



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:03 am BST

PDB ID : 5ZM6
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 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 : 2.11
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) : 2.11

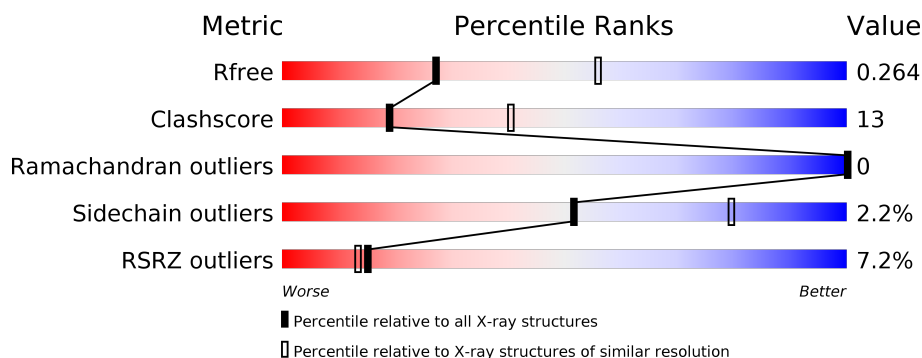
1 Overall quality at a glance

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 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 $\leq 5\%$. 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	<div> <div>7%</div> <div>67%</div> <div>22%</div> <div>10%</div> </div>
1	B	436	<div> <div>6%</div> <div>61%</div> <div>24%</div> <div>15%</div> </div>

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.

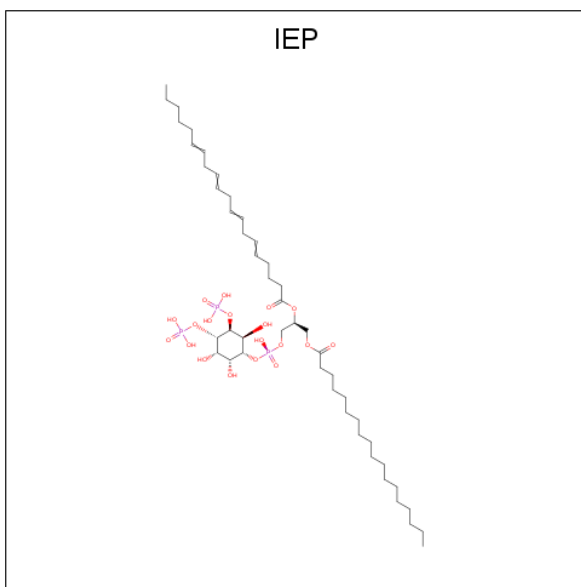
- Molecule 1 is a protein called Oxysterol-binding protein-related protein 1.

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] icosahexanoate (three-letter code: 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 (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

These plots are drawn for all protein, RNA and DNA 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.

Chain A:

7% 67% 22% 10%

MET ASP ALA LEU SER ASN GLY ILE LYS H533 H534 T535 S536 H544 H545 D546 F547 S548 T549 W550 G558 H559 E560 L561 L564 E572 P573 L574 S575 R579 L580 T581 E585 H586 A593 S594 D598 E601 R602 C605 V614 Q617 W618 G622 K623 D624

L629 Y630 Y633 L635 L644 I645 S646 E647 Q648 W649 P653 P654 L655 S656 A657 F658 Y674 K675 L676 L677 K678 F679 K682 S683 V684 E685 L689 E701 A702 Y703 N707 F708 C711 W712 H713 N714 I715 K719 L720 W721 I722 E723 Q724 Y725 V728 E729 I730 T731

T850 M854 V859 D860 K861 D862 M863 L867 L873 L874 R875 R876 D877 L878 L886 D887 Q888 L896 E897 Q900 R901 E911 D912 D913 W914 K915 T916 R917 W932 Y933 Y934 S935 G936 S937 Y938 N945 T949 L950 G951 H952 H953 H954 H955 H956 H957 H958 H959 H960 H961 H962 H963 H964 H965 H966 H967 H968 H969 H970 H971 H972 H973 H974 H975 H976 H977 H978 H979 H980 H981 H982 H983 H984 H985 H986 H987 H988 H989 H990 H991 H992 H993 H994 H995 H996 H997 H998 H999

