

Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2020 – 12:54 AM BST

PDB ID	:	6XUH
Title	:	Crystal structure of human phosphoglucose isomerase in complex with in-
		hibitor
Authors	:	Li de la Sierra-Gallay, I.; Ahmad, L.; Plancqueel, S.; van Tilbeurgh, H.;
		Salmon, L.
Deposited on	:	2020-01-20
Resolution	:	2.38 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity Mogul Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins)	: : : : : : : : : : : : : : : : : : :	4.02b-467 1.8.5 (274361), CSD as541be (2020) 1.13 2.13.1 1.1.7 (2018) 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001)
Ideal geometry (proteins) Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	:	Engh & Huber (2001) Parkinson et al. (1996) 2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.38 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R_{free}	130704	5509(2.40-2.36)
Clashscore	141614	6082(2.40-2.36)
Ramachandran outliers	138981	5973(2.40-2.36)
Sidechain outliers	138945	5975(2.40-2.36)
RSRZ outliers	127900	5397(2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	А	556	6% 	12%
1	В	556	5% 89%	11%
1	С	556	25% 89%	10%
1	D	556	19%	11%



6XUH

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18085 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		At	oms			ZeroOcc	AltConf	Trace
1	Δ	556	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	A	000	4437	2827	782	810	18	0	0	0
1	р	556	Total	С	Ν	Ο	S	0	0	0
	D	000	4437	2827	782	810	18	0	0	0
1	C	556	Total	С	Ν	Ο	S	0	0	0
		000	4437	2827	782	810	18	0	0	0
1	1 D	556	Total	С	Ν	Ο	S	0	0	0
	556	4437	2827	782	810	18	0		0	

• Molecule 1 is a protein called Glucose-6-phosphate isomerase.

• Molecule 2 is 5-PHOSPHOARABINONIC ACID (three-letter code: PA5) (formula: C₅H₁₁O₉P) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	А	1	Total 15	С 5	0 9	Р 1	0	0
2	С	1	Total 15	C 5	O 9	Р 1	0	0



• Molecule 3 is (2R,3R,4S)-5-((2-aminoethyl)amino)-2,3,4-trihydroxy-5-oxopentyl dihydrogen phosphate (three-letter code: O1B) (formula: C₇H₁₇N₂O₈P) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
3	В	1	Total	С	Ν	Ο	Р	0	0	
J	D	T	18	7	2	8	1	0	0	
9	р	1	Total	С	Ν	Ο	Р	0	0	
3 D	D	L	18	7	2	8	1	0	U	

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	87	Total O 87 87	0	0
4	В	96	Total O 96 96	0	0
4	С	41	Total O 41 41	0	0
4	D	47	$\begin{array}{cc} \text{Total} & \text{O} \\ 47 & 47 \end{array}$	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: Glucose-6-phosphate isomerase









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants	96.11Å 96.11 Å 271.45 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Posolution(A)	47.32 - 2.38	Depositor
Resolution (A)	47.32 - 2.38	EDS
% Data completeness	99.2 (47.32-2.38)	Depositor
(in resolution range)	99.1(47.32 - 2.38)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.15 (at 2.37 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
D D.	0.263 , 0.317	Depositor
Π, Π_{free}	0.268 , 0.318	DCC
R_{free} test set	4877 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	50.5	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.29 , 30.6	EDS
L-test for twinning ²	$< L >=0.41, < L^2>=0.24$	Xtriage
Estimated twinning fraction	0.146 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18085	wwPDB-VP
Average B, all atoms $(Å^2)$	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.

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: O1B, PA5 $\,$

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.53	0/4545	0.69	0/6154	
1	В	0.54	0/4545	0.70	1/6154~(0.0%)	
1	С	0.52	0/4545	0.69	1/6154~(0.0%)	
1	D	0.51	0/4545	0.67	0/6154	
All	All	0.53	0/18180	0.69	2/24616~(0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	520	LEU	CA-CB-CG	5.33	127.57	115.30
1	В	111	LEU	CB-CG-CD2	5.29	119.99	111.00

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	4437	0	4395	35	0
1	В	4437	0	4395	36	0
1	С	4437	0	4395	34	0
1	D	4437	0	4395	38	0
2	А	15	0	8	2	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	С	15	0	8	0	0
3	В	18	0	0	2	0
3	D	18	0	0	3	0
4	А	87	0	0	2	0
4	В	96	0	0	2	0
4	С	41	0	0	3	0
4	D	47	0	0	2	0
All	All	18085	0	17596	124	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 4.

All (124) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:272:ARG:HG2	3:D:600:O1B:N	1.89	0.87
1:C:513:GLY:H	1:D:392:GLN:HE22	1.31	0.75
1:B:209:SER:OG	3:B:600:O1B:O7	2.02	0.75
1:B:272:ARG:HG2	3:B:600:O1B:N	2.04	0.73
1:D:209:SER:OG	3:D:600:O1B:O6	2.01	0.72
1:B:92:THR:HB	1:B:512:TRP:CZ3	2.26	0.71
1:B:92:THR:HB	1:B:512:TRP:HZ3	1.60	0.63
1:C:513:GLY:H	1:D:392:GLN:NE2	1.95	0.62
1:D:14:GLN:HE22	1:D:17:ARG:HH11	1.49	0.60
1:B:405:PHE:HB3	1:B:428:PHE:CE1	2.39	0.58
1:D:405:PHE:HB3	1:D:428:PHE:CE1	2.39	0.57
1:B:294:GLN:HG3	4:B:785:HOH:O	2.03	0.57
1:A:230:GLN:HG3	4:A:736:HOH:O	2.05	0.56
1:B:523:LYS:HG3	1:B:524:ILE:HD12	1.88	0.56
1:C:186:ILE:HB	1:C:216:GLU:HG3	1.88	0.55
1:D:186:ILE:HB	1:D:216:GLU:HG3	1.89	0.55
1:D:249:THR:HA	1:D:262:MET:HE1	1.89	0.55
1:C:328:ASN:HD21	1:C:504:TRP:HE1	1.54	0.54
1:B:314:ASN:HB3	1:B:317:VAL:HB	1.90	0.54
1:A:186:ILE:HB	1:A:216:GLU:HG3	1.90	0.54
1:A:314:ASN:HB3	1:A:317:VAL:HB	1.90	0.54
1:C:392:GLN:HE22	1:D:513:GLY:H	1.55	0.53
1:D:314:ASN:HB3	1:D:317:VAL:HB	1.90	0.53
1:C:314:ASN:HB3	1:C:317:VAL:HB	1.90	0.53
1:B:186:ILE:HB	1:B:216:GLU:HG3	1.90	0.53
1:B:249:THR:HA	1:B:262:MET:HE1	1.92	0.52



