

Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 06:23 PM JST

PDB ID	:	7D56
Title	:	Structure of the peptidylarginine deiminase type III (PAD3) in complex with
		Cl-amidine
Authors	:	Funabashi, K.; Unno, M.
Deposited on	:	2020-09-25
Resolution	:	3.17 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	:	2.36
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: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.17 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574(3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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	664	80%	15%	•••
1	В	664	6%	18%	•••
1	С	664	9%	18%	•••

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	GOL	А	712	-	-	-	Х



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14956 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	640	Total	С	Ν	0	\mathbf{S}	0	1	0	
	040	4968	3174	837	922	35	0	L		
1	1 D	635	Total	С	Ν	0	S	0	1	0
I B	055	4931	3149	836	912	34	0		0	
1 A	637	Total	С	Ν	0	S	0	1	0	
	037	4939	3155	833	916	35	0			

• Molecule 1 is a protein called Protein-arginine deiminase type-3.

• Molecule 2 is N-[(1S)-1-(AMINOCARBONYL)-4-(ETHANIMIDOYLAMINO)BUTYL]BEN ZAMIDE (three-letter code: BFB) (formula: $C_{14}H_{20}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	С	1	Total C N O 20 14 4 2	0	0
2	В	1	Total C N O 20 14 4 2	0	0



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	Δ	1	Total	С	Ν	0	0	0
	17	1 I	20	14	4	2	0	

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	С	5	Total Ca 5 5	0	0
3	В	5	Total Ca 5 5	0	0
3	А	5	Total Ca 5 5	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	4	Total Cl 4 4	0	0
4	В	4	Total Cl 4 4	0	0
4	А	4	Total Cl 4 4	0	0

• Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	С	6	Total O 6 6	0	0
7	В	4	Total O 4 4	0	0
7	A	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: Protein-arginine deiminase type-3

 \bullet Molecule 1: Protein-arginine deiminase type-3



I 428 L 429 SER 1456 2457 GLU V554 L555 • Molecule 1: Protein-arginine deiminase type-3 10% Chain A: 80% 15% • • N124 CYS GLU GLY ARG GLN ASP ASP ASP VAL C337 P338 GLN ALA GLU ASN ASN ASN ASP 3301 1313 1314 ASP ARG SER P435 G436 G436 S437 SER SER GLY GLY R441 R441 V442 404 7455 7456 457 GLU GLN VED T575 E576 R577 K578 K578 1596 1597 1597 0586 N661 M662 V663 P664 G647 Tero



4 Data and refinement statistics (i)

Property	Value	Source	
Space group	C 1 2 1	Depositor	
Cell constants	199.58Å 115.34Å 127.84Å	Deperitor	
a, b, c, α , β , γ	90.00° 121.38° 90.00°	Depositor	
$\mathbf{B}_{\mathrm{ascolution}}\left(\overset{\mathrm{A}}{\mathbf{\lambda}}\right)$	49.36 - 3.17	Depositor	
Resolution (A)	49.36 - 3.17	EDS	
% Data completeness	99.3 (49.36-3.17)	Depositor	
(in resolution range)	99.2(49.36-3.17)	EDS	
R_{merge}	0.06	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$2.36 (at 3.19 \text{\AA})$	Xtriage	
Refinement program	PHENIX 1.14_3260	Depositor	
B B.	0.242 , 0.297	Depositor	
$\mathbf{n}, \mathbf{n}_{free}$	0.244 , 0.297	DCC	
R_{free} test set	2087 reflections $(5.00%)$	wwPDB-VP	
Wilson B-factor (Å ²)	89.3	Xtriage	
Anisotropy	0.456	Xtriage	
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.33, 51.2	EDS	
L-test for $twinning^2$	$< L > = 0.51, < L^2 > = 0.35$	Xtriage	
	0.459 for 1/2 *h + 3/2 *k, 1/2 *h - 1/2 *k, -1/2 *h-		
Estimated twinning fraction	$1/2^{*}k^{-1}$	Xtriage	
0	0.460 for $1/2^{h-3}/2^{k}, -1/2^{h-1}/2^{k}, -1/2^{h}$	11011050	
E.E. correlation	+1/2 K-1	EDG	
$\frac{\Gamma_0, \Gamma_c \text{ contention}}{\text{Total number of stores}}$	14056		
Access D all stores (⁸ 2)	01.0		
Average B, all atoms (A^2)	91.0	WWPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.24% 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: CL, GOL, BFB, CA, EDO

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
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.25	0/5065	0.45	0/6897
1	В	0.25	0/5056	0.44	0/6881
1	С	0.25	0/5097	0.45	0/6944
All	All	0.25	0/15218	0.45	0/20722

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	4939	0	4757	60	0
1	В	4931	0	4763	70	0
1	С	4968	0	4782	71	0
2	А	20	0	17	2	0
2	В	20	0	17	1	0
2	С	20	0	18	0	0
3	А	5	0	0	0	0
3	В	5	0	0	0	0
3	С	5	0	0	0	0
4	A	4	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	В	4	0	0	0	0
4	С	4	0	0	1	0
5	А	4	0	6	0	0
5	С	8	0	12	0	0
6	А	6	0	8	0	0
7	А	3	0	0	0	0
7	В	4	0	0	0	0
7	С	6	0	0	1	0
All	All	14956	0	14380	200	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 7.