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	188.66 Å 188.66 Å 64.58 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.03 – 2.70 35.03 – 2.68	Depositor EDS
% Data completeness (in resolution range)	96.5 (35.03-2.70) 96.4 (35.03-2.68)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.68 Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.245 , 0.264 0.245 , 0.264	Depositor DCC
R_{free} test set	1551 reflections (4.85%)	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)	0.26 , 26.3	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	0.88	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

5.1 Standard geometry

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	0.45	0/3276	0.59	0/4441
1	B	0.45	0/3122	0.60	0/4227
All	All	0.45	0/6398	0.59	0/8668

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

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	76	0
1	B	3038	0	2971	87	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
All	All	6382	0	6073	161	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 13.

All (161) 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: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:837:ALA:HB1	1:B:838:PRO:HD2	1.78	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: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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:740:VAL:O	1:A:758:GLY:HA3	2.06	0.55
1:A:649:VAL:HG11	1:A:932:TRP:CE3	2.42	0.55
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:A:645:ILE:O	1:A:645:ILE:HG23	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: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:B:695:GLU:OE2	1:B:926:TYR:OH	2.22	0.51
1:A:897:GLU:O	1:A:901:ARG:HG3	2.11	0.51
1:A:860:ASP:OD1	1:A:860:ASP:N	2.43	0.51
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:842:ASN:HB3	1:A:854:MET:HE1	1.95	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: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:723:GLU:HG2	1:A:725:TYR:CD2	2.50	0.46
1:A:629:LEU:N	1:A:900:GLN:OE1	2.45	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:HG2	1:A:911:GLU:O	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:HA	1:B:755:LYS:HD2	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:649:VAL:CG1	1:B:932:TRP:CZ3	3.00	0.45
1:B:696:LEU:HA	1:B:696:LEU:HD23	1.79	0.45
1:B:568:VAL:HG21	1:B:890:SER:HA	1.97	0.45
1:B:733:HIS:CD2	1:B:926:TYR:HB3	2.51	0.45
1:A:654:PRO:HD2	1:A:674:TYR:CE1	2.51	0.44
1:B:859:VAL:HA	1:B:863:MET:HE3	1.99	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:877:ASP:OD1	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: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: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:HA	1:A:707:ASN:HD22	1.73	0.41
1:A:845:GLN:OE1	1:A:845:GLN:N	2.53	0.41
1:B:712:VAL:HG22	1:B:722:ILE:HD13	2.02	0.41
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:B:838:PRO:O	1:B:851:SER:CB	2.68	0.40
1:B:568:VAL:CG2	1:B:893:LYS:HD3	2.49	0.40
1:A:682:LYS:HB3	1:A:714:ASN:HA	2.02	0.40
1:A:580:LEU:HD12	1:A:580:LEU:HA	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

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	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

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%)	344 (99%)	4 (1%)	73	90
1	B	333/393 (85%)	322 (97%)	11 (3%)	38	67
All	All	681/786 (87%)	666 (98%)	15 (2%)	52	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	534	ARG
1	A	835	ARG
1	A	839	ARG
1	A	887	ASP
1	B	534	ARG
1	B	580	LEU
1	B	665	ASN
1	B	674	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	679	PHE
1	B	689	LYS
1	B	724	GLN
1	B	860	ASP
1	B	888	GLN
1	B	901	ARG
1	B	917	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	713	HIS
1	A	724	GLN
1	B	571	ASN
1	B	888	GLN

5.3.3 RNA [i](#)

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 carbohydrates 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
3	ACT	B	1002	-	1,3,3	2.87	1 (100%)	0,3,3	0.00	-
2	IEP	A	1001	-	64,64,69	1.80	14 (21%)	78,82,87	2.24	21 (26%)
3	ACT	A	1002	-	1,3,3	2.84	1 (100%)	0,3,3	0.00	-
2	IEP	B	1001	-	59,59,69	1.92	13 (22%)	73,77,87	2.34	19 (26%)

