

Full wwPDB X-ray Structure Validation Report (i)

Sep 13, 2023 - 11:30 am BST

PDB ID	:	80KV
Title	:	lipoprotein BT2095 from Bacteroides thetaiotamicron bound to cyanocobal-
		amin CnCbl
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Deposited on	:	2023-03-29
Resolution	:	2.60 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 (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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.



Motric	Whole archive	Similar resolution
IVIETIC	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	333	85%	11%	•••
1	В	333	87%	10%	•••
1	С	333	84%	13%	•••
1	D	333	83%	12%	•••



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
2	CNC	А	401	X	-	-	-
2	CNC	В	401	Х	-	-	-
2	CNC	С	401	Х	-	-	-
2	CNC	D	401	Х	-	-	-



$80 \mathrm{KV}$

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 21033 atoms, of which 9944 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	р	220	Total	С	Η	Ν	0	\mathbf{S}	0	0	0
	D	550	5138	1739	2435	440	511	13	0	0	0
1	Δ	201	Total	С	Н	Ν	0	S	0	0	0
1	1 A	321	4992	1686	2373	418	502	13	0	0	0
1	C	327	Total	С	Η	Ν	0	S	0	0	0
1			5090	1721	2417	431	508	13		0	0
1	1 D	322	Total	С	Η	Ν	0	S	0	0	0
			5003	1689	2379	419	503	13	0	U	U

• Molecule 1 is a protein called Putative surface layer protein.

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	23	MET	-	initiating methionine	UNP Q8A5Z1
В	24	GLY	-	expression tag	UNP Q8A5Z1
В	25	HIS	-	expression tag	UNP Q8A5Z1
В	26	HIS	-	expression tag	UNP Q8A5Z1
В	27	HIS	-	expression tag	UNP Q8A5Z1
В	28	HIS	-	expression tag	UNP Q8A5Z1
В	29	HIS	-	expression tag	UNP Q8A5Z1
В	30	HIS	-	expression tag	UNP Q8A5Z1
А	23	MET	-	initiating methionine	UNP Q8A5Z1
А	24	GLY	-	expression tag	UNP Q8A5Z1
А	25	HIS	-	expression tag	UNP Q8A5Z1
А	26	HIS	-	expression tag	UNP Q8A5Z1
А	27	HIS	-	expression tag	UNP Q8A5Z1
А	28	HIS	-	expression tag	UNP Q8A5Z1
А	29	HIS	-	expression tag	UNP Q8A5Z1
А	30	HIS	-	expression tag	UNP Q8A5Z1
С	23	MET	-	initiating methionine	UNP Q8A5Z1
С	24	GLY	-	expression tag	UNP Q8A5Z1
С	25	HIS	-	expression tag	UNP Q8A5Z1
С	26	HIS	-	expression tag	UNP Q8A5Z1
С	27	HIS	-	expression tag	UNP Q8A5Z1



Chain	Residue	Modelled	Actual	Comment	Reference
С	28	HIS	-	expression tag	UNP Q8A5Z1
С	29	HIS	-	expression tag	UNP Q8A5Z1
С	30	HIS	-	expression tag	UNP Q8A5Z1
D	23	MET	-	initiating methionine	UNP Q8A5Z1
D	24	GLY	-	expression tag	UNP Q8A5Z1
D	25	HIS	-	expression tag	UNP Q8A5Z1
D	26	HIS	-	expression tag	UNP Q8A5Z1
D	27	HIS	-	expression tag	UNP Q8A5Z1
D	28	HIS	-	expression tag	UNP Q8A5Z1
D	29	HIS	-	expression tag	UNP Q8A5Z1
D	30	HIS	-	expression tag	UNP Q8A5Z1

• Molecule 2 is CYANOCOBALAMIN (three-letter code: CNC) (formula: $C_{63}H_{89}CoN_{14}O_{14}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
0	В	1	Total	С	Co	Η	Ν	Ο	Р	0	0
	D	1	178	63	1	85	14	14	1	0	0
0	2 A	1	Total	С	Co	Η	Ν	Ο	Р	0	0
		1	178	63	1	85	14	14	1	0	0
0	C	1	Total	С	Co	Η	Ν	Ο	Р	0	0
		L	178	63	1	85	14	14	1	0	0
0	п	1	Total	С	Co	Η	Ν	Ο	Р	0	0
		1	178	63	1	85	14	14	1	0	U

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	28	TotalO2828	0	0
3	А	28	TotalO2828	0	0
3	С	24	Total O 24 24	0	0
3	D	18	Total O 18 18	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: Putative surface layer protein

