



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 11:00 PM EDT

PDB ID : 6TWZ  
Title : 14-3-3 sigma complexed with a phosphorylated 16E6 peptide  
Authors : Gogl, G.; Cousido-Siah, A.; Sluchanko, N.N.; Trave, G.  
Deposited on : 2020-01-13  
Resolution : 2.80 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](mailto: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>.

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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 : 2.37.1  
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) : 2.37.1

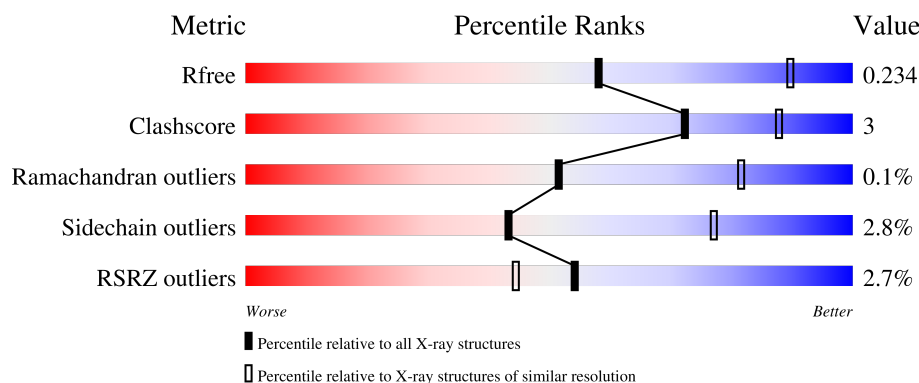
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	234	<div> <div>4%</div> <div>92%</div> <div>6%</div> </div>
1	B	234	<div> <div>2%</div> <div>91%</div> <div>6%</div> </div>
1	C	234	<div> <div>%</div> <div>90%</div> <div>9%</div> </div>
1	D	234	<div> <div>2%</div> <div>90%</div> <div>9%</div> </div>
2	D000	10	<div> <div>20%</div> <div>40%</div> <div>40%</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	10	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>10%50%30%20%</div>
2	F	10	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>10%30%20%30%20%</div>
2	G	10	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>40%30%10%20%</div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7586 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 14-3-3 protein sigma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1814	1132	308	365	9			
1	B	228	Total	C	N	O	S	0	0	0
			1790	1118	305	358	9			
1	C	231	Total	C	N	O	S	0	0	0
			1812	1131	308	363	10			
1	D	233	Total	C	N	O	S	0	0	0
			1817	1134	310	363	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P31947
A	-1	PRO	-	expression tag	UNP P31947
A	0	HIS	-	expression tag	UNP P31947
A	159	ALA	LYS	engineered mutation	UNP P31947
A	160	ALA	LYS	engineered mutation	UNP P31947
A	161	ALA	GLU	engineered mutation	UNP P31947
B	-2	GLY	-	expression tag	UNP P31947
B	-1	PRO	-	expression tag	UNP P31947
B	0	HIS	-	expression tag	UNP P31947
B	159	ALA	LYS	engineered mutation	UNP P31947
B	160	ALA	LYS	engineered mutation	UNP P31947
B	161	ALA	GLU	engineered mutation	UNP P31947
C	-2	GLY	-	expression tag	UNP P31947
C	-1	PRO	-	expression tag	UNP P31947
C	0	HIS	-	expression tag	UNP P31947
C	159	ALA	LYS	engineered mutation	UNP P31947
C	160	ALA	LYS	engineered mutation	UNP P31947
C	161	ALA	GLU	engineered mutation	UNP P31947
D	-2	GLY	-	expression tag	UNP P31947
D	-1	PRO	-	expression tag	UNP P31947
D	0	HIS	-	expression tag	UNP P31947

