Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2020 – 10:18 PM BST

PDB ID	:	6ZEG
Title	:	Structure of PP1-IRSp53 chimera [PP1(7-304) + linker (G/S)x9 + IRSp53(449-465)] bound to Phactr1 (516-580)
Authors	:	Mouilleron, S.; Treisman, R.; Fedoryshchak, R.; Lee, R.; Butler, A.M.; Prechova, M.
Deposited on	:	2020-06-16
Resolution	:	1.09 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:

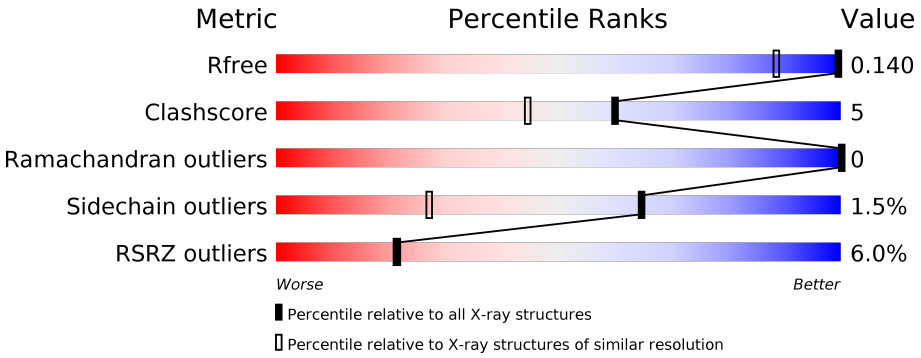
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.09 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	1619 (1.14-1.06)
Clashscore	141614	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (1.14-1.06)
RSRZ outliers	127900	1588 (1.14-1.06)

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 <=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	338	5% 84% 7% 8%
1	B	338	4% 83% 8% 9%
2	C	70	10% 84% 10% 6%
2	D	70	11% 86% 7% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13590 atoms, of which 6365 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 Serine/threonine-protein phosphatase PP1-alpha catalytic subunit,Brain-specific angiogenesis inhibitor 1-associated protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	311	Total	C	H	N	O	S	0	32	0
			5201	1666	2602	432	478	23			
1	B	308	Total	C	H	N	O	S	0	25	0
			5134	1652	2564	423	472	23			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP P62136
A	3	HIS	-	expression tag	UNP P62136
A	4	MET	-	expression tag	UNP P62136
A	5	GLY	-	expression tag	UNP P62136
A	6	SER	-	expression tag	UNP P62136
A	305	SER	-	linker	UNP P62136
A	306	GLY	-	linker	UNP P62136
A	307	SER	-	linker	UNP P62136
A	308	GLY	-	linker	UNP P62136
A	309	SER	-	linker	UNP P62136
A	310	GLY	-	linker	UNP P62136
A	311	SER	-	linker	UNP P62136
A	312	GLY	-	linker	UNP P62136
A	313	SER	-	linker	UNP P62136
A	314	GLY	-	linker	UNP P62136
A	315	SER	-	linker	UNP P62136
A	316	GLY	-	linker	UNP P62136
A	317	SER	-	linker	UNP P62136
A	318	GLY	-	linker	UNP P62136
A	319	SER	-	linker	UNP P62136
A	320	GLY	-	linker	UNP P62136
A	321	SER	-	linker	UNP P62136
A	322	GLY	-	linker	UNP P62136
B	2	GLY	-	expression tag	UNP P62136