Atom-1Atom-2InterferenceOterlan1:A:405:PHE:HB31:A:428:PHE:CE22.450.521:C:415:ILE:HD121:D:223:THR:HG211.920.521:C:249:THR:HA1:C:262:MET:HE11.910.511:B:80:ARG:HD21:B:307:ARG:HA1.930.511:D:437:ARG:HD24:D:732:HOH:O2.090.511:B:92:THR:CB1:B:512:TRP:HZ32.230.511:A:80:ARG:HD21:A:307:ARG:HA1.930.511:C:80:ARG:HD21:C:307:ARG:HA1.930.511:D:80:ARG:HD21:C:307:ARG:HA1.930.511:D:80:ARG:HD21:C:307:ARG:HA1.930.501:C:405:PHE:HB31:C:428:PHE:CE22.460.501:C:245:LEU:HD131:C:279:ILE:HA1.930.491:A:520:LEU:HD131:C:279:ILE:HA1.940.481:D:517:GLY:HA21:D:520:LEU:HD121.950.481:A:516:LEU:O1:A:519:GLN:HG22.130.48		ous page	Interatomic	Clash
1:A:405:PHE:HB31:A:428:PHE:CE22.450.521:C:415:ILE:HD121:D:223:THR:HG211.920.521:C:249:THR:HA1:C:262:MET:HE11.910.511:B:80:ARG:HD21:B:307:ARG:HA1.930.511:D:437:ARG:HD24:D:732:HOH:O2.090.511:B:92:THR:CB1:B:512:TRP:HZ32.230.511:A:80:ARG:HD21:A:307:ARG:HA1.930.511:C:80:ARG:HD21:A:307:ARG:HA1.930.511:C:80:ARG:HD21:C:307:ARG:HA1.930.511:C:80:ARG:HD21:D:307:ARG:HA1.930.501:C:405:PHE:HB31:C:428:PHE:CE22.460.501:C:405:PHE:HB31:C:428:PHE:CE22.460.501:C:245:LEU:HD131:C:279:ILE:HA1.930.491:A:520:LEU:HB31:B:430:ALA:HB11.940.481:D:517:GLY:HA21:D:520:LEU:HD121.950.481:A:516:LEU:O1:A:519:GLN:HG22.130.48	Atom-1	Atom-2	distance $(Å)$	overlap(Å)
1:R1:100:1 HE:HD01:R1:120:1 HE:OE22:100:021:C:415:ILE:HD121:D:223:THR:HG211.920.521:C:249:THR:HA1:C:262:MET:HE11.910.511:B:80:ARG:HD21:B:307:ARG:HA1.930.511:D:437:ARG:HD24:D:732:HOH:O2.090.511:B:92:THR:CB1:B:512:TRP:HZ32.230.511:A:80:ARG:HD21:A:307:ARG:HA1.930.511:C:80:ARG:HD21:C:307:ARG:HA1.940.511:D:80:ARG:HD21:C:307:ARG:HA1.930.501:C:405:PHE:HB31:C:428:PHE:CE22.460.501:C:405:PHE:HB31:C:428:PHE:CE22.460.501:C:245:LEU:HD131:C:279:ILE:HA1.930.491:A:520:LEU:HB31:B:430:ALA:HB11.940.481:D:517:GLY:HA21:D:520:LEU:HD121.950.481:A:516:LEU:O1:A:519:GLN:HG22.130.48	1·A·405·PHE·HB3	$1 \cdot A \cdot 428 \cdot PHE \cdot CE2$	2.45	0.52
1:0:1101111111111111111111111111111111	1:C:415:ILE:HD12	1:D:223:THR:HG21	1.92	0.52
1:0:10:11:11:11:11:11:11:11:11:11:11:11:	1·C·249·THB·HA	1.C·262·MET·HE1	1.92	0.51
1:D:30::Htte:HD21:D:30::Htte:HD21:D:30::Htte:HD21:D:437:ARG:HD24:D:732:HOH:O2.090.511:B:92:THR:CB1:B:512:TRP:HZ32.230.511:A:80:ARG:HD21:A:307:ARG:HA1.930.511:C:80:ARG:HD21:C:307:ARG:HA1.940.511:D:80:ARG:HD21:D:307:ARG:HA1.930.501:C:405:PHE:HB31:C:428:PHE:CE22.460.501:D:357:GLU:OE23:D:600:O1B:N12.440.501:C:245:LEU:HD131:C:279:ILE:HA1.930.491:A:520:LEU:HB31:B:430:ALA:HB11.940.481:D:517:GLY:HA21:D:520:LEU:HD121.950.481:A:516:LEU:O1:A:519:GLN:HG22.130.48	1.B.80.ABG.HD2	1.8.307.ABG.HA	1.01	0.51
1.D.101.111011102.000.011:B:92:THR:CB1:B:512:TRP:HZ32.230.511:A:80:ARG:HD21:A:307:ARG:HA1.930.511:C:80:ARG:HD21:C:307:ARG:HA1.940.511:D:80:ARG:HD21:D:307:ARG:HA1.930.501:C:405:PHE:HB31:C:428:PHE:CE22.460.501:D:357:GLU:OE23:D:600:O1B:N12.440.501:C:245:LEU:HD131:C:279:ILE:HA1.930.491:A:520:LEU:HB31:B:430:ALA:HB11.940.481:D:517:GLY:HA21:D:520:LEU:HD121.950.481:A:516:LEU:O1:A:519:GLN:HG22.130.48	1.D.437.ABG·HD2	4·D·732·HOH·O	2.09	0.51