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	A	1001	-	-	27/61/85/90	0/1/1/1
2	IEP	B	1001	-	-	31/56/80/90	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	IEP	O50-C49	5.66	1.39	1.22
2	B	1001	IEP	O19-C18	5.64	1.39	1.22
2	B	1001	IEP	P42-O41	-5.55	1.48	1.59
2	A	1001	IEP	O50-C49	5.46	1.38	1.22
2	A	1001	IEP	O19-C18	4.97	1.37	1.22
2	A	1001	IEP	O36-C33	-4.06	1.29	1.44
2	B	1001	IEP	C31-C32	3.92	1.62	1.52
2	A	1001	IEP	C64-C63	3.74	1.53	1.28
2	A	1001	IEP	C61-C60	3.60	1.52	1.31
2	B	1001	IEP	C33-C32	3.57	1.59	1.52
2	B	1001	IEP	C55-C54	3.56	1.52	1.31
2	A	1001	IEP	C23-C22	3.43	1.61	1.50
2	A	1001	IEP	C55-C54	3.40	1.51	1.31
2	B	1001	IEP	O48-C22	-3.32	1.38	1.46
2	A	1001	IEP	C58-C57	3.28	1.50	1.31
2	A	1001	IEP	C21-C22	3.27	1.60	1.50
2	B	1001	IEP	C57-C58	3.14	1.53	1.29
2	B	1001	IEP	C34-C29	3.13	1.60	1.52
3	B	1002	ACT	CH3-C	2.87	1.52	1.48
3	A	1002	ACT	CH3-C	2.84	1.52	1.48
2	B	1001	IEP	C34-C33	2.81	1.59	1.52
2	A	1001	IEP	O20-C21	-2.81	1.38	1.45
2	A	1001	IEP	C33-C32	-2.61	1.46	1.52
2	B	1001	IEP	O20-C18	2.54	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	IEP	O20-C18	2.51	1.40	1.33
2	B	1001	IEP	O35-C34	2.24	1.48	1.43
2	A	1001	IEP	P42-O41	-2.20	1.55	1.59
2	A	1001	IEP	O47-C30	-2.11	1.38	1.43
2	B	1001	IEP	P37-O36	-2.06	1.55	1.59

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	IEP	O48-C49-O50	-8.18	103.94	123.70
2	A	1001	IEP	O48-C49-O50	-7.74	104.99	123.70
2	B	1001	IEP	O41-C32-C31	7.73	126.64	108.66
2	A	1001	IEP	O41-C32-C33	6.78	124.67	108.69
2	A	1001	IEP	O20-C18-O19	-6.07	108.27	123.59
2	B	1001	IEP	O20-C18-O19	-5.95	108.56	123.59
2	B	1001	IEP	O36-C33-C32	5.61	121.92	108.69
2	B	1001	IEP	C33-C34-C29	4.98	119.28	108.96
2	B	1001	IEP	C30-C31-C32	4.62	120.23	109.68
2	A	1001	IEP	O41-C32-C31	4.31	118.69	108.66
2	A	1001	IEP	C31-C30-C29	4.13	119.11	109.68
2	B	1001	IEP	O19-C18-C17	-3.87	108.65	123.73
2	B	1001	IEP	O46-C31-C30	-3.86	101.43	110.35
2	B	1001	IEP	C31-C30-C29	3.85	118.48	109.68
2	A	1001	IEP	O19-C18-C17	-3.78	108.99	123.73
2	B	1001	IEP	O41-C32-C33	3.72	117.45	108.69
2	A	1001	IEP	O36-C33-C32	3.63	117.25	108.69
2	A	1001	IEP	C33-C34-C29	3.50	116.22	108.96
2	A	1001	IEP	C51-C52-C53	3.30	119.11	113.23
2	A	1001	IEP	C34-C29-C30	3.29	115.60	110.85
2	A	1001	IEP	C34-C33-C32	3.22	119.02	111.66
2	A	1001	IEP	O27-P25-O26	-3.19	96.49	112.24
2	A	1001	IEP	C23-C22-C21	3.08	119.08	111.79
2	A	1001	IEP	O48-C22-C23	3.02	119.35	108.40
2	A	1001	IEP	O36-C33-C34	2.95	115.52	108.66
2	B	1001	IEP	O46-C31-C32	-2.89	102.28	109.94
2	B	1001	IEP	O41-P42-O45	2.88	120.53	109.39
2	A	1001	IEP	O50-C49-C51	-2.88	112.49	123.73
2	A	1001	IEP	O38-P37-O40	-2.87	99.45	110.68
2	B	1001	IEP	O47-C30-C29	-2.79	102.55	109.94
2	B	1001	IEP	C34-C29-C30	2.69	114.73	110.85
2	B	1001	IEP	O39-P37-O40	-2.67	100.22	110.68
2	A	1001	IEP	C15-C16-C17	2.57	122.44	113.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	IEP	O36-C33-C34	2.33	114.09	108.66
2	B	1001	IEP	O50-C49-C51	-2.27	114.86	123.73
2	A	1001	IEP	O43-P42-O45	-2.24	101.91	110.68
2	B	1001	IEP	O28-C29-C30	-2.12	103.74	108.66
2	A	1001	IEP	C31-C32-C33	-2.07	106.93	111.66
2	A	1001	IEP	C22-O48-C49	-2.03	112.81	117.79
2	B	1001	IEP	C59-C58-C57	-2.00	109.84	126.37