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	HIS	-	expression tag	UNP P62136
B	4	MET	-	expression tag	UNP P62136
B	5	GLY	-	expression tag	UNP P62136
B	6	SER	-	expression tag	UNP P62136
B	305	SER	-	linker	UNP P62136
B	306	GLY	-	linker	UNP P62136
B	307	SER	-	linker	UNP P62136
B	308	GLY	-	linker	UNP P62136
B	309	SER	-	linker	UNP P62136
B	310	GLY	-	linker	UNP P62136
B	311	SER	-	linker	UNP P62136
B	312	GLY	-	linker	UNP P62136
B	313	SER	-	linker	UNP P62136
B	314	GLY	-	linker	UNP P62136
B	315	SER	-	linker	UNP P62136
B	316	GLY	-	linker	UNP P62136
B	317	SER	-	linker	UNP P62136
B	318	GLY	-	linker	UNP P62136
B	319	SER	-	linker	UNP P62136
B	320	GLY	-	linker	UNP P62136
B	321	SER	-	linker	UNP P62136
B	322	GLY	-	linker	UNP P62136

- Molecule 2 is a protein called Phosphatase and actin regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	66	Total	C	H	N	O	S	0	6	0
			1186	375	593	108	109	1			
2	D	65	Total	C	H	N	O	S	0	4	0
			1145	362	568	108	106	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	511	GLY	-	expression tag	UNP Q4VY12
C	512	PRO	-	expression tag	UNP Q4VY12
C	513	LEU	-	expression tag	UNP Q4VY12
C	514	GLY	-	expression tag	UNP Q4VY12
C	515	SER	-	expression tag	UNP Q4VY12
D	511	GLY	-	expression tag	UNP Q4VY12
D	512	PRO	-	expression tag	UNP Q4VY12
D	513	LEU	-	expression tag	UNP Q4VY12

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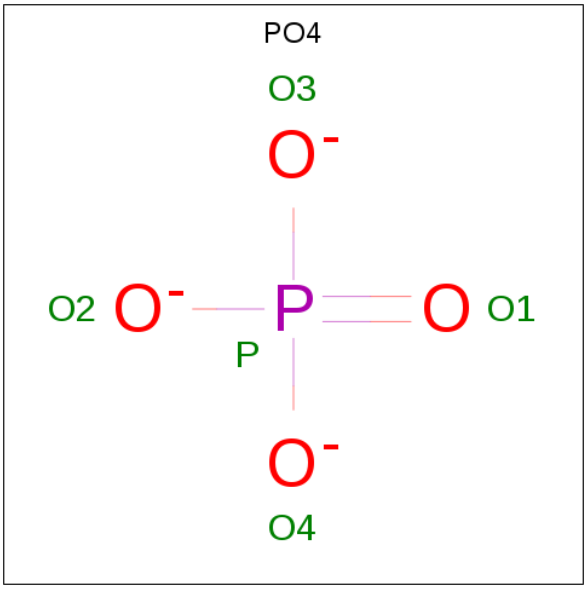
Chain	Residue	Modelled	Actual	Comment	Reference
D	514	GLY	-	expression tag	UNP Q4VY12
D	515	SER	-	expression tag	UNP Q4VY12

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

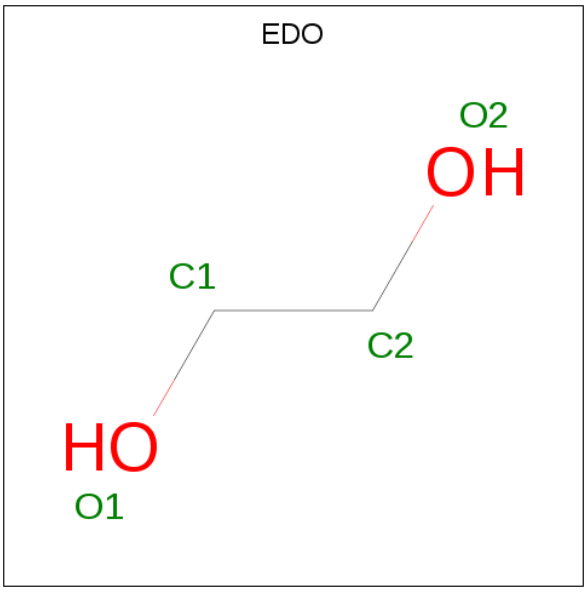
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mn 2 2	0	0
3	A	2	Total Mn 2 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