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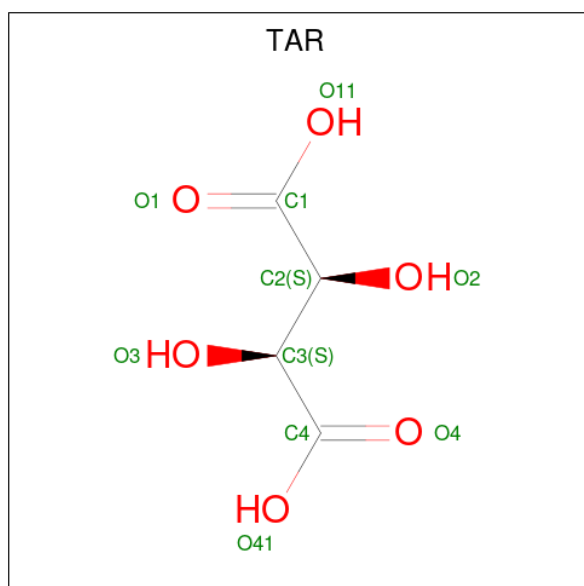
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Chain	Residue	Modelled	Actual	Comment	Reference
D	159	ALA	LYS	engineered mutation	UNP P31947
D	160	ALA	LYS	engineered mutation	UNP P31947
D	161	ALA	GLU	engineered mutation	UNP P31947

- Molecule 2 is a protein called phosphorylated 16E6 peptide.

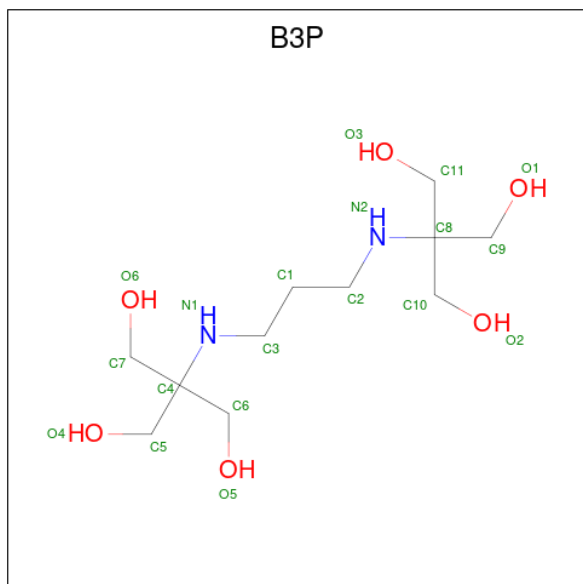
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	P	0	0	0
			72	39	15	17	1			
2	F	8	Total	C	N	O	P	0	0	0
			72	39	15	17	1			
2	G	8	Total	C	N	O	P	0	0	0
			78	42	18	17	1			
2	D000	8	Total	C	N	O	P	0	0	0
			72	39	15	17	1			

- Molecule 3 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula:  $C_4H_6O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		

- 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
			Total	C	N	O		
4	D	1	19	11	2	6	0	0

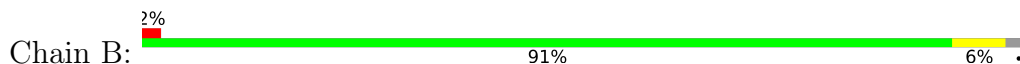
### 3 Residue-property plots [i](#)

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: 14-3-3 protein sigma



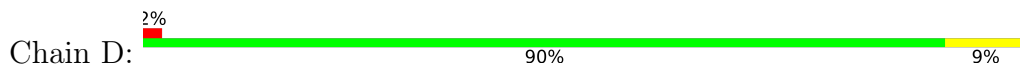
- Molecule 1: 14-3-3 protein sigma



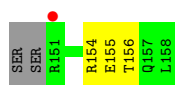
- Molecule 1: 14-3-3 protein sigma



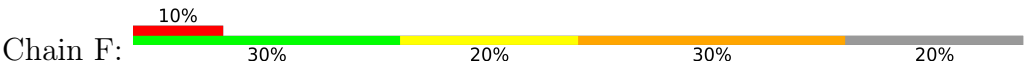
- Molecule 1: 14-3-3 protein sigma



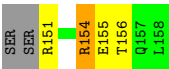
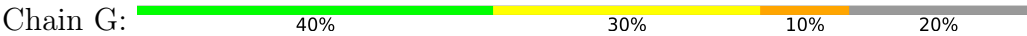
- Molecule 2: phosphorylated 16E6 peptide



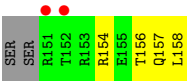
- Molecule 2: phosphorylated 16E6 peptide