All (200) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A + 1	A + a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:339:GLN:HG2	1:C:341:GLU:H	1.45	0.81
1:B:218:GLY:H	1:B:225:ALA:HB1	1.48	0.77
1:C:188:GLN:HG2	1:C:245:ASP:HB2	1.73	0.69
1:A:52:ILE:HD11	1:A:74:LEU:HD13	1.75	0.67
1:C:346:ARG:N	1:C:375:GLU:OE2	2.30	0.65
1:B:207:ASP:HB3	1:B:265:ILE:HG23	1.80	0.64
1:C:574:LYS:HG3	1:C:583:PHE:HA	1.81	0.62
1:A:433:ASN:ND2	1:A:436:GLY:O	2.33	0.62
1:C:313:VAL:HG12	1:C:316:ASN:HB2	1.82	0.62
1:B:152:VAL:O	1:B:166:ASN:ND2	2.33	0.61
1:C:385:LEU:HA	1:C:389:PHE:HB3	1.82	0.61
1:B:52:ILE:HD11	1:B:74:LEU:HD13	1.82	0.61
1:A:482:ASP:OD2	1:A:487:ARG:NH2	2.35	0.60
1:B:151:LEU:HD21	1:B:359:ALA:HB2	1.83	0.60
1:A:512:LEU:HB3	1:A:525:THR:HG22	1.82	0.60
1:C:512:LEU:HB3	1:C:525:THR:HG22	1.84	0.59
1:A:577:ARG:HG2	1:A:579:LYS:H	1.67	0.59
1:C:69:ARG:NH1	7:C:801:HOH:O	2.35	0.59
1:C:216:ILE:HD11	1:C:219:PRO:HA	1.83	0.59
1:B:512:LEU:HB3	1:B:525:THR:HG22	1.83	0.59
1:C:151:LEU:HD21	1:C:359:ALA:HB2	1.83	0.59
1:A:385:LEU:HA	1:A:389:PHE:HB3	1.85	0.58
1:B:385:LEU:HA	1:B:389:PHE:HB3	1.85	0.58
1:A:468:VAL:HG21	2:A:701:BFB:HAN2	1.86	0.58
1:C:27:VAL:HB	1:C:76:ILE:HG13	1.86	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:482:ASP:OD2	1:C:487:ARG:NH2	2.38	0.57
1:C:52:ILE:HD11	1:C:74:LEU:HD13	1.84	0.57
1:A:347:TRP:CE2	2:A:701:BFB:HAO1	2.40	0.56
1:B:346:ARG:N	1:B:375:GLU:OE2	2.39	0.56
1:B:597:LEU:HD12	1:B:628:CYS:HA	1.88	0.56
1:B:283:PRO:HG3	1:A:435:PRO:HG3	1.88	0.55
1:A:574:LYS:HG3	1:A:583:PHE:HA	1.89	0.55
1:B:27:VAL:HB	1:B:76:ILE:HG13	1.89	0.54
1:A:27:VAL:HB	1:A:76:ILE:HG13	1.88	0.54
1:B:349:GLN:NE2	1:B:349:GLN:O	2.41	0.54
1:B:468:VAL:HG21	2:B:701:BFB:HAO1	1.90	0.54
1:B:482:ASP:OD2	1:B:487:ARG:NH2	2.39	0.54
1:A:152:VAL:O	1:A:166:ASN:ND2	2.41	0.53
1:B:574:LYS:HG3	1:B:583:PHE:HA	1.90	0.53
1:A:575:THR:OG1	1:A:577:ARG:O	2.27	0.53
1:C:455:VAL:HG13	1:C:456:GLN:HG3	1.91	0.52
1:A:121:CYS:SG	1:A:122:ASP:N	2.82	0.52
1:A:441:ARG:HH12	1:A:447:ARG:NH1	2.07	0.52
1:A:151:LEU:HD21	1:A:359:ALA:HB2	1.90	0.52
1:A:455:VAL:HG13	1:A:456:GLN:HG3	1.91	0.52
1:C:575:THR:OG1	1:C:577:ARG:O	2.28	0.52
1:B:550:TRP:O	1:B:553[B]:GLU:HG2	2.10	0.52
1:B:455:VAL:HG13	1:B:456:GLN:HG3	1.92	0.51
1:A:308:VAL:HG21	1:A:593:LEU:HD21	1.93	0.51
1:B:537:LEU:O	1:B:541:ASN:ND2	2.41	0.50
1:B:329:LYS:HB3	1:B:596:HIS:CE1	2.46	0.50
1:A:115:VAL:HG22	1:A:117:ILE:HG13	1.93	0.50
1:B:196:ASP:OD1	1:B:275:SER:HB2	2.12	0.50
1:B:216:ILE:HD11	1:B:219:PRO:HA	1.94	0.50
1:A:15:THR:HB	1:A:110:LEU:HD12	1.93	0.50
1:A:432:GLY:HA3	1:A:441:ARG:HD3	1.93	0.50
1:A:550:TRP:O	1:A:553[B]:GLU:HG2	2.11	0.50
1:C:120:ASP:HB3	1:C:123:LEU:HD11	1.93	0.50
1:C:271:LEU:HD23	1:C:284:ILE:HD11	1.94	0.50
1:B:466:LEU:HB2	1:B:469:GLY:HA2	1.93	0.49
1:C:409:ASN:HA	1:C:471:VAL:H	1.77	0.49
1:B:18:VAL:HG22	1:B:113:THR:HB	1.94	0.49
1:B:378:ASP:O	1:B:382:LYS:HB2	2.12	0.49
1:B:222:VAL:HG22	1:B:225:ALA:H	1.77	0.49
1:C:407:PHE:HA	1:C:410:LEU:HB3	1.94	0.49
1:C:121:CYS:SG	1:C:122:ASP:N	2.86	0.49



