



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:04 AM UTC

PDB ID : 6Y7T / pdb_00006y7t
Title : Engineered conjugation of lysine-specific molecular tweezers with ExoS derived peptidic inhibitor enhance affinity towards target protein 14-3-3 through ditopic binding
Authors : Guillory, X.; Ottmann, C.
Deposited on : 2020-03-02
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

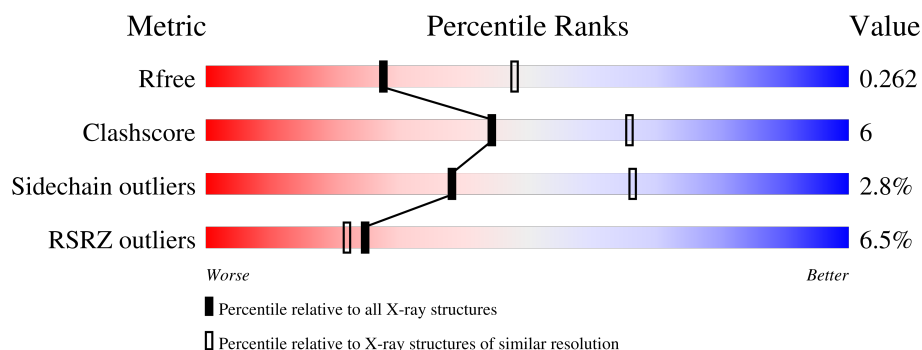
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	253	 2% 79% 10% • 9%
1	F	253	 3% 83% 7% • 9%
1	K	253	 3% 83% 8% 9%
1	P	253	 15% 75% 15% • 9%
2	D	11	 64% 36%

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Mol	Chain	Length	Quality of chain
2	E	11	18% 82% 9% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7941 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	230	Total	C	N	O	S	0	0	0
			1805	1127	307	360	11			
1	F	230	Total	C	N	O	S	0	5	0
			1844	1150	314	369	11			
1	K	231	Total	C	N	O	S	0	1	0
			1824	1137	309	367	11			
1	P	231	Total	C	N	O	S	0	2	0
			1813	1132	307	363	11			

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
F	-4	GLY	-	expression tag	UNP P31947
F	-3	ALA	-	expression tag	UNP P31947
F	-2	MET	-	expression tag	UNP P31947
F	-1	GLY	-	expression tag	UNP P31947
F	0	SER	-	expression tag	UNP P31947
K	-4	GLY	-	expression tag	UNP P31947
K	-3	ALA	-	expression tag	UNP P31947
K	-2	MET	-	expression tag	UNP P31947
K	-1	GLY	-	expression tag	UNP P31947
K	0	SER	-	expression tag	UNP P31947
P	-4	GLY	-	expression tag	UNP P31947
P	-3	ALA	-	expression tag	UNP P31947
P	-2	MET	-	expression tag	UNP P31947
P	-1	GLY	-	expression tag	UNP P31947
P	0	SER	-	expression tag	UNP P31947

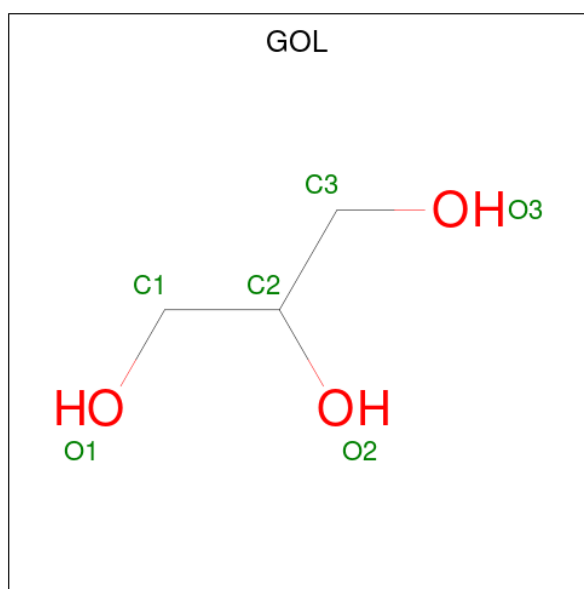
- Molecule 2 is a protein called Exoenzyme S.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	11	Total	C	N	O	0	0	1
			72	45	12	15			
2	E	11	Total	C	N	O	0	0	0
			75	48	12	15			

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	F	1	Total	Na	0	0
			1	1		
3	K	1	Total	Na	0	0
			1	1		
3	P	2	Total	Na	0	0
			2	2		

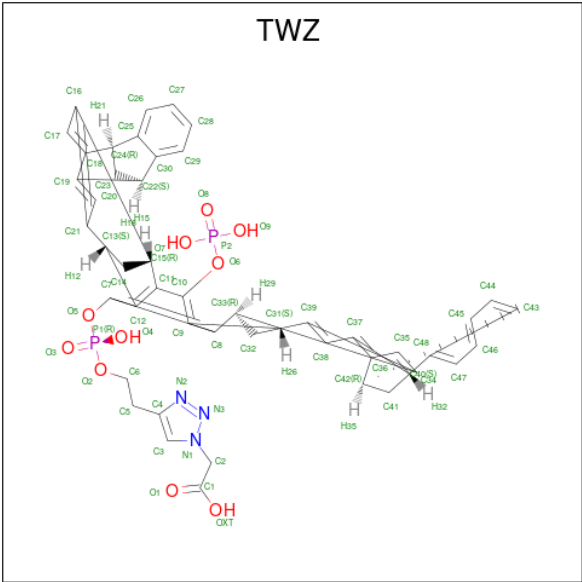
- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2-[4-[2-[hydroxy-[(1R,5S,9S,16R,20R,24S,28S,35R)-22-phosphonoxy-3-tridec

acyclo[22.14.1.15,20.19,16.128,35.02,23.04,21.06,19.08,17.010,15.025,38.027,36.029,34]dote traconta-2,4(21),6(19),7,10,12,14,17,22,25(38),26,29,31,33,36-pentadecaenyl]oxy]phosphor yl]oxyethyl]triazol-1-yl]acetic acid (CCD ID: TWZ) (formula: C₄₈H₃₉N₃O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			62	48	3	9	2		
5	E	1	Total	C	N	O	P	0	0
			62	48	3	9	2		