• Molecule 2: phosphorylated 16E6 peptide



• Molecule 2: phosphorylated 16E6 peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.58Å 107.42Å 79.60Å 90.00° 109.29° 90.00°	Depositor
Resolution (Å)	48.56 – 2.80 48.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.56-2.80) 92.3 (48.56-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.14_3260, PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.203 , 0.236 0.203 , 0.234	Depositor DCC
$R_{free}$ test set	1761 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.4	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7586	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TAR, B3P, TPO

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	0.23	0/1841	0.38	0/2482
1	B	0.24	0/1816	0.38	0/2446
1	C	0.23	0/1839	0.38	0/2476
1	D	0.24	0/1844	0.39	0/2484
2	D000	0.33	0/59	0.68	0/74
2	E	0.22	0/59	0.58	0/74
2	F	0.22	0/59	0.64	0/74
2	G	0.20	0/65	0.57	0/81
All	All	0.24	0/7582	0.39	0/10191

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	1814	0	1769	9	0
1	B	1790	0	1755	13	0
1	C	1812	0	1776	11	0
1	D	1817	0	1777	13	0
2	D000	72	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	72	0	64	1	0
2	F	72	0	64	3	0
2	G	78	0	75	2	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
4	D	19	0	26	3	0
All	All	7586	0	7322	46	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 3.

All (46) 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:B:224:ARG:HG2	1:B:224:ARG:HH11	1.29	0.96
1:D:222:LEU:HD22	2:G:155:GLU:HG2	1.71	0.72
1:B:224:ARG:HG2	1:B:224:ARG:NH1	2.05	0.69
1:B:222:LEU:HD22	2:E:155:GLU:HG2	1.76	0.67
1:A:208:LEU:HD22	1:A:212:SER:HB3	1.82	0.60
1:C:222:LEU:HD22	2:F:155:GLU:HG2	1.82	0.60
1:A:80:GLU:OE2	1:B:8:GLN:NE2	2.35	0.59
1:A:27:LYS:HG3	1:A:102:LEU:HD11	1.89	0.55
1:B:27:LYS:HG3	1:B:102:LEU:HD11	1.90	0.53
1:D:27:LYS:HG3	1:D:102:LEU:HD11	1.90	0.52
2:F:157:GLN:HG3	2:F:158:LEU:OXT	2.08	0.52
1:C:182:GLU:CD	2:F:154:ARG:HE	2.13	0.52
1:A:129:ARG:HG3	1:A:183:ILE:HG13	1.90	0.52
1:C:129:ARG:HG3	1:C:183:ILE:HG13	1.93	0.50
1:B:180:HIS:HA	1:B:184:ALA:HB3	1.93	0.49
1:A:138:ASP:N	1:A:138:ASP:OD1	2.44	0.49
1:C:126:ASP:OD1	1:C:151:TYR:OH	2.25	0.49
1:C:41:ARG:HD2	1:C:119:PHE:CD1	2.47	0.48
1:C:180:HIS:HA	1:C:184:ALA:HB3	1.96	0.47
1:D:-1:PRO:C	1:D:1:MET:H	2.18	0.46
1:D:180:HIS:HA	1:D:184:ALA:HB3	1.98	0.45
1:D:30:VAL:HG22	1:D:36:LEU:HD11	1.99	0.45
1:C:2:GLU:HG3	1:C:4:ALA:H	1.82	0.44
1:A:140:LYS:HE2	1:A:144:ILE:HD11	2.00	0.44
1:C:30:VAL:HG22	1:C:36:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:VAL:HG22	1:A:36:LEU:HD11	1.98	0.44
1:D:129:ARG:HG3	1:D:183:ILE:HG13	1.99	0.44
4:D:302:B3P:O6	4:D:302:B3P:O5	2.29	0.44
1:D:23:ALA:HB1	1:D:48:TYR:CZ	2.53	0.43
1:B:224:ARG:NH1	1:B:224:ARG:CG	2.73	0.43
1:D:182:GLU:CD	2:G:154:ARG:HE	2.21	0.43
4:D:302:B3P:H112	4:D:302:B3P:H21	1.60	0.43
1:B:30:VAL:HG22	1:B:36:LEU:HD11	2.00	0.43
1:C:12:LEU:HD11	1:D:81:VAL:HG22	2.01	0.43
1:C:205:LEU:HD23	1:C:205:LEU:HA	1.93	0.43
1:C:7:ILE:HD13	1:C:40:GLU:OE2	2.20	0.42
1:A:8:GLN:NE2	1:B:80:GLU:HB2	2.35	0.41
1:D:7:ILE:HD13	1:D:40:GLU:OE2	2.19	0.41
1:A:12:LEU:HD11	1:B:81:VAL:HG22	2.01	0.41
1:D:205:LEU:HD23	1:D:205:LEU:HA	1.93	0.41
1:B:139:ASP:OD1	1:B:142:ARG:NH2	2.53	0.41
1:B:224:ARG:O	1:B:224:ARG:HG3	2.21	0.41
1:D:0:HIS:ND1	1:D:0:HIS:C	2.73	0.41
1:D:59:TRP:CE2	1:D:134:VAL:HG12	2.56	0.41
4:D:302:B3P:H32	4:D:302:B3P:H71	1.87	0.40
1:B:208:LEU:HD23	1:B:208:LEU:HA	1.88	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	231/234 (99%)	226 (98%)	5 (2%)	0	100	100
1	B	224/234 (96%)	220 (98%)	4 (2%)	0	100	100
1	C	227/234 (97%)	224 (99%)	3 (1%)	0	100	100
1	D	229/234 (98%)	224 (98%)	4 (2%)	1 (0%)	34	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D000	5/10 (50%)	5 (100%)	0	0	100	100
2	E	5/10 (50%)	5 (100%)	0	0	100	100
2	F	5/10 (50%)	5 (100%)	0	0	100	100
2	G	5/10 (50%)	5 (100%)	0	0	100	100
All	All	931/976 (95%)	914 (98%)	16 (2%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	0	HIS

