



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2022 – 01:10 pm BST

PDB ID : 6YR6
Title : 14-3-3 sigma in complex with hDM2-186 peptide
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Deposited on : 2020-04-19
Resolution : 1.75 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

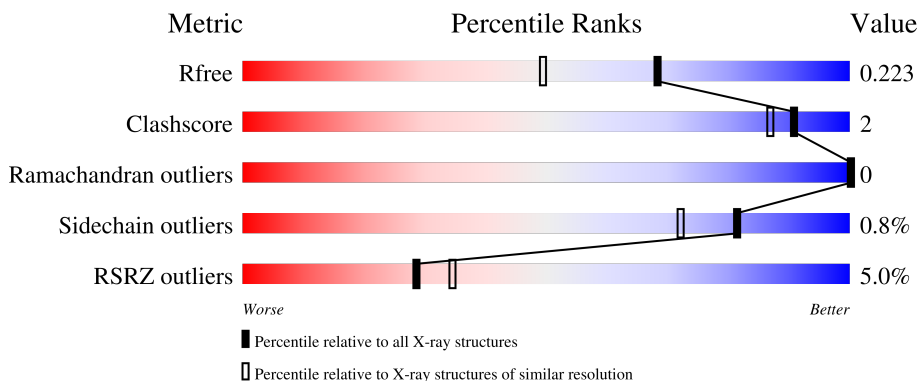
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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.



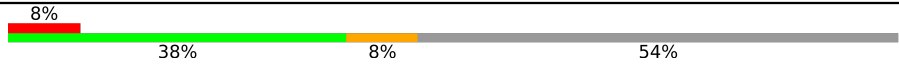


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	236	 5% 94%
1	C	236	 3% 93%
1	E	236	 3% 93%
1	G	236	 7% 94%
2	B	13	 38% 8% 54%

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Mol	Chain	Length	Quality of chain
2	D	13	 <p>8% 38% 8% 54%</p>
2	F	13	 <p>15% 31% 15% 54%</p>
2	H	13	 <p>8% 31% 15% 54%</p>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15129 atoms, of which 7091 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 14-3-3 protein sigma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	232	3589	1135	1769	311	361	13	0	10	0
1	C	229	3422	1092	1676	298	345	11	0	0	0
1	E	229	3472	1105	1707	301	348	11	0	4	0
1	G	226	3468	1098	1720	300	339	11	0	2	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P31947
A	-3	ALA	-	expression tag	UNP P31947
A	-2	MET	-	expression tag	UNP P31947
A	-1	GLY	-	expression tag	UNP P31947
A	0	SER	-	expression tag	UNP P31947
C	-4	GLY	-	expression tag	UNP P31947
C	-3	ALA	-	expression tag	UNP P31947
C	-2	MET	-	expression tag	UNP P31947
C	-1	GLY	-	expression tag	UNP P31947
C	0	SER	-	expression tag	UNP P31947
E	-4	GLY	-	expression tag	UNP P31947
E	-3	ALA	-	expression tag	UNP P31947
E	-2	MET	-	expression tag	UNP P31947
E	-1	GLY	-	expression tag	UNP P31947
E	0	SER	-	expression tag	UNP P31947
G	-4	GLY	-	expression tag	UNP P31947
G	-3	ALA	-	expression tag	UNP P31947
G	-2	MET	-	expression tag	UNP P31947
G	-1	GLY	-	expression tag	UNP P31947
G	0	SER	-	expression tag	UNP P31947