There are no chirality outliers.

All (58) 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
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	C29-O28-P25-O27
2	B	1001	IEP	C33-O36-P37-O39
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	B	1001	IEP	C07-C08-C09-C10
2	A	1001	IEP	C59-C60-C61-C62
2	A	1001	IEP	C13-C14-C15-C16
2	B	1001	IEP	C51-C49-O48-C22
2	A	1001	IEP	C23-O24-P25-O28
2	B	1001	IEP	C23-O24-P25-O28
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	A	1001	IEP	C51-C52-C53-C54
2	B	1001	IEP	C09-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1001	IEP	C08-C09-C10-C11
2	B	1001	IEP	C03-C04-C05-C06
2	B	1001	IEP	C51-C52-C53-C54
2	B	1001	IEP	C49-C51-C52-C53
2	A	1001	IEP	C22-C23-O24-P25
2	B	1001	IEP	C22-C23-O24-P25
2	B	1001	IEP	C29-O28-P25-O24
2	A	1001	IEP	C56-C57-C58-C59
2	B	1001	IEP	C29-O28-P25-O26
2	A	1001	IEP	C60-C61-C62-C63
2	B	1001	IEP	C54-C55-C56-C57
2	A	1001	IEP	C53-C54-C55-C56
2	A	1001	IEP	C32-O41-P42-O45
2	A	1001	IEP	O20-C21-C22-O48
2	A	1001	IEP	C03-C04-C05-C06
2	A	1001	IEP	C23-O24-P25-O26
2	A	1001	IEP	C61-C62-C63-C64
2	A	1001	IEP	O20-C21-C22-C23
2	A	1001	IEP	C04-C05-C06-C07
2	A	1001	IEP	C21-C22-C23-O24
2	A	1001	IEP	O48-C22-C23-O24
2	B	1001	IEP	C52-C53-C54-C55
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	B	1001	IEP	C32-O41-P42-O44