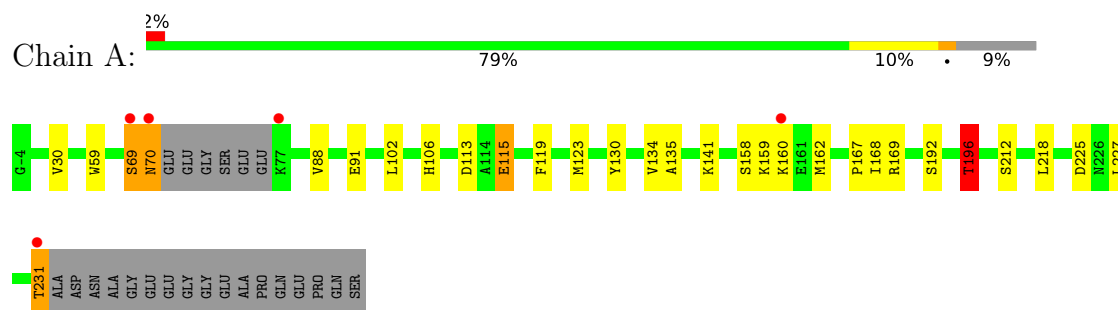
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	85	Total	O	0	0
			85	85		
6	D	13	Total	O	0	0
			13	13		
6	E	10	Total	O	0	0
			10	10		
6	F	90	Total	O	0	0
			90	90		
6	K	109	Total	O	0	0
			109	109		
6	P	60	Total	O	0	0
			60	60		

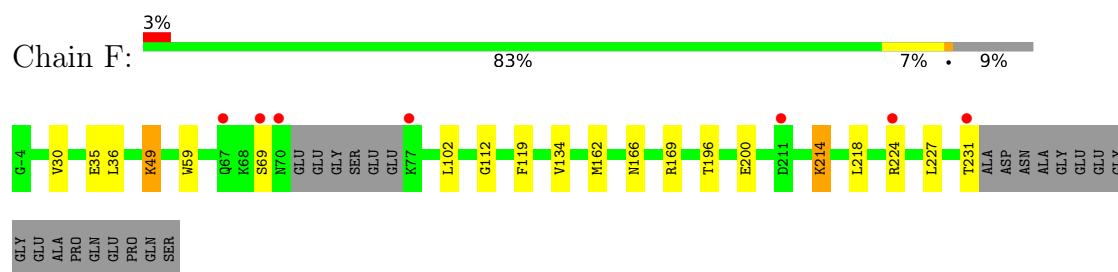
3 Residue-property plots [i](#)

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.

