

Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 02:05 PM EDT

PDB ID	:	7SVP
Title	:	Structure of compound 34 bound to human Phospholipase D2 catalytic domain
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Deposited on	:	2021-11-19
Resolution	:	2.90 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 (i) 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 (1)) 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	:	2.35
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)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.90 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.



Motrie	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	А	640	9%	14% •	13%
1	В	640	4% 71%	18%	10%
1	С	640	4%	14%	11%
1	D	640	5%	15%	14%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17334 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	C	571	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1		571	4453	2871	776	790	16	0		0
1	Δ	555	Total	С	Ν	0	S	0	0	0
1	A		4106	2626	724	740	16	0		
1	р	574	Total	С	Ν	0	S	0	1	0
1	ГБ	374	4412	2842	771	783	16		L	
1	1 D	550	Total	С	Ν	Ο	S	0	0	0
			4054	2606	712	723	13	0		

• Molecule 1 is a protein called Phospholipase D2.

• Molecule 2 is 1-(1-{(2S)-1-[(3R,5R)-3,5-dimethylpiperazin-1-yl]-1-oxopropan-2-yl}piperidi n-4-yl)-1,3-dihydro-2H-benzimidazol-2-one (three-letter code: CI0) (formula: C₂₁H₃₁N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	С	1	Total 28	C 21	N 5	O 2	0	0

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Continued	from	previous	page
	0	1	1 0

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
		1	Total	С	Ν	0	0	0	
	A	L	28	21	5	2	0	U	
0	В	1	Total	С	Ν	Ο	0	0	
	1	28	21	5	2	0	0		
0	Л	1	Total	С	Ν	0	0	0	
Z	D		28	21	5	2	0	0	

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	С	43	Total O 43 43	0	0
3	А	45	$\begin{array}{cc} \text{Total} & \text{O} \\ 45 & 45 \end{array}$	0	0
3	В	56	Total O 56 56	0	0
3	D	53	$\begin{array}{cc} \text{Total} & \text{O} \\ 53 & 53 \end{array}$	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Phospholipase D2

8894 7749 T1897 7756 LB16 7755 LB1 7755 PR0 1755 L175 1755 PR0 1775 L1769 1776 C17 1776 P28 771 P333 1779 P7193 1779 P7193 1779 P7193 1779 P7193 1779 P7193 1769 P7193 1769 P7193 1769 P7193 1779 P7193 1779 P7193 1779 P733 1769 P733 1769 P733 1769 P733 1769 P733 1769 P733 1770 P733 1770 P734 1789 P733 1783 P734 1783 P340 1783 P

• Molecule 1: Phospholipase D2









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	89.72Å 132.24Å 113.86Å	Depositor
a, b, c, α , β , γ	90.00° 100.65° 90.00°	Depositor
Besolution (Å)	111.00 - 2.90	Depositor
Resolution (A)	111.90 - 2.90	EDS
% Data completeness	99.2 (111.00-2.90)	Depositor
(in resolution range)	99.2 (111.90-2.90)	EDS
R _{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.09 (at 2.91 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
D D.	0.290 , 0.327	Depositor
II, II, <i>free</i>	0.297 , 0.334	DCC
R_{free} test set	2833 reflections $(4.93%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	60.8	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 64.8	EDS
L-test for twinning ²	$< L >=0.45, < L^2>=0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17334	wwPDB-VP
Average B, all atoms $(Å^2)$	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 61.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2774e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

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: ${\rm CI0}$

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).

Mal	Chain	Bond	lengths	Bond angles		
	Mol Chain		# Z > 5	RMSZ	# Z > 5	
1	А	0.24	0/4215	0.47	0/5770	
1	В	0.24	0/4528	0.48	0/6179	
1	С	0.24	0/4571	0.48	0/6232	
1	D	0.24	0/4159	0.47	0/5693	
All	All	0.24	0/17473	0.48	0/23874	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	4106	0	3664	56	0
1	В	4412	0	4171	80	0
1	С	4453	0	4267	56	0
1	D	4054	0	3592	60	0
2	А	28	0	0	0	0
2	В	28	0	0	1	0
2	С	28	0	0	1	0
2	D	28	0	0	0	0
3	A	45	0	0	7	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	56	0	0	17	0
3	С	43	0	0	8	0
3	D	53	0	0	15	0
All	All	17334	0	15694	249	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 8.