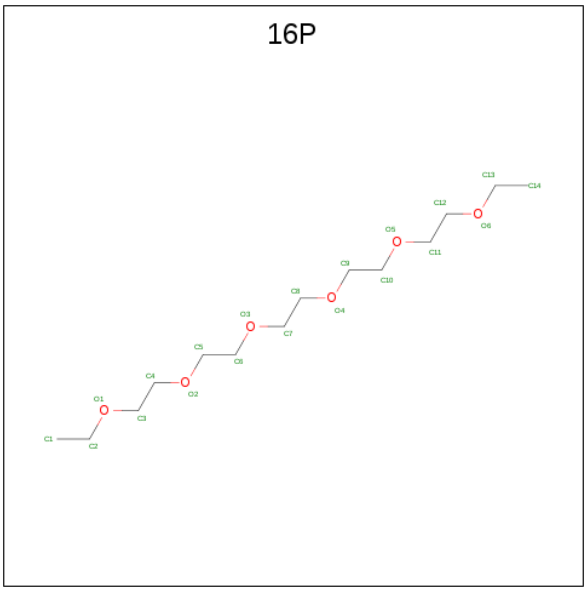
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is 3,6,9,12,15,18-HEXAOXAICOSANE (three-letter code: 16P) (formula: $C_{14}H_{30}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			36	10	20	6		

- Molecule 7 is water.

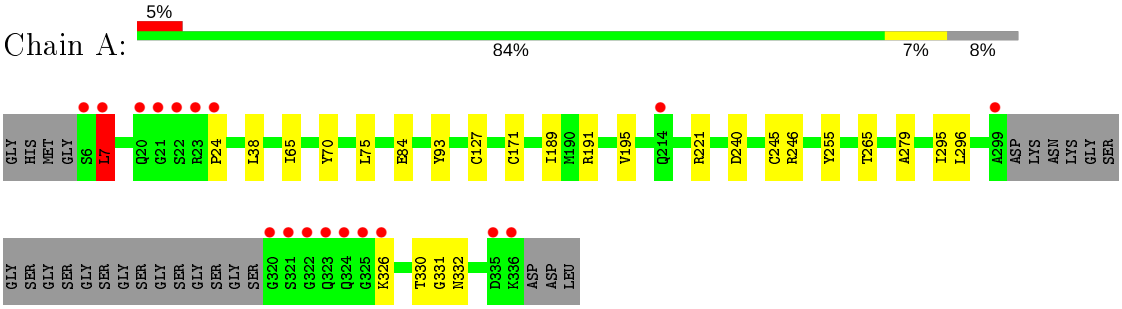
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	357	Total	O	0	2
			357	357		
7	C	115	Total	O	0	0
			115	115		
7	B	290	Total	O	0	6
			290	290		
7	D	82	Total	O	0	2
			82	82		

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.

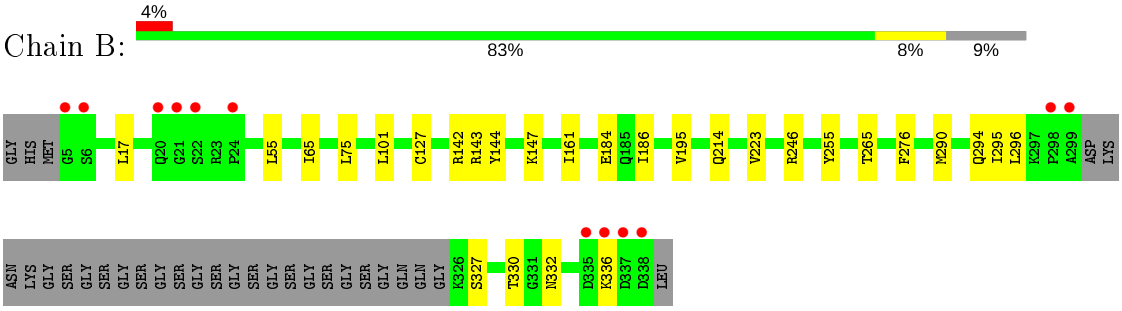
• Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit,Brain-specific angiogenesis inhibitor 1-associated protein 2

