

Full wwPDB X-ray Structure Validation Report (i)

Mar 11, 2024 - 06:07 pm GMT

PDB ID	:	8AJZ
Title	:	Serial femtosecond crystallography structure of CO bound ba3- type cy-
		to chrome c oxidase at 2 milliseconds after irradiation by a 532 nm laser
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		Bosman, R.; Dahl, P.; Nango, E.; Tanaka, R.; Zoric, D.; Svensson, E.; Nakane,
		T.; Iwata, S.; Neutze, R.; Branden, G.
Deposited on	:	2022-07-29
Resolution	:	2.00 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36



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 2.00 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\# {\rm Entries,\ resolution\ range}({\rm \AA})) \end{array}$			
R_{free}	130704	8085 (2.00-2.00)			
Clashscore	141614	9178 (2.00-2.00)			
Ramachandran outliers	138981	9054 (2.00-2.00)			
Sidechain outliers	138945	9053 (2.00-2.00)			
RSRZ outliers	127900	7900 (2.00-2.00)			

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	
			28%	
1	А	569	91%	5% • •
			17%	
2	В	168	89%	10% •••
			12%	
3	С	34	88%	• 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	HAS	А	603[A]	Х	-	-	-
6	HAS	А	603[B]	Х	-	-	-



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 6575 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	554	Total 4417	C 3000	N 707	0 694	S 16	0	6	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-6	MET	-	initiating methionine	UNP Q5SJ79
А	-5	HIS	-	expression tag	UNP Q5SJ79
А	-4	HIS	-	expression tag	UNP Q5SJ79
А	-3	HIS	-	expression tag	UNP Q5SJ79
А	-2	HIS	-	expression tag	UNP Q5SJ79
А	-1	HIS	-	expression tag	UNP Q5SJ79
А	0	HIS	-	expression tag	UNP Q5SJ79
А	1	HIS	-	expression tag	UNP Q5SJ79

• Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	167	Total 1301	C 846	N 216	O 235	$\frac{S}{4}$	0	0	0

• Molecule 3 is a protein called Cytochrome c oxidase polypeptide IIA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
3	С	31	Total 241	C 169	N 37	O 35	0	0	0

• Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Cu 2 2	0	1

• Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	А	1	Total 43	С 34	Fe 1	N 4	0 4	0	0

• Molecule 6 is HEME-AS (three-letter code: HAS) (formula: $C_{54}H_{64}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	А	1	Total 110	C 88	Fe 2	N 8	O 12	0	1

• Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	Total C O 23 19 4	0	0
7	А	1	Total C O 18 14 4	0	0
7	А	1	Total C O 17 13 4	0	0
7	А	1	Total C O 15 11 4	0	0
7	А	1	Total C O 18 14 4	0	0
7	А	1	Total C O 15 11 4	0	0
7	А	1	Total C O 20 16 4	0	0
7	А	1	Total C O 21 17 4	0	0
7	А	1	Total C 9 9	0	0
7	А	1	Total C 9 9	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
7	В	1	Total C O	0	0	
1	D	1	20 18 2	0	0	
7	В	1	Total C O	0	0	
1	D	T	25 21 4	0	0	
7	С	1	Total C O	0	0	
1	U	1	24 20 4	0	0	
7	С	1	Total C O	0	0	
1	U	T	15 11 4	0	0	
7	С	1	Total C O	0	0	
1	U	1	24 20 4	0	0	

• Molecule 8 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	А	1	Total C 4 2	O 2	0	1

• Molecule 9 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂) (labeled as "Ligand of Interest" by depositor).



CUA
CU1 <mark>Cu</mark> — <mark>Cu</mark> CU2

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	В	1	Total Cu 2 2	0	0

• Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	99	Total O 99 99	0	1
10	В	80	Total O 80 80	0	0
10	С	3	Total O 3 3	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: Cytochrome c oxidase subunit 1









4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	145.85Å 100.32Å 96.62Å	Depositor
a, b, c, α , β , γ	90.00° 126.76° 90.00°	Depositor
Bosolution(A)	38.70 - 2.00	Depositor
Resolution (A)	41.68 - 2.00	EDS
% Data completeness	99.9 (38.70-2.00)	Depositor
(in resolution range)	$100.0 \ (41.68-2.00)$	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.10 (at 2.00 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
P. P.	0.190 , 0.210	Depositor
II, II, <i>free</i>	0.187 , 0.212	DCC
R_{free} test set	3773 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	40.0	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35 , 85.7	EDS
L-test for $twinning^2$	$ < L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6575	wwPDB-VP
Average B, all atoms $(Å^2)$	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.17% 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: CU, HEM, OLC, CUA, HAS, CMO

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		
MIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.71	0/4595	0.82	0/6310	
2	В	0.72	0/1338	0.87	2/1828~(0.1%)	
3	С	0.71	0/247	0.71	0/335	
All	All	0.71	0/6180	0.82	2/8473~(0.0%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	1
2	В	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	3	ASP	O-C-N	-7.33	110.98	122.70
2	В	3	ASP	CA-C-N	5.11	128.43	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	516	GLU	Peptide
2	В	3	ASP	Mainchain