All (249) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom-2	Interatomic	Clash
Atom-1		distance (Å)	overlap (Å)
1:D:609:SER:O	1:D:785:SER:HA	1.60	1.00
1:C:361:ILE:O	3:C:1101:HOH:O	1.85	0.95
1:B:426:ASN:O	3:B:1101:HOH:O	1.84	0.94
1:B:609:SER:O	1:B:785:SER:HA	1.69	0.93
1:A:599:GLY:N	3:A:1101:HOH:O	2.04	0.89
1:D:470:TYR:O	3:D:1101:HOH:O	1.91	0.87
1:A:609:SER:O	1:A:785:SER:HA	1.77	0.84
1:D:881:VAL:N	3:D:1104:HOH:O	2.11	0.82
1:C:609:SER:O	1:C:785:SER:HA	1.79	0.82
1:B:608:ARG:O	3:B:1102:HOH:O	1.99	0.80
1:A:362:THR:HG22	1:A:400:LEU:HB2	1.64	0.80
1:D:902:HIS:ND1	3:D:1105:HOH:O	2.15	0.78
1:C:707:TYR:HB3	1:C:712:ARG:HG3	1.65	0.78
1:D:630:ILE:HD12	1:D:637:LEU:HD21	1.66	0.77
1:D:777:ARG:NH1	3:D:1107:HOH:O	2.18	0.77
1:B:397:VAL:N	3:B:1101:HOH:O	2.17	0.76
1:B:371:TYR:HB2	1:B:374:ARG:HE	1.50	0.76
1:A:406:GLU:O	3:A:1102:HOH:O	2.05	0.75
1:C:429:VAL:O	3:C:1102:HOH:O	2.04	0.74
1:D:647:CYS:O	3:D:1102:HOH:O	2.07	0.71
1:B:777[B]:ARG:NH1	1:B:784:ASP:OD2	2.23	0.71
1:B:929:LEU:O	3:B:1103:HOH:O	2.10	0.70
1:D:759:VAL:HG22	1:D:769:ILE:HG12	1.74	0.70
1:A:738:LEU:HD21	1:A:823:ILE:HG13	1.74	0.69
1:A:570:LYS:O	3:A:1103:HOH:O	2.09	0.69
1:B:532:ARG:NH1	3:B:1105:HOH:O	2.23	0.69
1:B:474:ASP:O	3:B:1105:HOH:O	2.12	0.68
1:B:424:HIS:O	3:B:1104:HOH:O	2.12	0.68
1:B:652:THR:O	3:B:1106:HOH:O	2.13	0.67
1:D:709:THR:OG1	3:D:1103:HOH:O	2.10	0.67



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Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:642:GLN:NE2	1:A:754:TYR:OH	2.26	0.66
1:B:427:ILE:O	3:B:1104:HOH:O	2.13	0.66
1:C:362:THR:HA	3:C:1101:HOH:O	1.94	0.65
1:B:442:HIS:HB2	1:B:777[B]:ARG:HH12	1.62	0.65
1:A:443:GLU:HG2	3:A:1107:HOH:O	1.98	0.63
1:B:374:ARG:NH2	3:B:1108:HOH:O	2.22	0.63
1:D:561:GLN:NE2	3:D:1113:HOH:O	2.32	0.62
1:B:711:CYS:HB3	1:B:718:LEU:HD12	1.82	0.61
1:D:404:GLU:HB3	1:D:411:ILE:HD11	1.82	0.61
1:A:676:ARG:NH2	1:A:840:ASP:OD1	2.31	0.61
1:C:609:SER:HB3	1:C:781:GLY:HA2	1.83	0.60
1:D:609:SER:HB3	1:D:781:GLY:HA2	1.84	0.60
1:C:438:LEU:HD21	1:D:438:LEU:HD21	1.84	0.60
1:A:627:LEU:O	3:A:1104:HOH:O	2.16	0.60
1:A:609:SER:HB3	1:A:781:GLY:HA2	1.83	0.60
1:B:777[B]:ARG:NH2	1:B:778:SER:OG	2.34	0.59
1:C:816:ARG:NH2	1:C:834:LEU:O	2.35	0.59
1:B:816:ARG:NH2	1:B:834:LEU:O	2.35	0.59
1:B:682:PRO:HD3	1:B:755:ILE:HB	1.84	0.58
1:C:627:LEU:HD22	1:C:660:GLU:HG3	1.84	0.58
1:C:640:GLU:HB3	1:C:759:VAL:HG13	1.86	0.58
1:C:374:ARG:NH2	3:C:1116:HOH:O	2.36	0.58
1:D:683:LEU:HB2	1:D:752:LEU:HD22	1.86	0.57
1:D:707:TYR:OH	3:D:1106:HOH:O	2.16	0.57
1:B:342:ALA:HA	1:B:465:TRP:NE1	2.20	0.57
1:C:361:ILE:HB	1:C:399:ILE:HG12	1.86	0.57
1:A:829:ARG:HB3	1:A:832:LEU:HD13	1.85	0.57
1:A:443:GLU:HB3	1:A:786:GLU:HA	1.86	0.57
1:D:802:ASN:HB2	1:D:838:ILE:HD11	1.85	0.57
1:D:626:TYR:O	1:D:630:ILE:HG12	2.05	0.57
1:D:455:LEU:HD11	1:D:789:VAL:HG13	1.87	0.56
1:B:648:SER:HA	1:B:653:VAL:HG23	1.87	0.56
1:B:685:PRO:HD2	1:B:699:ILE:HG13	1.86	0.56
1:B:795:GLU:OE1	1:B:810:ARG:NH1	2.38	0.56
1:A:442:HIS:O	1:A:444:LYS:NZ	2.38	0.56
1:B:509:LYS:NZ	1:B:527:GLU:O	2.37	0.56
1:D:641:ASN:HD21	1:D:773:ASN:HA	1.70	0.56
1:D:816:ARG:NH2	1:D:834:LEU:O	2.38	0.56
1:D:509:LYS:NZ	1:D:527:GLU:O	2.34	0.56
1:B:738:LEU:HD21	1:B:823:ILE:HG13	1.87	0.56
1:C:685:PRO:HD2	1:C:699:ILE:HG23	1.88	0.56