Chain A:



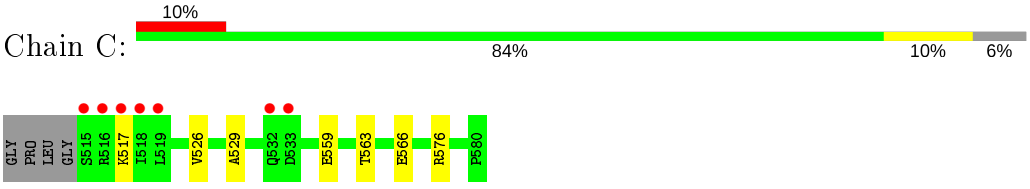
• Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit,Brain-specific angiogenesis inhibitor 1-associated protein 2

Chain B:



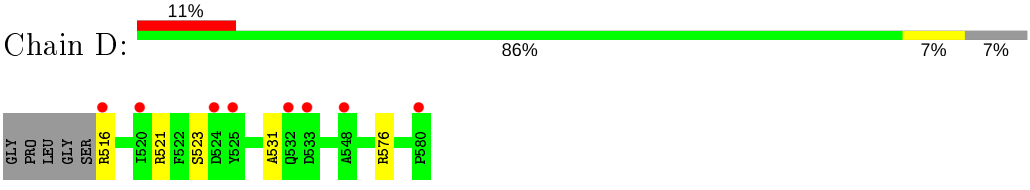
• Molecule 2: Phosphatase and actin regulator

Chain C:



• Molecule 2: Phosphatase and actin regulator

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.62Å 122.39Å 69.10Å 90.00° 92.22° 90.00°	Depositor
Resolution (Å)	37.18 – 1.09 37.18 – 1.09	Depositor EDS
% Data completeness (in resolution range)	99.2 (37.18-1.09) 99.2 (37.18-1.09)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 1.09Å)	Xtriage
Refinement program	PHENIX 1.18_3845, PHENIX 1.18_3845	Depositor
R, R_{free}	0.119 , 0.140 0.119 , 0.140	Depositor DCC
R_{free} test set	16711 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	10.8	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	13590	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MN, 16P, EDO

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	0.49	0/2754	0.71	2/3714 (0.1%)
1	B	0.51	0/2690	0.75	0/3634
2	C	0.50	0/620	0.67	0/833
2	D	0.49	0/601	0.68	0/807
All	All	0.50	0/6665	0.72	2/8988 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	7[A]	LEU	CA-CB-CG	-5.55	102.55	115.30
1	A	7[B]	LEU	CA-CB-CG	-5.55	102.55	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2599	2602	2540	24	0
1	B	2570	2564	2538	32	0
2	C	593	593	593	6	0
2	D	577	568	568	3	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	4	6	6	2	0
5	B	8	12	12	1	0
6	B	16	20	20	4	0
7	A	357	0	0	4	0
7	B	290	0	0	10	1
7	C	115	0	0	1	1
7	D	82	0	0	0	0
All	All	7225	6365	6277	59	1

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 5.