		Interatomic	Clash
Atom-1	Atom-1 Atom-2		overlap (Å)
1:B:121:CYS:SG	1:B:122:ASP:N	2.86	0.48
1:B:493:PRO:HB3	1:B:541:ASN:HB3	1.95	0.48
1:B:575:THR:OG1	1:B:577:ARG:O	2.31	0.48
1:C:600:PRO:HG3	1:C:644:VAL:HG12	1.96	0.48
1:C:493:PRO:HB3	1:C:541:ASN:HB3	1.94	0.48
1:A:58:ARG:HD3	1:A:58:ARG:HA	1.68	0.48
1:A:586:ASP:HB3	1:A:643:GLU:HG3	1.96	0.48
1:C:58:ARG:HD3	1:C:58:ARG:HA	1.64	0.47
1:B:367:VAL:HB	1:B:389:PHE:HE1	1.79	0.47
1:B:597:LEU:HD13	1:B:599:ILE:HD11	1.96	0.47
1:A:466:LEU:HB2	1:A:469:GLY:HA2	1.96	0.47
1:C:313:VAL:HG13	1:C:315:ASN:H	1.79	0.47
1:C:586:ASP:HB3	1:C:643:GLU:HG3	1.96	0.47
1:B:115:VAL:HG22	1:B:117:ILE:HG13	1.95	0.47
1:A:6:ILE:HG12	1:A:26:LEU:HB2	1.97	0.47
1:C:313:VAL:HG22	1:C:314:ARG:H	1.79	0.47
1:C:488:MET:SD	1:C:555:LEU:HD23	2.55	0.47
1:C:215:HIS:HE1	1:C:247:GLU:HB3	1.79	0.47
1:C:378:ASP:O	1:C:382:LYS:HB2	2.15	0.47
1:C:603:PHE:HD2	1:C:634:PHE:HD2	1.62	0.47
1:A:537:LEU:O	1:A:541:ASN:ND2	2.44	0.47
1:C:316:ASN:OD1	1:C:319:PHE:HB3	2.15	0.46
1:C:537:LEU:O	1:C:541:ASN:ND2	2.43	0.46
1:C:213:VAL:HB	1:C:230:LEU:HB2	1.96	0.46
1:B:577:ARG:HG2	1:B:579:LYS:H	1.79	0.46
1:C:622:GLU:N	1:C:623:PRO:HD2	2.30	0.46
1:A:597:LEU:HD13	1:A:599:ILE:HD11	1.96	0.46
1:B:385:LEU:H	1:B:385:LEU:HD23	1.81	0.46
1:A:329:LYS:HB3	1:A:596:HIS:CE1	2.50	0.46
1:C:466:LEU:HB2	1:C:469:GLY:HA2	1.96	0.46
1:B:492:SER:OG	1:B:545:GLN:OE1	2.30	0.46
1:A:589:ASN:OD1	1:A:643:GLU:HB2	2.16	0.46
1:B:429:LEU:HD13	1:B:475:LEU:HD21	1.98	0.46
1:B:58:ARG:HD3	1:B:58:ARG:HA	1.65	0.45
1:C:370:SER:OG	1:C:406:SER:HB3	2.15	0.45
1:C:199:LEU:HD23	1:C:239:VAL:HB	1.98	0.45
1:C:232:GLN:OE1	1:C:232:GLN:N	2.46	0.45
1:C:385:LEU:H	1:C:385:LEU:HD23	1.81	0.45
1:A:409:ASN:OD1	1:A:471:VAL:HG23	2.17	0.45
1:C:215:HIS:CE1	1:C:247:GLU:HB3	2.51	0.45
1:C:308:VAL:HG21	1:C:593:LEU:HD21	1.97	0.45