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	1.5	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:639:ILE:HG12	1:D:760:LEU:HD13	1.87	0.55
1:C:366:LEU:HD22	1:C:420:LEU:HD11	1.89	0.55
1:A:333:THR:HG21	1:A:551:PRO:HG2	1.89	0.55
1:C:738:LEU:HB3	1:C:753:ILE:HB	1.89	0.55
1:B:362:THR:HG23	1:B:445:LEU:HB3	1.89	0.54
1:B:532:ARG:NH2	3:B:1123:HOH:O	2.39	0.54
1:B:802:ASN:HB2	1:B:838:ILE:HD11	1.87	0.54
1:C:683:LEU:HB2	1:C:752:LEU:HD22	1.88	0.54
1:A:611:ASP:OD1	1:A:612:ARG:N	2.40	0.54
1:B:359:ILE:HB	1:B:397:VAL:HG22	1.90	0.54
1:D:541:ARG:NE	1:D:640:GLU:OE2	2.41	0.54
1:A:685:PRO:HD2	1:A:699:ILE:HG23	1.87	0.54
1:A:545:VAL:HG11	1:A:789:VAL:HG21	1.89	0.54
1:D:391:ALA:HB1	1:D:426:ASN:HB2	1.90	0.54
1:A:607:LEU:HD11	1:A:790:LEU:HB2	1.88	0.54
1:B:627:LEU:HD22	1:B:660:GLU:HG3	1.90	0.54
1:D:545:VAL:HG11	1:D:789:VAL:HG21	1.90	0.54
1:A:464:ARG:HB2	3:A:1111:HOH:O	2.08	0.53
1:C:927:ILE:HD13	1:D:927:ILE:HD13	1.90	0.53
1:A:364:TRP:CZ2	1:A:411:ILE:HD11	2.43	0.53
1:B:823:ILE:HG23	1:B:903:LEU:HB2	1.90	0.53
1:C:802:ASN:HB2	1:C:838:ILE:HD11	1.90	0.53
1:D:760:LEU:HD23	1:D:768:ILE:HD12	1.91	0.53
1:D:621:SER:N	3:D:1108:HOH:O	2.41	0.52
1:C:711:CYS:HB3	1:C:718:LEU:HD12	1.92	0.52
1:B:379:ASP:HB3	1:B:385:ILE:HG13	1.90	0.52
1:D:322:ARG:NH1	1:D:605:GLN:OE1	2.43	0.52
1:D:743:GLU:O	3:D:1109:HOH:O	2.19	0.52
1:C:400:LEU:HD23	1:C:430:MET:HB2	1.89	0.52
1:C:418:ARG:NH2	3:C:1118:HOH:O	2.41	0.52
1:A:464:ARG:HG3	1:A:540:TRP:NE1	2.25	0.52
1:C:833:ASP:OD1	1:C:835:ARG:NH1	2.43	0.52
1:C:634:GLN:HA	1:C:664:ARG:HH21	1.75	0.52
1:C:636:PHE:HB3	1:C:838:ILE:HG22	1.92	0.52
1:B:464:ARG:NH2	2:B:1001:CI0:O1	2.42	0.52
1:B:442:HIS:NE2	3:B:1118:HOH:O	2.31	0.51
1:C:676:ARG:NH1	1:C:731:ASP:O	2.40	0.51
1:A:640:GLU:HB2	1:A:759:VAL:HG12	1.93	0.51
1:B:676:ARG:NH1	1:B:731:ASP:O	2.44	0.51
1:C:823:ILE:HG23	1:C:903:LEU:HB2	1.93	0.51
1:D:333:THR:HG21	1:D:551:PRO:HG2	1.92	0.51