All (59) 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:294[B]:GLN:OE1	7:B:601[B]:HOH:O	1.80	0.98
1:B:127[B]:CYS:SG	1:B:195:VAL:HG21	2.08	0.93
1:B:214:GLN:O	7:B:602:HOH:O	1.92	0.86
1:A:127[B]:CYS:SG	1:A:195:VAL:HG21	2.15	0.85
1:B:75[B]:LEU:HD21	7:B:680:HOH:O	1.78	0.83
1:B:290[A]:MET:SD	2:D:523:SER:N	2.57	0.78
1:A:221:ARG:O	1:A:330[B]:THR:HG23	1.83	0.77
1:B:127[B]:CYS:SG	1:B:195:VAL:CG2	2.74	0.76
1:B:296[B]:LEU:HD22	2:D:531:ALA:HA	1.68	0.75
1:A:127[B]:CYS:SG	1:A:195:VAL:CG2	2.75	0.75
1:A:240:ASP:OD1	7:A:602:HOH:O	2.07	0.73
1:A:75[B]:LEU:HD21	7:A:763:HOH:O	1.87	0.72
1:B:255:TYR:HE1	1:B:295[B]:ILE:HD11	1.56	0.71
1:B:101[B]:LEU:CD1	1:B:143[B]:ARG:HG3	2.23	0.69
1:B:17:LEU:HD13	5:B:504:EDO:H11	1.76	0.67
1:A:295:ILE:HD12	2:C:526[A]:VAL:CG1	2.25	0.66
2:C:566[B]:GLU:OE1	7:C:601:HOH:O	2.13	0.64
1:A:7[A]:LEU:HG	7:A:720:HOH:O	1.97	0.64
1:A:326:LYS:NZ	7:A:604:HOH:O	2.31	0.64
1:B:55:LEU:HD23	6:B:505:16P:H101	1.81	0.63
1:B:255:TYR:CE1	1:B:295[B]:ILE:HD11	2.35	0.60
1:B:101[B]:LEU:HD12	1:B:143[B]:ARG:HG3	1.83	0.59
1:A:295:ILE:HD12	2:C:526[A]:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143[A]:ARG:HB3	1:B:144[A]:TYR:CD1	2.39	0.58
1:B:55:LEU:HB3	6:B:505:16P:H121	1.85	0.58
1:B:144[A]:TYR:OH	7:B:603:HOH:O	2.15	0.57
1:A:330[B]:THR:HG22	1:A:332[B]:ASN:H	1.71	0.56
1:B:223[A]:VAL:HG11	7:B:690:HOH:O	2.04	0.56
1:B:101[A]:LEU:CD2	1:B:144[A]:TYR:HE1	2.21	0.54
1:B:55:LEU:CD2	6:B:505:16P:H101	2.38	0.54
1:A:191:ARG:HE	5:A:504:EDO:C1	2.20	0.54
1:A:75[A]:LEU:C	1:A:75[A]:LEU:HD23	2.29	0.53
1:B:184:GLU:HG2	7:B:819:HOH:O	2.09	0.52
1:A:330[B]:THR:HG22	1:A:331:GLY:N	2.26	0.49
1:A:189:ILE:O	5:A:504:EDO:H11	2.13	0.48
1:B:143[A]:ARG:HB3	1:B:144[A]:TYR:CE1	2.48	0.48
1:A:24:PRO:HG3	1:A:70[B]:TYR:CE2	2.49	0.48
1:A:65[B]:ILE:HG23	1:A:93:TYR:HA	1.96	0.47
2:C:559:GLU:OE2	2:C:563:THR:HG21	2.15	0.47
1:B:101[B]:LEU:HD13	1:B:143[B]:ARG:HG3	1.96	0.46
1:A:295:ILE:CD1	2:C:526[A]:VAL:HG11	2.45	0.46
1:A:7[A]:LEU:HD21	1:A:38:LEU:HD23	1.97	0.46
1:A:65[B]:ILE:CG2	1:A:93:TYR:HA	2.46	0.46
1:A:296:LEU:HD13	2:C:529:ALA:HB3	1.98	0.46
1:B:296[B]:LEU:HD22	2:D:531:ALA:CA	2.41	0.46
1:A:84:GLU:CG	7:B:868:HOH:O	2.65	0.45
1:B:65:ILE:HD12	7:B:703:HOH:O	2.17	0.45
1:A:171:CYS:HA	1:A:245:CYS:O	2.17	0.44
1:B:276:PHE:CZ	1:B:327:SER:HB3	2.53	0.44
1:B:147:LYS:HE2	1:B:147:LYS:HB2	1.89	0.43
1:B:101[A]:LEU:CD2	1:B:144[A]:TYR:CE1	3.01	0.42
1:B:330:THR:HG22	1:B:332:ASN:H	1.85	0.42
1:B:161[A]:ILE:HD11	1:B:186:ILE:HG23	2.03	0.41
6:B:505:16P:C5	7:B:619:HOH:O	2.69	0.41
1:A:255:TYR:HA	1:A:265:THR:O	2.21	0.40
1:B:255:TYR:HA	1:B:265:THR:O	2.21	0.40
1:A:279:ALA:HB1	1:A:295:ILE:HG23	2.03	0.40
1:B:75[B]:LEU:HD11	7:B:680:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:668:HOH:O	7:B:815:HOH:O[2_546]	2.10	0.10