11.D.02.1110.0211.D.012.1101.111021.200.011:A:80:ARG:HD21:A:307:ARG:HA1.930.511:C:80:ARG:HD21:C:307:ARG:HA1.940.511:D:80:ARG:HD21:D:307:ARG:HA1.930.501:C:405:PHE:HB31:C:428:PHE:CE22.460.501:D:357:GLU:OE23:D:600:O1B:N12.440.501:C:245:LEU:HD131:C:279:ILE:HA1.930.491:A:520:LEU:HB31:B:430:ALA:HB11.940.481:D:517:GLY:HA21:D:520:LEU:HD121.950.481:A:516:LEU:O1:A:519:GLN:HG22.130.48	1·B·92·THB·CB	$1 \cdot B \cdot 512 \cdot TBP \cdot HZ3$	2.33	0.51
1:1:1:00:1:11:00:1:11:00:1:11:10:1:11:10:11:11	1:A:80:ABG:HD2	1.A.307.ABG.HA	1.93	0.51
1:0:30::RIC:MD21:0:30::RIC:MIC:MIX1:010.011:D:80:ARG:HD21:D:307:ARG:HA1.930.501:C:405:PHE:HB31:C:428:PHE:CE22.460.501:D:357:GLU:OE23:D:600:O1B:N12.440.501:C:245:LEU:HD131:C:279:ILE:HA1.930.491:A:520:LEU:HB31:B:430:ALA:HB11.940.481:D:517:GLY:HA21:D:520:LEU:HD121.950.481:A:516:LEU:O1:A:519:GLN:HG22.130.48	1:C:80:ARG:HD2	1:C:307:ABG:HA	1.90	0.51
1:D:357:GLU:OE2 1:C:428:PHE:CE2 2.46 0.50 1:D:357:GLU:OE2 3:D:600:O1B:N1 2.44 0.50 1:C:245:LEU:HD13 1:C:279:ILE:HA 1.93 0.49 1:A:520:LEU:HB3 1:B:430:ALA:HB1 1.94 0.48 1:D:517:GLY:HA2 1:D:520:LEU:HD12 1.95 0.48 1:A:516:LEU:O 1:A:519:GLN:HG2 2.13 0.48	1:D:80:ARG:HD2	1:D:307:ABG:HA	1.91	0.50
1:0:1001 HEHEO 1:0:1201 HEEO2 2:10 0:00 1:D:357:GLU:OE2 3:D:600:O1B:N1 2.44 0.50 1:C:245:LEU:HD13 1:C:279:ILE:HA 1.93 0.49 1:A:520:LEU:HB3 1:B:430:ALA:HB1 1.94 0.48 1:D:517:GLY:HA2 1:D:520:LEU:HD12 1.95 0.48 1:A:516:LEU:O 1:A:519:GLN:HG2 2.13 0.48	$1 \cdot C \cdot 405 \cdot PHE \cdot HB3$	$1 \cdot C \cdot 428 \cdot PHE \cdot CE2$	2.46	0.50
1:D:501:GE0:0E12 0:D:000:0E1D:1(1) 2:11 0:00 1:C:245:LEU:HD13 1:C:279:ILE:HA 1.93 0.49 1:A:520:LEU:HB3 1:B:430:ALA:HB1 1.94 0.48 1:D:517:GLY:HA2 1:D:520:LEU:HD12 1.95 0.48 1:A:516:LEU:O 1:A:519:GLN:HG2 2.13 0.48	1.D.357.GLU.OE2	3·D·600·01B·N1	2.10	0.50
1:A:520:LEU:HB3 1:B:430:ALA:HB1 1.94 0.48 1:D:517:GLY:HA2 1:D:520:LEU:HD12 1.95 0.48 1:A:516:LEU:O 1:A:519:GLN:HG2 2.13 0.48	1.C.245.LEU.HD13	1.C.279.ILE.HA	1.93	0.50
1:D:517:GLY:HA2 1:D:520:LEU:HD12 1.95 0.48 1:A:516:LEU:O 1:A:519:GLN:HG2 2.13 0.48	1.A.520.LEU.HB3	1.B.430.ALA.HB1	1.90	0.19
1:A:516:LEU:O 1:A:519:GLN:HG2 2.13 0.48	1.D:517.GLY.HA2	1.D.520.LEU.HD12	1.91	0.10
	1.A.516.LEU.O	1:A:519:GLN:HG2	2.13	0.10
1:C:556:VAL:HG11 $1:D:48:GLV:HA2$ 1.96 0.48	1.C:556:VAL:HG11	1.D.48.GLV·HA2	1.96	0.48
$1.0.553 \cdot \text{GLU} + \text{HB}_3 = 4 \cdot \text{C} \cdot 701 \cdot \text{HOH} \cdot \text{O} = 2.13 = 0.47$	1.C.553.GLU.HB3	4·C·701·HOH·O	2.30	0.40
$\frac{1.8.535.616.1105}{1.8.517.617.617.617.617.617.617.617.617.617.6$	$1 \cdot B \cdot 517 \cdot GLV \cdot HA2$	1.B.520.LEU.HD12	1.96	0.47
1.5.917.011.1112 1.5.920.0100.11012 1.50 0.47 $1.4.920.000000000000000000000000000000000$	$1 \cdot \Delta \cdot 2/9 \cdot \text{THB} \cdot \text{HG} 23$	$\frac{1.0.020.\text{DEC.IID12}}{1.4.969.\text{MET-HE1}}$	1.96	0.47
