



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:58 PM UTC

PDB ID : 5ZM6 / pdb_00005zm6
Title : Crystal structure of ORP1-ORD in complex with PI(4,5)P2
Authors : Dong, J.; Wang, J.; Luo, Z.; Wu, J.W.
Deposited on : 2018-04-01
Resolution : 2.70 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

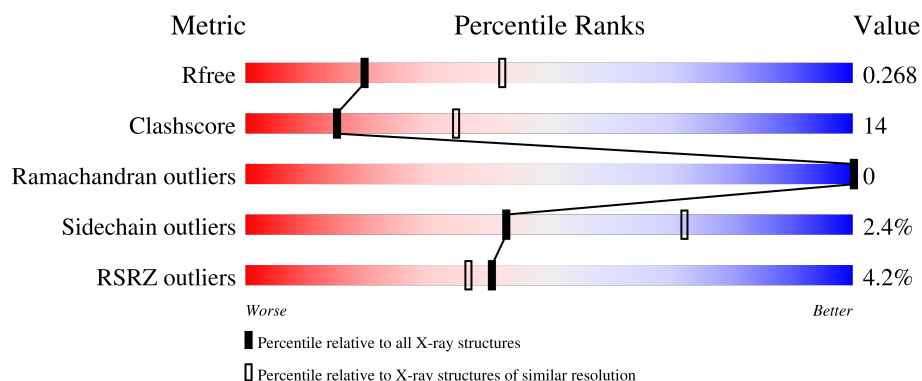
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	436	
1	B	436	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6382 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.

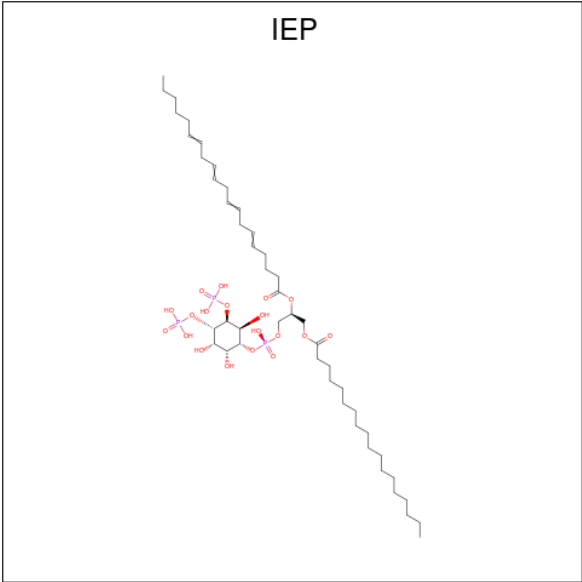
- Molecule 1 is a protein called Oxysterol-binding protein-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	1	0
			3185	2043	540	584	18			
1	B	372	Total	C	N	O	S	0	0	0
			3038	1948	520	553	17			

There are 18 discrepancies between the modelled and reference sequences:

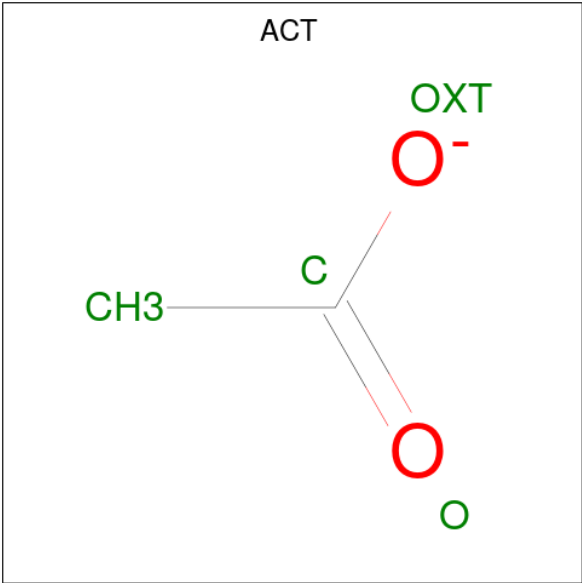
Chain	Residue	Modelled	Actual	Comment	Reference
A	523	MET	-	initiating methionine	UNP Q9BXW6
A	951	LEU	-	expression tag	UNP Q9BXW6
A	952	GLU	-	expression tag	UNP Q9BXW6
A	953	HIS	-	expression tag	UNP Q9BXW6
A	954	HIS	-	expression tag	UNP Q9BXW6
A	955	HIS	-	expression tag	UNP Q9BXW6
A	956	HIS	-	expression tag	UNP Q9BXW6
A	957	HIS	-	expression tag	UNP Q9BXW6
A	958	HIS	-	expression tag	UNP Q9BXW6
B	523	MET	-	initiating methionine	UNP Q9BXW6
B	951	LEU	-	expression tag	UNP Q9BXW6
B	952	GLU	-	expression tag	UNP Q9BXW6
B	953	HIS	-	expression tag	UNP Q9BXW6
B	954	HIS	-	expression tag	UNP Q9BXW6
B	955	HIS	-	expression tag	UNP Q9BXW6
B	956	HIS	-	expression tag	UNP Q9BXW6
B	957	HIS	-	expression tag	UNP Q9BXW6
B	958	HIS	-	expression tag	UNP Q9BXW6

- Molecule 2 is [(2 {S})-1-octadecanoyloxy-3-[oxidanyl-[(1 {R},2 {R},3 {S},4 {S},5 {S},6 {S})-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] icosan-5,8,11,14-tetraenoate (CCD ID: IEP) (formula: C₄₇H₈₅O₁₉P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			64	42	19	3		
2	B	1	Total	C	O	P	0	0
			59	37	19	3		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).