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	338/338 (100%)	326 (96%)	12 (4%)	0	100	100
1	B	329/338 (97%)	316 (96%)	13 (4%)	0	100	100
2	C	70/70 (100%)	69 (99%)	1 (1%)	0	100	100
2	D	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
All	All	804/816 (98%)	777 (97%)	27 (3%)	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	295/289 (102%)	292 (99%)	3 (1%)	76	44
1	B	288/289 (100%)	284 (99%)	4 (1%)	67	30
2	C	64/61 (105%)	62 (97%)	2 (3%)	40	7
2	D	61/61 (100%)	58 (95%)	3 (5%)	25	2
All	All	708/700 (101%)	696 (98%)	12 (2%)	65	23

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7[A]	LEU
1	A	7[B]	LEU

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Mol	Chain	Res	Type
1	A	246	ARG
2	C	517	LYS
2	C	576	ARG
1	B	142[A]	ARG
1	B	142[B]	ARG
1	B	246	ARG
1	B	336	LYS
2	D	516	ARG
2	D	521	ARG
2	D	576	ARG

Some 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 monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
5	EDO	B	506	-	3,3,3	0.41	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	16P	B	505	-	15,15,19	0.46	0	14,14,18	0.69	0
5	EDO	A	504	-	3,3,3	0.36	0	2,2,2	0.70	0
5	EDO	B	504	-	3,3,3	0.47	0	2,2,2	0.23	0
4	PO4	A	503	3	4,4,4	1.33	0	6,6,6	1.26	1 (16%)
4	PO4	B	503	3	4,4,4	0.76	0	6,6,6	1.12	0

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
5	EDO	B	506	-	-	1/1/1/1	-
6	16P	B	505	-	-	8/13/13/17	-
5	EDO	A	504	-	-	0/1/1/1	-
5	EDO	B	504	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503	PO4	O3-P-O2	2.18	114.96	107.97

There are no chirality outliers.

All (9) torsion outliers are listed below:

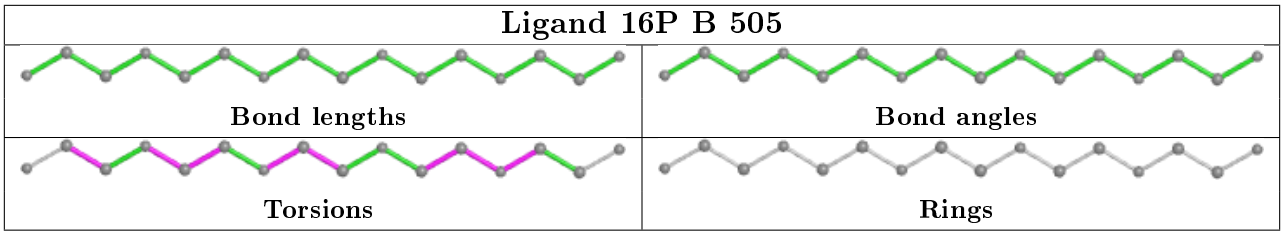
Mol	Chain	Res	Type	Atoms
6	B	505	16P	C3-C4-O2-C5
6	B	505	16P	O5-C10-C9-O4
5	B	506	EDO	O1-C1-C2-O2
6	B	505	16P	C9-C10-O5-C11
6	B	505	16P	O5-C11-C12-O6
6	B	505	16P	C7-C8-O4-C9
6	B	505	16P	C6-C5-O2-C4
6	B	505	16P	O2-C5-C6-O3
6	B	505	16P	O3-C7-C8-O4