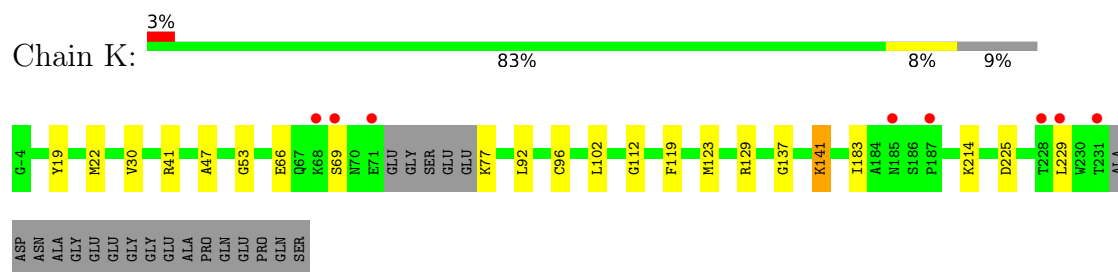
- Molecule 1: 14-3-3 protein sigma



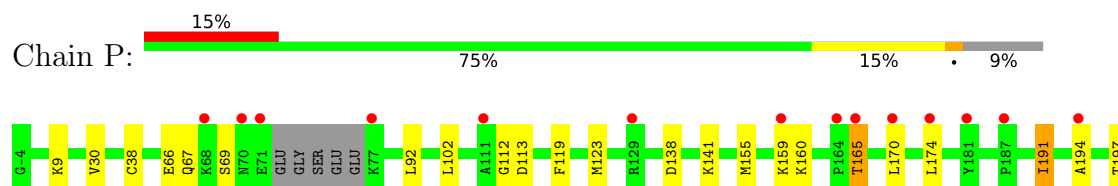
- Molecule 1: 14-3-3 protein sigma

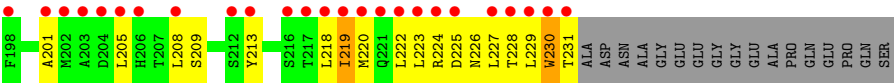


- Molecule 1: 14-3-3 protein sigma



- Molecule 1: 14-3-3 protein sigma

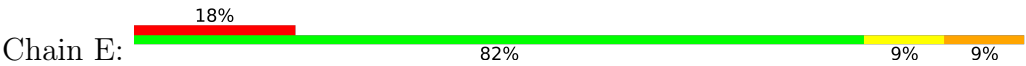




● Molecule 2: Exoenzyme S



● Molecule 2: Exoenzyme S



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.15Å 63.12Å 167.02Å 90.00° 101.29° 90.00°	Depositor
Resolution (Å)	59.90 – 2.50 59.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (59.90-2.50) 99.8 (59.90-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.219 , 0.268 (Not available) , 0.262	Depositor DCC
R_{free} test set	2689 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7941	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.08% 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: NA, CSO, TWZ, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.23	2/1822 (0.1%)	1.63	5/2448 (0.2%)
1	F	1.18	0/1860	1.59	3/2499 (0.1%)
1	K	1.22	1/1841 (0.1%)	1.63	5/2474 (0.2%)
1	P	1.15	1/1829 (0.1%)	1.63	3/2458 (0.1%)
2	D	1.34	0/71	1.89	2/96 (2.1%)
2	E	1.09	0/74	1.50	1/100 (1.0%)
All	All	1.20	4/7497 (0.1%)	1.62	19/10075 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	ASP	C-O	5.45	1.30	1.24
1	A	106	HIS	CE1-NE2	5.34	1.37	1.32
1	K	96	CYS	C-O	5.06	1.29	1.24
1	P	9	LYS	C-O	5.02	1.30	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	427	ASP	CA-CB-CG	6.24	118.83	112.60
1	F	112	GLY	CA-C-O	-6.19	117.63	122.52
1	P	112	GLY	CA-C-O	-5.89	117.86	122.52
1	F	119	PHE	N-CA-C	-5.89	104.86	111.28
1	P	230	TRP	N-CA-C	-5.70	106.95	114.31
1	K	214	LYS	CA-C-O	-5.42	115.13	120.82
2	E	427	ASP	CA-CB-CG	5.29	117.89	112.60
1	F	35	GLU	CB-CA-C	-5.28	100.96	109.72
1	A	113	ASP	CA-CB-CG	5.26	117.86	112.60
1	K	19	TYR	CB-CA-C	5.21	119.44	110.79
1	A	196	THR	CA-CB-CG2	5.16	119.28	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ALA	CA-C-O	-5.16	115.63	121.72
1	K	53	GLY	CA-C-N	5.16	125.68	120.00
1	K	53	GLY	C-N-CA	5.16	125.68	120.00
1	P	113	ASP	CA-CB-CG	5.11	117.71	112.60
1	K	112	GLY	CA-C-O	-5.05	118.53	122.52
2	D	427	ASP	N-CA-C	-5.03	104.30	111.24
1	A	88	VAL	CA-C-N	5.00	126.94	120.44
1	A	88	VAL	C-N-CA	5.00	126.94	120.44