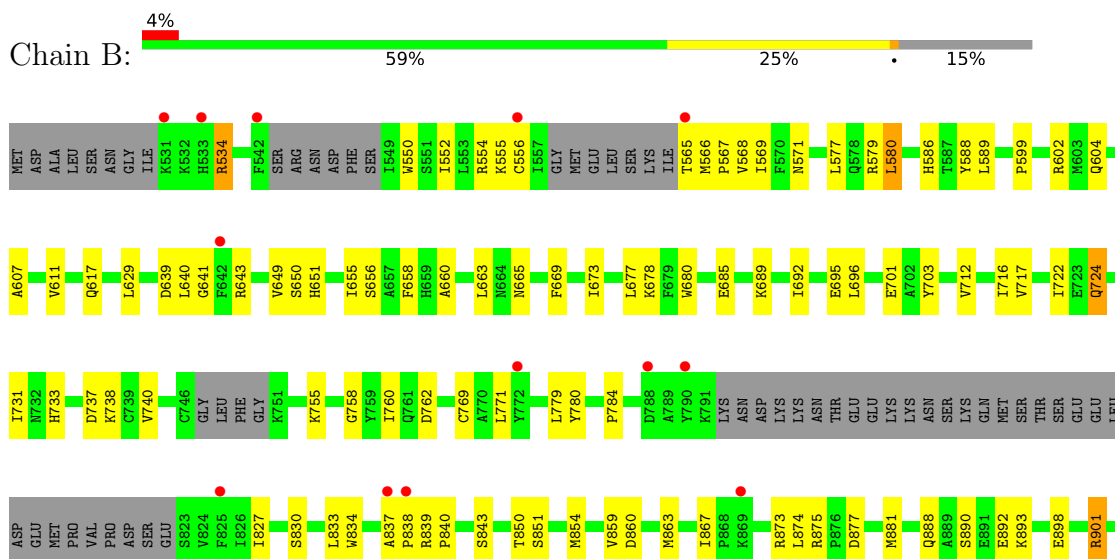


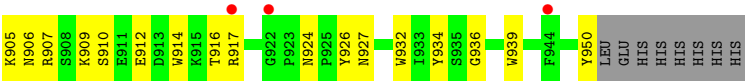
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total 10	O 10	0	0
4	B	18	Total 18	O 18	0	0

- Molecule 1: Oxysterol-binding protein-related protein 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	188.66Å 188.66Å 64.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.03 – 2.70 35.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (35.03-2.70) 96.5 (35.03-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.68Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.245 , 0.264 0.244 , 0.268	Depositor DCC
R_{free} test set	1559 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 16.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6382	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: IEP, ACT

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	0.38	0/3276	0.58	0/4441
1	B	0.39	0/3122	0.62	1/4227 (0.0%)
All	All	0.39	0/6398	0.60	1/8668 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	901	ARG	N-CA-C	-5.11	105.62	111.14

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	3185	0	3096	82	0
1	B	3038	0	2971	90	0
2	A	64	0	0	1	0
2	B	59	0	0	1	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	10	0	0	1	0
4	B	18	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6382	0	6073	170	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 14.