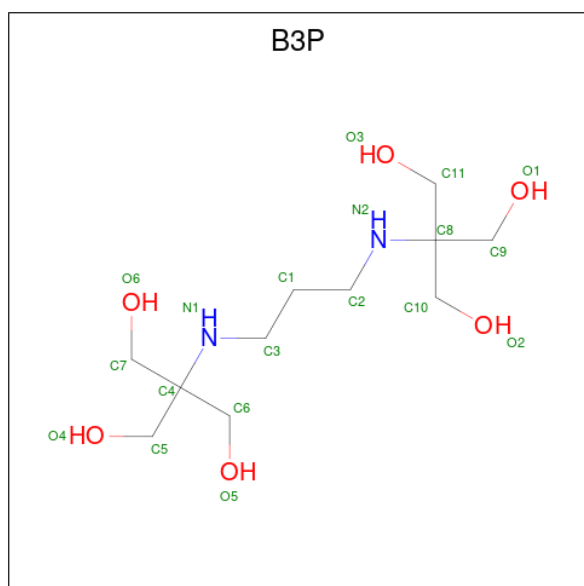
- Molecule 2 is a protein called hDM2-186.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	B	6	Total	C	H	N	O	P	0	2	0
			122	34	57	16	14	1			
2	D	6	Total	C	H	N	O	P	0	0	0
			98	28	44	12	13	1			
2	F	6	Total	C	H	N	O	P	0	0	0
			81	25	33	9	13	1			
2	H	6	Total	C	H	N	O	P	0	0	0
			83	25	33	11	13	1			

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
3	A	3	Total	I	0	0
			3	3		
3	C	2	Total	I	0	0
			2	2		
3	E	3	Total	I	0	0
			3	3		
3	G	3	Total	I	0	0
			3	3		

- Molecule 4 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	H	N	O	0	0
			45	11	26	2	6		
4	G	1	Total	C	H	N	O	0	0
			45	11	26	2	6		

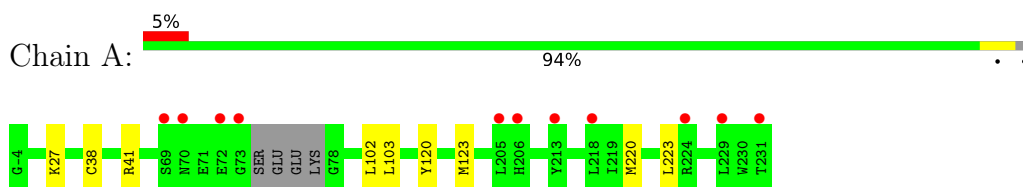
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	177	Total	O	0	0
			177	177		
5	B	9	Total	O	0	0
			9	9		
5	C	170	Total	O	0	0
			170	170		
5	D	3	Total	O	0	0
			3	3		
5	E	184	Total	O	0	0
			184	184		
5	F	6	Total	O	0	0
			6	6		
5	G	139	Total	O	0	0
			139	139		
5	H	5	Total	O	0	0
			5	5		

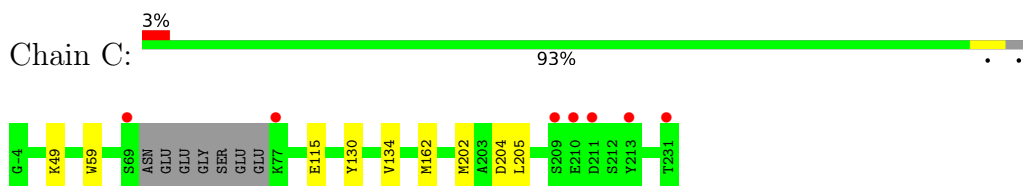
3 Residue-property plots [i](#)

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.