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	4417	0	4511	27	0
2	В	1301	0	1278	17	0
3	С	241	0	267	1	0
4	А	2	0	0	0	0
5	А	43	0	30	2	0
6	А	110	0	62	4	0
7	А	165	0	229	0	0
7	В	45	0	68	0	0
7	С	63	0	89	1	0
8	А	4	0	0	0	0
9	В	2	0	0	0	0
10	А	99	0	0	2	0
10	В	80	0	0	5	0
10	С	3	0	0	0	0
All	All	6575	0	6534	48	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 (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
2:B:140:LYS:HE3	2:B:140:LYS:HA	1.66	0.76
5:A:602:HEM:HMC2	5:A:602:HEM:HBC2	1.69	0.74
1:A:332:LEU:HD23	1:A:333:PHE:CE2	2.28	0.69
2:B:49:LYS:O	2:B:49:LYS:HD2	1.97	0.65
2:B:140:LYS:HA	2:B:140:LYS:CE	2.27	0.64
1:A:519:ARG:O	1:A:519:ARG:HD3	1.99	0.62
2:B:141:ARG:HD3	10:B:361:HOH:O	1.98	0.62
2:B:2:VAL:HG22	2:B:3:ASP:H	1.64	0.62
6:A:603[B]:HAS:HMC1	6:A:603[B]:HAS:HBC1	1.83	0.60
1:A:519:ARG:HD3	1:A:519:ARG:C	2.21	0.60
2:B:47:ALA:HB3	2:B:49:LYS:HE3	1.85	0.56
1:A:332:LEU:HD23	1:A:333:PHE:CZ	2.42	0.54
6:A:603[A]:HAS:HBC1	6:A:603[A]:HAS:HMC1	1.88	0.53



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Interatomic Clash								
Atom-1	Atom-2	distance $\begin{pmatrix} \lambda \end{pmatrix}$	$\operatorname{Clash}_{\operatorname{overlap}}(\lambda)$					
9.D.47.ALA.UD1	2.D.40.IVS.UC2		$\frac{0.52}{0.52}$					
2.D.47.ALA.IID1 5.A.602.HEM.HBC2	2.D.49.L15.HG5 5.A.602.HFM.CMC	1.90	0.55					
$\frac{1.4.411.1}{1.4.411.1}$	5.A.002.HEM.CMC	2.37	0.52					
1:A:411:LYS:HE2	I:A:494:5ER:U	2.11	0.50					
1:A:282[B]:HIS:CD2	6:A:603[B]:HAS:OMD	2.65	0.49					
1:A:33:1LE:U	1:A:37:LEU:HG	2.13	0.49					
1:A:355:GLY:HA3	1:A:433:MET:HE1	1.96	0.48					
1:A:400:SER:HB3	10:A:740:HOH:O	2.13	0.47					
2:B:95:1LE:HG23	10:B:376:HOH:O	2.15	0.47					
1:A:516:GLU:OE2	10:A:701:HOH:O	2.20	0.47					
1:A:337:ARG:HB3	1:A:337:ARG:CZ	2.45	0.46					
1:A:400:SER:HA	1:A:403:TRP:NE1	2.31	0.46					
2:B:144:GLU:HG2	2:B:165:VAL:HG22	1.97	0.45					
1:A:37:LEU:HD23	1:A:481:LEU:HD21	1.98	0.45					
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.51	0.45					
3:C:13:LEU:HD13	7:C:103:OLC:H12	1.98	0.45					
2:B:47:ALA:CB	2:B:49:LYS:HE3	2.47	0.45					
2:B:104:VAL:HG22	2:B:136:ARG:HG2	1.99	0.45					
2:B:15:GLU:O	2:B:19:LEU:HG	2.17	0.44					
1:A:307:VAL:N	1:A:308:PRO:HD2	2.33	0.43					
1:A:282[B]:HIS:CG	6:A:603[B]:HAS:OMD	2.71	0.43					
1:A:411:LYS:CE	1:A:494:SER:O	2.67	0.43					
1:A:52:TYR:N	1:A:53:PRO:CD	2.82	0.42					
1:A:411:LYS:HZ3	1:A:497:ARG:CZ	2.32	0.42					
1:A:223:VAL:HG21	1:A:553:LEU:CD2	2.50	0.42					
2:B:59:ARG:NH1	10:B:307:HOH:O	2.53	0.42					
1:A:241:LEU:HD12	1:A:241:LEU:HA	1.84	0.41					
1:A:562:TRP:HA	2:B:155:LEU:HG	2.02	0.41					
2:B:103:ILE:O	2:B:136:ARG:HA	2.20	0.41					
1:A:29:PHE:CE2	1:A:401:LEU:HD21	2.55	0.41					
1:A:348:ALA:HB3	1:A:349:PRO:HD3	2.03	0.41					
1:A:387:LEU:CD2	1:A:433:MET:CE	3.00	0.41					
1:A:302:THR:O	1:A:305:VAL:HG12	2.20	0.40					
1:A:387:LEU:HD22	1:A:433:MET:HE1	2.03	0.40					
2:B:159:ASN:ND2	10:B:301:HOH:O	2.23	0.40					
2:B:52:ARG:NH2	10:B:303:HOH:O	2.44	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	558/569~(98%)	539~(97%)	18 (3%)	1 (0%)	47	44
2	В	165/168~(98%)	163 (99%)	2(1%)	0	100	100
3	С	29/34~(85%)	29 (100%)	0	0	100	100
All	All	752/771~(98%)	731 (97%)	20 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type	
1	А	369	PHE	