All (170) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:ILE:HD13	1:A:938:TYR:CE2	1.82	1.13
1:A:558:GLY:HA3	1:B:717:VAL:HG21	1.47	0.92
1:A:645:ILE:CD1	1:A:938:TYR:CZ	2.54	0.90
1:A:645:ILE:HD13	1:A:938:TYR:CZ	2.10	0.86
1:B:859:VAL:HG12	1:B:860:ASP:N	1.94	0.82
1:A:645:ILE:HD11	1:A:938:TYR:CZ	2.17	0.80
1:B:839:ARG:CG	1:B:850:THR:HA	2.13	0.77
1:B:839:ARG:HG3	1:B:850:THR:HG22	1.68	0.74
1:A:647:GLU:O	1:A:649:VAL:HG23	1.91	0.71
1:B:859:VAL:HA	1:B:863:MET:HE3	1.74	0.70
1:A:579:ARG:HH21	1:A:624:PRO:HD3	1.57	0.69
1:A:645:ILE:CD1	1:A:938:TYR:CE2	2.66	0.69
1:A:684:VAL:HG23	1:A:715:ILE:HG21	1.73	0.69
1:B:924:ASN:HB3	1:B:927:ASN:OD1	1.93	0.68
1:B:839:ARG:HG2	1:B:850:THR:HA	1.76	0.67
1:B:859:VAL:CG1	1:B:860:ASP:N	2.58	0.67
1:B:660:ALA:HB3	1:B:669:PHE:HB3	1.76	0.66
1:B:839:ARG:HG3	1:B:850:THR:HA	1.74	0.66
1:B:580:LEU:HD11	1:B:673:ILE:HG13	1.77	0.66
1:B:649:VAL:HG11	1:B:932:TRP:CH2	2.31	0.66
1:B:586:HIS:CD2	1:B:834:TRP:HE1	2.15	0.65
1:B:568:VAL:HG22	1:B:893:LYS:HD3	1.77	0.65
1:B:649:VAL:HG11	1:B:932:TRP:CZ2	2.31	0.65
1:B:837:ALA:HB1	1:B:838:PRO:HD2	1.78	0.65
1:A:676:LYS:HE3	1:A:689:LYS:HG3	1.79	0.65
1:B:839:ARG:CG	1:B:850:THR:HG22	2.26	0.65
1:B:716:ILE:HG22	1:B:717:VAL:HG23	1.79	0.64
1:A:579:ARG:HH11	1:A:617:GLN:HE22	1.45	0.64
1:B:617:GLN:NE2	1:B:724:GLN:OE1	2.31	0.63
1:A:846:MET:CB	1:A:854:MET:HE2	2.29	0.62
1:A:579:ARG:NH2	1:A:624:PRO:HD3	2.14	0.62
1:B:649:VAL:CG1	1:B:932:TRP:CH2	2.83	0.62
1:A:645:ILE:HD11	1:A:938:TYR:CE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:LYS:HE3	4:A:1105:HOH:O	2.01	0.61
1:A:876:PRO:HG2	1:A:896:LEU:HD11	1.83	0.59
1:B:859:VAL:CG1	1:B:860:ASP:H	2.15	0.59
1:A:730:ILE:HB	1:A:739:CYS:HB3	1.84	0.59
1:B:579:ARG:NH1	1:B:617:GLN:OE1	2.37	0.58
1:A:598:ASP:HB3	1:A:601:GLU:HB2	1.85	0.58
1:B:649:VAL:HG11	1:B:932:TRP:CE2	2.39	0.57
1:A:917:ARG:NH1	1:A:945:ASN:O	2.37	0.57
1:B:550:TRP:CE2	1:B:554:ARG:HB2	2.40	0.57
1:B:565:THR:HG22	1:B:566:MET:N	2.19	0.57
1:A:875:ARG:HD3	1:A:878:ILE:HD12	1.86	0.55
1:B:859:VAL:HG12	1:B:860:ASP:H	1.66	0.55
1:B:650:SER:OG	1:B:655:ILE:HD12	2.06	0.55
1:A:676:LYS:HG2	1:B:680:TRP:HE1	1.72	0.55
1:B:839:ARG:HD2	1:B:850:THR:HG22	1.88	0.55
1:B:731:ILE:HD13	1:B:738:LYS:HG3	1.89	0.55
1:B:859:VAL:CG2	1:B:873:ARG:HB3	2.37	0.55
1:B:673:ILE:HD11	1:B:692:ILE:HD11	1.88	0.55
1:B:867:ILE:HD11	1:B:874:LEU:HD21	1.88	0.55
1:A:649:VAL:HG11	1:A:932:TRP:CE3	2.42	0.55
1:A:740:VAL:O	1:A:758:GLY:HA3	2.06	0.55
1:A:842:ASN:HB3	1:A:854:MET:HE1	1.89	0.54
1:A:572:GLU:O	1:A:574:LEU:N	2.40	0.54
1:B:906:ASN:HA	1:B:909:LYS:HE2	1.88	0.54
1:B:571:ASN:O	1:B:881:MET:HE1	2.07	0.54
1:A:645:ILE:HG23	1:A:645:ILE:O	2.08	0.54
1:A:617:GLN:HG3	1:A:724:GLN:OE1	2.08	0.54
1:A:579:ARG:HH11	1:A:617:GLN:NE2	2.06	0.54
1:B:695:GLU:OE2	1:B:926:TYR:OH	2.22	0.53
1:B:649:VAL:HG11	1:B:932:TRP:CZ3	2.44	0.53
1:A:708:PRO:HD3	1:A:728:VAL:HG21	1.91	0.53
1:B:651:HIS:CE1	2:B:1001:IEP:C31	2.91	0.53
1:A:711:CYS:SG	1:A:713:HIS:CE1	3.02	0.52
1:A:752:GLU:OE1	1:A:755:LYS:HD3	2.08	0.52
1:B:840:PRO:O	1:B:843:SER:HB2	2.08	0.52
1:B:838:PRO:O	1:B:851:SER:HB2	2.08	0.52
1:B:839:ARG:CD	1:B:850:THR:HG22	2.40	0.51
1:A:649:VAL:HG21	1:A:657:ALA:HB3	1.91	0.51
1:A:746:CYS:SG	1:A:750:GLY:HA2	2.50	0.51
1:A:897:GLU:O	1:A:901:ARG:HG3	2.11	0.51
1:A:860:ASP:N	1:A:860:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:905:LYS:O	1:B:909:LYS:HG2	2.11	0.51
1:B:914:TRP:HZ3	1:B:916:THR:HG22	1.75	0.51
1:B:859:VAL:HG22	1:B:873:ARG:HB3	1.93	0.50
1:B:737:ASP:OD1	1:B:762:ASP:HA	2.12	0.50
1:B:769:CYS:HA	1:B:784:PRO:HD3	1.93	0.50
1:A:859:VAL:CG2	1:A:873:ARG:HB3	2.42	0.50
1:A:549:ILE:HG23	1:A:550:TRP:CD1	2.47	0.49
1:B:552:ILE:HA	1:B:555:LYS:HE2	1.94	0.49
1:B:641:GLY:HA2	1:B:663:LEU:HD12	1.93	0.49
1:A:679[B]:PHE:CE1	1:A:715:ILE:HD11	2.47	0.49
1:A:614:VAL:HG23	1:A:724:GLN:HE22	1.77	0.49
1:B:850:THR:O	1:B:854:MET:HG2	2.13	0.49
1:A:756:VAL:O	1:A:772:TYR:HA	2.12	0.48
1:B:740:VAL:O	1:B:758:GLY:HA3	2.14	0.48
1:A:703:TYR:HA	1:A:731:ILE:O	2.13	0.48
1:B:678:LYS:HD2	4:B:1111:HOH:O	2.13	0.48
1:A:713:HIS:CD2	1:A:721:TRP:CH2	3.02	0.48
1:A:934:TYR:CE2	1:A:936:GLY:HA2	2.49	0.48
1:B:875:ARG:HG3	1:B:950:TYR:CE1	2.48	0.47
1:A:602:ARG:NH1	1:A:701:GLU:OE2	2.42	0.47
1:A:712:VAL:HG22	1:A:722:ILE:HD13	1.95	0.47
1:A:566:MET:HE2	1:A:570:PHE:HB2	1.96	0.46
1:B:577:LEU:HD23	1:B:656:SER:HB3	1.98	0.46
1:A:653:PRO:HG2	1:A:655:ILE:HD11	1.98	0.46
1:A:897:GLU:O	1:A:901:ARG:NH1	2.49	0.46
1:B:779:LEU:HD23	1:B:833:LEU:HD12	1.97	0.46
1:A:629:LEU:N	1:A:900:GLN:OE1	2.45	0.46
1:A:723:GLU:HG2	1:A:725:TYR:CD2	2.50	0.46
1:B:580:LEU:HD21	1:B:658:PHE:CD1	2.50	0.46
1:B:604:GLN:HB3	1:B:833:LEU:HD22	1.98	0.46
1:A:911:GLU:O	1:A:911:GLU:HG2	2.16	0.46
1:B:934:TYR:CE2	1:B:936:GLY:HA2	2.51	0.45
1:A:618:TRP:O	1:A:839:ARG:NH2	2.50	0.45
1:B:755:LYS:HD2	1:B:755:LYS:HA	1.70	0.45
1:A:579:ARG:NH2	1:A:622:GLY:O	2.49	0.45
1:A:623:LYS:HE2	2:A:1001:IEP:O24	2.15	0.45
1:B:568:VAL:HG21	1:B:890:SER:HA	1.97	0.45
1:B:649:VAL:CG1	1:B:932:TRP:CZ3	3.00	0.45
1:B:696:LEU:HD23	1:B:696:LEU:HA	1.79	0.45
1:A:647:GLU:CD	1:A:916:THR:HG23	2.42	0.45
1:B:733:HIS:CD2	1:B:926:TYR:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:ASP:C	1:A:640:LEU:HD23	2.41	0.45
1:A:654:PRO:HD2	1:A:674:TYR:CE1	2.51	0.44
1:A:579:ARG:NH1	1:A:617:GLN:OE1	2.50	0.44
1:A:677:LEU:HA	1:A:685:GLU:O	2.17	0.44
1:A:846:MET:HB2	1:A:854:MET:HE2	1.98	0.44
1:B:599:PRO:HA	1:B:602:ARG:HB2	1.99	0.44
1:B:586:HIS:HD2	1:B:588:TYR:OH	2.01	0.43
1:A:534:ARG:HG3	1:A:536:SER:O	2.18	0.43
1:A:756:VAL:HG21	1:A:775:TRP:HB3	1.99	0.43
1:B:649:VAL:HG11	1:B:932:TRP:CD2	2.53	0.43
1:B:643:ARG:HB2	1:B:939:TRP:CZ2	2.53	0.43
1:B:589:LEU:HD11	1:B:834:TRP:CD1	2.54	0.43
1:A:839:ARG:HG3	1:A:850:THR:HG22	1.99	0.43
1:B:877:ASP:OD1	1:B:877:ASP:N	2.34	0.43
1:A:593:ALA:HB2	1:A:605:CYS:HB2	2.01	0.43
1:A:877:ASP:OD1	1:A:877:ASP:N	2.51	0.42
1:B:565:THR:CG2	1:B:566:MET:N	2.81	0.42
1:B:629:LEU:HD11	1:B:649:VAL:O	2.19	0.42
1:B:649:VAL:HG13	1:B:916:THR:HG21	2.00	0.42
1:B:701:GLU:OE2	1:B:703:TYR:OH	2.31	0.42
1:A:875:ARG:HD3	1:A:878:ILE:CD1	2.49	0.42
1:B:580:LEU:HD11	1:B:673:ILE:CG1	2.47	0.42
1:B:863:MET:O	1:B:867:ILE:HG12	2.19	0.42
1:A:581:THR:HG23	1:A:644:LEU:HD13	2.00	0.42
1:B:907:ARG:HG2	1:B:912:GLU:HB2	2.02	0.42
1:B:827:ILE:O	1:B:830:SER:OG	2.28	0.42
1:B:607:ALA:O	1:B:611:VAL:HG23	2.19	0.42
1:B:760:ILE:HD12	1:B:769:CYS:SG	2.59	0.42
1:A:561:LEU:O	1:A:564:ILE:HG12	2.20	0.42
1:B:567:PRO:HB2	1:B:569:ILE:HG22	2.02	0.42
1:A:580:LEU:HD21	1:A:658:PHE:CD2	2.55	0.41
1:A:875:ARG:HG2	1:A:877:ASP:OD1	2.19	0.41
1:B:555:LYS:HG3	1:B:556:CYS:SG	2.60	0.41
1:B:660:ALA:N	1:B:669:PHE:O	2.50	0.41
1:A:633:TYR:CE2	1:A:635:LEU:HB2	2.55	0.41
1:B:771:LEU:HA	1:B:780:TYR:O	2.20	0.41
1:A:580:LEU:HD21	1:A:658:PHE:HD2	1.84	0.41
1:B:909:LYS:HG3	1:B:910:SER:H	1.85	0.41
1:A:707:ASN:HD22	1:A:707:ASN:HA	1.73	0.41
1:A:845:GLN:N	1:A:845:GLN:OE1	2.53	0.41
1:B:712:VAL:HG22	1:B:722:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:ARG:HB3	1:A:843:SER:HB2	2.02	0.41
1:B:649:VAL:HG11	1:B:932:TRP:CE3	2.56	0.41
1:A:574:LEU:HD23	1:A:574:LEU:HA	1.87	0.41
1:B:677:LEU:HA	1:B:685:GLU:O	2.21	0.41
1:B:639:ASP:OD1	1:B:640:LEU:N	2.49	0.40
1:A:846:MET:HB3	1:A:854:MET:HE2	2.02	0.40
1:B:568:VAL:CG2	1:B:893:LYS:HD3	2.49	0.40
1:B:838:PRO:O	1:B:851:SER:CB	2.68	0.40
1:A:682:LYS:HB3	1:A:714:ASN:HA	2.02	0.40
1:A:580:LEU:HA	1:A:580:LEU:HD12	1.88	0.40
1:A:585:GLU:HB3	1:A:586:HIS:CD2	2.57	0.40
1:A:679[A]:PHE:HD1	1:A:684:VAL:HG22	1.86	0.40
1:A:863:MET:O	1:A:867:ILE:HG12	2.22	0.40
1:B:534:ARG:O	1:B:534:ARG:HG2	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	389/436 (89%)	368 (95%)	21 (5%)	0	100	100
1	B	362/436 (83%)	341 (94%)	21 (6%)	0	100	100
All	All	751/872 (86%)	709 (94%)	42 (6%)	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	348/393 (88%)	342 (98%)	6 (2%)	53	79
1	B	333/393 (85%)	323 (97%)	10 (3%)	36	66
All	All	681/786 (87%)	665 (98%)	16 (2%)	43	73