$1:\Delta \cdot 377 \cdot 11 \text{ E \cdot HD 12} 1 \cdot \text{R} \cdot 300 \cdot 1 \cdot \text{VS \cdot HD 3} 1.95 0.47$	$1 \cdot \Delta \cdot 377 \cdot \text{ILE} \cdot \text{HD} 12$	1.R.202.ME1.HE1 1.R.200.LVS.HD2	1.95	0.47
1.11 + 1.11 +	1.M.077.HEB.HD12 $1.D.262.MET.HE3$	4·D·704·HOH·O	2 14	0.47
$1 \cdot B \cdot 104 \cdot THB \cdot HC22 = 1 \cdot B \cdot 108 \cdot LEU \cdot HD11 = 1.96 = 0.46$	1.B.104.THB.HC22	1.B.108.LEU.HD11	1.96	0.41
$1:C:195:LEU:H\Delta = 1:C:198:LEU:HD12 = 1.97 = 0.46$	1.C.195.LEU·HΔ	1.C.198.LEU.HD12	1.90	0.40
1.0.195.1100.11X 1.0.195.1110112 1.97 0.46	1.0.199.DD0.III 1.D.194.THB.HG22	1.0.198.LEU.HD12	1.97	0.40
$1:C \cdot 194 \cdot THR \cdot HG22 = 1:C \cdot 198 \cdot LEU \cdot HD11 = 1.91 = 0.46$	1.C.194.THR.HG22	1.C.198.LEU.HD11	1.97	0.46
$1:D:195:LEU:H\Delta = 1:D:198:LEU:HD12 = 1.98 = 0.46$	1.0.194.1110.1022 $1.0.195.LEU.H\Delta$	1.0.198.LEU.HD12	1.90	0.40
$1.5.155.112 \cdot 1.55.112 \cdot 1.55 \cdot 112 \cdot 1.55$	1.A.157.GLV.HA3	$2 \cdot A \cdot 600 \cdot PA 5 \cdot O2$	2 15	0.46
$1 \cdot \Delta \cdot 517 \cdot \text{GLV} \cdot \text{H} \Delta 2 = 1 \cdot \Delta \cdot 520 \cdot \text{LEU} \cdot \text{HD} 12 = 1.97 = 0.46$	$1 \cdot \Lambda \cdot 517 \cdot \text{GLV} \cdot \text{H} \Lambda 2$	$\frac{1 \cdot \Delta \cdot 520 \cdot \text{LEU} \cdot \text{HD} 12}{1 \cdot \Delta \cdot 520 \cdot \text{LEU} \cdot \text{HD} 12}$	1.97	0.40
1:A:209:SEB:OG 2:A:600:PA5:O1P 2 18 0.46	$1 \cdot A \cdot 209 \cdot \text{SEB} \cdot \text{OG}$	$2 \cdot A \cdot 600 \cdot PA 5 \cdot O1P$	2.18	0.40
1·D·98·LEU·HB2 1·D·268·TBP·CE3 2.51 0.46	1.D.98.LEU.HB2	1.D.268.TRP.CE3	2.10	0.10
1·B·98·LEU·HB2 1·B·268·TBP·CE3 2.51 0.46	1.B.98.LEU.HB2	$1 \cdot B \cdot 268 \cdot TBP \cdot CE3$	2.51	0.46
1:C:514:VAL:HB 1:D:388:HIS:HA 1.98 0.46	1:C:514:VAL:HB	1.D.388.HIS.HA	1.98	0.10
1:C:98:LEU:HB2 1:C:268:TBP:CE3 2.51 0.46	1.C.98.LEU.HB2	$1 \cdot C \cdot 268 \cdot TRP \cdot CE3$	2.51	0.46
$1 \cdot 4 \cdot 414 \cdot PRO \cdot HD2 = 4 \cdot 4 \cdot 778 \cdot HOH \cdot O = 2.51 = 0.10$	$1 \cdot A \cdot 414 \cdot PBO \cdot HD2$	4·A·778·HOH·O	2.01	0.10
1:A:195:LEU:HA = 1:A:198:LEU:HD12 = 1.98 = 0.46	1.A.195.LEU.HA	1·A·198·LEU·HD12	1.98	0.46
$1 \cdot A \cdot 194 \cdot THR \cdot HG22 = 1 \cdot A \cdot 198 \cdot LEU \cdot HD11 = 1.97 = 0.45$	$1 \cdot A \cdot 194 \cdot \text{THR} \cdot \text{HG} \cdot 92$	1.A.198.LEU.HD11	1.90	0.45
$1 \cdot C \cdot 169 \cdot A \downarrow A \cdot H A = 1 \cdot C \cdot 343 \cdot T \vee R \cdot H R3 = 1.98 = 0.45$	$1 \cdot C \cdot 169 \cdot \Delta I \cdot \Delta \cdot H \Delta$	1.C·343·TVR·HR3	1.01	0.45
1·B·195·LEU·HA 1·B·198·LEU·HD12 1.99 0.45	$\frac{1 \cdot B \cdot 105 \cdot I \cdot E I \cdot H \Lambda}{1 \cdot B \cdot 195 \cdot I \cdot E I \cdot H \Lambda}$	1.B.198.LEII.HD19	1 99	0.45
$1 \cdot B \cdot 245 \cdot L E U \cdot H D 13 \qquad 1 \cdot B \cdot 270 \cdot U E \cdot H A \qquad 1.08 \qquad 0.45$	1.B.245.LEU.HD12	1·B·270·Π Ε·H Δ	1.00	0.45
$1 \cdot B \cdot 481 \cdot L \cdot EU \cdot H D \cdot 23 \qquad 4 \cdot B \cdot 744 \cdot H \cap H \cdot O \qquad 2 \cdot 17 \qquad 0 \cdot 45$	1.B.481.LEU.HD93	4·B·744·HOH·O	<u> </u>	0.45