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	453/463~(98%)	446 (98%)	7~(2%)	65	69	
2	В	136/138~(99%)	135~(99%)	1 (1%)	84	88	
3	С	24/27~(89%)	24 (100%)	0	100	100	
All	All	613/628~(98%)	605~(99%)	8 (1%)	71	74	

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	133[A]	TYR
1	А	133[B]	TYR



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Mol	Chain	Res	Type
1	А	230	TRP
1	А	241	LEU
1	А	369	PHE
1	А	411	LYS
1	А	519	ARG
2	В	49	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Turne	Chain	Dec	Tink	В	ond leng	gths	Bo	ond ang	les
	туре	Unam	nes	LIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	OLC	А	606	-	16,16,24	0.34	0	17,17,25	0.31	0
7	OLC	А	611	-	20,20,24	0.27	0	21,21,25	0.23	0
6	HAS	А	603[B]	1	69,72,72	<mark>3.13</mark>	31 (44%)	73,109,109	2.94	27 (36%)
7	OLC	А	609	-	14,14,24	0.26	0	15,15,25	0.28	0



Mal	Tuno	Chain	Dog	Link	В	ond leng	gths	Bo	ond ang	es
	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
8	CMO	А	614[B]	4	$0,\!1,\!1$	-	-	-		
7	OLC	А	607	-	14,14,24	0.22	0	$15,\!15,\!25$	0.27	0
7	OLC	А	605	-	17,17,24	0.27	0	$18,\!18,\!25$	0.33	0
7	OLC	В	201	-	19,19,24	0.24	0	$19,\!19,\!25$	0.19	0
7	OLC	А	610	-	$19,\!19,\!24$	0.27	0	$20,\!20,\!25$	0.29	0
9	CUA	В	203	2	$0,\!1,\!1$	-	-	-		
5	HEM	А	602	1	41,50,50	1.53	7 (17%)	45,82,82	1.88	11 (24%)
7	OLC	В	202	-	24,24,24	0.29	0	$25,\!25,\!25$	0.25	0
7	OLC	А	604	-	22,22,24	0.23	0	$23,\!23,\!25$	0.42	0
7	OLC	А	613	-	8,8,24	0.16	0	7,7,25	0.18	0
6	HAS	А	603[A]	1	69,72,72	2.18	21 (30%)	73,109,109	2.31	22 (30%)
7	OLC	С	102	-	14,14,24	0.27	0	$15,\!15,\!25$	0.39	0
8	CMO	А	614[A]	4	$0,\!1,\!1$	-	-	-		
7	OLC	А	608	-	17,17,24	0.41	0	$18,\!18,\!25$	0.39	0
7	OLC	A	612	-	8,8,24	0.18	0	7,7,25	0.15	0
7	OLC	С	101	-	23,23,24	0.22	0	24,24,25	0.26	0
7	OLC	С	103	-	23,23,24	0.34	0	24,24,25	0.21	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OLC	А	613	-	-	2/6/6/24	-
7	OLC	А	607	-	-	8/14/14/24	-
7	OLC	А	605	-	-	5/17/17/24	-
6	HAS	А	603[A]	1	1/1/8/18	6/40/82/82	-
7	OLC	А	606	-	-	7/16/16/24	-
7	OLC	В	201	-	-	10/18/18/24	-
7	OLC	А	610	-	-	8/19/19/24	-
7	OLC	А	611	-	-	7/20/20/24	-
7	OLC	С	102	-	-	9/14/14/24	-
6	HAS	А	603[B]	1	1/1/8/18	8/40/82/82	-
5	HEM	А	602	1	-	1/12/54/54	-
7	OLC	А	608	-	-	5/17/17/24	-
7	OLC	А	612	-	-	4/6/6/24	-
7	OLC	С	101	-	-	11/23/23/24	-
7	OLC	А	609	-	-	5/14/14/24	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OLC	В	202	-	-	9/24/24/24	-
7	OLC	С	103	-	-	9/23/23/24	-
7	OLC	А	604	-	-	5/22/22/24	-