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	534	ARG
1	A	698	GLU
1	A	835	ARG
1	A	839	ARG
1	A	887	ASP
1	A	911	GLU
1	B	534	ARG
1	B	580	LEU
1	B	665	ASN
1	B	689	LYS
1	B	724	GLN
1	B	888	GLN
1	B	892	GLU
1	B	898	GLU
1	B	901	ARG
1	B	917	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	707	ASN
1	A	713	HIS
1	B	571	ASN
1	B	626	ASN
1	B	670	HIS
1	B	707	ASN
1	B	888	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
2	IEP	B	1001	-	59,59,69	1.96	13 (22%)	74,77,87	2.43	23 (31%)
2	IEP	A	1001	-	64,64,69	1.83	15 (23%)	79,82,87	2.35	22 (27%)
3	ACT	A	1002	-	3,3,3	0.82	0	3,3,3	1.46	0
3	ACT	B	1002	-	3,3,3	0.90	0	3,3,3	1.51	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
2	IEP	B	1001	-	-	29/56/80/90	0/1/1/1
2	IEP	A	1001	-	-	27/61/85/90	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	IEP	P42-O41	-6.10	1.48	1.59
2	B	1001	IEP	O50-C49	5.65	1.39	1.22
2	B	1001	IEP	O19-C18	5.62	1.39	1.22
2	A	1001	IEP	O50-C49	5.45	1.38	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	IEP	O19-C18	4.96	1.37	1.22
2	A	1001	IEP	O36-C33	-4.32	1.29	1.44
2	B	1001	IEP	C31-C32	3.88	1.62	1.52
2	A	1001	IEP	C64-C63	3.83	1.53	1.29
2	A	1001	IEP	C61-C60	3.68	1.52	1.31
2	B	1001	IEP	C55-C54	3.65	1.52	1.31
2	B	1001	IEP	C33-C32	3.60	1.59	1.52
2	B	1001	IEP	O48-C22	-3.54	1.38	1.46
2	A	1001	IEP	C55-C54	3.48	1.51	1.31
2	A	1001	IEP	C58-C57	3.36	1.50	1.31
2	A	1001	IEP	C23-C22	3.32	1.61	1.50
2	B	1001	IEP	C57-C58	3.24	1.53	1.29
2	A	1001	IEP	C21-C22	3.17	1.60	1.50
2	B	1001	IEP	C34-C29	3.10	1.60	1.52
2	A	1001	IEP	O20-C21	-2.87	1.38	1.45
2	B	1001	IEP	C34-C33	2.80	1.59	1.52
2	A	1001	IEP	C33-C32	-2.65	1.46	1.52
2	B	1001	IEP	O20-C18	2.54	1.40	1.33
2	A	1001	IEP	O20-C18	2.51	1.40	1.33
2	A	1001	IEP	P42-O41	-2.50	1.55	1.59
2	B	1001	IEP	P37-O36	-2.34	1.55	1.59
2	B	1001	IEP	O35-C34	2.14	1.48	1.43
2	A	1001	IEP	P37-O36	-2.06	1.55	1.59
2	A	1001	IEP	O47-C30	-2.00	1.38	1.43