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	505	16P	4	0
5	A	504	EDO	2	0
5	B	504	EDO	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 then 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, 95^{th} 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	311/338 (92%)	0.19	18 (5%)	23	22	7, 12, 27, 33	1 (0%)
1	B	308/338 (91%)	0.09	12 (3%)	39	36	7, 12, 25, 40	0
2	C	66/70 (94%)	0.30	7 (10%)	6	7	11, 15, 28, 38	0
2	D	65/70 (92%)	0.46	8 (12%)	4	5	11, 20, 29, 34	0
All	All	750/816 (91%)	0.18	45 (6%)	21	21	7, 13, 27, 40	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	GLY	11.1
2	C	515	SER	10.1
1	B	5	GLY	8.2
1	B	299	ALA	7.8
1	B	337	ASP	7.4
1	A	299	ALA	6.9
1	B	338	ASP	5.8
1	A	324	GLN	5.8
1	A	21[A]	GLY	5.5
2	D	580	PRO	5.2
1	A	24	PRO	5.0
2	C	517	LYS	5.0
1	A	325	GLY	4.8
1	A	214	GLN	4.6
2	D	533	ASP	4.5
1	A	322	GLY	4.4
1	A	323	GLN	4.3
1	A	320	GLY	4.2
1	B	336	LYS	4.0
1	A	7[A]	LEU	3.8
2	C	518	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
2	C	533	ASP	3.7
2	D	532	GLN	3.6
1	A	336	LYS	3.6
2	C	519	LEU	3.2
1	B	20	GLN	3.1
2	C	516	ARG	3.0
1	B	335	ASP	2.6
1	A	335	ASP	2.6
2	D	520	ILE	2.6
2	C	532	GLN	2.5
2	D	516	ARG	2.5
2	D	525[A]	TYR	2.4
1	B	24	PRO	2.3
1	A	6	SER	2.3
1	A	22	SER	2.3
2	D	548	ALA	2.3
1	B	22	SER	2.3
1	A	23	ARG	2.2
1	A	20[A]	GLN	2.2
1	B	298	PRO	2.2
2	D	524[A]	ASP	2.2
1	B	6	SER	2.2
1	A	326	LYS	2.1
1	A	321	SER	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 monosaccharides in this entry.