### 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	189/195 (97%)	184 (97%)	5 (3%)	46	79
1	B	188/195 (96%)	185 (98%)	3 (2%)	62	88
1	C	191/195 (98%)	189 (99%)	2 (1%)	76	93
1	D	190/195 (97%)	187 (98%)	3 (2%)	62	88
2	D000	6/9 (67%)	3 (50%)	3 (50%)	0	0
2	E	6/9 (67%)	5 (83%)	1 (17%)	2	6
2	F	6/9 (67%)	3 (50%)	3 (50%)	0	0
2	G	7/9 (78%)	5 (71%)	2 (29%)	0	1
All	All	783/816 (96%)	761 (97%)	22 (3%)	43	77

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	ASP
1	A	176	PHE
1	A	204	ASP

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Mol	Chain	Res	Type
1	A	210	GLU
1	A	212	SER
1	B	76	GLU
1	B	176	PHE
1	B	224	ARG
1	C	72	GLU
1	C	176	PHE
1	D	0	HIS
1	D	176	PHE
1	D	204	ASP
2	E	154	ARG
2	F	154	ARG
2	F	155	GLU
2	F	157	GLN
2	G	151	ARG
2	G	154	ARG
2	D000	154	ARG
2	D000	157	GLN
2	D000	158	LEU

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 ⓘ

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	TPO	F	156	2	8,10,11	1.58	1 (12%)	10,14,16	1.72	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TPO	G	156	2	8,10,11	1.61	1 (12%)	10,14,16	1.75	2 (20%)
2	TPO	E	156	2	8,10,11	1.09	0	10,14,16	1.77	2 (20%)
2	TPO	D000	156	2	8,10,11	1.49	2 (25%)	10,14,16	1.04	1 (10%)

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	TPO	F	156	2	-	2/9/11/13	-
2	TPO	G	156	2	-	2/9/11/13	-
2	TPO	E	156	2	-	1/9/11/13	-
2	TPO	D000	156	2	-	1/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	156	TPO	P-O1P	3.38	1.61	1.50
2	G	156	TPO	P-O1P	3.32	1.61	1.50
2	D000	156	TPO	P-O3P	-2.54	1.45	1.54
2	D000	156	TPO	P-O2P	-2.43	1.45	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	156	TPO	P-OG1-CB	-4.61	109.28	123.21
2	G	156	TPO	P-OG1-CB	-4.31	110.18	123.21
2	F	156	TPO	P-OG1-CB	-4.22	110.45	123.21
2	G	156	TPO	CG2-CB-CA	-2.66	107.92	113.16
2	D000	156	TPO	O-C-CA	-2.61	117.95	124.78
2	E	156	TPO	CG2-CB-CA	-2.40	108.42	113.16
2	F	156	TPO	CG2-CB-CA	-2.39	108.45	113.16