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	IEP	O41-C32-C31	8.46	126.64	108.73
2	B	1001	IEP	O48-C49-O50	-8.45	103.94	123.70
2	A	1001	IEP	O48-C49-O50	-8.01	104.99	123.70
2	A	1001	IEP	O41-C32-C33	7.48	124.67	108.76
2	B	1001	IEP	O36-C33-C32	6.18	121.92	108.76
2	A	1001	IEP	O20-C18-O19	-6.14	108.27	123.63
2	B	1001	IEP	O20-C18-O19	-6.02	108.56	123.63
2	B	1001	IEP	C33-C34-C29	5.02	119.28	109.11
2	A	1001	IEP	O41-C32-C31	4.70	118.69	108.73
2	B	1001	IEP	C30-C31-C32	4.65	120.23	109.68
2	A	1001	IEP	P37-O36-C33	4.63	135.79	123.43
2	A	1001	IEP	C31-C30-C29	4.16	119.11	109.68
2	B	1001	IEP	O41-C32-C33	4.09	117.45	108.76
2	A	1001	IEP	O36-C33-C32	3.99	117.25	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	IEP	C31-C30-C29	3.88	118.48	109.68
2	B	1001	IEP	O19-C18-C17	-3.87	108.65	123.78
2	B	1001	IEP	O46-C31-C30	-3.80	101.43	110.38
2	A	1001	IEP	O19-C18-C17	-3.78	108.99	123.78
2	A	1001	IEP	C33-C34-C29	3.51	116.22	109.11
2	A	1001	IEP	O27-P25-O26	-3.43	96.49	112.44
2	A	1001	IEP	C34-C29-C30	3.41	115.60	110.86
2	A	1001	IEP	C34-C33-C32	3.25	119.02	111.72
2	A	1001	IEP	O36-C33-C34	3.20	115.52	108.73
2	B	1001	IEP	O41-P42-O45	3.14	120.53	109.33
2	A	1001	IEP	C23-C22-C21	3.13	119.08	111.78
2	A	1001	IEP	O48-C22-C23	3.07	119.35	108.34
2	B	1001	IEP	O46-C31-C32	-2.99	102.28	109.94
2	A	1001	IEP	O38-P37-O40	-2.92	99.45	110.83
2	A	1001	IEP	O50-C49-C51	-2.89	112.49	123.78
2	B	1001	IEP	O47-C30-C29	-2.88	102.55	109.94
2	B	1001	IEP	C34-C29-C30	2.79	114.73	110.86
2	B	1001	IEP	O39-P37-O40	-2.72	100.22	110.83
2	A	1001	IEP	C51-C52-C53	2.64	119.11	113.35
2	A	1001	IEP	C15-C16-C17	2.53	122.44	113.13
2	B	1001	IEP	O36-C33-C34	2.53	114.09	108.73
2	B	1001	IEP	O28-C29-C30	-2.36	103.74	108.73
2	A	1001	IEP	O43-P42-O45	-2.29	101.91	110.83
2	B	1001	IEP	O50-C49-C51	-2.28	114.86	123.78
2	A	1001	IEP	C31-C32-C33	-2.13	106.93	111.72
2	B	1001	IEP	C59-C58-C57	-2.12	109.84	126.43
2	B	1001	IEP	O28-P25-O26	2.12	116.58	109.81
2	B	1001	IEP	O39-P37-O36	2.10	114.03	105.85
2	A	1001	IEP	C22-O48-C49	-2.09	112.81	117.80
2	B	1001	IEP	O35-C34-C29	2.03	115.14	109.94
2	B	1001	IEP	C23-C22-C21	-2.01	107.11	111.78