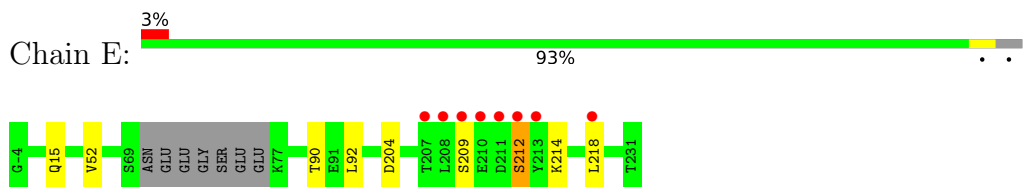
- Molecule 1: 14-3-3 protein sigma



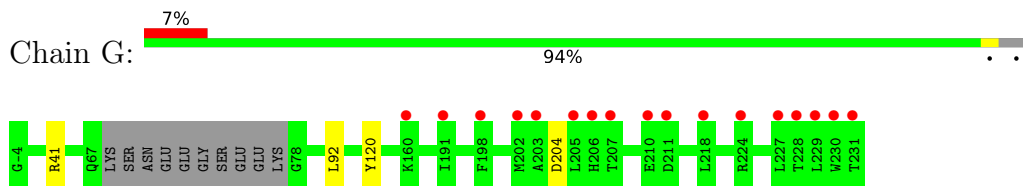
- Molecule 1: 14-3-3 protein sigma



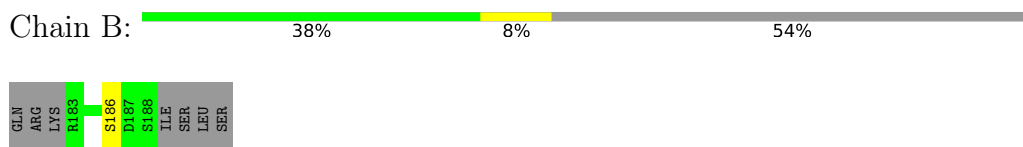
- Molecule 1: 14-3-3 protein sigma



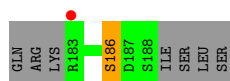
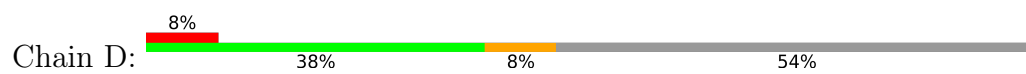
- Molecule 1: 14-3-3 protein sigma



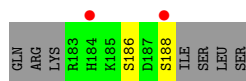
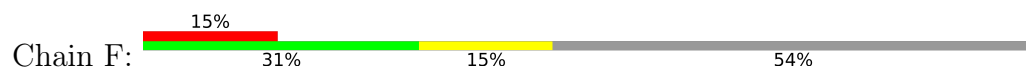
- Molecule 2: hDM2-186



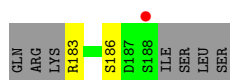
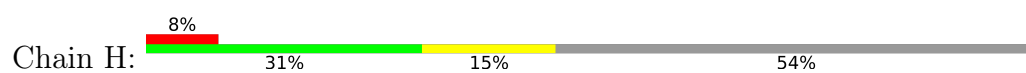
- Molecule 2: hDM2-186



- Molecule 2: hDM2-186



- Molecule 2: hDM2-186



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.23Å 74.57Å 77.97Å 98.43° 111.09° 93.12°	Depositor
Resolution (Å)	56.90 – 1.75 73.26 – 1.75	Depositor EDS
% Data completeness (in resolution range)	94.9 (56.90-1.75) 90.0 (73.26-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.75Å)	Xtrriage
Refinement program	PHENIX 1.12_2829, REFMAC 5.8.0238	Depositor
R, R_{free}	0.199 , 0.224 0.198 , 0.223	Depositor DCC
R_{free} test set	6318 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtrriage
Anisotropy	0.241	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	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	0.94	EDS
Total number of atoms	15129	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.64% 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: SEP, IOD, B3P

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	0.29	0/1894	0.45	0/2549
1	C	0.27	0/1771	0.44	0/2392
1	E	0.30	0/1807	0.46	0/2439
1	G	0.27	0/1781	0.42	0/2400
2	B	0.24	0/65	0.51	0/82
2	D	0.24	0/43	0.52	0/53
2	F	0.20	0/37	0.33	0/46
2	H	0.21	0/39	0.47	0/49
All	All	0.28	0/7437	0.44	0/10010