R242 1256 1256 1256 1256 1256 1256 1256 1256 1266 1266 1266 1265 1266 1280 1322 1323 1323 1322 1323 1322 1323 1322 1323



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	74.77Å 131.04Å 179.38Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	74.12 - 2.60	Depositor
Resolution (A)	74.01 - 2.60	EDS
% Data completeness	99.3 (74.12-2.60)	Depositor
(in resolution range)	99.3 (74.01-2.60)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.75 (at 2.62 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
B B.	0.218 , 0.276	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.225 , 0.276	DCC
R_{free} test set	2675 reflections $(4.90%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	56.5	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.36 , 53.4	EDS
L-test for $twinning^2$	$ < L >=0.52, < L^2>=0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21033	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 3.99% 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: CNC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bo	ond lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.66	2/2686~(0.1%)	1.07	7/3646~(0.2%)	
1	В	0.68	3/2777~(0.1%)	1.13	12/3770~(0.3%)	
1	С	0.64	2/2744~(0.1%)	1.07	7/3725~(0.2%)	
1	D	0.74	4/2691~(0.1%)	1.14	10/3653~(0.3%)	
All	All	0.68	11/10898~(0.1%)	1.10	36/14794~(0.2%)	

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	3
1	В	0	6
1	С	0	2
1	D	0	7
All	All	0	18

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	264	GLU	CD-OE2	14.63	1.41	1.25
1	А	164	GLU	CD-OE1	8.77	1.35	1.25
1	С	264	GLU	CD-OE1	8.47	1.34	1.25
1	В	264	GLU	CD-OE2	7.81	1.34	1.25
1	А	169	GLU	CD-OE2	7.27	1.33	1.25
1	D	264	GLU	CB-CG	6.72	1.65	1.52
1	D	169	GLU	CD-OE2	-5.96	1.19	1.25
1	В	264	GLU	CB-CG	5.80	1.63	1.52
1	C	264	GLU	CB-CG	5.56	1.62	1.52
1	D	264	GLU	CD-OE1	-5.50	1.19	1.25



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	44	GLU	CD-OE2	5.44	1.31	1.25

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	313	ASN	CB-CA-C	-7.96	94.48	110.40
1	D	99	HIS	CB-CA-C	7.80	126.00	110.40
1	С	29	HIS	CA-CB-CG	7.52	126.38	113.60
1	С	313	ASN	CB-CA-C	-7.47	95.46	110.40
1	В	33	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	А	283	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	D	264	GLU	CB-CA-C	7.20	124.79	110.40
1	В	53	THR	CA-CB-OG1	-7.18	93.92	109.00
1	А	313	ASN	CB-CA-C	-7.16	96.09	110.40
1	D	313	ASN	CB-CA-C	-7.13	96.14	110.40
1	А	242	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	В	264	GLU	CB-CA-C	6.88	124.15	110.40
1	D	133	TYR	CB-CG-CD1	6.70	125.02	121.00
1	D	99	HIS	CA-CB-CG	6.63	124.87	113.60
1	С	188	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	В	188	ARG	CG-CD-NE	6.61	125.68	111.80
1	А	46	ASN	CB-CA-C	6.37	123.14	110.40
1	С	264	GLU	CB-CA-C	6.33	123.06	110.40
1	D	264	GLU	CG-CD-OE2	6.07	130.44	118.30
1	В	264	GLU	CB-CG-CD	5.95	130.25	114.20
1	В	30	HIS	CB-CA-C	-5.92	98.56	110.40
1	D	46	ASN	CB-CA-C	5.83	122.06	110.40
1	В	46	ASN	CB-CA-C	5.78	121.96	110.40
1	С	30	HIS	CB-CA-C	-5.67	99.06	110.40
1	А	133	TYR	CB-CG-CD1	5.53	124.32	121.00
1	D	34	ALA	CB-CA-C	5.50	118.35	110.10
1	В	33	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	А	219	LYS	CB-CA-C	5.21	120.83	110.40
1	А	195	THR	CA-CB-CG2	5.17	119.63	112.40
1	С	150	TYR	CB-CG-CD1	5.16	124.10	121.00
1	С	46	ASN	CB-CA-C	5.14	120.69	110.40
1	В	$\overline{28}$	HIS	CB-CA-C	-5.09	100.22	110.40
1	В	322	ILE	CB-CA-C	-5.08	101.45	111.60
1	D	195	THR	CA-CB-CG2	5.05	119.47	112.40
1	D	133	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	В	315	ASP	CB-CG-OD2	-5.01	113.79	118.30



There are no chirality outliers.