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	IEP	C31-C32-O41-P42
2	A	1001	IEP	C32-C33-O36-P37
2	A	1001	IEP	C57-C58-C59-C60
2	A	1001	IEP	C23-O24-P25-O27
2	B	1001	IEP	C17-C18-O20-C21
2	B	1001	IEP	C31-C32-O41-P42

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Mol	Chain	Res	Type	Atoms
2	B	1001	IEP	C32-C33-O36-P37
2	B	1001	IEP	O50-C49-O48-C22
2	B	1001	IEP	C56-C57-C58-C59
2	B	1001	IEP	C23-O24-P25-O26
2	B	1001	IEP	C23-O24-P25-O27
2	B	1001	IEP	C23-O24-P25-O28
2	B	1001	IEP	C29-O28-P25-O27
2	B	1001	IEP	O19-C18-O20-C21
2	A	1001	IEP	O19-C18-O20-C21
2	A	1001	IEP	O50-C49-O48-C22
2	A	1001	IEP	C17-C18-O20-C21
2	A	1001	IEP	C59-C60-C61-C62
2	B	1001	IEP	C07-C08-C09-C10
2	B	1001	IEP	C51-C49-O48-C22
2	A	1001	IEP	C13-C14-C15-C16
2	B	1001	IEP	C06-C07-C08-C09
2	B	1001	IEP	C14-C15-C16-C17
2	A	1001	IEP	C08-C09-C10-C11
2	B	1001	IEP	C02-C03-C04-C05
2	B	1001	IEP	C12-C13-C14-C15
2	B	1001	IEP	C09-C10-C11-C12
2	A	1001	IEP	C51-C52-C53-C54
2	B	1001	IEP	C08-C09-C10-C11
2	A	1001	IEP	C56-C57-C58-C59
2	A	1001	IEP	C22-C23-O24-P25
2	B	1001	IEP	C22-C23-O24-P25
2	B	1001	IEP	C03-C04-C05-C06
2	B	1001	IEP	C51-C52-C53-C54
2	A	1001	IEP	C53-C54-C55-C56
2	A	1001	IEP	C60-C61-C62-C63
2	B	1001	IEP	C54-C55-C56-C57
2	B	1001	IEP	C49-C51-C52-C53
2	A	1001	IEP	O20-C21-C22-O48
2	B	1001	IEP	C29-O28-P25-O26
2	A	1001	IEP	C03-C04-C05-C06
2	A	1001	IEP	C61-C62-C63-C64
2	A	1001	IEP	O20-C21-C22-C23
2	B	1001	IEP	C52-C53-C54-C55
2	A	1001	IEP	C23-O24-P25-O26
2	A	1001	IEP	C23-O24-P25-O28
2	A	1001	IEP	C21-C22-C23-O24
2	A	1001	IEP	O48-C22-C23-O24