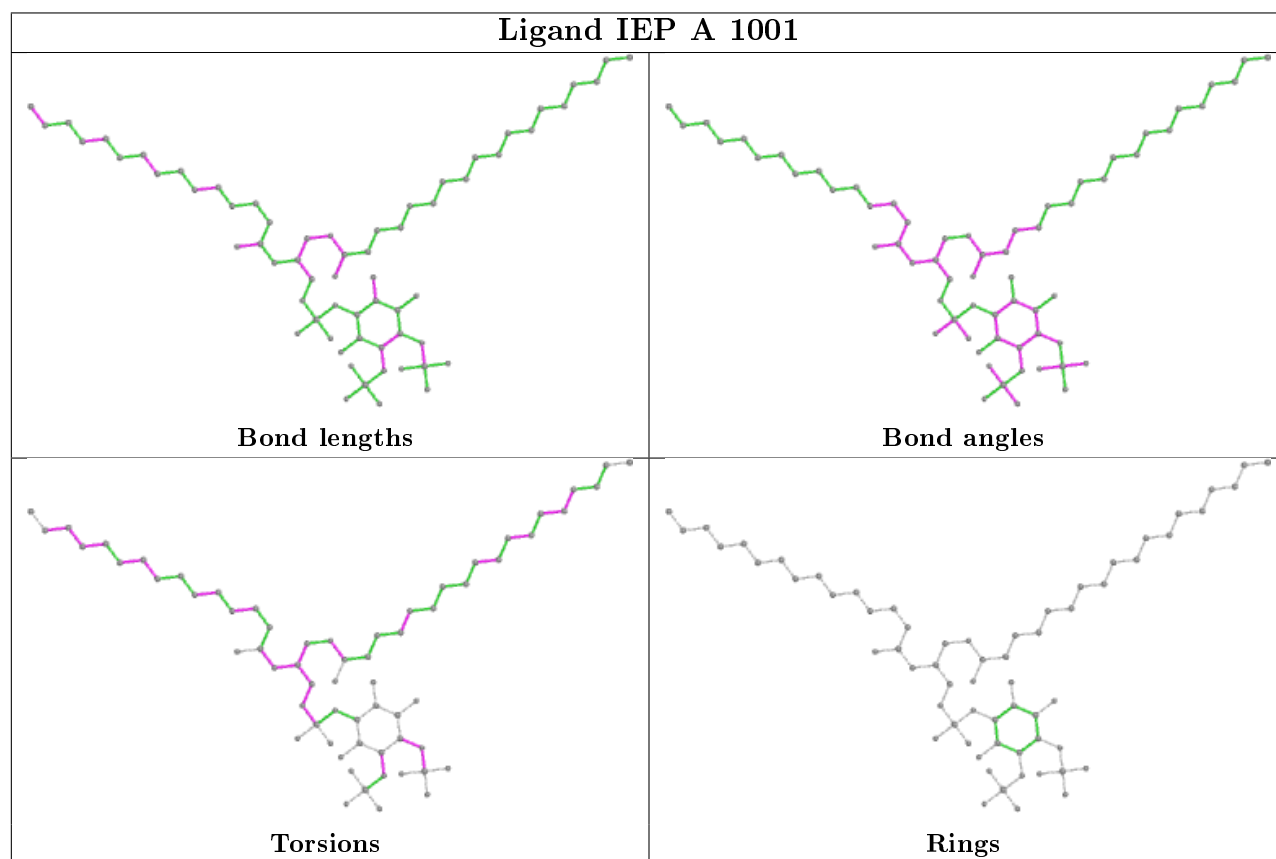
There are no ring outliers.