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	1805	0	1786	16	0
1	F	1844	0	1813	13	0
1	K	1824	0	1796	14	0
1	P	1813	0	1780	43	0
2	D	72	0	72	4	0
2	E	75	0	74	3	0
3	A	1	0	0	0	0
3	F	1	0	0	0	0
3	K	1	0	0	0	0
3	P	2	0	0	0	0
4	A	6	0	8	0	0
4	P	6	0	8	0	0
5	D	62	0	0	3	0
5	E	62	0	0	2	0
6	A	85	0	0	1	0
6	D	13	0	0	1	0
6	E	10	0	0	0	0
6	F	90	0	0	1	0
6	K	109	0	0	5	0
6	P	60	0	0	1	0
All	All	7941	0	7337	90	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (90) 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:P:201:ALA:HB1	1:P:220:MET:CE	1.74	1.16
1:P:201:ALA:HB1	1:P:220:MET:HE3	1.15	1.13
1:P:201:ALA:CB	1:P:220:MET:CE	2.36	1.03
1:P:194:ALA:HB3	1:P:227:LEU:HD21	1.50	0.93
1:P:194:ALA:CB	1:P:227:LEU:HD21	1.99	0.92
1:P:191:ILE:HD11	1:P:230:TRP:HB3	1.50	0.90
1:A:227:LEU:O	1:A:231:THR:HB	1.75	0.85
1:P:201:ALA:HB3	1:P:220:MET:HE2	1.57	0.84
1:P:223:LEU:O	1:P:227:LEU:HG	1.78	0.84
1:P:165:THR:CG2	1:P:208:LEU:HD13	2.08	0.83
1:P:201:ALA:CB	1:P:220:MET:HE2	2.08	0.83
1:P:218:LEU:O	1:P:222:LEU:HD13	1.81	0.80
1:F:162:MET:HE2	1:F:169:ARG:HB2	1.62	0.80
5:D:501:TWZ:O8	1:F:214:LYS:NZ	2.16	0.79
1:P:170:LEU:HB3	1:P:219:ILE:HG21	1.61	0.79
1:A:192:SER:O	1:A:196:THR:HG23	1.83	0.78
1:P:165:THR:HG21	1:P:208:LEU:HD13	1.67	0.76
1:P:201:ALA:CB	1:P:220:MET:HE3	2.02	0.75
1:P:191:ILE:HD11	1:P:230:TRP:CB	2.17	0.75
1:A:158:SER:HB2	1:A:162:MET:HE2	1.69	0.74
1:P:224:ARG:O	1:P:224:ARG:HG3	1.87	0.73
2:D:424:ASP:OD1	1:F:49:LYS:HE2	1.89	0.70
1:A:115:GLU:HG3	1:A:168:ILE:HD12	1.74	0.70
1:P:38:CSO:OD	6:P:401:HOH:O	2.10	0.69
1:P:165:THR:HG22	1:P:208:LEU:HD13	1.76	0.68
1:A:70:ASN:H	1:A:70:ASN:ND2	1.89	0.68
1:A:162:MET:HE3	1:A:169:ARG:HB2	1.75	0.68
1:P:194:ALA:HB3	1:P:227:LEU:CD2	2.24	0.67
1:A:162:MET:CE	1:A:169:ARG:HB2	2.25	0.67
1:A:115:GLU:HG3	1:A:168:ILE:CD1	2.26	0.65
2:D:423:LEU:HD21	1:F:218[A]:LEU:HD13	1.78	0.64
2:E:420:GLN:HA	5:E:501:TWZ:N3	2.12	0.64
1:K:77:LYS:CB	6:K:409:HOH:O	2.46	0.63
1:P:194:ALA:HB1	1:P:227:LEU:HD21	1.81	0.62
1:K:129:ARG:NH2	6:K:403:HOH:O	2.34	0.59
1:F:162:MET:HE3	1:F:166:ASN:OD1	2.03	0.58
1:K:225:ASP:O	1:K:229:LEU:HD13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:209:SER:O	1:P:213:TYR:CB	2.51	0.58
1:K:30:VAL:HG11	1:K:102:LEU:HD22	1.87	0.57
1:P:30:VAL:HG11	1:P:102:LEU:HD22	1.85	0.56
1:P:225:ASP:O	1:P:229:LEU:HG	2.05	0.56
1:P:226:ASN:HA	1:P:229:LEU:HD12	1.87	0.56
1:P:222:LEU:HD12	1:P:222:LEU:N	2.22	0.55
2:D:420:GLN:HG3	5:D:501:TWZ:N3	2.21	0.55
1:F:30:VAL:HG11	1:F:102:LEU:HD22	1.89	0.55
1:A:30:VAL:HG11	1:A:102:LEU:HD22	1.90	0.53
2:E:420:GLN:HG3	5:E:501:TWZ:N3	2.23	0.53
1:K:66:GLU:O	1:K:69:SER:HB3	2.08	0.53
1:A:130:TYR:OH	2:E:427:ASP:OD2	2.27	0.53
1:P:191:ILE:CD1	1:P:230:TRP:HE3	2.22	0.52
1:A:158:SER:CB	1:A:162:MET:HE2	2.36	0.52
1:P:170:LEU:HB3	1:P:219:ILE:CG2	2.35	0.52
1:F:227:LEU:O	1:F:231[A]:THR:HB	2.10	0.52
1:P:191:ILE:CD1	1:P:230:TRP:CB	2.88	0.51
1:P:191:ILE:CD1	1:P:230:TRP:CE3	2.94	0.50
1:F:196:THR:O	1:F:200:GLU:HG3	2.12	0.49
5:D:501:TWZ:N2	6:D:602:HOH:O	2.34	0.49
1:P:138:ASP:HA	1:P:141:LYS:HG2	1.94	0.49
1:A:69:SER:O	1:A:69:SER:OG	2.05	0.48
1:P:194:ALA:CB	1:P:227:LEU:CD2	2.84	0.48
1:P:197:THR:HG22	1:P:223:LEU:HD11	1.95	0.48
1:K:92:LEU:C	1:K:92:LEU:HD23	2.39	0.48
1:A:119:PHE:CE2	1:A:123:MET:HE2	2.49	0.48
1:P:191:ILE:HD12	1:P:230:TRP:HE3	1.79	0.48
2:D:423:LEU:HD11	1:F:218[A]:LEU:HD22	1.95	0.48
1:P:191:ILE:N	1:P:191:ILE:HD13	2.29	0.47
1:A:59:TRP:CE2	1:A:134:VAL:HG12	2.50	0.47
1:A:91:GLU:OE1	6:A:401:HOH:O	2.20	0.47
1:P:222:LEU:N	1:P:222:LEU:CD1	2.78	0.47
1:P:174:LEU:C	1:P:174:LEU:HD23	2.39	0.47
1:F:162:MET:CE	1:F:169:ARG:HB2	2.40	0.47
1:K:141:LYS:HE2	6:K:441:HOH:O	2.15	0.46
1:P:224:ARG:HA	1:P:227:LEU:HD12	1.98	0.46
1:P:66:GLU:O	1:P:69:SER:HB3	2.17	0.45
1:K:137:GLY:O	1:K:141:LYS:HD3	2.17	0.44
1:F:30:VAL:HG22	1:F:36:LEU:HD11	2.00	0.43
1:K:141:LYS:CE	6:K:441:HOH:O	2.66	0.43
1:P:208:LEU:HG	1:P:213:TYR:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:77:LYS:N	6:K:409:HOH:O	2.51	0.43
1:F:59:TRP:CE2	1:F:134:VAL:HG12	2.54	0.42
1:P:92:LEU:C	1:P:92:LEU:HD23	2.44	0.42
1:P:197:THR:CG2	1:P:223:LEU:HD11	2.50	0.42
1:A:167:PRO:HD3	1:A:212:SER:HB2	2.00	0.41
1:P:155:MET:HE3	1:P:155:MET:HB3	1.96	0.41
1:K:41:ARG:HD3	1:K:119:PHE:CD1	2.55	0.41
1:P:119:PHE:CE1	1:P:123:MET:CE	3.03	0.41
1:K:129:ARG:HG3	1:K:183:ILE:HG13	2.02	0.41
1:K:119:PHE:CE1	1:K:123:MET:CE	3.04	0.40
1:F:224[A]:ARG:NH2	6:F:410:HOH:O	2.54	0.40
1:K:22:MET:HG2	1:K:47:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	191/208 (92%)	182 (95%)	9 (5%)	23	47
1	F	194/208 (93%)	191 (98%)	3 (2%)	57	80
1	K	193/208 (93%)	192 (100%)	1 (0%)	81	92
1	P	188/208 (90%)	179 (95%)	9 (5%)	23	46
2	D	7/8 (88%)	7 (100%)	0	100	100
2	E	7/8 (88%)	7 (100%)	0	100	100
All	All	780/848 (92%)	758 (97%)	22 (3%)	38	66

