1.41	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	GSP	C1'-N9-C4	10.35	144.82	126.64
3	A	801	5W3	O10-S8-O9	-9.59	107.76	119.55
3	A	801	5W3	O17-C5-C6	8.71	123.25	116.50
4	B	301	GSP	N3-C2-N1	-5.37	120.06	127.22
3	A	801	5W3	C7-C2-C1	4.88	125.29	119.65
3	A	801	5W3	C26-C25-N24	-4.69	118.14	125.03
3	A	801	5W3	C2-C1-N22	-4.12	117.36	123.37
3	A	801	5W3	C26-C25-CL	4.09	123.98	118.88
4	B	301	GSP	C2-N3-C4	4.08	120.01	115.36
3	A	801	5W3	O17-C5-C4	-3.95	117.61	124.37
3	A	801	5W3	C31-N32-C33	3.91	128.58	122.56
3	A	801	5W3	C25-C26-C27	3.82	122.52	116.85
3	A	801	5W3	C18-O17-C5	3.79	123.25	117.53
3	A	801	5W3	C11-N11-S8	-3.72	108.40	120.41
3	A	801	5W3	C6-S8-N11	3.69	112.61	107.82
4	B	301	GSP	O4'-C1'-C2'	-3.48	101.85	106.93
3	A	801	5W3	C31-C30-N29	3.37	118.50	111.46
3	A	801	5W3	C19-N21-C23	3.25	109.32	103.59
4	B	301	GSP	PA-O3A-PB	-2.80	123.23	132.83
3	A	801	5W3	C7-C6-C5	-2.76	117.36	120.04
4	B	301	GSP	C4-C5-N7	-2.71	106.58	109.40
3	A	801	5W3	C3-C2-C1	-2.67	116.30	120.24
3	A	801	5W3	CL-C25-N24	2.63	117.88	115.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	5W3	C7-C6-S8	2.45	122.82	118.51
3	A	801	5W3	C30-N29-C27	-2.43	119.25	123.28
4	B	301	GSP	C5-C6-N1	-2.35	120.22	123.43
4	B	301	GSP	C5'-C4'-C3'	-2.32	106.50	115.18
4	B	301	GSP	O5'-PA-O1A	-2.31	100.02	109.07
3	A	801	5W3	O9-S8-C6	2.20	111.28	107.66
4	B	301	GSP	C6-N1-C2	2.17	119.38	115.93
4	B	301	GSP	N2-C2-N1	2.06	120.46	117.25

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	GSP	O4'-C4'-C5'-O5'
3	A	801	5W3	C6-C5-O17-C18
3	A	801	5W3	C23-C27-N29-C30
3	A	801	5W3	C26-C27-N29-C30
3	A	801	5W3	C34-C33-N32-C31
3	A	801	5W3	O35-C33-N32-C31
4	B	301	GSP	C3'-C4'-C5'-O5'
3	A	801	5W3	N29-C30-C31-N32
3	A	801	5W3	C4-C5-O17-C18
4	B	301	GSP	PB-O3A-PA-O1A

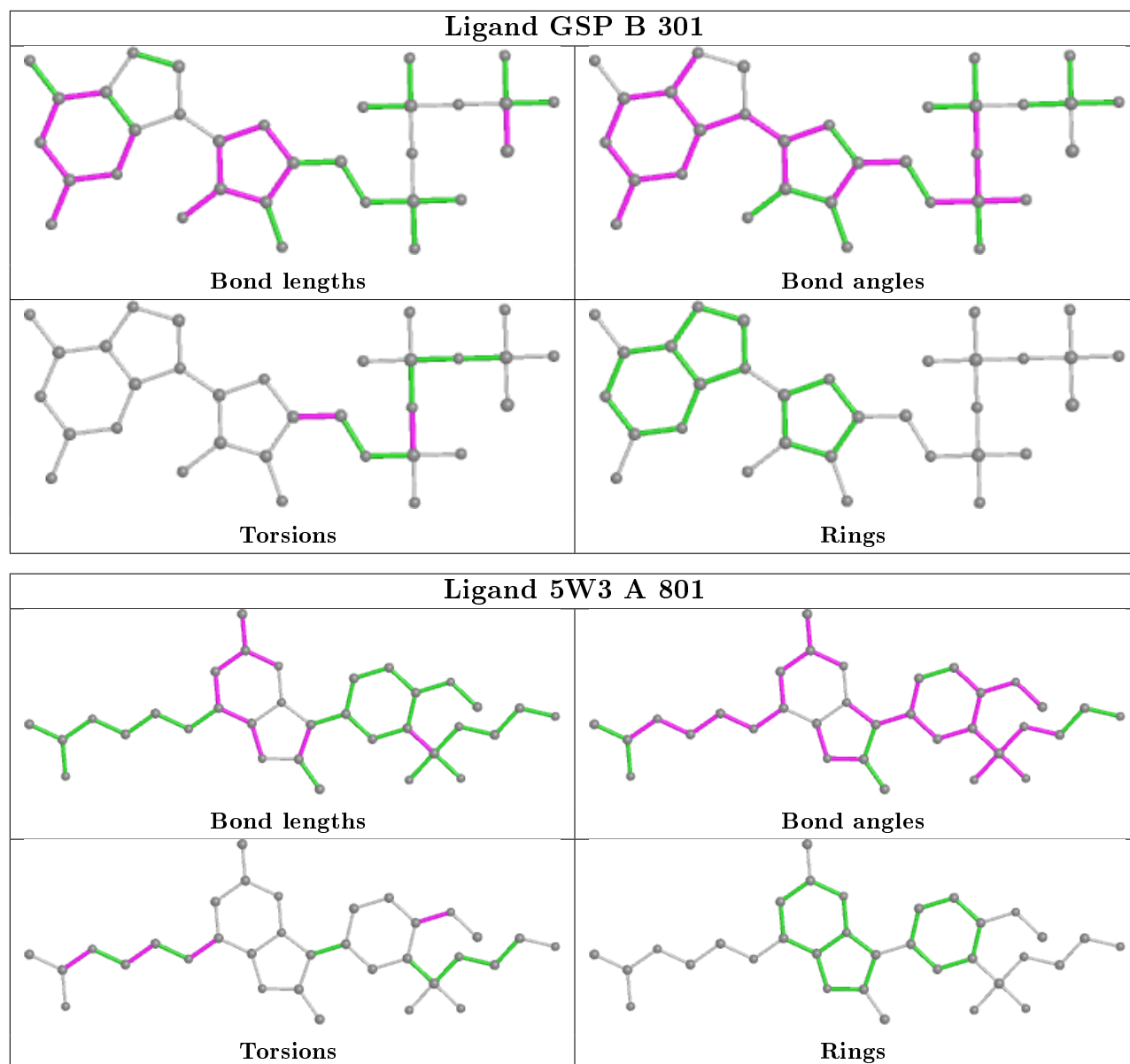
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	GSP	6	0
3	A	801	5W3	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	465/572 (81%)	0.30	9 (1%) 66 64	64, 98, 126, 153	0
2	B	167/221 (75%)	0.33	3 (1%) 68 66	89, 114, 141, 150	0
All	All	632/793 (79%)	0.31	12 (1%) 66 64	64, 104, 132, 153	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	119	ILE	3.7
1	A	533	LEU	3.4
1	A	708	PHE	3.3
1	A	406	ASN	3.2
2	B	142	PHE	2.4
1	A	383	LEU	2.3
1	A	307	LEU	2.3
2	B	147	GLY	2.3
1	A	531	VAL	2.3
1	A	328	PRO	2.2
1	A	306	ARG	2.2
1	A	630	LEU	2.2