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Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:608:ARG:O	3:D:1108:HOH:O	2.19	0.51
1:A:365:TRP:CD1	1:A:411:ILE:HG23	2.46	0.51
1:B:773:ASN:HD22	1:B:777[B]:ARG:HH21	1.59	0.51
1:A:759:VAL:HG23	1:A:769:ILE:HG12	1.93	0.51
1:A:802:ASN:HB2	1:A:838:ILE:HD11	1.92	0.51
1:C:825:GLY:O	1:C:829:ARG:N	2.44	0.51
1:D:641:ASN:HA	1:D:757:SER:O	2.12	0.50
1:D:738:LEU:HD21	1:D:823:ILE:HG13	1.94	0.50
1:D:901:GLY:O	3:D:1105:HOH:O	2.20	0.50
1:C:721:LEU:O	1:C:725:MET:HG2	2.12	0.49
1:A:374:ARG:NH2	1:A:510:ASP:OD2	2.45	0.49
1:B:761:ILE:HG12	1:B:767:VAL:HG22	1.95	0.49
1:C:509:LYS:NZ	1:C:527:GLU:O	2.36	0.49
1:A:639:ILE:HG12	1:A:760:LEU:HD12	1.94	0.48
1:B:560:ILE:HG12	1:B:581:LEU:HB3	1.95	0.48
1:B:366:LEU:HD22	1:B:420:LEU:HD11	1.94	0.48
1:B:523:ASP:OD1	1:B:523:ASP:N	2.45	0.48
1:D:384:ASP:HB2	1:D:423:LEU:HD21	1.95	0.48
1:D:432:HIS:CG	1:D:433:PRO:HA	2.48	0.48
1:A:793:ASP:OD2	1:A:811:PHE:N	2.43	0.48
1:A:825:GLY:O	1:A:829:ARG:N	2.46	0.48
1:B:499:LEU:N	3:B:1130:HOH:O	2.47	0.48
1:D:758:LYS:HD3	1:D:771:SER:HA	1.96	0.48
1:D:823:ILE:HG23	1:D:903:LEU:HB2	1.96	0.48
1:C:400:LEU:O	3:C:1101:HOH:O	2.20	0.48
1:C:432:HIS:CG	1:C:433:PRO:HA	2.49	0.48
1:A:682:PRO:HD3	1:A:755:ILE:HB	1.95	0.48
1:A:894:SER:O	1:A:897:THR:OG1	2.32	0.48
1:B:333:THR:HG21	1:B:551:PRO:HG2	1.96	0.48
1:A:441:HIS:CE1	1:A:562:ARG:HH12	2.31	0.47
1:A:561:GLN:HE21	1:A:615:ALA:HB1	1.79	0.47
1:B:441:HIS:HE1	1:B:614:SER:HB2	1.80	0.47
1:D:676:ARG:NH1	1:D:731:ASP:O	2.46	0.47
1:C:464:ARG:NH2	2:C:1001:CI0:O1	2.45	0.47
1:C:684:LEU:HG	1:C:865:PRO:HD3	1.96	0.47
1:B:758:LYS:HB2	1:B:770:GLY:O	2.15	0.47
1:D:758:LYS:HB2	1:D:770:GLY:O	2.14	0.47
1:A:758:LYS:HB2	1:A:770:GLY:O	2.15	0.46
1:B:721:LEU:O	1:B:725:MET:HG2	2.16	0.46
1:A:391:ALA:HB1	1:A:426:ASN:HB2	1.98	0.46
1:A:758:LYS:HD3	1:A:771:SER:HA	1.98	0.46