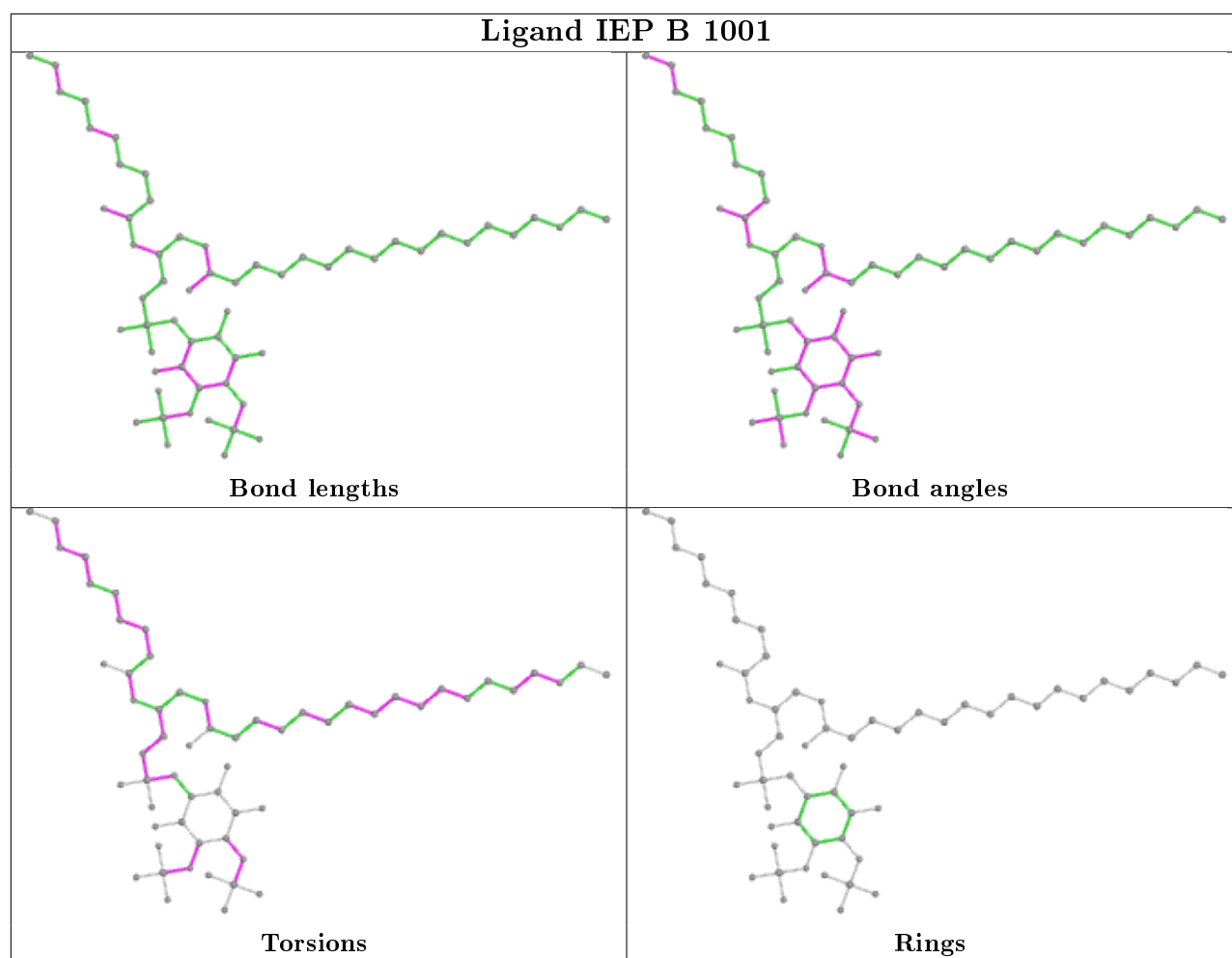
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	IEP	1	0
2	B	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%)	0.37	30 (7%) 13 11	39, 56, 104, 164	0
1	B	372/436 (85%)	0.40	25 (6%) 17 16	37, 55, 92, 117	0
All	All	764/872 (87%)	0.39	55 (7%) 15 13	37, 55, 100, 164	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	825	PHE	6.4
1	A	545	ASN	6.1
1	A	549	ILE	4.9
1	A	790	TYR	4.3
1	B	552	ILE	4.1
1	B	542	PHE	4.0
1	A	548	SER	3.9
1	A	547	PHE	3.9
1	B	764	SER	3.9
1	B	751	LYS	3.8
1	B	555	LYS	3.7
1	B	531	LYS	3.7
1	A	546	ASP	3.7
1	A	914	TRP	3.6
1	A	768	LEU	3.6
1	B	790	TYR	3.2
1	B	557	ILE	3.2
1	A	544	ARG	3.2
1	A	911	GLU	3.1
1	B	895	ARG	3.1
1	A	719	LYS	3.1
1	A	912	GLU	3.1
1	B	837	ALA	3.0
1	B	680	TRP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	915	LYS	2.9
1	A	594	SER	2.8
1	B	772	TYR	2.7
1	B	894	LYS	2.7
1	B	549	ILE	2.7
1	A	949	ILE	2.7
1	B	550	TRP	2.6
1	A	580	LEU	2.6
1	B	838	PRO	2.5
1	A	749	PHE	2.5
1	A	550	TRP	2.5
1	B	917	ARG	2.4
1	A	860	ASP	2.4
1	B	580	LEU	2.3
1	A	859	VAL	2.3
1	A	593	ALA	2.3
1	B	911	GLU	2.3
1	A	861	LYS	2.2
1	B	738	LYS	2.2
1	A	575	SER	2.2
1	A	863	MET	2.2
1	B	575	SER	2.2
1	A	559	MET	2.2
1	A	601	GLU	2.1
1	B	928	GLY	2.1
1	B	752	GLU	2.1
1	A	886	ILE	2.1
1	A	645	ILE	2.1
1	A	916	THR	2.0
1	A	888	GLN	2.0
1	B	734	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