1·A·98·LEU·HB2 1·A·268·TRP·CE3 2.52 0.45	1.A.98.LEU.HR9	1·A·268·TRP·CE3	2.11	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:169:ALA:HA	1:A:343:TYR:HB3	1.98	0.45
1:A:245:LEU:HD13	1:A:279:ILE:HA	1.97	0.45
1:A:392:GLN:OE1	1:B:512:TRP:O	2.35	0.45
1:A:86:GLY:HA2	1:A:98:LEU:HD21	1.99	0.45
1:B:86:GLY:HA2	1:B:98:LEU:HD21	1.99	0.45
1:D:245:LEU:HD13	1:D:279:ILE:HA	1.97	0.45
1:A:249:THR:HA	1:A:262:MET:HE1	1.99	0.45
1:B:352:GLN:O	1:B:356:MET:HB2	2.18	0.44
1:A:376:PRO:HA	1:B:399:LYS:HE2	1.98	0.44
1:D:169:ALA:HA	1:D:343:TYR:HB3	1.98	0.44
1:B:169:ALA:HA	1:B:343:TYR:HB3	1.99	0.44
1:B:1:ALA:HB2	1:B:370:VAL:HA	2.00	0.44
1:C:104:ASN:HA	1:C:300:HIS:CD2	2.53	0.44
1:D:86:GLY:HA2	1:D:98:LEU:HD21	2.00	0.44
1:A:1:ALA:HB2	1:A:370:VAL:HA	2.00	0.43
1:A:252:VAL:HG11	1:A:262:MET:HG3	2.00	0.43
1:C:352:GLN:O	1:C:356:MET:HB2	2.19	0.43
1:D:1:ALA:HB2	1:D:370:VAL:HA	2.00	0.43
1:A:388:HIS:HA	1:B:514:VAL:HB	2.00	0.43
1:D:252:VAL:HG11	1:D:262:MET:HG3	2.01	0.43
1:A:104:ASN:HA	1:A:300:HIS:CD2	2.53	0.43
1:A:352:GLN:O	1:A:356:MET:HB2	2.18	0.43
1:B:249:THR:HG23	1:B:262:MET:HE1	2.00	0.43
1:D:163:PRO:HB2	1:D:182:TYR:HE2	1.84	0.43
1:C:1:ALA:HB2	1:C:370:VAL:HA	2.00	0.43
1:C:252:VAL:HG11	1:C:262:MET:HG3	2.00	0.43
1:A:163:PRO:HB2	1:A:182:TYR:HE2	1.84	0.43
1:D:352:GLN:O	1:D:356:MET:HB2	2.18	0.43
1:A:399:LYS:HG3	1:B:373:GLN:OE1	2.19	0.42
1:B:82:ARG:NH1	1:B:89:ILE:HG22	2.34	0.42
1:C:249:THR:HG23	1:C:262:MET:HE1	2.01	0.42
1:C:343:TYR:CZ	1:D:189:THR:HG23	2.53	0.42
1:C:79:ALA:HB2	4:C:739:HOH:O	2.20	0.42
1:C:86:GLY:HA2	1:C:98:LEU:HD21	2.02	0.42
1:C:41:LEU:HD11	1:C:318:LEU:HD12	2.02	0.42
1:C:399:LYS:HD3	1:D:377:ILE:HD12	2.01	0.42
1:D:16:TYR:O	1:D:20:ARG:HB2	2.20	0.41
1:A:6:ASP:HA	1:A:7:PRO:HD3	1.97	0.41
1:C:163:PRO:HB2	1:C:182:TYR:HE2	1.84	0.41
1:A:430:ALA:HB1	1:B:520:LEU:HB3	2.02	0.41
1:C:388:HIS:HA	1:D:514:VAL:HB	2.02	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:16:TYR:O	1:A:20:ARG:HB2	2.21	0.41
1:B:41:LEU:HD11	1:B:318:LEU:HD12	2.03	0.41
4:C:705:HOH:O	1:D:410:GLN:HG2	2.20	0.41
1:D:41:LEU:HD11	1:D:318:LEU:HD12	2.02	0.41
1:B:6:ASP:HA	1:B:7:PRO:HD3	1.96	0.41
1:B:92:THR:HB	1:B:512:TRP:CH2	2.56	0.41
1:B:14:GLN:HE22	1:B:17:ARG:HH11	1.68	0.41
1:A:14:GLN:HE22	1:A:17:ARG:HH11	1.69	0.41
1:B:252:VAL:HG11	1:B:262:MET:HG3	2.03	0.41
1:C:516:LEU:HD13	1:D:467:PHE:CE1	2.56	0.41
1:D:249:THR:HG23	1:D:262:MET:HE1	2.01	0.40
1:A:417:LYS:HE3	1:A:417:LYS:HB3	1.91	0.40
1:C:520:LEU:HD12	1:D:430:ALA:HB1	2.02	0.40
1:C:392:GLN:NE2	1:D:513:GLY:H	2.17	0.40
1:A:41:LEU:HD11	1:A:318:LEU:HD12	2.03	0.40
1:C:528:LEU:HD23	1:C:545:ILE:HG23	2.04	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	\mathbf{ntiles}
1	А	554/556~(100%)	530~(96%)	23~(4%)	1 (0%)	47	61
1	В	554/556~(100%)	529~(96%)	24 (4%)	1 (0%)	47	61
1	С	554/556~(100%)	531~(96%)	22 (4%)	1 (0%)	47	61
1	D	554/556~(100%)	531~(96%)	22 (4%)	1 (0%)	47	61
All	All	2216/2224~(100%)	2121~(96%)	91 (4%)	4 (0%)	47	61