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		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:444:LYS:NZ	1:C:459:ASP:OD2	2.48	0.46	
1:A:432:HIS:CG	1:A:433:PRO:HA	2.51	0.46	
1:C:333:THR:HG21	1:C:551:PRO:HG2	1.98	0.46	
1:C:711:CYS:HA	1:C:718:LEU:HB2	1.97	0.46	
1:B:434:ASP:N	3:B:1120:HOH:O	2.36	0.46	
1:B:359:ILE:O	1:B:397:VAL:HA	2.15	0.46	
1:C:738:LEU:HD11	1:C:823:ILE:HG13	1.96	0.46	
1:D:894:SER:O	1:D:897:THR:OG1	2.34	0.46	
1:B:418:ARG:O	1:B:421:MET:HG3	2.16	0.45	
1:A:638:TYR:OH	1:A:640:GLU:OE2	2.20	0.45	
1:B:825:GLY:O	1:B:829:ARG:N	2.48	0.45	
1:C:767:VAL:HG12	1:C:769:ILE:HG13	1.99	0.45	
1:B:420:LEU:HB2	1:B:429:VAL:HG21	1.99	0.45	
1:C:449:ASP:O	1:C:451:VAL:HG23	2.16	0.45	
1:B:374:ARG:NH2	1:B:510:ASP:OD2	2.36	0.45	
1:B:542:ASP:OD2	1:B:756:HIS:ND1	2.42	0.45	
1:D:768:ILE:HG12	1:D:790:LEU:HD13	1.97	0.45	
1:D:374:ARG:NH2	1:D:510:ASP:OD2	2.49	0.45	
1:B:439:TRP:HB3	1:B:783:ARG:O	2.16	0.45	
1:C:596:LEU:N	3:C:1123:HOH:O	2.50	0.45	
1:B:874:THR:O	1:B:878:TYR:HB2	2.17	0.45	
1:D:714:GLU:HA	1:D:719:HIS:ND1	2.32	0.45	
1:D:885:ALA:HA	1:D:892:ALA:HB2	1.98	0.45	
1:D:424:HIS:CG	1:D:425:PRO:HD2	2.51	0.45	
1:C:355:ALA:HB3	1:C:390:LYS:HZ3	1.82	0.45	
1:C:910:PHE:CZ	1:C:911:LEU:HD23	2.52	0.45	
1:D:682:PRO:HD3	1:D:755:ILE:HB	1.98	0.44	
1:C:682:PRO:HB3	1:C:755:ILE:H	1.82	0.44	
1:B:548:HIS:NE2	1:B:597:PRO:HD2	2.33	0.44	
1:C:682:PRO:HD3	1:C:755:ILE:HB	1.99	0.44	
1:B:639:ILE:HG12	1:B:760:LEU:HD12	2.00	0.44	
1:D:902:HIS:HA	3:D:1105:HOH:O	2.16	0.44	
1:A:506:TRP:HB3	1:A:510:ASP:HB3	2.00	0.44	
1:B:656:LYS:NZ	3:B:1127:HOH:O	2.44	0.44	
1:B:417:LYS:HD3	1:B:431:ARG:HD3	2.00	0.44	
1:D:924:GLU:N	3:D:1123:HOH:O	2.51	0.44	
1:C:567:LYS:HE2	1:C:578:TYR:O	2.18	0.44	
1:A:468:LEU:HD23	1:A:822:VAL:HG22	2.00	0.44	
1:B:758:LYS:HD3	1:B:771:SER:HA	2.00	0.44	
1:C:662:VAL:HG22	1:C:717:ILE:HG23	2.00	0.43	
1:B:748:PRO:HG2	1:B:892:ALA:HB3	2.00	0.43	