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

Mol	Chain	Res	Type
1	A	69	SER
1	A	70	ASN
1	A	115	GLU
1	A	141	LYS
1	A	159	LYS
1	A	160	LYS
1	A	196	THR
1	A	218	LEU
1	A	231	THR
1	F	49	LYS
1	F	69	SER
1	F	214	LYS
1	K	141	LYS
1	P	67	GLN
1	P	159	LYS
1	P	160	LYS
1	P	165	THR
1	P	191	ILE
1	P	205	LEU
1	P	219	ILE
1	P	228	THR
1	P	231	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	185	ASN
1	F	206	HIS
1	P	70	ASN
1	P	175	ASN

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	$\# Z > 2$
1	CSO	K	38	1	3,6,7	0.51	0	1,6,8	0.36	0
1	CSO	F	38	1	3,6,7	0.94	0	1,6,8	1.85	0
1	CSO	P	38	1	3,6,7	0.67	0	1,6,8	0.57	0
1	CSO	A	38	1	3,6,7	0.71	0	1,6,8	1.31	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
1	CSO	K	38	1	-	0/1/5/7	-
1	CSO	F	38	1	-	1/1/5/7	-
1	CSO	P	38	1	-	0/1/5/7	-
1	CSO	A	38	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	38	CSO	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	38	CSO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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	TWZ	D	501	2	75,75,76	1.06	3 (4%)	119,122,124	1.27	17 (14%)
5	TWZ	E	501	2	75,75,76	0.98	0	119,122,124	1.16	16 (13%)
4	GOL	P	303	-	5,5,5	0.07	0	5,5,5	0.34	0
4	GOL	A	302	-	5,5,5	0.12	0	5,5,5	0.21	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	TWZ	D	501	2	-	7/19/100/101	0/1/14/14
5	TWZ	E	501	2	-	8/19/100/101	0/1/14/14
4	GOL	P	303	-	-	2/4/4/4	-
4	GOL	A	302	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	TWZ	C2-N1	-2.56	1.45	1.47
5	D	501	TWZ	C8-C33	-2.20	1.49	1.52
5	D	501	TWZ	C9-C31	-2.08	1.49	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	TWZ	O6-C10-C11	5.37	124.36	118.34
5	D	501	TWZ	O5-C7-C12	3.97	122.78	118.34
5	E	501	TWZ	O6-C10-C11	3.95	122.76	118.34
5	E	501	TWZ	O5-C7-C12	2.85	121.54	118.34
5	D	501	TWZ	C28-C29-C30	-2.57	117.91	120.99
5	D	501	TWZ	C43-C42-C36	2.56	108.17	105.39
5	D	501	TWZ	C48-C40-C37	2.55	108.17	105.39
5	E	501	TWZ	C27-C26-C25	-2.51	117.98	120.99
5	E	501	TWZ	C21-C20-C19	-2.51	118.98	123.16
5	E	501	TWZ	C39-C38-C37	-2.48	119.02	123.16
5	D	501	TWZ	C42-C41-C40	-2.44	92.91	94.42
5	E	501	TWZ	C28-C29-C30	-2.42	118.09	120.99
5	D	501	TWZ	C27-C26-C25	-2.40	118.11	120.99
5	E	501	TWZ	C36-C35-C34	-2.35	119.25	123.16
5	D	501	TWZ	C21-C20-C19	-2.34	119.27	123.16
5	D	501	TWZ	C46-C47-C48	-2.33	118.20	120.99
5	E	501	TWZ	C46-C47-C48	-2.32	118.21	120.99
5	E	501	TWZ	O9-P2-O6	2.26	112.01	105.32
5	E	501	TWZ	C18-C17-C16	-2.26	119.40	123.16
5	D	501	TWZ	C39-C38-C37	-2.25	119.42	123.16
5	E	501	TWZ	C45-C44-C43	-2.23	118.32	120.99
5	D	501	TWZ	C18-C17-C16	-2.22	119.47	123.16
5	D	501	TWZ	C36-C35-C34	-2.16	119.56	123.16
5	D	501	TWZ	C45-C44-C43	-2.16	118.40	120.99
5	D	501	TWZ	C44-C43-C42	2.15	132.71	129.39
5	E	501	TWZ	C26-C25-C24	2.09	132.61	129.39
5	D	501	TWZ	C47-C48-C40	2.06	132.56	129.39
5	E	501	TWZ	C44-C43-C42	2.05	132.55	129.39
5	E	501	TWZ	C11-C15-C16	2.04	107.17	104.71
5	D	501	TWZ	C26-C25-C24	2.04	132.54	129.39
5	E	501	TWZ	C42-C41-C40	-2.03	93.16	94.42
5	D	501	TWZ	C11-C15-C16	2.02	107.15	104.71
5	E	501	TWZ	C47-C48-C40	2.02	132.50	129.39