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All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	А	603[B]	HAS	CBA-CGA	10.22	1.74	1.50
6	А	603[B]	HAS	CHD-C4A	8.14	1.46	1.35
6	А	603[A]	HAS	CHD-C4A	7.75	1.46	1.35
6	А	603[B]	HAS	FE-NA	6.75	2.21	1.95
6	А	603[B]	HAS	C3B-C2B	5.74	1.47	1.34
6	А	603[B]	HAS	CHC-C4B	5.58	1.49	1.35
6	А	603[B]	HAS	C3C-C2C	5.53	1.48	1.40
6	А	603[B]	HAS	CHB-C1D	5.38	1.49	1.38
6	А	603[A]	HAS	C3C-C2C	5.26	1.47	1.40
6	А	603[B]	HAS	C12-C11	5.22	1.61	1.52
6	А	603[B]	HAS	C4D-C3D	5.05	1.53	1.45
6	А	603[B]	HAS	C4B-C3B	4.94	1.52	1.44
6	А	603[B]	HAS	CHA-C1A	4.86	1.47	1.38
6	А	603[A]	HAS	C3B-C2B	4.85	1.45	1.34
5	А	602	HEM	C1B-NB	-4.78	1.32	1.40
6	А	603[A]	HAS	CHC-C4B	4.46	1.46	1.35
6	А	603[A]	HAS	C1D-ND	-4.26	1.33	1.40
6	А	603[B]	HAS	C2A-C3A	4.20	1.45	1.36
6	А	603[A]	HAS	C2A-C3A	3.99	1.45	1.36
6	А	603[B]	HAS	CHB-C1B	3.95	1.48	1.39
6	А	603[B]	HAS	CHA-C4D	3.91	1.48	1.39
6	А	603[B]	HAS	C1B-C2B	3.85	1.52	1.44
6	А	603[B]	HAS	C1C-CHC	3.77	1.51	1.41
5	А	602	HEM	C4D-ND	-3.71	1.33	1.40
6	А	603[B]	HAS	FE-ND	3.60	2.16	1.97
6	А	603[A]	HAS	C4B-NB	-3.50	1.34	1.40
6	А	603[A]	HAS	CHB-C1D	3.50	1.45	1.38
6	А	603[B]	HAS	O1A-CGA	3.46	1.33	1.22
6	А	603[A]	HAS	CHA-C1A	3.45	1.45	1.38
6	А	603[A]	HAS	FE-NA	3.34	2.08	1.95
6	А	603[B]	HAS	C1D-ND	-3.28	1.34	1.40
6	А	603[A]	HAS	C4A-NA	-3.26	1.33	1.39
6	А	603[B]	HAS	C1A-C2A	3.25	1.51	1.45
6	А	603[A]	HAS	C1B-NB	-3.19	1.32	1.38
6	А	603[B]	HAS	C4B-NB	-3.14	1.34	1.40



Mol	Chain	Res	Type	Atoms		Observed(A)	Ideal(A)
6	А	603[B]	HAS	C4A-NA	-3.11	1.33	1.39
6	А	603[B]	HAS	CBD-CGD	3.03	1.57	1.50
6	А	603[B]	HAS	FE-NB	2.96	2.13	1.97
5	А	602	HEM	CHB-C1B	2.95	1.42	1.35
6	А	603[B]	HAS	C4A-C3A	2.94	1.51	1.45
5	А	602	HEM	FE-NB	2.86	2.11	1.96
6	А	603[A]	HAS	CHA-C4D	2.84	1.45	1.39
6	А	603[A]	HAS	CHB-C1B	2.68	1.45	1.39
6	А	603[B]	HAS	C1B-NB	-2.62	1.33	1.38
6	А	603[A]	HAS	C2D-C3D	2.52	1.42	1.36
6	А	603[A]	HAS	FE-NB	2.35	2.10	1.97
5	А	602	HEM	C1A-NA	2.32	1.41	1.36
6	А	603[B]	HAS	C1A-NA	-2.32	1.35	1.39
6	А	603[A]	HAS	C4A-C3A	2.31	1.49	1.45
6	А	603[B]	HAS	CBD-CAD	2.31	1.59	1.52
6	А	603[A]	HAS	C1A-NA	-2.29	1.35	1.39
6	А	603[A]	HAS	C1C-CHC	2.27	1.47	1.41
6	А	603[A]	HAS	C4D-C3D	2.25	1.48	1.45
6	А	603[B]	HAS	C2D-C1D	2.22	1.49	1.44
6	А	603[B]	HAS	C2D-C3D	2.21	1.41	1.36
5	А	602	HEM	C4B-NB	-2.14	1.34	1.38
6	А	603[A]	HAS	FE-ND	2.12	2.08	1.97
6	A	603[B]	HAS	FE-NC	2.07	2.13	1.96
5	A	602	HEM	$\overline{C3C-C2C}$	-2.07	1.37	1.40

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All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	А	603[B]	HAS	C2D-C3D-C4D	-10.60	98.93	106.49
6	А	603[B]	HAS	CAD-C3D-C4D	9.65	141.53	124.66
6	А	603[A]	HAS	C2D-C3D-C4D	-7.63	101.05	106.49
6	А	603[B]	HAS	CAA-CBA-CGA	-7.04	98.46	113.60
5	А	602	HEM	CHC-C4B-NB	5.65	130.57	124.43
6	А	603[B]	HAS	OMD-CMD-C2D	-5.53	113.19	125.69
6	А	603[B]	HAS	C2A-C1A-NA	5.47	115.65	110.32
6	А	603[B]	HAS	C2B-C1B-NB	5.32	116.25	109.88
6	А	603[A]	HAS	C2A-C1A-NA	4.99	115.17	110.32
6	А	603[A]	HAS	C3B-C4B-NB	4.95	115.70	109.84
6	А	603[A]	HAS	C3D-C4D-ND	4.90	115.11	110.36
6	А	603[B]	HAS	CBD-CAD-C3D	-4.85	99.16	112.63
6	А	603[A]	HAS	CAD-C3D-C4D	4.67	132.82	124.66
6	А	603[A]	HAS	C2B-C1B-NB	4.56	115.34	109.88