	h + O	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:600:PRO:HG3	1:B:644:VAL:HG12	1.98	0.45	
1:A:622:GLU:N	1:A:623:PRO:HD2	2.31	0.45	
1:B:488:MET:SD	1:B:555:LEU:HD23	2.57	0.45	
1:A:185:LEU:HD21	1:A:199:LEU:HD21	1.97	0.45	
1:A:493:PRO:HB3	1:A:541:ASN:HB3	1.99	0.45	
1:C:115:VAL:HG22	1:C:117:ILE:HG13	1.97	0.45	
1:A:301:SER:HA	1:A:652:ARG:NE	2.32	0.45	
1:A:421:LYS:HB3	1:A:421:LYS:HE3	1.68	0.45	
1:A:488:MET:SD	1:A:555:LEU:HD23	2.57	0.45	
1:A:600:PRO:HG3	1:A:644:VAL:HG12	1.98	0.45	
1:B:622:GLU:N	1:B:623:PRO:HD2	2.31	0.45	
1:A:487:ARG:HG2	1:A:567:ILE:HD13	1.99	0.45	
1:B:251:VAL:HG21	1:B:267:PHE:HE2	1.82	0.45	
1:B:334:LEU:HG	1:B:336:ILE:HD11	1.98	0.45	
1:B:301:SER:HA	1:B:652:ARG:NE	2.31	0.44	
1:B:325:GLU:O	1:B:329:LYS:NZ	2.24	0.44	
1:B:603:PHE:HD2	1:B:634:PHE:HD2	1.65	0.44	
1:C:301:SER:HA	1:C:652:ARG:NE	2.32	0.44	
1:C:152:VAL:O	1:C:166:ASN:ND2	2.45	0.44	
1:C:409:ASN:OD1	1:C:471:VAL:HG23	2.17	0.44	
1:C:492:SER:OG	1:C:545:GLN:OE1	2.28	0.44	
1:B:599:ILE:O	1:B:630:PHE:HA	2.17	0.44	
1:B:266:SER:HB3	1:B:268:HIS:CE1	2.52	0.44	
1:B:409:ASN:HA	1:B:471:VAL:H	1.82	0.44	
1:C:203:THR:HB	1:C:267:PHE:HD1	1.82	0.44	
1:C:274:ASP:HA	1:C:281:ALA:HA	1.99	0.43	
1:B:347:TRP:CZ3	1:B:642:GLY:HA3	2.53	0.43	
1:B:26:LEU:HD23	1:B:77:ILE:HG13	1.99	0.43	
1:A:603:PHE:HD2	1:A:634:PHE:HD2	1.66	0.43	
1:C:434:LEU:HB3	1:C:435:PRO:HD3	2.00	0.43	
1:C:491:ALA:O	1:C:548:ILE:HG21	2.18	0.43	
1:C:339:GLN:HG2	1:C:341:GLU:N	2.24	0.43	
1:A:251:VAL:HG21	1:A:267:PHE:HE2	1.84	0.43	
1:A:491:ALA:O	1:A:548:ILE:HG21	2.18	0.43	
1:B:271:LEU:HD23	1:B:284:ILE:HD11	2.01	0.43	
1:B:423:TYR:HE2	1:B:457:PRO:HG2	1.83	0.43	
1:A:347:TRP:CZ3	1:A:642:GLY:HA3	2.53	0.43	
1:B:213:VAL:HB	1:B:230:LEU:HB2	2.00	0.43	
1:B:313:VAL:HG22	1:B:314:ARG:H	1.83	0.43	
1:B:475:LEU:HD22	1:B:555:LEU:HD21	2.01	0.43	
1:A:215:HIS:HE1	1:A:247:GLU:HB3	1.83	0.43	