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	303	GOL	C1-C2-C3-O3
4	P	303	GOL	O2-C2-C3-O3
5	D	501	TWZ	C3-C4-C5-C6
5	D	501	TWZ	C4-C5-C6-O2
5	D	501	TWZ	C6-O2-P1-O3

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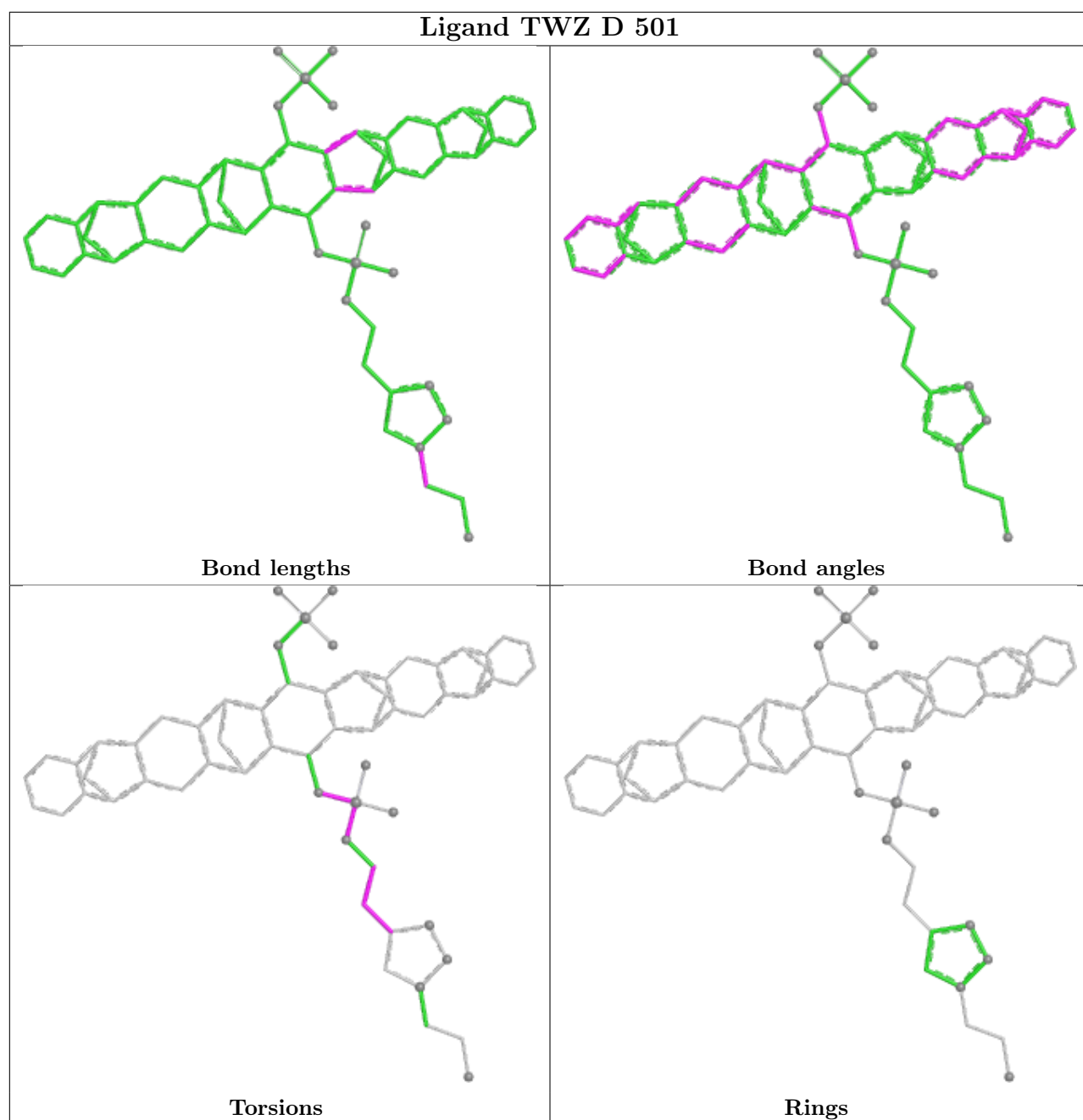
Mol	Chain	Res	Type	Atoms
5	D	501	TWZ	C6-O2-P1-O5
5	E	501	TWZ	C4-C5-C6-O2
5	E	501	TWZ	C6-O2-P1-O3
5	E	501	TWZ	C7-O5-P1-O4
4	A	302	GOL	C1-C2-C3-O3
4	A	302	GOL	O2-C2-C3-O3
5	E	501	TWZ	C10-O6-P2-O8
5	E	501	TWZ	C7-O5-P1-O2
5	E	501	TWZ	C3-C4-C5-C6
5	D	501	TWZ	C6-O2-P1-O4
5	E	501	TWZ	C6-O2-P1-O5
5	D	501	TWZ	C7-O5-P1-O4
5	E	501	TWZ	C11-C10-O6-P2
5	D	501	TWZ	N2-C4-C5-C6