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$		
5	А	602	HEM	C1B-NB-C4B	4.45	109.67	105.07		
6	А	603[B]	HAS	C3D-C4D-ND	4.43	114.64	110.36		
6	А	603[A]	HAS	CMC-C2C-C3C	4.43	132.96	124.68		
6	А	603[A]	HAS	CAA-CBA-CGA	-4.42	104.09	113.60		
6	А	603[B]	HAS	C1B-C2B-C3B	-4.38	101.57	106.80		
5	А	602	HEM	CHD-C1D-ND	4.12	128.91	124.43		
6	А	603[B]	HAS	C1D-C2D-C3D	4.00	110.29	107.11		
6	А	603[B]	HAS	C3B-C4B-NB	3.91	114.47	109.84		
6	А	603[B]	HAS	C3A-C4A-NA	3.85	116.79	109.69		
6	А	603[A]	HAS	C3C-C4C-NC	3.82	114.15	109.21		
6	А	603[B]	HAS	C13-C12-C11	-3.74	108.72	114.35		
6	А	603[B]	HAS	O11-C11-C12	3.58	119.41	109.42		
6	А	603[B]	HAS	CMC-C2C-C3C	3.55	131.31	124.68		
6	А	603[B]	HAS	C4A-C3A-C2A	-3.49	101.85	106.94		
6	А	603[B]	HAS	C1A-C2A-C3A	-3.47	102.60	107.13		
6	А	603[B]	HAS	CHA-C4D-ND	-3.43	120.69	124.42		
6	А	603[A]	HAS	C13-C12-C11	-3.30	109.39	114.35		
6	А	603[A]	HAS	C4B-C3B-C2B	-3.20	101.95	107.41		
5	А	602	HEM	CHC-C4B-C3B	-3.16	119.72	124.57		
6	А	603[A]	HAS	OMD-CMD-C2D	-3.15	118.56	125.69		
6	А	603[A]	HAS	C1B-C2B-C3B	-3.10	103.09	106.80		
6	А	603[A]	HAS	C1A-C2A-C3A	-3.06	103.13	107.13		
5	А	602	HEM	CHD-C1D-C2D	-2.95	120.37	124.98		
6	А	603[A]	HAS	CMA-C3A-C4A	2.92	129.86	124.71		
6	А	603[B]	HAS	O1A-CGA-CBA	-2.89	113.79	123.08		
6	А	603[A]	HAS	C4A-C3A-C2A	-2.79	102.87	106.94		
6	А	603[B]	HAS	C4A-NA-C1A	-2.77	102.64	105.35		
6	А	603[A]	HAS	CAA-C2A-C1A	2.73	130.03	124.89		
6	А	603[B]	HAS	C4B-C3B-C2B	-2.67	102.84	107.41		
6	А	603[A]	HAS	CMB-C2B-C1B	2.67	129.10	125.04		
6	А	603[A]	HAS	C3A-C4A-NA	2.64	114.56	109.69		
5	А	602	HEM	O2A-CGA-CBA	2.64	122.50	114.03		
6	А	603[B]	HAS	O2D-CGD-CBD	2.61	122.41	114.03		
5	А	602	HEM	O2D-CGD-O1D	-2.51	117.05	123.30		
5	А	602	HEM	CHA-C4D-C3D	-2.50	120.63	125.33		
6	А	603[B]	HAS	O2D-CGD-O1D	-2.50	117.07	123.30		
6	А	603[A]	HAS	O1D-CGD-CBD	-2.47	115.16	123.08		
6	А	603[B]	HAS	CHB-C1B-C2B	-2.46	121.14	124.98		
6	А	603[B]	HAS	CHA-C1A-C2A	-2.45	120.97	124.94		
6	А	603[A]	HAS	CHA-C1A-C2A	-2.37	121.10	124.94		
6	А	603[A]	HAS	CHB-C1B-C2B	-2.33	121.34	124.98		
6	А	603[B]	HAS	O2A-CGA-CBA	2.30	121.43	114.03		



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$					
5	А	602	HEM	CHA-C4D-ND	2.16	127.05	124.38					
5	А	602	HEM	C3C-C4C-NC	-2.13	106.92	110.94					
5	А	602	HEM	CAB-C3B-C2B	2.07	135.44	128.60					
6	А	603[B]	HAS	CAA-C2A-C1A	2.03	128.71	124.89					

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All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	А	603[A]	HAS	NA
6	А	603[B]	HAS	NA