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	A L D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:432:HIS:CG	1:B:433:PRO:HA	2.54	0.43
1:B:741:HIS:CD2	1:B:896:LEU:HD13	2.52	0.43
1:C:371:TYR:O	1:C:374:ARG:NE	2.49	0.43
1:B:777[A]:ARG:HD2	1:B:931:VAL:O	2.19	0.43
1:D:646:SER:HA	1:D:655:ASN:HD21	1.84	0.43
1:A:366:LEU:HD22	1:A:420:LEU:HD11	2.01	0.43
1:D:907:PRO:HG2	3:D:1106:HOH:O	2.18	0.43
1:C:640:GLU:HG2	1:C:757:SER:HB2	2.01	0.42
1:A:439:TRP:CD2	1:A:783:ARG:HB3	2.53	0.42
1:C:607:LEU:HD11	1:C:790:LEU:HB2	2.01	0.42
1:C:875:LEU:HD22	1:C:911:LEU:HD21	2.02	0.42
1:D:636:PHE:HB3	1:D:838:ILE:HG22	2.02	0.42
1:A:443:GLU:HA	1:A:771:SER:OG	2.19	0.42
1:B:409:LEU:HD23	1:B:409:LEU:HA	1.74	0.42
1:A:644:PHE:HB3	1:A:681:LEU:HD21	2.02	0.42
1:C:623:LEU:HD13	1:C:779:LEU:HB3	2.01	0.42
1:D:763:ASP:O	1:D:765:ARG:HG3	2.20	0.42
1:C:374:ARG:HD3	1:C:465:TRP:CE2	2.54	0.42
1:D:400:LEU:HD12	1:D:400:LEU:HA	1.92	0.42
1:B:362:THR:CG2	1:B:445:LEU:HB3	2.48	0.42
1:B:441:HIS:CE1	1:B:614:SER:HB2	2.54	0.42
1:B:445:LEU:HD11	1:B:555:LEU:HD13	2.02	0.42
1:C:860:ILE:HG23	1:C:892:ALA:HB1	2.02	0.42
1:B:739:ARG:HA	1:B:752:LEU:HA	2.01	0.42
1:B:775:ASN:HB2	1:B:933:THR:C	2.41	0.42
1:D:558:HIS:CD2	1:D:787:LEU:HD21	2.54	0.42
1:B:327:ALA:HA	1:B:328:PRO:HD3	1.94	0.42
1:A:337:TRP:HD1	1:A:811:PHE:CE1	2.38	0.41
1:C:664:ARG:HA	1:C:664:ARG:HD2	1.89	0.41
1:A:777:ARG:O	1:A:784:ASP:HB2	2.20	0.41
1:D:555:LEU:HD13	1:D:555:LEU:HA	1.90	0.41
1:D:654:LEU:N	1:D:776:ASP:OD2	2.48	0.41
1:C:362:THR:OG1	1:C:445:LEU:HB3	2.21	0.41
1:A:767:VAL:HG12	1:A:769:ILE:HG13	2.03	0.41
1:B:532:ARG:HD3	3:B:1105:HOH:O	2.20	0.41
1:B:374:ARG:HG2	1:B:505:PHE:O	2.21	0.41
1:B:400:LEU:HD23	1:B:430:MET:HB3	2.03	0.41
1:B:777[A]:ARG:HG3	1:B:933:THR:O	2.21	0.41
1:A:555:LEU:HD13	1:A:555:LEU:HA	1.90	0.41
1:A:607:LEU:HB2	1:A:622:ILE:HG22	2.02	0.41
1:B:662:VAL:HG22	1:B:717:ILE:HG23	2.02	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:443:GLU:HG3	1:A:787:LEU:HG	2.02	0.41
1:A:622:ILE:HG13	1:A:623:LEU:N	2.36	0.41
1:A:647:CYS:O	3:A:1105:HOH:O	2.22	0.41
1:A:761:ILE:HD11	1:A:815:LEU:HD23	2.01	0.41
1:B:933:THR:N	3:B:1103:HOH:O	2.45	0.41
1:D:661:ILE:O	1:D:665:ILE:HG12	2.21	0.41
1:B:738:LEU:HD12	1:B:755:ILE:HD11	2.02	0.41
1:B:813:LEU:HD11	1:B:817:LYS:HE3	2.02	0.41
1:B:640:GLU:HG2	1:B:757:SER:HB2	2.03	0.40
1:A:377:HIS:HB3	1:B:835:ARG:NH1	2.36	0.40
1:D:539:PRO:HB2	1:D:753:ILE:HG23	2.02	0.40
1:A:374:ARG:NH1	1:A:505:PHE:O	2.54	0.40
1:B:535:THR:HA	1:B:536:PRO:HD3	1.96	0.40
1:C:601:CYS:SG	3:C:1106:HOH:O	2.63	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	Perce	ntiles
1	А	547/640~(86%)	529~(97%)	18 (3%)	0	100	100
1	В	565/640~(88%)	551 (98%)	14~(2%)	0	100	100
1	\mathbf{C}	561/640~(88%)	546~(97%)	15 (3%)	0	100	100
1	D	532/640~(83%)	511 (96%)	20~(4%)	1 (0%)	47	78
All	All	2205/2560 (86%)	2137 (97%)	67(3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	406	GLU