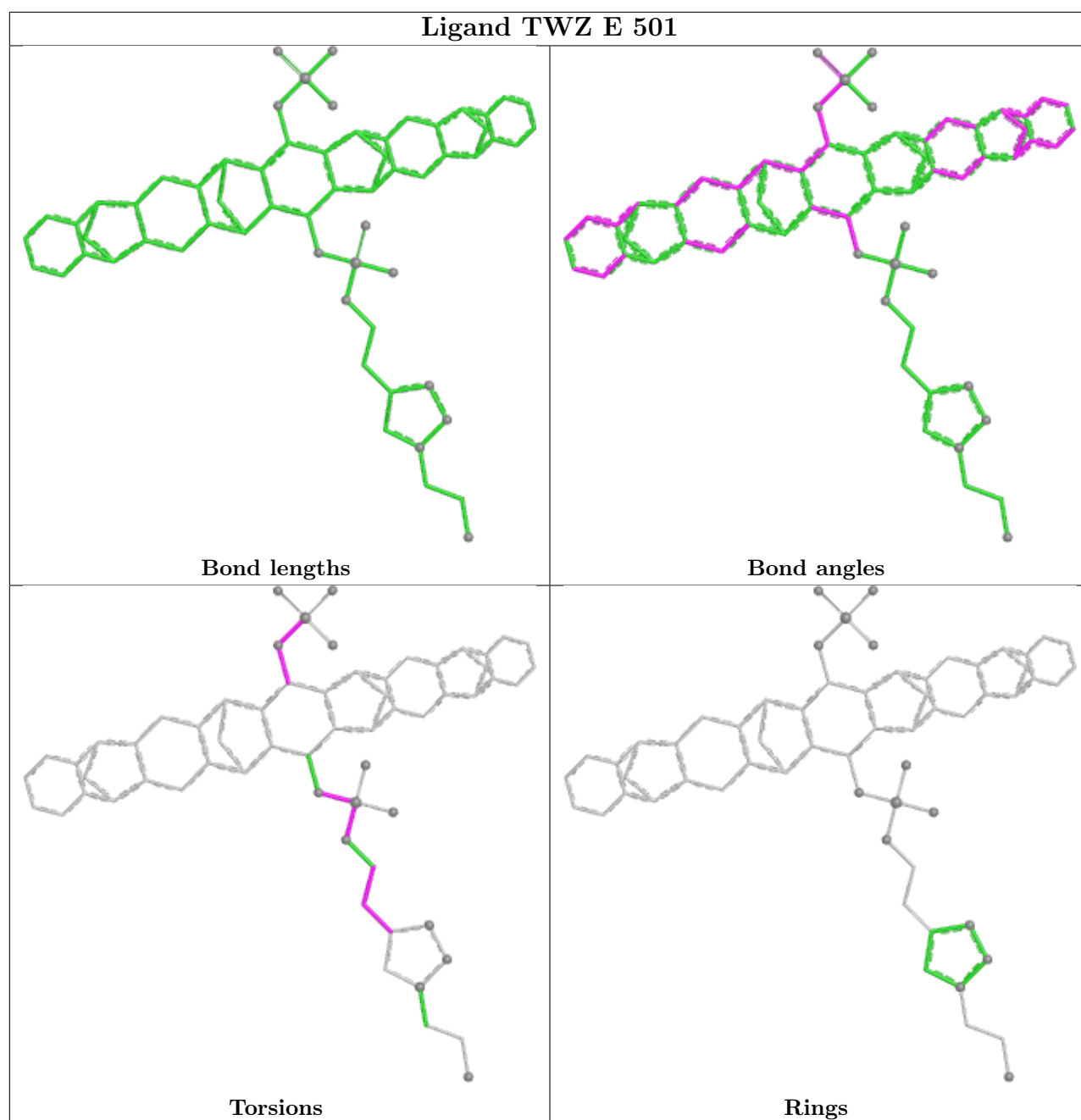
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501	TWZ	3	0
5	E	501	TWZ	2	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, 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	229/253 (90%)	0.24	5 (2%) 62 58	30, 41, 64, 88	0
1	F	229/253 (90%)	0.24	7 (3%) 51 47	18, 41, 63, 85	5 (2%)
1	K	230/253 (90%)	0.28	8 (3%) 47 42	21, 46, 77, 106	1 (0%)
1	P	230/253 (90%)	0.90	39 (16%) 4 3	23, 52, 121, 134	2 (0%)
2	D	11/11 (100%)	0.51	0 100 100	35, 45, 56, 76	0
2	E	11/11 (100%)	1.13	2 (18%) 3 2	32, 40, 51, 58	0
All	All	940/1034 (90%)	0.42	61 (6%) 25 22	18, 44, 90, 134	8 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	430	SER	7.0
1	F	231[A]	THR	6.6
1	A	70	ASN	5.4
1	F	70	ASN	5.3
1	P	223	LEU	5.2
1	P	231	THR	4.7
1	P	225	ASP	4.6
1	P	218	LEU	4.5
1	P	71	GLU	4.4
1	K	71	GLU	4.3
1	P	203	ALA	4.2
1	P	77	LYS	4.2
1	P	224	ARG	4.1
1	P	229	LEU	4.0
1	F	224[A]	ARG	4.0
1	P	217	THR	4.0
1	P	222	LEU	4.0
1	P	159	LYS	3.8
1	P	230	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	K	231	THR	3.7
1	P	213	TYR	3.5
1	K	228	THR	3.5
1	P	219	ILE	3.4
1	P	201	ALA	3.4
1	K	69	SER	3.4
1	F	77	LYS	3.3
1	P	228	THR	3.3
1	P	187	PRO	3.2
1	P	221	GLN	3.1
1	A	231	THR	3.1
1	P	202	MET	3.0
1	P	220	MET	3.0
1	P	205	LEU	3.0
1	A	77	LYS	3.0
1	P	212	SER	3.0
1	K	185	ASN	2.9
1	P	164	PRO	2.8
1	P	68	LYS	2.7
1	P	170	LEU	2.7
1	P	206	HIS	2.7
1	P	198	PHE	2.6
1	A	69	SER	2.6
1	P	216	SER	2.6
1	P	227	LEU	2.6
1	P	174	LEU	2.6
1	P	70	ASN	2.6
1	F	67	GLN	2.6
1	F	211	ASP	2.5
1	K	229	LEU	2.5
1	P	204	ASP	2.4
1	K	187	PRO	2.4
1	P	194	ALA	2.4
1	P	129[A]	ARG	2.3
1	P	181	TYR	2.3
1	K	68	LYS	2.3
1	F	69	SER	2.3
1	P	208	LEU	2.3
2	E	420	GLN	2.2
1	A	160	LYS	2.2
1	P	111	ALA	2.1
1	P	165	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($\text{\AA}^2$)	Q<0.9
1	CSO	F	38	7/8	0.81	0.17	43,47,62,69	0
1	CSO	A	38	7/8	0.83	0.17	43,47,69,69	0
1	CSO	K	38	7/8	0.86	0.11	47,50,55,62	0
1	CSO	P	38	7/8	0.92	0.12	46,47,49,52	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