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 monosaccharides in this entry.

6.4 Ligands ⓘ

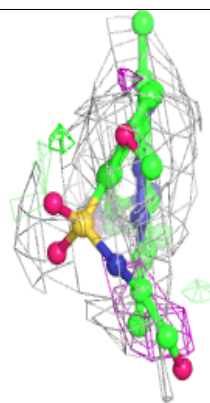
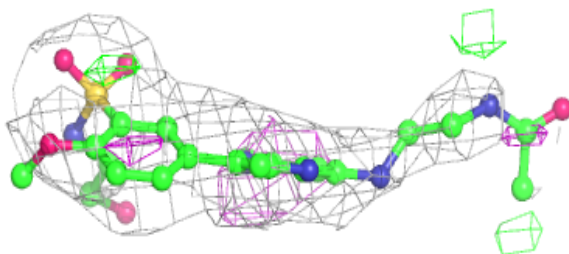
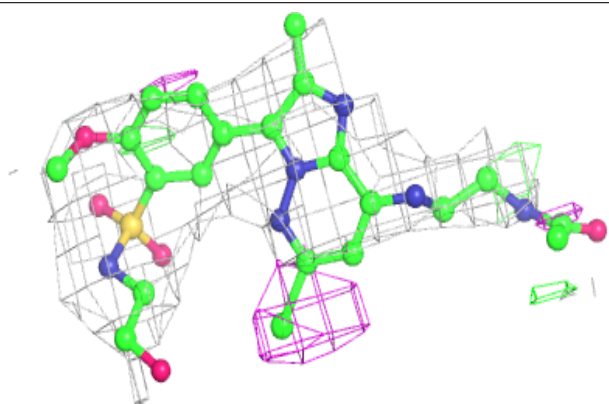
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	5W3	A	801	33/33	0.84	0.35	81,94,106,122	0
4	GSP	B	301	32/32	0.92	0.18	84,100,121,129	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.

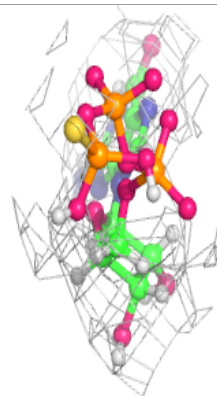
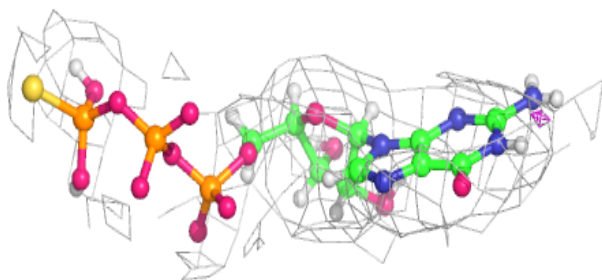
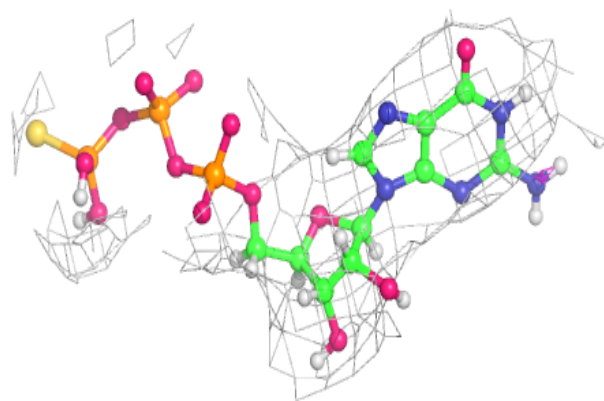
Electron density around 5W3 A 801:

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 GSP B 301:

$2mF_o-DF_c$ (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.