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	156	TPO	O-C-CA-CB
2	F	156	TPO	CB-OG1-P-O2P

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Mol	Chain	Res	Type	Atoms
2	G	156	TPO	CB-OG1-P-O3P
2	F	156	TPO	O-C-CA-CB
2	G	156	TPO	O-C-CA-CB
2	D000	156	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 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	$\# Z  > 2$
3	TAR	B	301	-	9,9,9	1.01	0	12,12,12	1.37	2 (16%)
3	TAR	A	301	-	9,9,9	1.19	0	12,12,12	0.95	0
4	B3P	D	302	-	18,18,18	0.54	0	21,23,23	1.40	2 (9%)
3	TAR	C	301	-	9,9,9	1.00	0	12,12,12	1.31	2 (16%)
3	TAR	D	301	-	9,9,9	1.45	3 (33%)	12,12,12	1.50	3 (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
3	TAR	B	301	-	-	6/12/12/12	-
3	TAR	A	301	-	-	10/12/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	B3P	D	302	-	-	9/28/28/28	-
3	TAR	C	301	-	-	8/12/12/12	-
3	TAR	D	301	-	-	6/12/12/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	TAR	C3-C4	-2.17	1.49	1.52
3	D	301	TAR	O41-C4	-2.16	1.23	1.30
3	D	301	TAR	C2-C1	-2.11	1.49	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	302	B3P	C3-N1-C4	-3.95	110.47	116.08
4	D	302	B3P	C2-N2-C8	-2.99	111.84	116.08
3	B	301	TAR	O41-C4-C3	2.63	120.37	113.27
3	B	301	TAR	O11-C1-C2	2.60	120.31	113.27
3	C	301	TAR	O41-C4-C3	2.50	120.02	113.27
3	C	301	TAR	O11-C1-C2	2.47	119.96	113.27
3	D	301	TAR	O41-C4-C3	2.29	119.47	113.27
3	D	301	TAR	O3-C3-C4	-2.25	105.94	110.66
3	D	301	TAR	O11-C1-C2	2.06	118.83	113.27

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	TAR	O1-C1-C2-O2
3	C	301	TAR	O1-C1-C2-O2
3	C	301	TAR	O11-C1-C2-O2
3	A	301	TAR	O11-C1-C2-O2
3	A	301	TAR	O3-C3-C4-O4
3	A	301	TAR	O3-C3-C4-O41
3	C	301	TAR	O3-C3-C4-O4
3	C	301	TAR	O3-C3-C4-O41
3	C	301	TAR	O1-C1-C2-C3
3	C	301	TAR	O11-C1-C2-C3
3	A	301	TAR	O2-C2-C3-O3
3	A	301	TAR	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	B	301	TAR	O3-C3-C4-O4
3	B	301	TAR	O3-C3-C4-O41
3	D	301	TAR	O3-C3-C4-O4
3	D	301	TAR	O3-C3-C4-O41
3	C	301	TAR	C2-C3-C4-O41
4	D	302	B3P	C1-C2-N2-C8
3	C	301	TAR	C2-C3-C4-O4
3	A	301	TAR	C1-C2-C3-O3
3	A	301	TAR	O2-C2-C3-C4
4	D	302	B3P	N1-C4-C6-O5
4	D	302	B3P	O2-C10-C8-N2
4	D	302	B3P	C1-C3-N1-C4
3	A	301	TAR	C2-C3-C4-O4
3	B	301	TAR	O1-C1-C2-C3
3	A	301	TAR	C2-C3-C4-O41
4	D	302	B3P	C3-C1-C2-N2
3	B	301	TAR	C1-C2-C3-C4
3	D	301	TAR	O1-C1-C2-C3
3	B	301	TAR	O11-C1-C2-C3
3	B	301	TAR	O2-C2-C3-O3
3	D	301	TAR	O11-C1-C2-C3
4	D	302	B3P	C5-C4-C6-O5
4	D	302	B3P	O2-C10-C8-C9
4	D	302	B3P	C2-C1-C3-N1
3	D	301	TAR	O1-C1-C2-O2
3	D	301	TAR	O11-C1-C2-O2
4	D	302	B3P	C11-C8-N2-C2