All (119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	А	603[B]	HAS	C1D-C2D-CMD-OMD
6	А	603[B]	HAS	C3D-C2D-CMD-OMD
7	А	607	OLC	C21-C22-C24-O25
7	А	610	OLC	O20-C21-C22-C24
7	С	102	OLC	C21-C22-C24-O25
7	С	102	OLC	O23-C22-C24-O25
7	С	101	OLC	C2-C1-O20-C21
7	С	101	OLC	O19-C1-O20-C21
7	С	102	OLC	C2-C1-O20-C21
7	А	606	OLC	O20-C21-C22-O23
7	А	610	OLC	O20-C21-C22-O23
7	С	102	OLC	O19-C1-O20-C21
7	А	608	OLC	C2-C1-O20-C21
7	В	202	OLC	O20-C21-C22-C24
7	А	608	OLC	O19-C1-O20-C21
7	С	103	OLC	O20-C21-C22-O23
7	А	607	OLC	O23-C22-C24-O25
7	С	102	OLC	C1-C2-C3-C4
7	В	202	OLC	O20-C21-C22-O23
7	С	102	OLC	O20-C21-C22-O23
7	С	103	OLC	C2-C1-O20-C21
7	А	610	OLC	C5-C6-C7-C8
7	С	103	OLC	O20-C21-C22-C24
7	A	610	OLC	C2-C3-C4-C5
7	С	103	OLC	C11-C12-C13-C14
7	С	103	OLC	C2-C3-C4-C5
7	С	101	OLC	C3-C4-C5-C6
7	А	607	OLC	C2-C3-C4-C5



Mol	Chain	Res	Type	Atoms
7	А	605	OLC	C21-C22-C24-O25
7	А	609	OLC	C21-C22-C24-O25
7	А	611	OLC	C21-C22-C24-O25
7	С	103	OLC	O19-C1-O20-C21
7	В	202	OLC	C5-C6-C7-C8
7	А	612	OLC	C12-C13-C14-C15
7	А	610	OLC	C3-C4-C5-C6
7	В	201	OLC	C3-C4-C5-C6
7	С	101	OLC	C13-C14-C15-C16
7	А	606	OLC	C5-C6-C7-C8
7	А	609	OLC	C4-C5-C6-C7
7	А	605	OLC	O23-C22-C24-O25
7	В	201	OLC	C6-C7-C8-C9
7	В	202	OLC	C3-C4-C5-C6
7	А	606	OLC	O20-C21-C22-C24
7	А	608	OLC	C2-C3-C4-C5
7	А	604	OLC	C11-C12-C13-C14
7	А	612	OLC	C14-C15-C16-C17
7	А	607	OLC	C5-C6-C7-C8
7	А	612	OLC	C10-C11-C12-C13
7	А	607	OLC	C2-C1-O20-C21
7	В	201	OLC	C1-C2-C3-C4
7	В	201	OLC	C2-C1-O20-C21
7	А	611	OLC	C3-C4-C5-C6
7	В	201	OLC	C11-C12-C13-C14
7	А	611	OLC	O20-C21-C22-C24
7	А	606	OLC	C3-C4-C5-C6
7	С	102	OLC	C4-C5-C6-C7
7	В	202	OLC	C13-C14-C15-C16
7	С	103	OLC	C12-C13-C14-C15
7	A	607	OLC	O19-C1-O20-C21
7	C	101	OLC	C6-C7-C8-C9
7	В	202	OLC	C11-C12-C13-C14
7	В	202	OLC	C4-C5-C6-C7
7	В	201	OLC	C2-C3-C4-C5
7	С	102	OLC	C2-C3-C4-C5
7	С	102	OLC	O20-C21-C22-C24
7	В	201	OLC	C14-C15-C16-C17
7	A	610	OLC	C4-C5-C6-C7
7	A	606	OLC	C7-C8-C9-C10
7	A	605	OLC	C2-C3-C4-C5
7	А	604	OLC	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
7	А	613	OLC	C11-C12-C13-C14
6	А	603[B]	HAS	C11-C12-C13-C14
7	В	201	OLC	O19-C1-O20-C21
7	А	605	OLC	C4-C5-C6-C7
7	А	608	OLC	C3-C4-C5-C6
7	А	611	OLC	C9-C10-C11-C12
7	В	202	OLC	C9-C10-C11-C12
7	А	608	OLC	C7-C8-C9-C10
7	С	101	OLC	C11-C12-C13-C14
7	А	609	OLC	C5-C6-C7-C8
7	В	202	OLC	C10-C11-C12-C13
6	А	603[A]	HAS	C23-C24-C28-C29
6	А	603[B]	HAS	C23-C24-C28-C29
6	А	603[A]	HAS	CAD-CBD-CGD-O1D
7	В	201	OLC	C10-C11-C12-C13
7	А	604	OLC	C12-C13-C14-C15
6	А	603[B]	HAS	CAD-CBD-CGD-O1D
7	В	201	OLC	C12-C13-C14-C15
6	А	603[B]	HAS	CAA-CBA-CGA-O1A
7	С	101	OLC	C9-C10-C11-C12
6	А	603[A]	HAS	C3D-C2D-CMD-OMD
6	А	603[B]	HAS	CAD-CBD-CGD-O2D
6	А	603[A]	HAS	CAA-CBA-CGA-O1A
6	А	603[A]	HAS	CAA-CBA-CGA-O2A
7	С	101	OLC	C1-C2-C3-C4
6	А	603[A]	HAS	CAD-CBD-CGD-O2D
7	С	101	OLC	C5-C6-C7-C8
6	А	603[B]	HAS	CAA-CBA-CGA-O2A
7	А	610	OLC	C9-C10-C11-C12
7	А	609	OLC	O23-C22-C24-O25
7	A	607	OLC	O20-C1-C2-C3
7	A	606	OLC	O20-C1-C2-C3
7	A	604	OLC	C10-C11-C12-C13
7	С	103	OLC	C7-C8-C9-C10
7	A	604	OLC	C7-C8-C9-C10
7	C	101	OLC	C7-C8-C9-C10
7	A	609	OLC	C1-C2-C3-C4
7	A	610	$OL\overline{C}$	C7-C8-C9-C10
7	A	611	OLC	C7-C8-C9-C10
7	C	101	OLC	O20-C21-C22-C24
7	С	103	OLC	C3-C4-C5-C6
7	A	611	OLC	O20-C21-C22-O23