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	D	277	SER
1	А	277	SER
1	В	277	SER
1	С	277	SER

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	Percentile	es
1	А	475/475~(100%)	463~(98%)	12 (2%)	47 65	
1	В	475/475~(100%)	460 (97%)	15~(3%)	39 56	
1	С	475/475~(100%)	461 (97%)	14(3%)	42 60	
1	D	475/475~(100%)	462~(97%)	13 (3%)	44 62	
All	All	1900/1900~(100%)	1846~(97%)	54 (3%)	43 61	

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	22	GLU
1	А	33	LYS
1	А	103	ARG
1	А	133	GLN
1	А	212	PHE
1	А	251	LYS
1	А	436	MET
1	А	437	ARG
1	А	505	ASP
1	А	514	VAL
1	А	522	LYS
1	А	523	LYS
1	В	22	GLU
1	В	26	ARG
1	В	33	LYS
1	В	103	ARG
1	В	123	LYS
1	В	133	GLN



Mol	Chain	Res	Type
1	В	212	PHE
1	В	251	LYS
1	В	264	GLU
1	В	417	LYS
1	В	437	ARG
1	В	505	ASP
1	В	514	VAL
1	В	523	LYS
1	В	552	ARG
1	С	26	ARG
1	С	33	LYS
1	С	103	ARG
1	С	126	ASP
1	С	133	GLN
1	С	212	PHE
1	С	251	LYS
1	С	417	LYS
1	С	433	GLU
1	С	437	ARG
1	С	505	ASP
1	С	514	VAL
1	С	520	LEU
1	С	523	LYS
1	D	22	GLU
1	D	26	ARG
1	D	33	LYS
1	D	103	ARG
1	D	133	GLN
1	D	212	PHE
1	D	251	LYS
1	D	433	GLU
1	D	437	ARG
1	D	505	ASP
1	D	507	ASN
1	D	514	VAL
1	D	523	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	14	GLN
1	А	300	HIS



	9	1	1 0
Mol	Chain	Res	Type
1	В	14	GLN
1	В	500	GLN
1	С	14	GLN
1	С	57	ASN
1	С	104	ASN
1	С	300	HIS
1	С	328	ASN
1	С	392	GLN
1	С	551	GLN
1	D	14	GLN
1	D	392	GLN
1	D	507	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 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).

Mal	Type	Chain	Dec	Dec Link	Bond lengths			Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	O1B	В	600	-	17,17,17	1.10	2 (11%)	21,23,23	1.23	2 (9%)
2	PA5	А	600	-	11,14,14	0.85	0	$16,\!20,\!20$	1.07	0



Mol	Type	Chain	Dec	Tinl	Bond lengths			Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	O1B	D	600	-	17,17,17	0.67	1 (5%)	21,23,23	0.78	0
2	PA5	С	600	-	11,14,14	0.94	1 (9%)	16,20,20	1.99	4 (25%)

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
3	O1B	В	600	-	-	5/22/22/22	-
2	PA5	А	600	-	-	5/14/18/18	-
3	O1B	D	600	-	-	4/22/22/22	-
2	PA5	С	600	-	-	0/14/18/18	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
3	В	600	O1B	P-O6	3.18	1.60	1.50
3	В	600	O1B	P-07	-2.78	1.44	1.54
3	D	600	O1B	P-O6	-2.53	1.42	1.50
2	С	600	PA5	C3-C2	-2.04	1.51	1.53

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	600	PA5	C4-C3-C2	-4.72	103.97	112.10
2	С	600	PA5	O3P-P-O5	-3.45	97.54	106.73
3	В	600	O1B	C4-C3-C2	-3.03	102.52	109.91
2	С	600	PA5	O3P-P-O2P	2.97	118.97	107.64
3	В	600	O1B	P-O4-C6	-2.90	110.30	118.30
2	С	600	PA5	O2P-P-O5	-2.74	99.44	106.73

All (6) bond angle outliers are listed below:

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	В	600	O1B	O3-C5-C6-O4
3	В	600	O1B	C6-O4-P-O5
3	В	600	O1B	C3-C2-N1-C1
2	А	600	PA5	C3-C4-C5-O5



		1	1 0	
Mol	Chain	\mathbf{Res}	Type	Atoms
2	А	600	PA5	O4-C4-C5-O5
2	А	600	PA5	C5-O5-P-O1P
2	А	600	PA5	C5-O5-P-O2P
2	А	600	PA5	C5-O5-P-O3P
3	D	600	O1B	C3-C2-N1-C1
3	D	600	O1B	O-C2-N1-C1
3	В	600	O1B	O-C2-N1-C1
3	В	600	O1B	C-C1-N1-C2
3	D	600	O1B	N-C-C1-N1
3	D	600	O1B	C6-O4-P-O6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	600	O1B	2	0
2	А	600	PA5	2	0
3	D	600	O1B	3	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	556/556~(100%)	0.50	31 (5%) 24 27	30, 59, 105, 183	0
1	В	556/556~(100%)	0.38	28 (5%) 28 31	30, 52, 98, 184	0
1	С	556/556~(100%)	1.46	140 (25%) 0 0	39, 83, 161, 216	0
1	D	556/556~(100%)	1.15	108 (19%) 1 1	37, 78, 147, 184	0
All	All	2224/2224~(100%)	0.87	307 (13%) 2 3	30, 67, 141, 216	0