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:347:TRP:CZ3	1:C:642:GLY:HA3	2.54	0.42
1:A:334:LEU:HG	1:A:336:ILE:HD11	2.01	0.42
1:C:154:CYS:HB3	1:C:391:TYR:H	1.83	0.42
1:A:358:GLN:HA	1:A:363:THR:HB	2.01	0.42
1:C:187:THR:HG21	1:C:199:LEU:HD21	2.00	0.42
1:B:384:ILE:HD12	1:B:384:ILE:HA	1.83	0.42
1:A:385:LEU:HD23	1:A:385:LEU:H	1.84	0.42
1:B:203:THR:HB	1:B:267:PHE:HD1	1.84	0.42
1:B:266:SER:HB3	1:B:268:HIS:HE1	1.84	0.42
1:C:367:VAL:HB	1:C:389:PHE:HE1	1.84	0.42
1:C:423:TYR:HE2	1:C:457:PRO:HG2	1.85	0.42
1:B:409:ASN:OD1	1:B:471:VAL:HG23	2.19	0.42
1:A:140:VAL:HG23	1:A:145:GLY:HA2	2.02	0.42
1:B:309:TYR:O	1:B:648:THR:HA	2.20	0.42
1:B:379:PHE:HB3	1:B:380:PRO:HD3	2.02	0.42
1:B:224:GLU:H	1:B:224:GLU:HG2	1.53	0.42
1:B:484:LYS:HE2	1:B:565:ASP:OD2	2.19	0.42
1:A:313:VAL:HG22	1:A:314:ARG:H	1.84	0.42
1:A:442:VAL:HG13	1:A:447:ARG:HG3	2.01	0.42
1:C:100:HIS:HB3	1:C:101:GLU:OE1	2.20	0.42
1:C:429:LEU:HD13	1:C:475:LEU:HD21	2.02	0.42
1:B:298:MET:HE1	1:B:428:ILE:HG12	2.02	0.42
1:B:586:ASP:HB3	1:B:643:GLU:HG3	2.02	0.42
1:A:26:LEU:HD23	1:A:77:ILE:HG13	2.02	0.42
1:C:218:GLY:HA2	1:C:219:PRO:HD3	1.81	0.41
1:B:20:VAL:HG21	1:B:285:PHE:CG	2.55	0.41
1:A:203:THR:HB	1:A:267:PHE:HD1	1.85	0.41
1:A:154:CYS:HB3	1:A:391:TYR:H	1.85	0.41
1:A:409:ASN:HA	1:A:471:VAL:H	1.85	0.41
1:C:7:VAL:HG13	4:C:707:CL:CL	2.57	0.41
1:C:26:LEU:HD23	1:C:77:ILE:HG13	2.02	0.41
1:A:218:GLY:HA2	1:A:219:PRO:HD3	1.76	0.41
1:C:394:ARG:HA	1:C:394:ARG:HD3	1.94	0.41
1:C:163:VAL:HG12	1:C:164:GLN:H	1.86	0.41
1:C:274:ASP:HB3	1:C:281:ALA:HB2	2.01	0.41
1:B:199:LEU:HD23	1:B:239:VAL:HB	2.03	0.41
1:C:578:LYS:HE2	1:C:578:LYS:HB3	1.91	0.41
1:C:607:ILE:H	1:C:607:ILE:HG13	1.69	0.41
1:B:589:ASN:OD1	1:B:643:GLU:HB2	2.21	0.41
1:B:659:TRP:O	1:B:662:MET:HB2	2.21	0.41
1:A:329:LYS:HZ2	1:A:329:LYS:N	2.19	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:GLN:HA	1:C:363:THR:HB	2.03	0.41
1:C:597:LEU:HD13	1:C:599:ILE:HD11	2.03	0.41
1:C:309:TYR:CE2	1:C:384:ILE:HD11	2.56	0.40
1:C:329:LYS:HB3	1:C:596:HIS:CE1	2.55	0.40
1:B:100:HIS:HB3	1:B:101:GLU:OE1	2.20	0.40
1:A:359:ALA:H	1:A:363:THR:HG22	1.85	0.40
1:A:423:TYR:HE2	1:A:457:PRO:HG2	1.86	0.40
1:C:526:ILE:HD13	1:C:583:PHE:CZ	2.56	0.40
1:B:457:PRO:HA	1:B:458:PRO:HD3	1.93	0.40
1:A:199:LEU:HD23	1:A:239:VAL:HB	2.02	0.40
1:A:213:VAL:HB	1:A:230:LEU:HB2	2.02	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	622/664~(94%)	586 (94%)	36~(6%)	0	100	100
1	В	620/664~(93%)	583 (94%)	37~(6%)	0	100	100
1	С	629/664~(95%)	586~(93%)	43 (7%)	0	100	100
All	All	1871/1992~(94%)	1755 (94%)	116 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was



Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	543/588~(92%)	524 (96%)	19 (4%)	36	68	
1	В	542/588~(92%)	522 (96%)	20 (4%)	34	67	
1	С	545/588~(93%)	524 (96%)	21 (4%)	32	65	
All	All	1630/1764~(92%)	1570 (96%)	60 (4%)	34	67	

analysed, and the total number of residues.

All (60) residues with a non-rotameric sidechain are listed below:

\mathbf{Mol}	Chain	\mathbf{Res}	Type
1	С	25	THR
1	С	35	GLU
1	С	69	ARG
1	С	86	ASP
1	С	110	LEU
1	С	139	TRP
1	С	163	VAL
1	С	258	ASP
1	С	265	ILE
1	С	314	ARG
1	С	329	LYS
1	С	372	ARG
1	С	381	TYR
1	С	389	PHE
1	С	521	GLU
1	С	577	ARG
1	С	593	LEU
1	С	597	LEU
1	С	634	PHE
1	С	635	THR
1	С	663	VAL
1	В	15	THR
1	В	69	ARG
1	В	86	ASP
1	В	110	LEU
1	В	139	TRP
1	В	222	VAL
1	В	224	GLU
1	В	329	LYS
1	В	349	GLN
1	В	372	ARG
1	В	389	PHE