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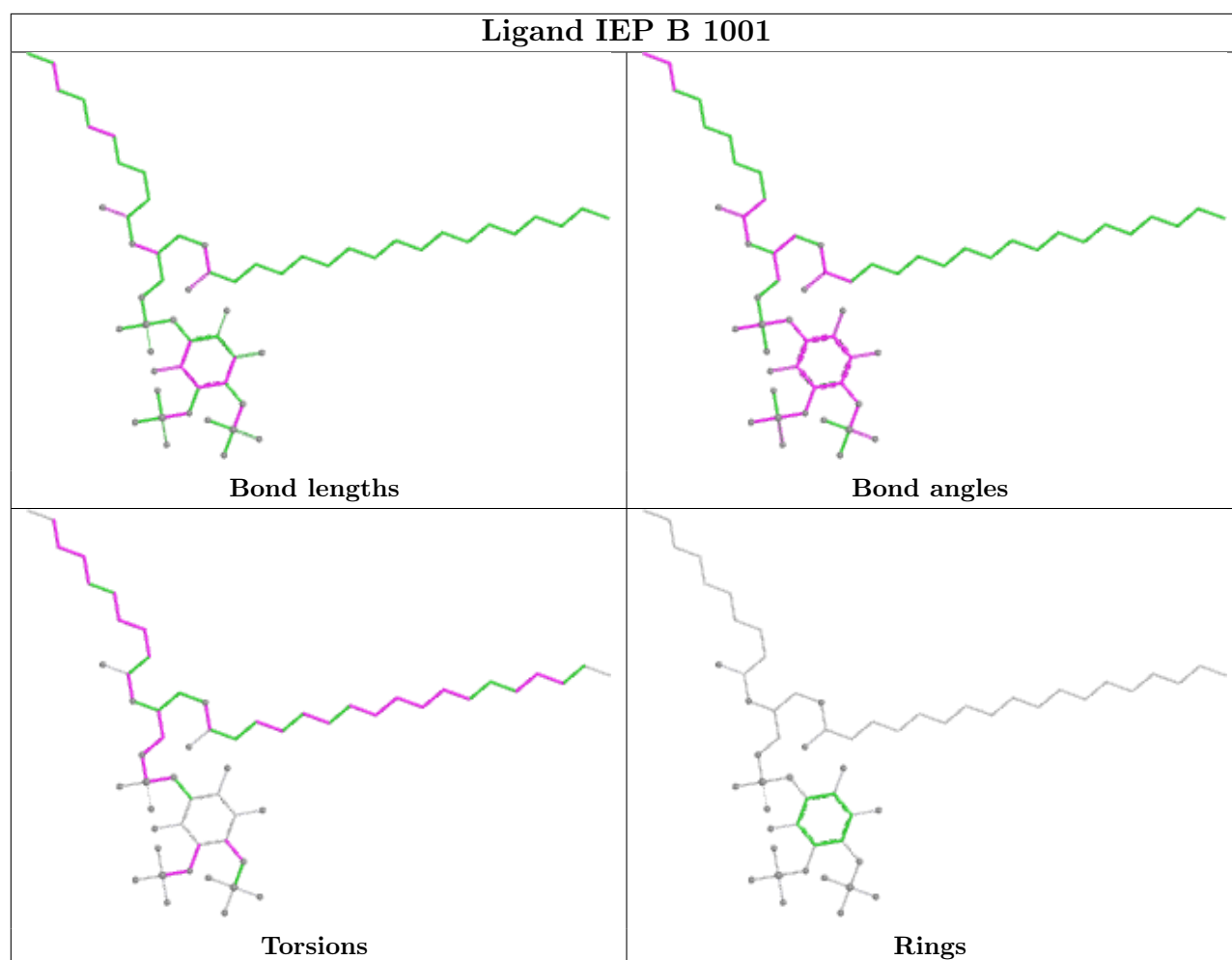
Mol	Chain	Res	Type	Atoms
2	A	1001	IEP	C04-C05-C06-C07
2	B	1001	IEP	C33-O36-P37-O39
2	A	1001	IEP	C21-C22-O48-C49
2	B	1001	IEP	C55-C56-C57-C58
2	B	1001	IEP	C10-C11-C12-C13
2	A	1001	IEP	C06-C07-C08-C09
2	B	1001	IEP	C21-C22-C23-O24
2	A	1001	IEP	C32-O41-P42-O45

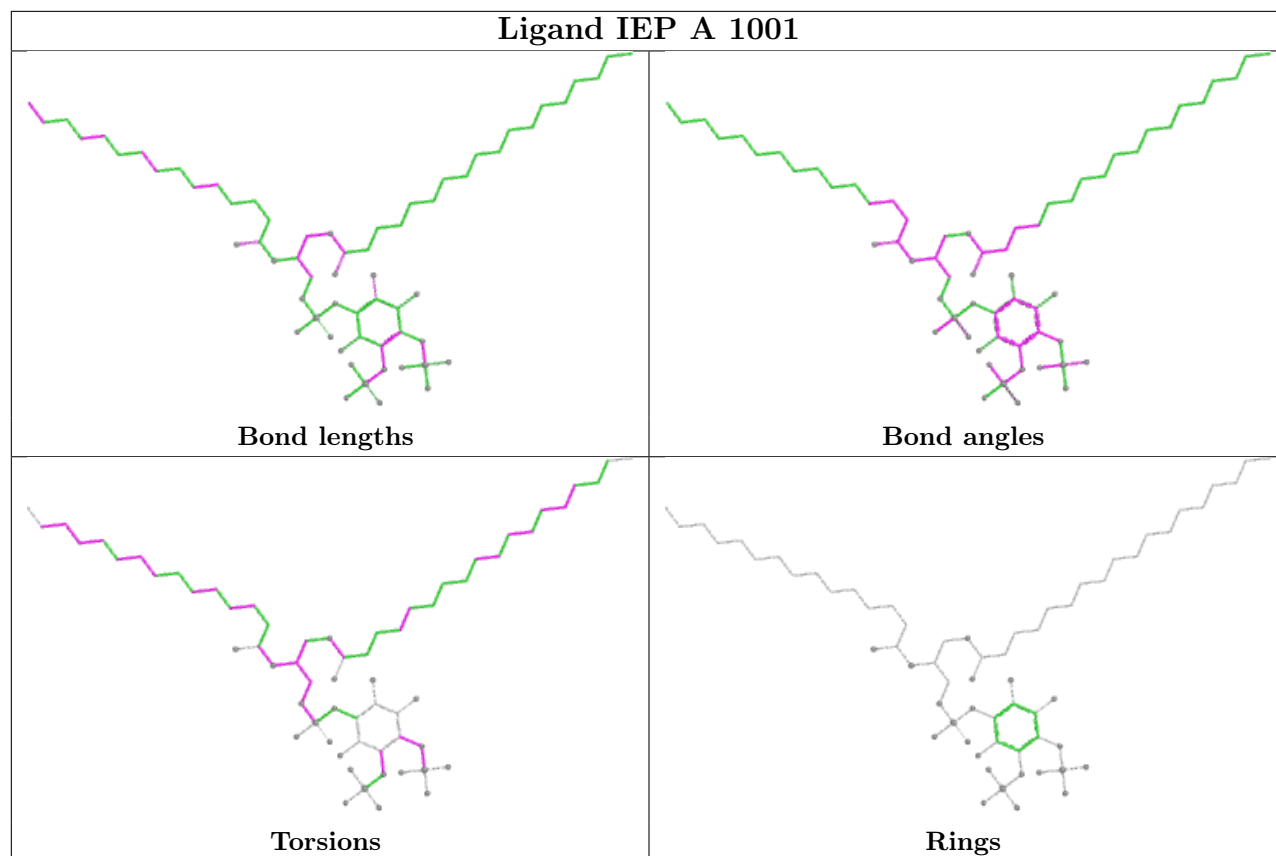
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	IEP	1	0
2	A	1001	IEP	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 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	392/436 (89%)	0.38	16 (4%) 41 37	28, 56, 104, 164	1 (0%)
1	B	372/436 (85%)	0.35	16 (4%) 40 36	37, 55, 92, 117	0
All	All	764/872 (87%)	0.36	32 (4%) 40 37	28, 55, 100, 164	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	679[A]	PHE	6.4
1	A	914	TRP	3.6
1	B	542	PHE	3.5
1	A	916	THR	3.4
1	A	790	TYR	3.4
1	B	772	TYR	3.3
1	B	825	PHE	3.1
1	B	565	THR	2.8
1	A	898	GLU	2.8
1	A	563	LYS	2.7
1	B	838	PRO	2.7
1	A	597	SER	2.6
1	B	531	LYS	2.6
1	B	837	ALA	2.5
1	A	547	PHE	2.5
1	A	564	ILE	2.4
1	A	628	LEU	2.4
1	B	788	ASP	2.4
1	A	590	ILE	2.3
1	B	556	CYS	2.2
1	B	944	PHE	2.2
1	A	601	GLU	2.2
1	B	922	GLY	2.2
1	B	790	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	645	ILE	2.1
1	A	949	ILE	2.1
1	B	642	PHE	2.1
1	B	917	ARG	2.0
1	B	869	LYS	2.0
1	A	841	PRO	2.0
1	A	630	GLY	2.0
1	B	533	HIS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