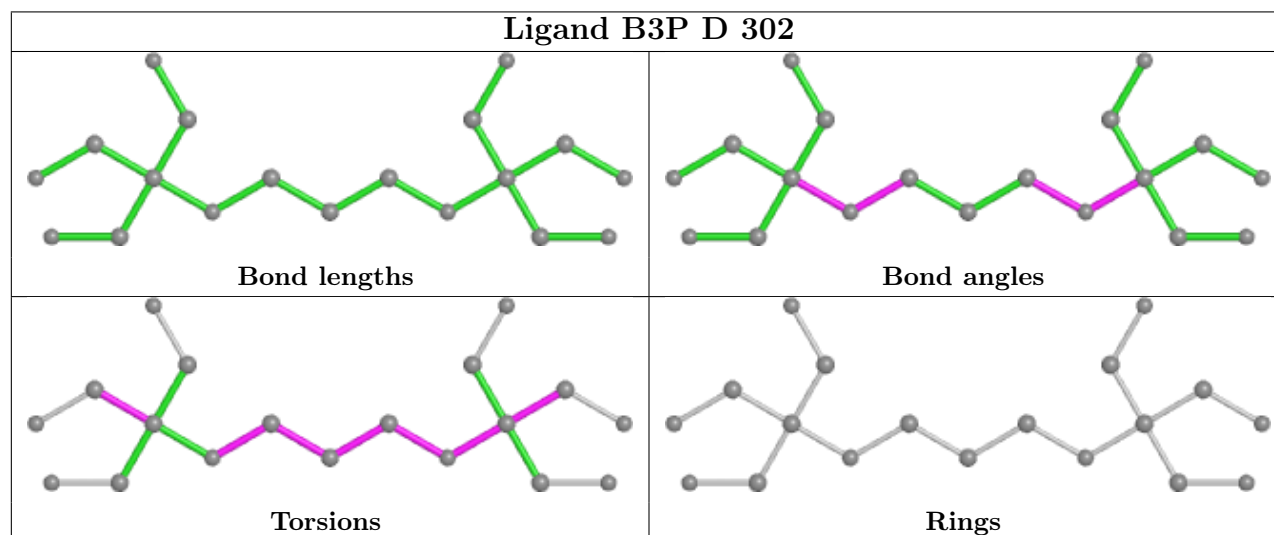
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	302	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	233/234 (99%)	0.21	10 (4%) 35 25	56, 89, 161, 221	0
1	B	228/234 (97%)	0.08	4 (1%) 68 61	48, 85, 139, 193	0
1	C	231/234 (98%)	-0.01	3 (1%) 77 72	46, 72, 124, 163	0
1	D	233/234 (99%)	0.07	5 (2%) 63 54	43, 77, 136, 179	0
2	D000	7/10 (70%)	0.95	2 (28%) 0 0	79, 105, 146, 183	0
2	E	7/10 (70%)	0.51	1 (14%) 2 1	75, 90, 144, 161	0
2	F	7/10 (70%)	0.74	1 (14%) 2 1	75, 99, 153, 161	0
2	G	7/10 (70%)	-0.01	0 100 100	60, 78, 116, 130	0
All	All	953/976 (97%)	0.10	26 (2%) 54 44	43, 81, 143, 221	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	SER	4.5
1	B	69	SER	3.9
1	C	-1	PRO	3.6
1	A	76	GLU	3.4
1	D	1	MET	3.2
2	E	151	ARG	3.0
1	A	74	SER	3.0
1	B	136	THR	2.9
2	F	158	LEU	2.8
1	B	65	ILE	2.5
1	D	210	GLU	2.5
1	A	77	LYS	2.5
1	A	0	HIS	2.4
1	A	73	GLY	2.4
1	A	72	GLU	2.4
1	C	69	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	70	ASN	2.3
1	B	141	LYS	2.3
2	D000	152	THR	2.3
1	D	112	GLY	2.3
1	A	71	GLU	2.3
1	C	67	GLN	2.1
1	D	117	ARG	2.1
1	A	229	LEU	2.0
1	D	111	ALA	2.0
2	D000	151	ARG	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	TPO	E	156	11/12	0.97	0.19	52,64,80,82	0
2	TPO	G	156	11/12	0.97	0.23	48,61,76,91	0
2	TPO	F	156	11/12	0.98	0.16	56,62,89,96	0
2	TPO	D000	156	11/12	0.98	0.14	61,68,91,104	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, 95<sup>th</sup> 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.