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	1820	1769	1720	5	0
1	C	1746	1676	1676	5	0
1	E	1765	1707	1691	7	0
1	G	1748	1720	1713	2	0
2	B	65	57	49	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	54	44	44	1	0
2	F	48	33	33	0	0
2	H	50	33	33	1	0
3	A	3	0	0	0	0
3	C	2	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	C	19	26	26	3	0
4	G	19	26	26	3	0
5	A	177	0	0	0	0
5	B	9	0	0	0	0
5	C	170	0	0	0	0
5	D	3	0	0	0	0
5	E	184	0	0	1	0
5	F	6	0	0	0	0
5	G	139	0	0	0	0
5	H	5	0	0	1	0
All	All	8038	7091	7011	24	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 2.

All (24) 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:E:15:GLN:NE2	5:E:401:HOH:O	2.19	0.75
1:A:38[B]:CYS:SG	1:A:41[B]:ARG:NH1	2.60	0.74
2:H:183:ARG:NH1	5:H:201:HOH:O	2.29	0.64
4:C:303:B3P:O3	4:C:303:B3P:H22	1.97	0.64
1:E:212:SER:O	1:E:212:SER:OG	2.13	0.62
1:C:202:MET:HE3	1:C:205:LEU:CB	2.39	0.53
1:A:220:MET:HA	1:A:223:LEU:HD12	1.94	0.50
1:C:115:GLU:HA	1:C:162:MET:HE3	1.95	0.48
4:C:303:B3P:H91	4:C:303:B3P:H31	1.95	0.48
1:E:52:VAL:HG23	1:E:92[B]:LEU:HD12	1.97	0.46
4:G:304:B3P:O3	4:G:304:B3P:O1	2.30	0.46
1:E:90:THR:CG2	4:G:304:B3P:H111	2.46	0.46
1:A:103:LEU:HD11	1:A:123[B]:MET:HG2	1.98	0.45
1:C:49:LYS:NZ	2:D:186:SEP:O3P	2.46	0.45
4:C:303:B3P:H51	4:C:303:B3P:H12	1.98	0.45
1:A:41[B]:ARG:HG2	1:A:120:TYR:OH	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:92:LEU:C	1:G:92:LEU:HD23	2.39	0.42
1:A:27:LYS:HG3	1:A:102:LEU:HD21	2.02	0.42
1:C:49:LYS:HE2	1:C:130:TYR:OH	2.20	0.42
1:C:59:TRP:CE2	1:C:134:VAL:HG12	2.55	0.41
1:E:52:VAL:HG23	1:E:92[B]:LEU:CD1	2.51	0.41
1:E:90:THR:HG23	4:G:304:B3P:H111	2.02	0.41
1:G:41:ARG:HG2	1:G:120:TYR:OH	2.21	0.40
1:E:214:LYS:O	1:E:218:LEU:HB2	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	A	239/236 (101%)	235 (98%)	4 (2%)	0	100	100
1	C	225/236 (95%)	223 (99%)	2 (1%)	0	100	100
1	E	229/236 (97%)	224 (98%)	5 (2%)	0	100	100
1	G	224/236 (95%)	221 (99%)	3 (1%)	0	100	100
2	B	4/13 (31%)	4 (100%)	0	0	100	100
2	D	3/13 (23%)	3 (100%)	0	0	100	100
2	F	3/13 (23%)	3 (100%)	0	0	100	100
2	H	3/13 (23%)	3 (100%)	0	0	100	100
All	All	930/996 (93%)	916 (98%)	14 (2%)	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	A	192/198 (97%)	192 (100%)	0	100	100
1	C	176/198 (89%)	175 (99%)	1 (1%)	86	79
1	E	181/198 (91%)	178 (98%)	3 (2%)	60	42
1	G	180/198 (91%)	179 (99%)	1 (1%)	86	79
2	B	7/12 (58%)	7 (100%)	0	100	100
2	D	5/12 (42%)	5 (100%)	0	100	100
2	F	4/12 (33%)	3 (75%)	1 (25%)	0	0
2	H	4/12 (33%)	4 (100%)	0	100	100
All	All	749/840 (89%)	743 (99%)	6 (1%)	81	72