5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percen	tiles
1	А	377/554~(68%)	366~(97%)	11 (3%)	42	76
1	В	436/554~(79%)	425~(98%)	11 (2%)	47	78
1	С	451/554~(81%)	440 (98%)	11 (2%)	49	79
1	D	365/554~(66%)	363 (100%)	2(0%)	88	96
All	All	1629/2216 (74%)	1594 (98%)	35 (2%)	53	81

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	357	GLU
1	С	362	THR
1	С	382	ARG
1	С	413	SER
1	С	607	LEU
1	С	782	LYS
1	С	801	MET
1	С	829	ARG
1	С	872	LEU
1	С	882	GLU
1	С	905	HIS
1	А	421	MET
1	А	443	GLU
1	А	445	LEU
1	А	510	ASP
1	А	514	LEU
1	А	523	ASP
1	А	555	LEU
1	А	607	LEU
1	А	622	ILE
1	А	669	HIS
1	A	869	THR
1	В	362	THR
1	В	421	MET



Mol	Chain	Res	Type
1	В	423	LEU
1	В	438	LEU
1	В	514	LEU
1	В	534	THR
1	В	607	LEU
1	В	699	ILE
1	В	801	MET
1	В	872	LEU
1	В	905	HIS
1	D	607	LEU
1	D	869	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	513	ASN
1	В	642	GLN
1	В	773	ASN

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 monosaccharides 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



Mal	Turne	Chain	Dec	Bond lengths			B	ond ang	gles	
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CI0	А	1001	-	31,31,31	0.28	0	44,45,45	0.45	0
2	CI0	С	1001	-	31,31,31	0.32	0	44,45,45	0.45	0
2	CI0	D	1001	-	31,31,31	0.32	0	44,45,45	0.55	0
2	CI0	В	1001	-	31,31,31	0.28	0	44,45,45	0.44	0

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).

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	CI0	А	1001	-	-	4/16/38/38	0/4/4/4
2	CI0	С	1001	-	-	4/16/38/38	0/4/4/4
2	CI0	D	1001	-	-	4/16/38/38	0/4/4/4
2	CI0	В	1001	-	-	4/16/38/38	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	1001	CI0	C3-C2-N1-C21
2	В	1001	CIO	O1-C2-N1-C21
2	В	1001	CI0	C3-C2-N1-C1
2	В	1001	CI0	O1-C2-N1-C1
2	С	1001	CI0	O1-C2-C3-C4
2	С	1001	CI0	N1-C2-C3-C4
2	А	1001	CI0	N1-C2-C3-C4
2	D	1001	CI0	N1-C2-C3-C4
2	D	1001	CI0	O1-C2-C3-N2
2	С	1001	CI0	N1-C2-C3-N2
2	А	1001	CI0	N1-C2-C3-N2
2	D	1001	CI0	N1-C2-C3-N2
2	А	1001	CI0	O1-C2-C3-C4
2	D	1001	CI0	O1-C2-C3-C4



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Mol	Chain	Res	Type	Atoms
2	С	1001	CI0	O1-C2-C3-N2
2	А	1001	CI0	O1-C2-C3-N2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	1001	CI0	1	0
2	В	1001	CI0	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers (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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	< RSRZ >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	555/640~(86%)	0.68	55~(9%) 7 5	55, 75, 98, 116	0
1	В	574/640~(89%)	0.53	27 (4%) 31 28	45, 59, 78, 93	0
1	С	571/640~(89%)	0.48	27 (4%) 31 28	31, 53, 76, 109	0
1	D	550/640~(85%)	0.52	32 (5%) 23 19	44, 68, 93, 117	0
All	All	2250/2560~(87%)	0.55	141 (6%) 20 16	31, 64, 91, 117	0

All (141) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	С	692	SER	6.8
1	С	576	PRO	6.6
1	D	678	TYR	6.2
1	D	734	SER	5.9
1	А	863	CYS	5.7
1	В	616	GLY	5.4
1	С	573	TYR	5.2
1	В	915	SER	4.9
1	А	440	ALA	4.8
1	В	916	LEU	4.5
1	А	650	GLY	4.3
1	D	864	LEU	4.1
1	В	384	ASP	4.0
1	А	695	GLY	3.7
1	А	505	PHE	3.6
1	А	651	ARG	3.6
1	А	725	MET	3.6
1	D	933	THR	3.6
1	D	440	ALA	3.6
1	В	647	CYS	3.6
1	А	724	ALA	3.5