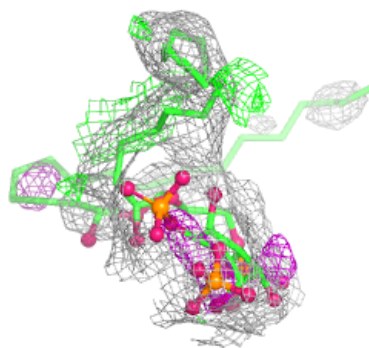
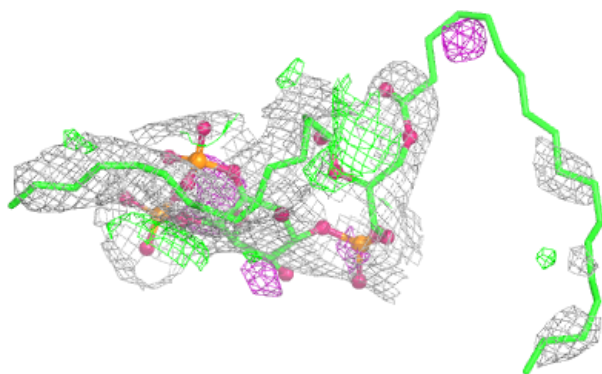
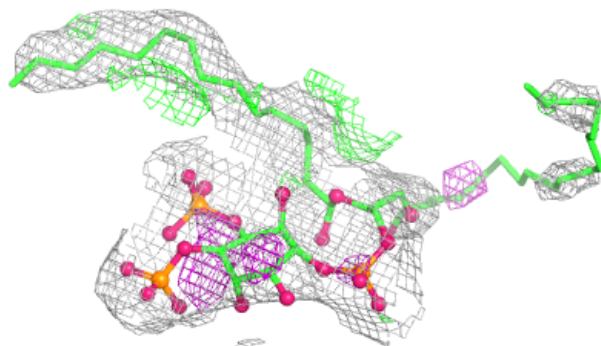
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	ACT	B	1002	4/4	0.31	0.30	63,63,63,63	0
3	ACT	A	1002	4/4	0.55	0.31	63,63,63,63	0
2	IEP	A	1001	64/69	0.69	0.22	53,93,105,115	0
2	IEP	B	1001	59/69	0.72	0.17	48,81,115,127	0

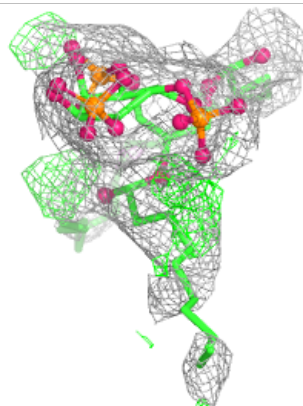
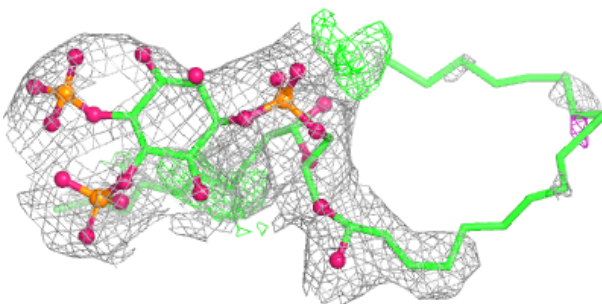
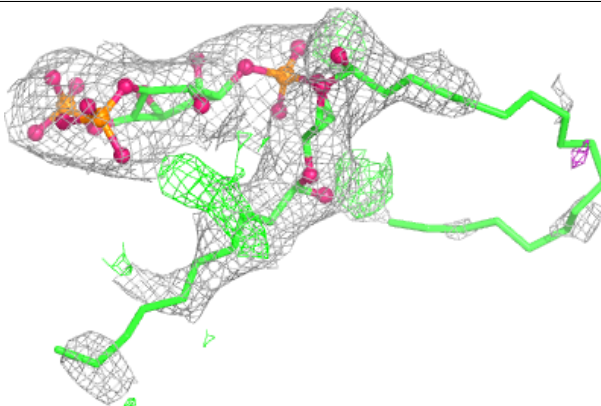
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IEP A 1001:

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

**Electron density around IEP B 1001:**

$2mF_o-DF_c$ (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.