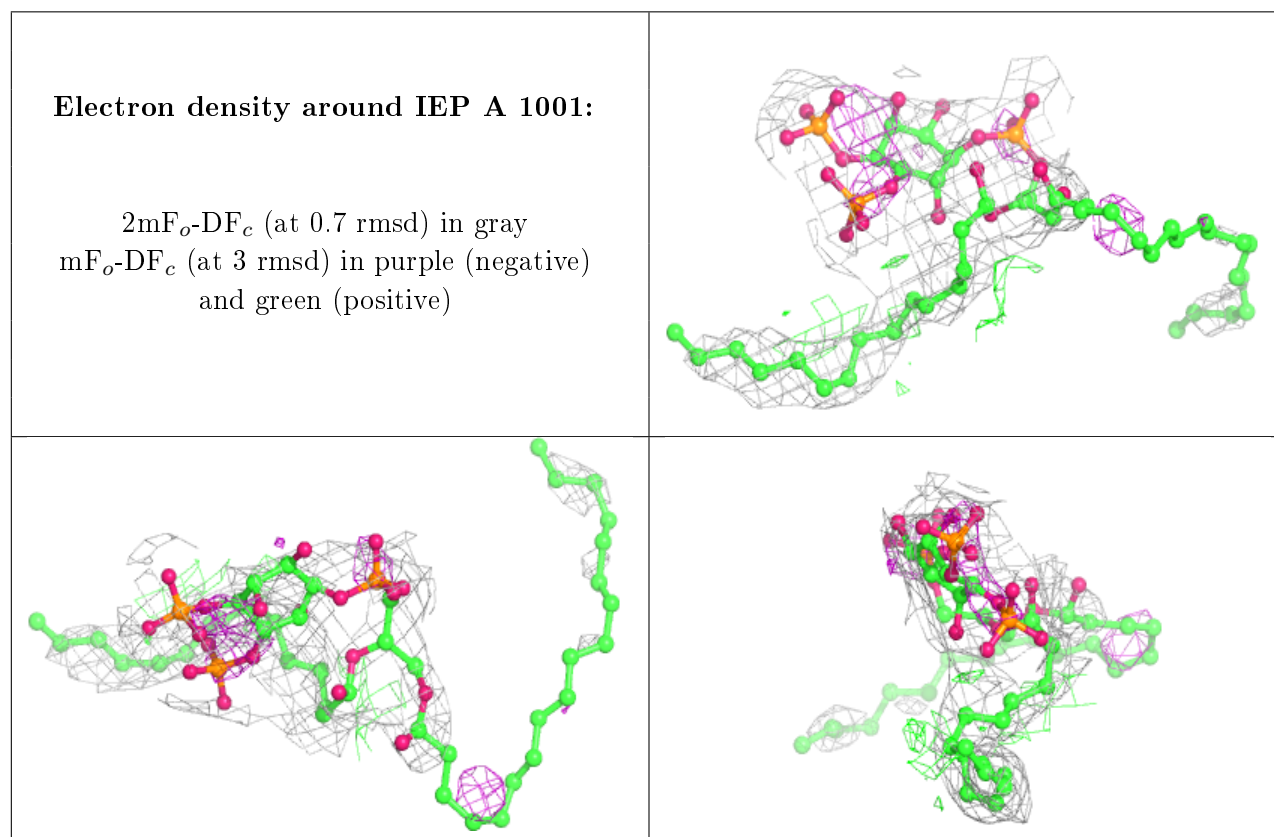
There are no carbohydrates in this entry.