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	204	ASP
1	E	204	ASP
1	E	209	SER
1	E	212	SER
2	F	188	SER
1	G	204	ASP

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
2	SEP	D	186	2	8,9,10	1.44	1 (12%)	8,12,14	1.54	2 (25%)
2	SEP	F	186	2	8,9,10	1.45	1 (12%)	8,12,14	0.93	0
2	SEP	B	186	2	8,9,10	1.45	1 (12%)	8,12,14	1.37	2 (25%)
2	SEP	H	186	2	8,9,10	1.50	1 (12%)	8,12,14	1.51	2 (25%)

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
2	SEP	D	186	2	-	0/5/8/10	-
2	SEP	F	186	2	-	0/5/8/10	-
2	SEP	B	186	2	-	0/5/8/10	-
2	SEP	H	186	2	-	0/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	186	SEP	P-O1P	3.18	1.60	1.50
2	D	186	SEP	P-O1P	3.09	1.60	1.50
2	B	186	SEP	P-O1P	3.09	1.60	1.50
2	F	186	SEP	P-O1P	2.97	1.60	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	186	SEP	OG-CB-CA	3.22	111.28	108.14
2	D	186	SEP	P-OG-CB	-2.82	110.53	118.30
2	H	186	SEP	P-OG-CB	-2.36	111.80	118.30
2	B	186	SEP	P-OG-CB	-2.36	111.80	118.30
2	B	186	SEP	OG-CB-CA	2.29	110.38	108.14
2	D	186	SEP	OG-CB-CA	2.24	110.33	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	186	SEP	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 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$
4	B3P	G	304	-	18,18,18	1.49	2 (11%)	21,23,23	1.28	2 (9%)
4	B3P	C	303	-	18,18,18	1.84	3 (16%)	21,23,23	1.22	2 (9%)

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	B3P	G	304	-	-	8/28/28/28	-
4	B3P	C	303	-	-	7/28/28/28	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	303	B3P	C2-N2	5.93	1.54	1.46
4	G	304	B3P	C2-N2	3.89	1.51	1.46
4	G	304	B3P	C9-C8	3.50	1.57	1.53
4	C	303	B3P	C9-C8	2.59	1.56	1.53
4	C	303	B3P	C11-C8	2.28	1.56	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	304	B3P	C3-N1-C4	-2.92	111.94	116.08
4	G	304	B3P	C2-N2-C8	-2.20	112.96	116.08
4	C	303	B3P	O4-C5-C4	-2.14	107.30	111.63
4	C	303	B3P	C7-C4-C5	-2.12	105.55	110.04

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	303	B3P	C1-C3-N1-C4
4	C	303	B3P	C5-C4-N1-C3
4	C	303	B3P	C6-C4-N1-C3
4	C	303	B3P	C7-C4-N1-C3
4	G	304	B3P	N2-C8-C9-O1
4	G	304	B3P	C10-C8-C9-O1
4	G	304	B3P	C11-C8-C9-O1
4	G	304	B3P	C3-C1-C2-N2
4	C	303	B3P	C1-C2-N2-C8
4	G	304	B3P	O3-C11-C8-C9
4	G	304	B3P	O3-C11-C8-C10
4	G	304	B3P	C1-C2-N2-C8
4	C	303	B3P	C3-C1-C2-N2
4	G	304	B3P	O3-C11-C8-N2
4	C	303	B3P	C11-C8-N2-C2