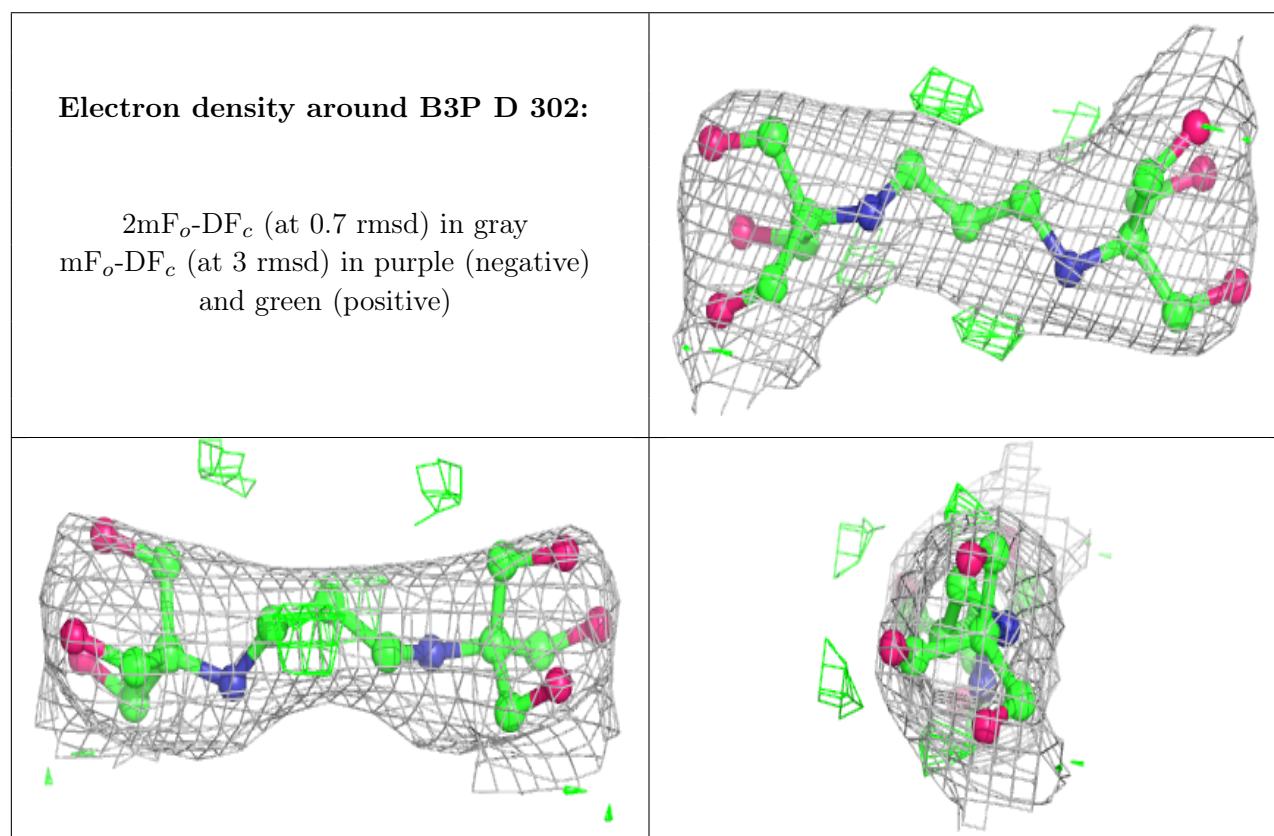
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	TAR	B	301	10/10	0.70	0.37	110,132,136,139	0
3	TAR	C	301	10/10	0.71	0.36	119,134,140,146	0
3	TAR	D	301	10/10	0.79	0.33	109,126,133,143	0
3	TAR	A	301	10/10	0.88	0.29	122,130,159,161	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	B3P	D	302	19/19	0.89	0.25	86,95,99,99	19

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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.