Mol	Chain	Res	Type
1	В	397	ARG
1	В	401	VAL
1	В	404	LEU
1	В	441	ARG
1	В	577	ARG
1	В	593	LEU
1	В	597	LEU
1	В	634	PHE
1	В	635	THR
1	А	35	GLU
1	А	69	ARG
1	А	86	ASP
1	А	110	LEU
1	А	139	TRP
1	А	173	CYS
1	А	222	VAL
1	А	317	THR
1	А	329	LYS
1	А	372	ARG
1	А	389	PHE
1	А	404	LEU
1	А	421	LYS
1	A	440	ARG
1	А	441	ARG
1	А	577	ARG
1	А	597	LEU
1	А	634	PHE
1	А	635	THR

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:

Mol	Chain	Res	Type
1	С	268	HIS
1	А	268	HIS

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 34 ligands modelled in this entry, 27 are monoatomic - leaving 7 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	Mol Type Chain	nain Ros Lini		Bond lengths			Bond angles			
INIOI	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	А	712	-	$5,\!5,\!5$	0.96	0	$5,\!5,\!5$	0.90	0
2	BFB	А	701	1	20,20,20	2.20	5 (25%)	$22,\!25,\!25$	1.36	3 (13%)
5	EDO	A	711	-	3,3,3	0.49	0	2,2,2	0.26	0
5	EDO	C	712	-	3,3,3	0.46	0	2,2,2	0.34	0
2	BFB	В	701	1	20,20,20	2.18	5 (25%)	$22,\!25,\!25$	1.82	4 (18%)
5	EDO	С	711	-	3,3,3	0.47	0	2,2,2	0.30	0
2	BFB	С	701	1	20,20,20	2.19	5 (25%)	22,25,25	1.36	1 (4%)

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
6	GOL	А	712	-	-	0/4/4/4	-
2	BFB	А	701	1	-	6/18/19/19	0/1/1/1
5	EDO	А	711	-	-	0/1/1/1	-
5	EDO	С	712	-	-	0/1/1/1	-
2	BFB	В	701	1	-	6/18/19/19	0/1/1/1
5	EDO	С	711	-	-	0/1/1/1	-
2	BFB	С	701	1	-	8/18/19/19	0/1/1/1



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	701	BFB	CAW-NAS	5.41	1.45	1.34
2	С	701	BFB	CAW-NAS	5.29	1.45	1.34
2	В	701	BFB	CAW-NAS	5.28	1.45	1.34
2	С	701	BFB	CAV-NAR	5.12	1.46	1.35
2	А	701	BFB	CAV-NAR	5.10	1.46	1.35
2	В	701	BFB	CAV-NAR	5.04	1.45	1.35
2	С	701	BFB	CAU-NAA	5.01	1.45	1.32
2	В	701	BFB	CAU-NAA	5.00	1.45	1.32
2	А	701	BFB	CAU-NAA	5.00	1.45	1.32
2	В	701	BFB	OAE-CAU	-2.57	1.18	1.23
2	А	701	BFB	OAE-CAU	-2.57	1.18	1.23
2	С	701	BFB	OAE-CAU	-2.55	1.19	1.23
2	С	701	BFB	OAF-CAW	-2.20	1.18	1.23
2	А	701	BFB	OAF-CAW	-2.19	1.18	1.23
2	В	701	BFB	OAF-CAW	-2.17	1.18	1.23

All (15) bond length outliers are listed below:

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	701	BFB	CAP-CAV-NAR	6.19	122.17	114.24
2	С	701	BFB	CAP-CAV-NAR	4.95	120.58	114.24
2	А	701	BFB	CAP-CAV-NAR	4.50	120.01	114.24
2	В	701	BFB	CAX-CAW-NAS	2.48	121.83	117.06
2	В	701	BFB	CAO-CAZ-CAU	-2.37	104.72	110.21
2	А	701	BFB	CAX-CAW-NAS	2.17	121.22	117.06
2	А	701	BFB	CAZ-CAU-NAA	2.10	120.28	116.69
2	В	701	BFB	CAZ-NAS-CAW	-2.03	116.63	121.60

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	С	701	BFB	CAM-CAO-CAZ-CAU
2	С	701	BFB	CAM-CAO-CAZ-NAS
2	В	701	BFB	CAM-CAO-CAZ-CAU
2	В	701	BFB	CAM-CAO-CAZ-NAS
2	С	701	BFB	NAS-CAW-CAX-CAL
2	С	701	BFB	OAF-CAW-CAX-CAL
2	В	701	BFB	NAS-CAW-CAX-CAL
2	В	701	BFB	OAF-CAW-CAX-CAK
2	В	701	BFB	OAF-CAW-CAX-CAL



Mol	Chain	Res	Type	Atoms
2	С	701	BFB	OAF-CAW-CAX-CAK
2	В	701	BFB	NAS-CAW-CAX-CAK
2	А	701	BFB	OAF-CAW-CAX-CAL
2	С	701	BFB	NAS-CAW-CAX-CAK
2	А	701	BFB	NAS-CAW-CAX-CAK
2	А	701	BFB	NAS-CAW-CAX-CAL
2	А	701	BFB	OAF-CAW-CAX-CAK
2	А	701	BFB	CAO-CAM-CAN-NAR
2	С	701	BFB	CAO-CAM-CAN-NAR
2	А	701	BFB	CAN-CAM-CAO-CAZ
2	С	701	BFB	CAN-CAM-CAO-CAZ

Continued from previous page...