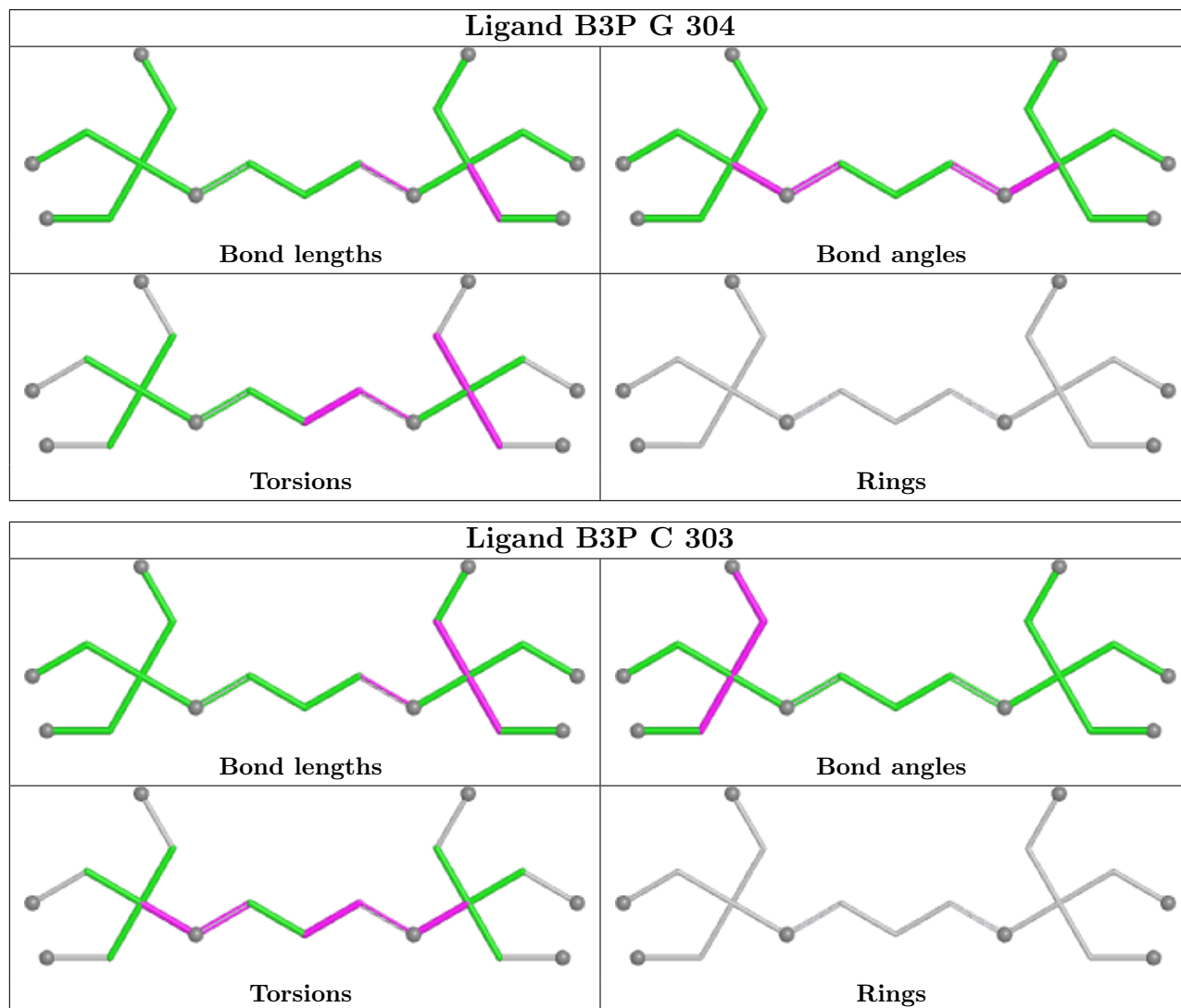
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	304	B3P	3	0
4	C	303	B3P	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	232/236 (98%)	0.44	11 (4%) 31 37	21, 31, 60, 102	0
1	C	229/236 (97%)	0.37	7 (3%) 49 55	22, 32, 58, 94	0
1	E	229/236 (97%)	0.39	8 (3%) 44 50	22, 31, 57, 86	0
1	G	226/236 (95%)	0.67	17 (7%) 14 19	24, 39, 72, 93	0
2	B	5/13 (38%)	0.87	0 100 100	42, 43, 48, 58	0
2	D	5/13 (38%)	1.40	1 (20%) 1 1	42, 49, 60, 72	0
2	F	5/13 (38%)	1.66	2 (40%) 0 0	41, 52, 60, 62	0
2	H	5/13 (38%)	1.07	1 (20%) 1 1	46, 52, 62, 67	0
All	All	936/996 (93%)	0.48	47 (5%) 28 34	21, 33, 64, 102	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	206	HIS	5.4
1	E	211	ASP	5.2
1	G	230	TRP	5.1
1	C	213	TYR	5.0
1	G	202	MET	4.9
1	A	206	HIS	4.5
1	E	209	SER	4.5
1	G	207	THR	4.2
1	G	205	LEU	4.2
2	D	183	ARG	4.2
1	G	229	LEU	4.1
1	G	231	THR	4.0
1	E	213	TYR	3.9
1	G	191	ILE	3.5
1	G	198	PHE	3.4
1	C	210	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	69	SER	3.3
1	C	231	THR	3.2
1	A	72	GLU	3.2
1	G	228	THR	2.9
1	C	211	ASP	2.9
1	A	205	LEU	2.9
2	F	188	SER	2.9
1	G	160	LYS	2.9
1	A	70	ASN	2.8
1	A	213	TYR	2.8
1	G	210	GLU	2.8
1	E	212	SER	2.7
1	G	227	LEU	2.7
1	E	210	GLU	2.7
1	C	209	SER	2.7
1	A	224	ARG	2.6
1	G	218	LEU	2.5
1	A	73	GLY	2.5
2	F	184	HIS	2.4
1	C	77	LYS	2.4
1	A	218	LEU	2.4
2	H	188	SER	2.3
1	G	211	ASP	2.3
1	G	203	ALA	2.2
1	G	224	ARG	2.2
1	A	229	LEU	2.2
1	E	208	LEU	2.2
1	C	69	SER	2.1
1	E	218	LEU	2.1
1	E	207	THR	2.0
1	A	231	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	SEP	H	186	10/11	0.96	0.12	34,41,49,51	0
2	SEP	D	186	10/11	0.97	0.10	25,29,37,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SEP	B	186	10/11	0.97	0.10	25,31,36,41	0
2	SEP	F	186	10/11	0.98	0.10	25,30,36,37	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