Mol	Chain	Res	Type	RSRZ
1	А	738	LEU	3.4
1	В	684	LEU	3.4
1	С	545	VAL	3.3
1	А	671	GLN	3.3
1	В	530	ILE	3.3
1	А	686	GLY	3.3
1	А	693	THR	3.2
1	D	362	THR	3.2
1	А	555	LEU	3.2
1	А	750	SER	3.1
1	А	864	LEU	3.1
1	В	545	VAL	3.1
1	D	905	HIS	3.1
1	D	474	ASP	3.1
1	С	744	LEU	3.1
1	С	553	ARG	3.0
1	С	578	TYR	3.0
1	С	793	ASP	3.0
1	С	647	CYS	3.0
1	А	678	TYR	3.0
1	В	607	LEU	3.0
1	С	726	GLY	3.0
1	В	401	LEU	2.9
1	А	616	GLY	2.9
1	С	684	LEU	2.9
1	С	525	PRO	2.9
1	А	702	ILE	2.8
1	А	726	GLY	2.8
1	А	649	ASP	2.8
1	А	825	GLY	2.7
1	А	719	HIS	2.7
1	D	738	LEU	2.7
1	А	461	ALA	2.7
1	С	401	LEU	2.7
1	С	673	TRP	2.7
1	С	717	ILE	2.7
1	A	737	GLY	2.7
1	D	727	THR	2.6
1	C	535	THR	2.6
1	В	566	THR	2.6
1	B	526	PHE	2.6
1	А	749	VAL	2.6



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Mol	Chain	Res	Type	RSRZ
1	А	745	GLY	2.6
1	D	398	SER	2.6
1	D	461	ALA	2.6
1	С	526	PHE	2.6
1	D	644	PHE	2.6
1	А	740	THR	2.6
1	D	604	VAL	2.5
1	В	669	HIS	2.5
1	В	598	GLY	2.5
1	В	692	SER	2.5
1	D	694	GLY	2.5
1	А	834	LEU	2.5
1	В	789	VAL	2.5
1	D	830	PRO	2.5
1	С	580	TYR	2.5
1	А	399	ILE	2.5
1	В	550	LEU	2.5
1	А	519	TRP	2.5
1	D	932	TRP	2.4
1	А	928	PRO	2.4
1	А	398	SER	2.4
1	С	616	GLY	2.4
1	В	615	ALA	2.4
1	D	713	GLY	2.4
1	D	514	LEU	2.4
1	А	932	TRP	2.4
1	А	408	ALA	2.4
1	D	391	ALA	2.4
1	В	884	LEU	2.4
1	D	507	LEU	2.4
1	D	526	PHE	2.4
1	А	384	ASP	2.4
1	D	856	ILE	2.4
1	D	674	CYS	2.3
1	A	468	LEU	2.3
1	А	679	VAL	2.3
1	А	647	CYS	2.3
1	С	416	SER	2.3
1	А	629	THR	2.3
1	В	617	THR	2.3
1	С	780	LEU	2.3
1	В	731	ASP	2.3



7SVP

Mol	Chain	Res	Type	RSRZ
1	А	723	ALA	2.3
1	D	860	ILE	2.3
1	В	929	LEU	2.2
1	А	762	ALA	2.2
1	С	715	TYR	2.2
1	А	638	TYR	2.2
1	А	350	ASP	2.2
1	В	573	TYR	2.2
1	D	752	LEU	2.2
1	D	367	SER	2.2
1	D	924	GLU	2.2
1	D	927	ILE	2.1
1	А	694	GLY	2.1
1	А	734	SER	2.1
1	С	933	THR	2.1
1	D	462	TYR	2.1
1	С	615	ALA	2.1
1	В	686	GLY	2.1
1	С	530	ILE	2.1
1	D	762	ALA	2.1
1	С	680	LEU	2.1
1	А	414	GLY	2.1
1	А	615	ALA	2.1
1	D	688	GLU	2.1
1	А	362	THR	2.1
1	А	604	VAL	2.1
1	С	360	PHE	2.1
1	А	711	CYS	2.1
1	А	411	ILE	2.0
1	А	885	ALA	2.0
1	А	601	CYS	2.0
1	А	466	ASP	2.0
1	А	415	TYR	2.0
1	В	534	THR	2.0
1	В	681	LEU	2.0
1	В	685	PRO	2.0

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

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



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	CIO	D	1001	28/28	0.83	0.36	45,58,65,72	0
2	CI0	А	1001	28/28	0.85	0.30	47,58,69,72	0
2	CI0	С	1001	28/28	0.86	0.32	39,48,57,60	0
2	CIO	В	1001	28/28	0.87	0.33	39,55,68,72	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.