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	701	BFB	2	0
2	В	701	BFB	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	637/664~(95%)	0.64	65 (10%) 6 3	47, 87, 142, 189	0
1	В	635/664~(95%)	0.55	37 (5%) 23 12	49, 88, 137, 176	0
1	С	640/664~(96%)	0.62	58 (9%) 9 5	48, 87, 140, 185	0
All	All	1912/1992~(95%)	0.60	160 (8%) 11 6	47, 88, 140, 189	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	628	CYS	6.6
1	А	200	VAL	6.4
1	В	17	ALA	5.8
1	В	664	PRO	5.8
1	С	326	LEU	5.7
1	В	599	ILE	5.7
1	В	239	VAL	5.5
1	В	598	GLY	5.3
1	С	322	ALA	5.2
1	А	463	VAL	5.0
1	В	561	LEU	5.0
1	А	359	ALA	4.8
1	А	154	CYS	4.8
1	А	655	PHE	4.8
1	С	551	ASN	4.7
1	В	154	CYS	4.7
1	В	53	SER	4.7
1	С	190	PRO	4.6
1	А	358	GLN	4.5
1	С	136	LYS	4.4
1	С	525	THR	4.3
1	А	134	VAL	4.3
1	С	489	LEU	4.3



Mol	Chain	Res	Type	RSRZ
1	А	188	GLN	4.2
1	В	560	GLY	4.1
1	А	326	LEU	4.1
1	С	139	TRP	4.0
1	А	647	GLY	4.0
1	С	475	LEU	3.8
1	С	597	LEU	3.8
1	С	334	LEU	3.5
1	А	311	CYS	3.5
1	С	249	PHE	3.5
1	В	392	VAL	3.5
1	А	198	LYS	3.4
1	С	268	HIS	3.4
1	С	135	ASP	3.3
1	А	374	GLY	3.3
1	В	211	ALA	3.2
1	А	319	PHE	3.2
1	В	18	VAL	3.2
1	А	184	VAL	3.2
1	А	559	LEU	3.2
1	С	335	THR	3.2
1	А	118	SER	3.1
1	С	554	VAL	3.0
1	В	597	LEU	3.0
1	А	364	LEU	3.0
1	А	553[A]	GLU	3.0
1	В	229	VAL	3.0
1	В	275	SER	3.0
1	A	270	THR	3.0
1	A	199	LEU	3.0
1	C	542	LYS	3.0
1	B	219	PRO	3.0
1	С	567	ILE	2.9
1	В	593	LEU	2.9
1	А	624	LEU	2.9
1	A	412	VAL	2.9
1	A	516	GLY	2.9
1	A	310	VAL	2.9
1	A	362	LYS	2.9
1	С	143	PRO	2.8
1	A	376	LEU	2.8
1	В	212	GLN	2.8



Mol	Chain	Res	Type	RSRZ
1	С	541	541 ASN	
1	С	407	407 PHE	
1	А	115	VAL	2.8
1	А	612	CYS	2.8
1	А	588	VAL	2.8
1	А	298	MET	2.7
1	А	225	ALA	2.7
1	С	355	GLY	2.7
1	А	254	LEU	2.6
1	С	351	GLU	2.6
1	С	173	CYS	2.6
1	С	358	GLN	2.6
1	А	635	THR	2.6
1	В	662	MET	2.6
1	C	187	THR	2.6
1	А	309	TYR	2.6
1	В	609	GLY	2.6
1	А	172	HIS	2.6
1	С	619	SER	2.6
1	А	396	PRO	2.6
1	В	250	PHE	2.5
1	А	431	GLY	2.5
1	А	177	LEU	2.5
1	В	319	PHE	2.5
1	С	161	CYS	2.5
1	С	553[A]	GLU	2.5
1	С	524	LYS	2.5
1	В	230	LEU	2.5
1	A	578	LYS	2.5
1	В	4	GLN	2.5
1	В	657	PHE	2.5
1	В	391	TYR	2.5
1	B	155	ASP	2.5
1	С	661	ASN	2.4
1	A	664	PRO	2.4
1	C	367	VAL	2.4
1	A	661	ASN	2.4
1	С	490	LEU	2.4
1	A	658	LYS	2.4
1	A	603	PHE	2.4
1	С	324	ALA	2.4
1	A	626	LEU	2.4