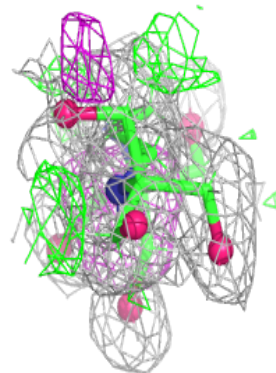
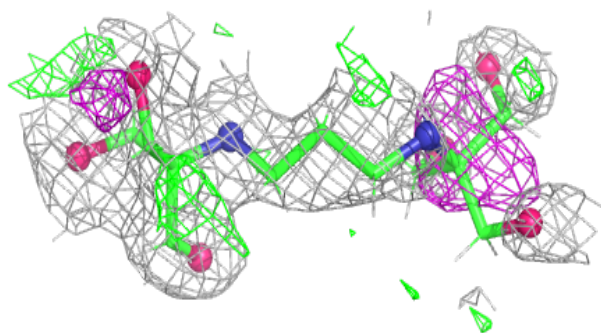
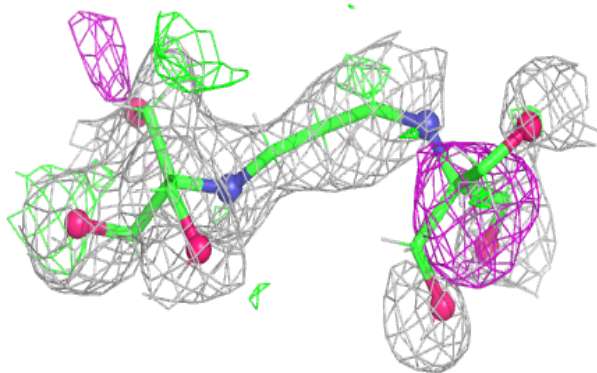
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	B3P	G	304	19/19	0.64	0.30	35,58,84,89	0
4	B3P	C	303	19/19	0.83	0.17	28,43,57,60	0
3	IOD	G	303	1/1	0.89	0.08	101,101,101,101	0
3	IOD	A	301	1/1	0.90	0.07	85,85,85,85	0
3	IOD	E	303	1/1	0.95	0.06	74,74,74,74	0
3	IOD	E	302	1/1	0.98	0.04	45,45,45,45	0
3	IOD	G	301	1/1	0.99	0.15	29,29,29,29	0
3	IOD	G	302	1/1	0.99	0.06	56,56,56,56	0
3	IOD	E	301	1/1	0.99	0.16	26,26,26,26	0
3	IOD	A	303	1/1	0.99	0.05	45,45,45,45	0
3	IOD	C	302	1/1	0.99	0.04	49,49,49,49	0
3	IOD	C	301	1/1	1.00	0.17	28,28,28,28	0
3	IOD	A	302	1/1	1.00	0.15	27,27,27,27	0