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Mol	Chain	Res	Type	Atoms
7	А	606	OLC	O19-C1-C2-C3
7	А	607	OLC	O19-C1-C2-C3
7	А	612	OLC	C15-C16-C17-C18
7	А	613	OLC	C14-C15-C16-C17
7	А	605	OLC	C5-C6-C7-C8
7	А	611	OLC	O23-C22-C24-O25
5	А	602	HEM	CAD-CBD-CGD-O1D

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There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	А	603[B]	HAS	3	0
5	А	602	HEM	2	0
6	А	603[A]	HAS	1	0
7	С	103	OLC	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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	554/569~(97%)	1.54	157 (28%) 0 0	26, 39, 65, 105	0
2	В	167/168~(99%)	1.19	29 (17%) 1 1	28, 39, 64, 109	0
3	С	31/34~(91%)	1.10	4 (12%) 3 3	33, 39, 49, 72	0
All	All	752/771~(97%)	1.44	190 (25%) 0 0	26, 39, 65, 109	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	2	VAL	15.0
1	А	331	GLY	6.9
1	А	495	ARG	6.8
2	В	3	ASP	6.6
1	А	333	PHE	6.3
1	А	515	PRO	5.8
2	В	5	HIS	5.8
1	А	496	GLU	5.6
1	А	494	SER	5.5
1	А	9	SER	5.2
1	А	519	ARG	5.2
1	А	175	PRO	5.1
1	А	241	LEU	4.8
1	А	172	ALA	4.7
1	А	389	VAL	4.7
1	А	240	LEU	4.7
1	А	235	ILE	4.7
1	А	518	ARG	4.6
2	В	76	PRO	4.5
1	A	393	VAL	4.5
1	А	11	VAL	4.5
1	A	176	GLY	4.4
1	А	57	ARG	4.4



Mol	Chain	Res	Type	RSRZ
1	А	54	LEU	4.4
1	А	551	GLY	4.3
1	А	133[A]	TYR	4.3
1	А	238	PHE	4.1
1	А	174	ASN	4.1
1	А	392	LEU	4.1
1	А	236	VAL	4.1
1	А	10	ARG	4.0
1	А	246	ILE	4.0
1	А	247	ILE	4.0
1	А	78	ILE	4.0
1	А	330	ARG	4.0
1	А	326	LEU	3.9
1	А	239	TRP	3.9
1	А	491	VAL	3.9
1	А	60	PRO	3.8
1	А	332	LEU	3.7
1	А	88	ILE	3.7
1	А	514	GLY	3.7
1	А	488	LEU	3.7
1	А	522	LEU	3.7
1	А	499	PRO	3.7
1	А	32	LEU	3.5
1	А	337	ARG	3.5
1	А	536	ILE	3.5
1	А	58	LEU	3.5
1	А	396	THR	3.4
1	A	500	GLU	3.4
1	A	244	TYR	3.3
1	А	385	PHE	3.3
1	A	492	LEU	3.3
1	А	124	LEU	3.3
1	А	504	ALA	3.2
1	А	486	TYR	3.2
1	А	513	SER	3.2
1	А	520	LEU	3.2
2	В	153	CYS	3.2
1	А	527	ILE	3.2
1	А	498	LYS	3.2
1	А	15	TYR	3.1
2	В	84	LEU	3.1
1	А	53	PRO	3.1



Mol	Chain	Res Type		RSRZ
1	А	552	HIS	3.1
1	А	404	LEU	3.1
1	А	353	LEU	3.1
1	А	381	VAL	3.1
1	А	217	GLU	3.1
1	А	245	ALA	3.1
1	А	501	LEU	3.1
2	В	168	GLU	3.1
1	А	493	LEU	3.0
1	А	548	GLN	3.0
1	А	98	ASN	3.0
1	А	132	LEU	3.0
2	В	90	TYR	3.0
1	A	25	LEU	3.0
1	A	69	LEU	3.0
1	А	497	ARG	2.9
1	A	517	ASP	2.9
1	А	533	VAL	2.9
1	А	334	GLY	2.9
2	В	85	ALA	2.9
1	А	329	GLY	2.9
2	В	75	GLY	2.9
1	А	415	ASP	2.9
1	А	516	GLU	2.9
1	А	328	GLY	2.9
1	А	77	ALA	2.9
2	В	112	VAL	2.8
3	С	11	VAL	2.8
1	А	173	ALA	2.8
1	A	307	VAL	2.8
1	A	269	PHE	2.8
2	В	39	THR	2.8
1	A	12	TYR	2.8
1	А	59	LEU	2.8
1	А	242	PRO	2.8
2	В	88	PHE	2.8
1	A	55	LEU	2.8
1	A	532	ALA	2.7
1	А	412	PRO	2.7
1	A	489	PHE	2.7
1	А	84	PHE	2.7
1	A	189	PHE	2.7