Mol	Chain	Res	Type	RSRZ
1	С	182	VAL	2.4
1	С	189	GLY	2.3
1	С	630	PHE	2.3
1	С	528	ILE	2.3
1	В	610	CYS	2.3
1	С	356	TYR	2.3
1	А	637	TYR	2.3
1	А	430	ILE	2.3
1	В	354	LEU	2.3
1	С	462	PHE	2.3
1	С	488	MET	2.3
1	А	144	SER	2.3
1	В	6	ILE	2.3
1	А	297	ILE	2.3
1	С	250	PHE	2.3
1	В	379	PHE	2.3
1	A	459	VAL	2.3
1	С	285	PHE	2.3
1	С	381	TYR	2.2
1	А	555	LEU	2.2
1	А	187	THR	2.2
1	А	1	MET	2.2
1	С	596	HIS	2.2
1	С	517 VAL		2.2
1	А	636	PRO	2.2
1	С	321	ASP	2.2
1	A	441	ARG	2.2
1	А	9	VAL	2.2
1	А	235	VAL	2.2
1	С	425	LEU	2.2
1	В	397	ARG	2.2
1	A	186	ARG	2.2
1	В	52	ILE	2.1
1	A	307	GLU	2.1
1	А	662	MET	2.1
1	A	500	PHE	2.1
1	В	140	VAL	2.1
1	С	288	THR	2.1
1	A	121	CYS	2.1
1	C	310	VAL	2.1
1	C	617	VAL	2.1
1	А	201	LEU	2.1



Mol	Chain	Res	Type	RSRZ
1	В	523	VAL	2.1
1	С	364	LEU	2.1
1	А	648	THR	2.1
1	С	269	VAL	2.1
1	С	160	SER	2.1
1	С	591	LEU	2.0
1	С	476	SER	2.0
1	В	313	VAL	2.0
1	C	214	PHE	2.0
1	В	562	ALA	2.0
1	А	253	GLY	2.0

Continued from previous page...

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	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
6	GOL	А	712	6/6	0.44	0.48	92,99,101,103	0
4	CL	В	708	1/1	0.51	0.23	106,106,106,106	0
4	CL	В	710	1/1	0.55	0.29	97,97,97,97	0
4	CL	А	708	1/1	0.63	0.24	102,102,102,102	0
4	CL	С	710	1/1	0.69	0.29	100,100,100,100	0
4	CL	А	709	1/1	0.71	0.18	91,91,91,91	0
5	EDO	А	711	4/4	0.76	0.30	80,82,86,86	0
4	CL	А	710	1/1	0.78	0.38	84,84,84,84	0
4	CL	В	709	1/1	0.79	0.23	80,80,80,80	0
4	CL	С	709	1/1	0.80	0.37	88,88,88,88	0
4	CL	А	707	1/1	0.82	0.54	80,80,80,80	0
2	BFB	С	701	20/20	0.82	0.43	84,92,101,102	0



7D56

			Der	^ + ~	Deco	DCD	\mathbf{D} for the matrix $\begin{pmatrix} \mathbf{A} \\ \mathbf{A} \end{pmatrix}$	O < 0.0
IVIOI	Type	Chain	Res	Atoms	RSCC	RSR	$B-Iactors(A^2)$	Q<0.9
4	CL	C	707	1/1	0.84	0.47	$83,\!83,\!83,\!83$	0
2	BFB	А	701	20/20	0.84	0.29	$83,\!91,\!103,\!103$	0
3	CA	В	705	1/1	0.84	0.10	84,84,84,84	0
2	BFB	В	701	20/20	0.86	0.39	87,100,113,119	0
3	CA	В	702	1/1	0.87	0.20	60,60,60,60	0
5	EDO	С	711	4/4	0.87	0.38	61,64,65,67	0
4	CL	В	707	1/1	0.88	0.26	87,87,87,87	0
3	CA	В	706	1/1	0.89	0.12	94,94,94,94	0
3	CA	В	704	1/1	0.90	0.11	87,87,87,87	0
3	CA	С	703	1/1	0.91	0.08	84,84,84,84	0
3	CA	А	703	1/1	0.92	0.19	81,81,81,81	0
3	CA	А	704	1/1	0.92	0.23	79,79,79,79	0
5	EDO	С	712	4/4	0.93	0.22	$53,\!53,\!53,\!54$	0
3	CA	А	705	1/1	0.94	0.12	76, 76, 76, 76, 76	0
4	CL	С	708	1/1	0.94	0.14	81,81,81,81	0
3	CA	В	703	1/1	0.96	0.07	$77,\!77,\!77,\!77$	0
3	CA	С	704	1/1	0.96	0.06	83,83,83,83	0
3	CA	А	702	1/1	0.96	0.17	$59,\!59,\!59,\!59$	0
3	CA	А	706	1/1	0.96	0.20	82,82,82,82	0
3	CA	C	706	1/1	0.97	0.19	85,85,85,85	0
3	CA	С	705	1/1	0.98	0.08	82,82,82,82	0
3	CA	С	702	1/1	0.98	0.17	$6\overline{4,}64,\!64,\!64$	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.