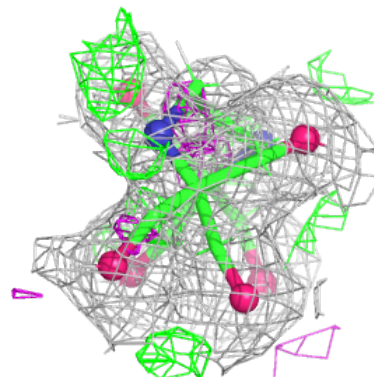
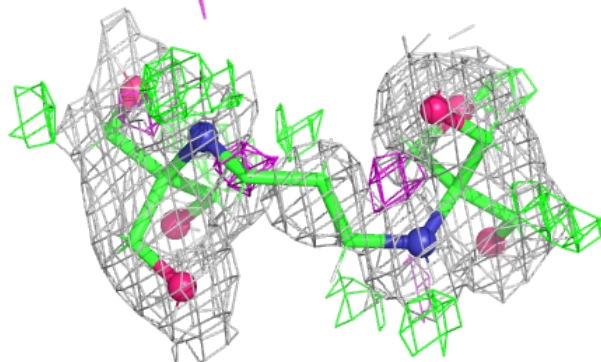
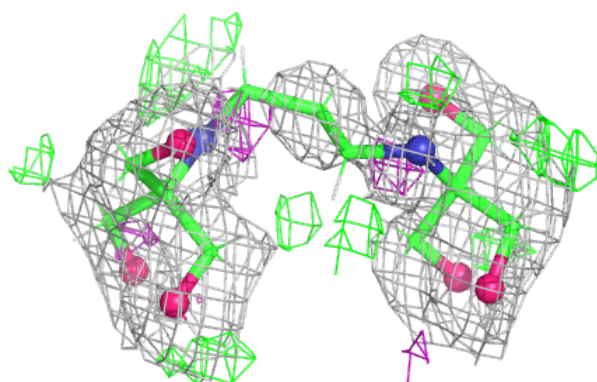
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around B3P G 304:

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

**Electron density around B3P C 303:**

$2mF_o-DF_c$ (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.