Mol	Chain	Res	Type	RSRZ
2	В	141	ARG	2.7
1	А	490	SER	2.7
1	А	92	LEU	2.7
1	А	237[A]	TYR	2.7
1	А	248	TYR	2.7
1	А	272	PHE	2.7
1	А	83	LEU	2.7
1	А	356	PHE	2.6
1	А	164	LEU	2.6
1	А	405	LEU	2.6
1	А	561	LEU	2.6
1	А	153	VAL	2.6
1	А	170	TRP	2.6
1	A	168	ARG	2.6
1	А	316	VAL	2.6
1	А	80	PHE	2.6
1	А	81	THR	2.6
1	А	305	VAL	2.5
2	В	152	TYR	2.5
1	А	503	GLU	2.5
1	А	134	THR	2.5
2	В	113	ILE	2.5
1	А	547	VAL	2.5
1	А	163	VAL	2.4
1	А	546	LEU	2.4
2	В	77	ASN	2.4
1	А	414	SER	2.4
1	А	243	ALA	2.4
1	А	271	LEU	2.4
3	C	12	ILE	2.4
1	A	139	LEU	2.4
1	А	395	LEU	2.4
1	А	549	LEU	2.3
2	В	140	LYS	2.3
1	A	259	LEU	2.3
1	A	152	PHE	2.3
1	A	303	LEU	2.3
1	A	208	LEU	2.3
1	А	411	LYS	2.3
1	А	506	LEU	2.3
1	А	193	TRP	2.3
1	А	388	GLN	2.3



Mol	Chain	Res	Type	RSRZ
2	В	11	ILE	2.3
1	А	325	ARG	2.3
1	А	413	ILE	2.3
1	А	181	LEU	2.2
2	В	74	THR	2.2
1	А	229	TRP	2.2
1	А	387	LEU	2.2
2	В	50	LEU	2.2
2	В	142	PRO	2.2
3	С	5	PRO	2.2
1	А	16	PRO	2.2
1	А	185	MET	2.2
1	А	324	GLY	2.2
2	В	107	ILE	2.1
1	А	79	VAL	2.1
1	А	364	ILE	2.1
1	А	75	LEU	2.1
3	С	15	LEU	2.1
1	А	178	VAL	2.1
1	А	29	PHE	2.1
1	А	135	PHE	2.1
2	В	86	PHE	2.1
1	А	308	PRO	2.1
1	А	406	PRO	2.1
1	А	417	GLN	2.1
1	А	264	MET	2.1
1	А	74	VAL	2.1
1	A	410	GLY	2.1
2	В	6	LYS	2.1
1	А	408	LEU	2.0
1	А	462	HIS	2.0
1	А	545	THR	2.0
2	В	127	VAL	2.0
1	А	228	PHE	2.0
1	А	33	ILE	2.0
1	А	219	VAL	2.0
2	В	40	HIS	2.0
2	В	87	ALA	2.0
2	В	123	ILE	2.0
1	A	279	VAL	2.0
1	А	526	ARG	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	$B-factors(Å^2)$	Q<0.9
7	OLC	A	607	15/25	0.23	0.37	76,92,106,110	0
7	OLC	С	101	24/25	0.42	0.27	58,67,97,100	0
7	OLC	С	102	15/25	0.42	0.32	66,88,97,99	0
7	OLC	В	202	25/25	0.55	0.23	66,70,94,101	0
7	OLC	А	608	18/25	0.56	0.23	57,71,93,93	0
7	OLC	А	609	15/25	0.57	0.20	78,85,90,91	0
7	OLC	А	611	21/25	0.62	0.25	60,82,94,108	0
7	OLC	А	610	20/25	0.62	0.20	71,81,90,101	0
7	OLC	А	606	17/25	0.63	0.22	67,76,87,96	0
7	OLC	А	605	18/25	0.64	0.25	60,77,91,106	0
7	OLC	А	613	9/25	0.65	0.23	66,70,75,76	0
7	OLC	В	201	20/25	0.67	0.17	77,85,95,102	0
7	OLC	С	103	24/25	0.69	0.23	67,80,103,110	0
5	HEM	А	602	43/43	0.76	0.26	27,29,32,41	0
7	OLC	А	604	23/25	0.78	0.16	49,58,92,94	0
6	HAS	А	603[A]	65/65	0.79	0.29	26,31,45,52	45
6	HAS	А	603[B]	65/65	0.79	0.29	27,45,52,62	45
7	OLC	А	612	9/25	0.83	0.13	67,71,82,84	0
8	CMO	А	614[A]	2/2	0.86	0.28	26,26,26,28	2
8	CMO	А	614[B]	2/2	0.86	0.28	35,35,35,43	2
9	CUA	В	203	2/2	0.99	0.10	33,33,33,34	0
4	CU	A	601[B]	1/1	1.00	0.13	46,46,46,46	1
4	CU	A	601[A]	1/1	1.00	0.13	30,30,30,30	1

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.