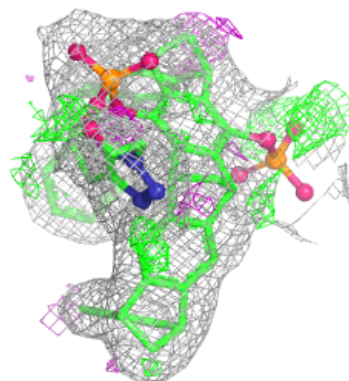
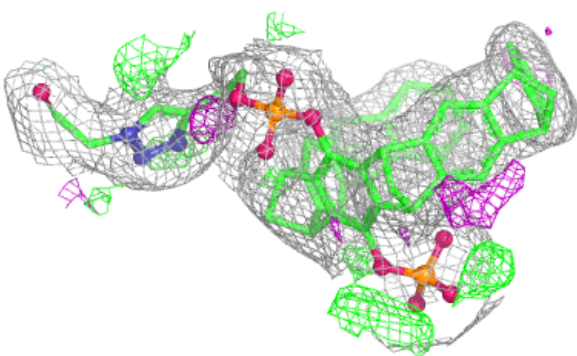
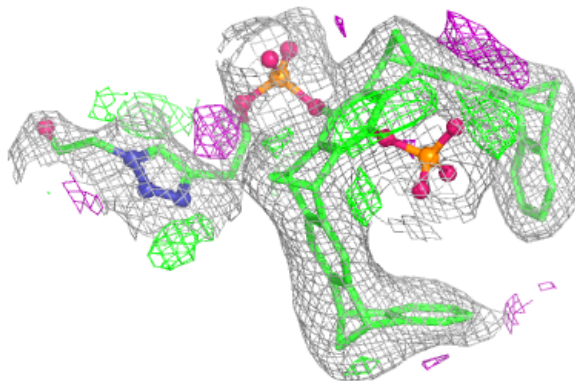
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	P	303	6/6	0.81	0.17	51,58,61,67	0
4	GOL	A	302	6/6	0.83	0.23	79,82,85,88	0
5	TWZ	E	501	62/63	0.85	0.14	40,53,85,93	0
5	TWZ	D	501	62/63	0.88	0.14	32,55,102,110	0
3	NA	A	301	1/1	0.96	0.06	33,33,33,33	0
3	NA	K	301	1/1	0.97	0.07	31,31,31,31	0
3	NA	P	302	1/1	0.97	0.07	42,42,42,42	0
3	NA	P	301	1/1	0.99	0.04	28,28,28,28	0
3	NA	F	301	1/1	0.99	0.07	31,31,31,31	0

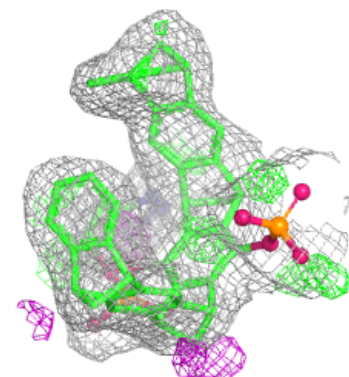
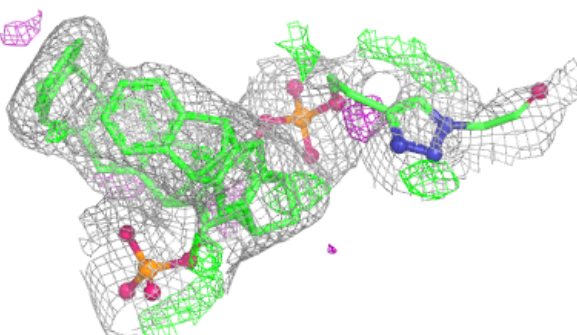
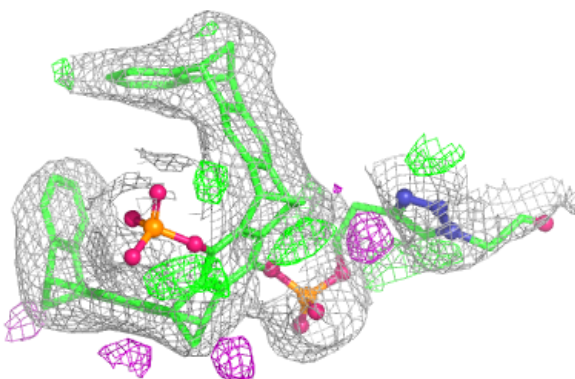
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TWZ E 501:

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

**Electron density around TWZ D 501:**

$2mF_o-DF_c$ (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.