All (307) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	455	PRO	19.5
1	С	63	VAL	14.8
1	С	372	HIS	13.8
1	В	452	GLY	12.0
1	С	318	LEU	11.2
1	С	12	LEU	10.8
1	С	59	VAL	10.6
1	С	466	VAL	10.0
1	С	67	LEU	8.5
1	С	21	SER	8.4
1	С	31	ALA	7.9
1	С	60	THR	7.9
1	D	368	THR	7.5
1	В	453	LYS	7.4
1	С	76	VAL	7.3
1	А	455	PRO	7.3
1	С	504	TRP	7.2
1	D	12	LEU	7.1
1	С	329	CYS	7.0
1	D	554	ALA	6.8
1	С	23	LEU	6.8



Mol	Chain	Res	Type	RSRZ
1	С	29	PHE	6.6
1	D	466	VAL	6.6
1	С	467	PHE	6.6
1	D	453	LYS	6.6
1	С	362	TYR	6.5
1	С	311	LEU	6.4
1	С	363	ILE	6.2
1	С	556	VAL	6.0
1	С	371	ASP	5.8
1	А	450	ALA	5.8
1	D	372	HIS	5.7
1	В	1	ALA	5.7
1	В	460	ARG	5.6
1	D	454	SER	5.6
1	В	456	GLU	5.6
1	D	445	ARG	5.6
1	С	51	LEU	5.6
1	D	1	ALA	5.4
1	D	369	ARG	5.3
1	С	4	THR	5.2
1	D	534	VAL	5.2
1	D	547	PHE	5.2
1	D	10	GLN	5.2
1	С	312	GLU	5.1
1	В	448	LEU	5.1
1	В	458	LEU	5.1
1	D	448	LEU	5.1
1	D	29	PHE	5.0
1	С	41	LEU	4.9
1	D	23	LEU	4.9
1	D	451	ALA	4.9
1	D	461	LEU	4.9
1	С	16	TYR	4.9
1	D	462	LEU	4.9
1	D	449	GLN	4.8
1	С	7	PRO	4.8
1	D	5	ARG	4.7
1	D	204	LEU	4.7
1	С	462	LEU	4.7
1	D	30	ASP	4.7
1	А	453	LYS	4.6
1	D	119	PRO	4.6



Mol	Chain	Res	Type	RSRZ
1	D	255	PHE	4.6
1	С	22	GLU	4.6
1	D	456	GLU	4.6
1	D	58	LEU	4.5
1	D	14	GLN	4.5
1	В	58	LEU	4.5
1	С	50	ILE	4.5
1	В	451	ALA	4.4
1	С	435	LEU	4.4
1	D	528	LEU	4.4
1	D	535	THR	4.4
1	В	461	LEU	4.4
1	C	9	PHE	4.3
1	С	330	PHE	4.3
1	С	447	GLU	4.3
1	А	31	ALA	4.2
1	D	317	VAL	4.2
1	D	455	PRO	4.2
1	С	58	LEU	4.1
1	С	503	ILE	4.1
1	D	232	ALA	4.1
1	А	363	ILE	4.0
1	D	92	THR	4.0
1	С	321	LEU	4.0
1	С	310	PRO	4.0
1	С	8	GLN	4.0
1	D	519	GLN	4.0
1	С	65	ARG	3.9
1	D	39	PHE	3.9
1	С	66	MET	3.9
1	С	89	ILE	3.9
1	C	322	LEU	3.9
1	D	9	PHE	3.9
1	С	336	ALA	3.9
1	C	395	HIS	3.9
1	C	324	ILE	3.8
1	D	555	ARG	3.8
1	D	363	ILE	3.8
1	D	27	ARG	3.7
1	C	461	LEU	3.7
1	D	529	ASP	3.7
1	C	394	ILE	3.7



Mol	Chain	Res	Type	RSRZ	
1	D	502	ILE	3.7	
1	D	218	ILE	3.6	
1	С	17	ARG	3.6	
1	В	462	LEU	3.6	
1	С	547	PHE	3.5	
1	С	360	GLY	3.5	
1	С	454	SER	3.5	
1	D	370	VAL	3.5	
1	А	22	GLU	3.5	
1	А	114	GLY	3.5	
1	С	139	ASP	3.5	
1	С	438	GLY	3.5	
1	С	64	MET	3.5	
1	D	318	LEU	3.5	
1	D	28	LEU	3.5	
1	D	470	ASN	3.5	
1	С	456	GLU	3.4	
1	С	61	GLU	3.4	
1	В	449	GLN	3.4	
1	С	27	ARG	3.4	
1	D	227	TRP	3.4	
1	С	464	HIS	3.4	
1	D	522	LYS	3.4	
1	D	541	THR	3.3	
1	С	448	LEU	3.3	
1	С	10	GLN	3.3	
1	D	457	ASP	3.3	
1	D	458	LEU	3.3	
1	С	365	LYS	3.3	
1	D	91	TYR	3.2	
1	D	18	GLU	3.2	
1	C	15	TRP	3.2	
1	C	28	LEU	3.2	
1	D	459	GLU	3.2	
1	D	524	ILE	3.2	
1	C	370	VAL	3.2	
1	D	21	SER	3.1	
1	С	43	LEU	3.1	
1	С	112	VAL	3.1	
1	С	439	LYS	3.1	
1	С	14	GLN	3.1	
1	D	542	ASN	3.1	