6.4 Ligands (i)

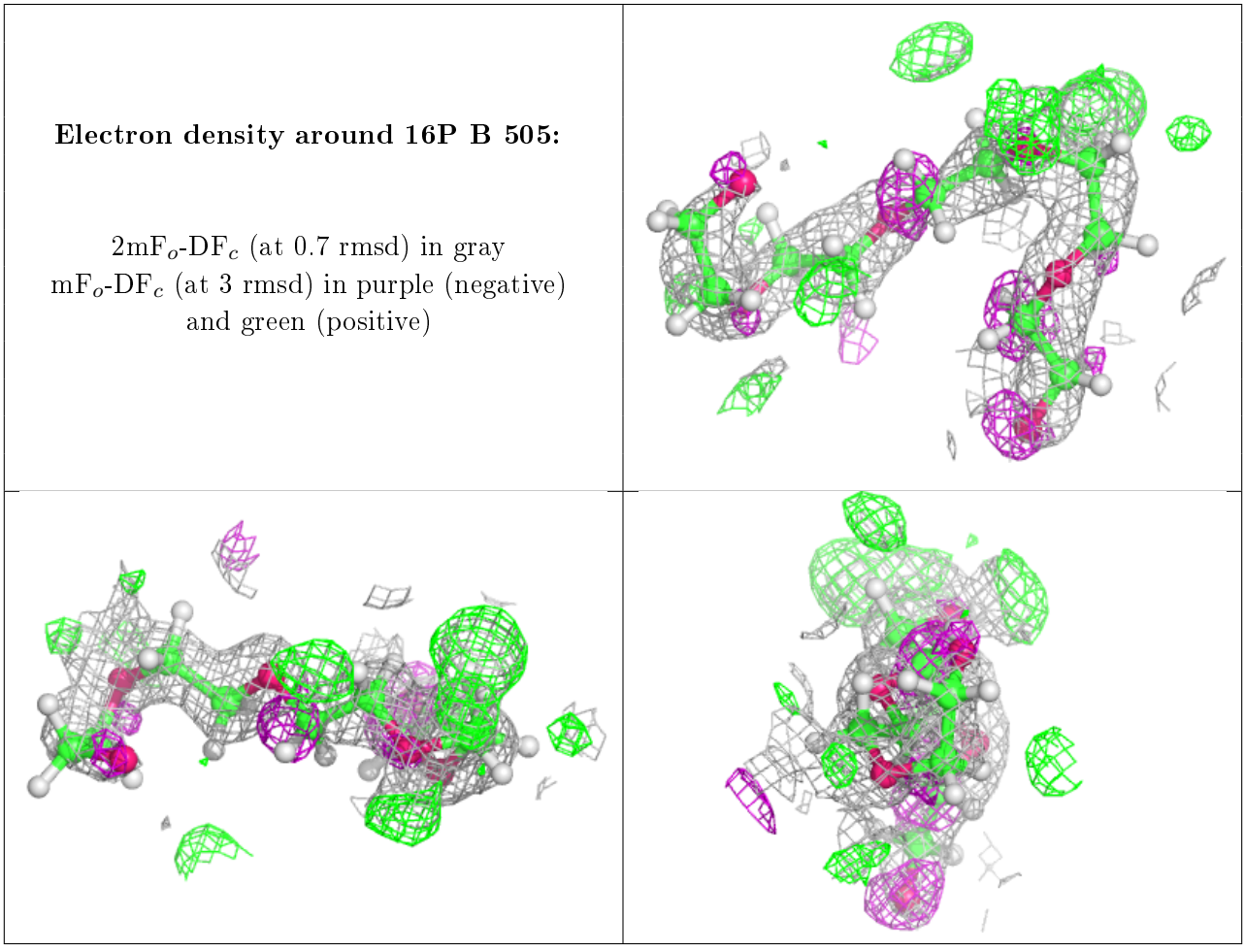
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	EDO	B	506	4/4	0.75	0.21	33,40,41,41	0
6	16P	B	505	16/20	0.81	0.24	27,36,43,45	0
5	EDO	B	504	4/4	0.84	0.28	33,40,41,44	0
5	EDO	A	504	4/4	0.90	0.19	11,14,20,25	10
3	MN	B	502	1/1	1.00	0.07	8,8,8,8	0
3	MN	A	502	1/1	1.00	0.07	6,6,6,6	0
4	PO4	A	503	5/5	1.00	0.10	7,7,8,9	0
4	PO4	B	503	5/5	1.00	0.08	8,8,9,10	0
3	MN	B	501	1/1	1.00	0.08	7,7,7,7	0
3	MN	A	501	1/1	1.00	0.08	6,6,6,6	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 16P B 505:

$2mF_o$-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.