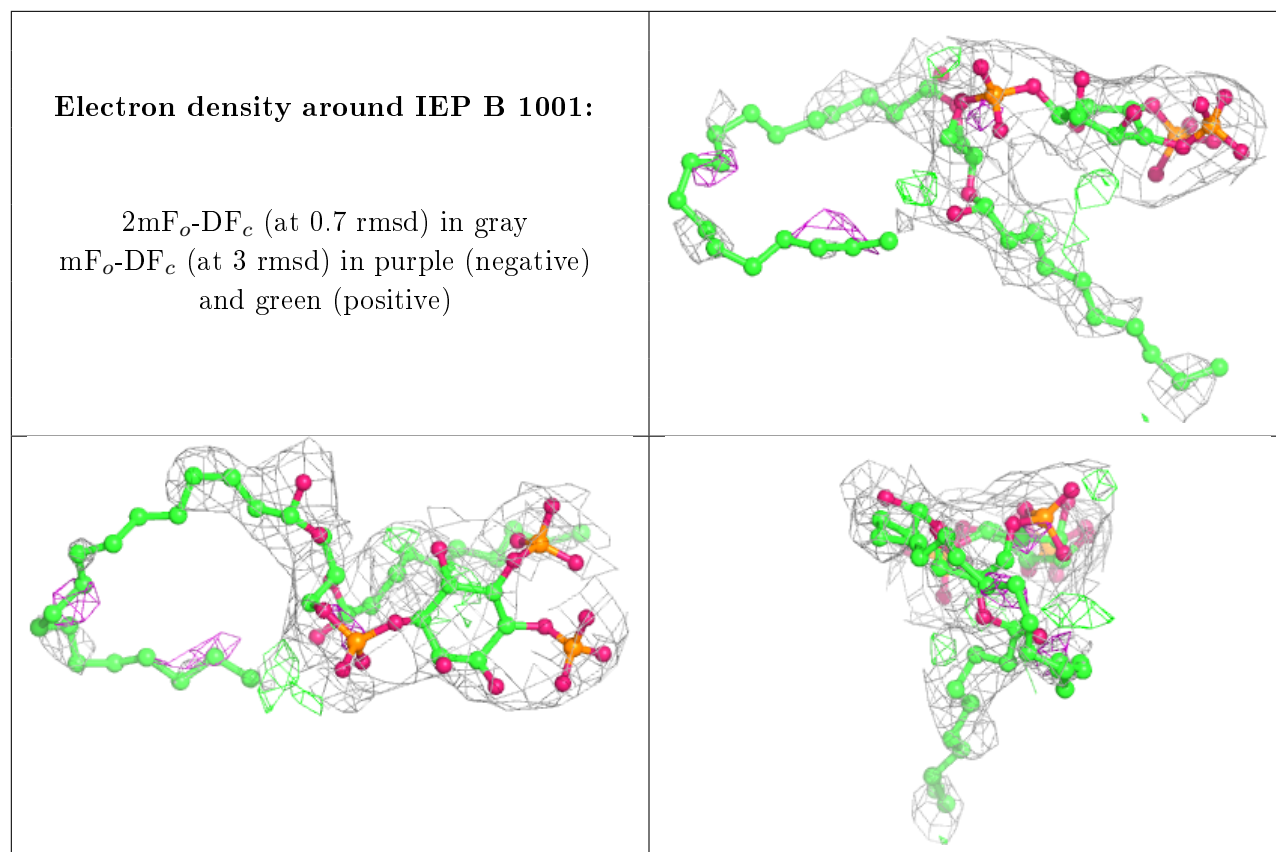
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
3	ACT	B	1002	4/4	0.69	0.29	63,63,63,63	0
2	IEP	A	1001	64/69	0.78	0.28	53,93,105,115	0
2	IEP	B	1001	59/69	0.82	0.26	48,81,115,127	0
3	ACT	A	1002	4/4	0.85	0.26	63,63,63,63	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.