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Mol	Chain	Res	Type	RSRZ	
1	D	377	ILE	3.0	
1	С	361	LYS	3.0	
1	D	545	ILE	3.0	
1	D	54	TYR	3.0	
1	С	319	LEU	3.0	
1	С	396	GLN	3.0	
1	С	111	LEU	3.0	
1	С	555	ARG	3.0	
1	А	515	GLU	3.0	
1	С	375	GLY	3.0	
1	D	33	LYS	2.9	
1	С	470	ASN	2.9	
1	С	84	PHE	2.9	
1	С	34	ASP	2.9	
1	С	55	SER	2.9	
1	С	3	LEU	2.9	
1	С	232	ALA	2.9	
1	В	457	ASP	2.9	
1	D	76	VAL	2.9	
1	D	393	LEU	2.9	
1	С	54	TYR	2.9	
1	D	505	ASP	2.9	
1	С	228	PHE	2.9	
1	D	111	LEU	2.9	
1	С	359	ASN	2.8	
1	D	212	PHE	2.8	
1	D	436	MET	2.8	
1	С	19	HIS	2.8	
1	D	463	PRO	2.8	
1	С	68	VAL	2.8	
1	С	25	LEU	2.8	
1	C	401	ILE	2.8	
1	D	362	TYR	2.8	
1	C	325	TRP	2.8	
1	A	109	PRO	2.7	
1	D	112	VAL	2.7	
1	D	224	ALA	2.7	
1	C	70	LEU	2.7	
1	С	98	LEU	2.7	
1	C	314	ASN	2.7	
1	C _	301	TRP	2.7	
1	C	42	THR	2.7	



Mol	Chain	Res	Type	RSRZ	
1	D	452	GLY	2.7	
1	С	434	ALA	2.7	
1	С	35	ARG	2.7	
1	А	110	ILE	2.7	
1	В	454	SER	2.7	
1	А	369	ARG	2.7	
1	А	260	GLN	2.7	
1	D	20	ARG	2.7	
1	D	526	PRO	2.7	
1	А	206	ILE	2.7	
1	D	464	HIS	2.7	
1	С	52	VAL	2.7	
1	D	143	TYR	2.6	
1	С	122	ASN	2.6	
1	В	512	TRP	2.6	
1	С	374	THR	2.6	
1	D	230	GLN	2.6	
1	А	456	GLU	2.6	
1	С	433	GLU	2.6	
1	В	29	PHE	2.6	
1	С	267	ASP	2.6	
1	D	530	GLY	2.6	
1	С	453	LYS	2.6	
1	А	461	LEU	2.6	
1	А	242	PHE	2.6	
1	D	533	GLN	2.6	
1	В	450	ALA	2.6	
1	С	2	ALA	2.6	
1	С	323	GLY	2.5	
1	С	416	ARG	2.5	
1	D	74	ARG	2.5	
1	С	432	THR	2.5	
1	D	358	SER	2.5	
1	D	257	ILE	2.5	
1	С	5	ARG	2.5	
1	С	369	ARG	2.5	
1	С	471	ARG	2.5	
1	A	454	SER	2.5	
1	D	3	LEU	2.5	
1	D	228	PHE	2.4	
1	D	325	TRP	2.4	
1	С	40	SER	2.4	



Mol	Chain	Res	Type	RSRZ	
1	D	71	ALA	2.4	
1	С	238	VAL	2.4	
1	С	306	PHE	2.4	
1	D	8	GLN	2.4	
1	D	89	ILE	2.4	
1	D	394	ILE	2.4	
1	D	446	LYS	2.4	
1	А	289	PHE	2.4	
1	В	112	VAL	2.4	
1	В	14	GLN	2.3	
1	С	309	THR	2.3	
1	С	39	PHE	2.3	
1	С	242	PHE	2.3	
1	D	329	CYS	2.3	
1	D	207	ILE	2.3	
1	А	446	LYS	2.3	
1	D	437	ARG	2.3	
1	D	546	ASN	2.3	
1	С	45	THR	2.3	
1	С	131	PHE	2.3	
1	С	378	VAL	2.3	
1	D	243	VAL	2.3	
1	С	449	GLN	2.3	
1	А	506	ILE	2.3	
1	В	23	LEU	2.3	
1	D	236	SER	2.3	
1	С	38	HIS	2.3	
1	С	531	SER	2.3	
1	В	12	LEU	2.2	
1	С	364	THR	2.2	
1	A	513	GLY	2.2	
1	D	443	GLU	2.2	
1	C	268	TRP	2.2	
1	В	21	SER	2.2	
1	В	369	ARG	2.2	
1	С	423	ILE	2.2	
1	A	91	TYR	2.2	
1	В	8	GLN	2.2	
1	С	463	PRO	2.2	
1	В	555	ARG	2.2	
1	D	438	GLY	2.2	
1	С	451	ALA	2.2	



Mol	Chain	Res	Type	RSRZ	
1	D	41	LEU	2.2	
1	С	91	TYR	2.2	
1	С	96	ALA	2.2	
1	С	458	LEU	2.2	
1	А	457	ASP	2.2	
1	С	308	THR	2.2	
1	D	539	ALA	2.2	
1	С	1	ALA	2.1	
1	D	548	ILE	2.1	
1	D	552	ARG	2.1	
1	D	84	PHE	2.1	
1	А	253	LYS	2.1	
1	С	506	ILE	2.1	
1	В	20	ARG	2.1	
1	D	442	GLU	2.1	
1	А	556	VAL	2.1	
1	С	460	ARG	2.1	
1	А	204	LEU	2.1	
1	С	499	VAL	2.1	
1	D	205 PHI		2.1	
1	В	41	LEU	2.1	
1	D	321	LEU	2.1	
1	D	233	LYS	2.1	
1	А	8	GLN	2.0	
1	В	33	LYS	2.0	
1	С	426	ALA	2.0	
1	С	72	LYS	2.0	
1	А	532	ALA	2.0	
1	А	20	ARG	2.0	
1	С	505	ASP	2.0	
1	A	228	228 PHE		
1	А	458	LEU	2.0	
1	С	377	ILE	2.0	
1	С	442	GLU	2.0	

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

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



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	O1B	D	600	18/18	0.91	0.16	$63,\!92,\!109,\!109$	0
2	PA5	A	600	15/15	0.93	0.12	48,60,62,67	0
2	PA5	С	600	15/15	0.93	0.15	46,59,67,67	0
3	O1B	В	600	18/18	0.96	0.14	35,43,54,57	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.