\mathbf{Mol}	Chain	\mathbf{Res}	Type	Group
1	А	242	ARG	Sidechain
1	А	283	ARG	Sidechain
1	А	294	ARG	Sidechain
1	В	188	ARG	Sidechain
1	В	226	GLY	Peptide
1	В	283	ARG	Sidechain
1	В	290	ARG	Sidechain
1	В	33	ARG	Sidechain
1	В	71	ARG	Sidechain
1	С	242	ARG	Sidechain
1	С	36	GLY	Peptide
1	D	242	ARG	Sidechain
1	D	283	ARG	Sidechain
1	D	290	ARG	Sidechain
1	D	294	ARG	Sidechain
1	D	300	ARG	Sidechain
1	D	313	ASN	Mainchain
1	D	71	ARG	Sidechain

All (18) planarity outliers are listed below:

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	2619	2373	2526	19	0
1	В	2703	2435	2595	13	0
1	С	2673	2417	2574	26	0
1	D	2624	2379	2531	18	0
2	А	93	85	86	9	0
2	В	93	85	86	6	0
2	С	93	85	87	9	0
2	D	93	85	87	8	0
3	А	28	0	0	3	0
3	В	28	0	0	1	0
3	С	24	0	0	1	0
3	D	18	0	0	0	0
All	All	11089	9944	10572	101	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 5.

All (101) 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)
2:C:401:CNC:H362	2:C:401:CNC:H351	1.55	0.88
2:D:401:CNC:H362	2:D:401:CNC:H351	1.55	0.88
1:A:264:GLU:OE1	3:A:501:HOH:O	1.93	0.87
2:B:401:CNC:H351	2:B:401:CNC:H362	1.58	0.85
1:D:96:ASN:HD21	2:D:401:CNC:H331	1.22	0.84
1:B:133:TYR:HB2	1:B:171:MET:HE1	1.61	0.80
1:C:189:ILE:HD11	1:C:222:THR:HG21	1.64	0.80
2:A:401:CNC:H362	2:A:401:CNC:H351	1.63	0.78
1:D:228:TYR:O	1:D:229:LYS:HB2	1.86	0.74
2:A:401:CNC:H531	2:A:401:CNC:H552	1.68	0.74
1:A:122:ARG:HH22	2:A:401:CNC:H292	1.36	0.72
1:C:130:GLU:HG3	3:C:508:HOH:O	1.91	0.70
1:D:133:TYR:HB2	1:D:171:MET:HE1	1.73	0.70
2:A:401:CNC:H531	2:A:401:CNC:C55	2.23	0.69
1:A:303:LYS:HD3	1:A:324:TYR:CE2	2.28	0.69
1:A:264:GLU:OE1	3:A:503:HOH:O	2.11	0.68
2:C:401:CNC:H543	2:C:401:CNC:H531	1.77	0.66
2:C:401:CNC:H351	2:C:401:CNC:C36	2.26	0.66
1:A:252:LYS:NZ	3:A:504:HOH:O	2.32	0.63
1:B:33:ARG:HH11	1:B:33:ARG:HG3	1.64	0.63
1:B:287:ASP:O	1:B:288:GLU:HB3	1.99	0.62
1:D:193:ASP:OD1	1:D:195:THR:HB	2.00	0.61
1:B:133:TYR:HB2	1:B:171:MET:CE	2.31	0.60
2:A:401:CNC:H351	2:A:401:CNC:C36	2.32	0.60
1:A:96:ASN:HD21	2:A:401:CNC:H331	1.48	0.60
2:B:401:CNC:H552	2:B:401:CNC:H531	1.85	0.59
2:A:401:CNC:H533	2:A:401:CNC:H482	1.84	0.59
1:A:193:ASP:OD1	1:A:195:THR:HB	2.03	0.58
2:D:401:CNC:H351	2:D:401:CNC:C36	2.27	0.58
2:A:401:CNC:H252	2:A:401:CNC:N62	2.19	0.58
1:C:313:ASN:HB2	1:C:315:ASP:H	1.68	0.57
1:D:281:ILE:HD12	1:D:304:TYR:CD2	2.40	0.57
1:D:300:ARG:NH1	1:D:304:TYR:OH	2.39	0.56
1:A:87:ARG:HH11	1:A:87:ARG:HG3	1.71	0.55
1:C:228:TYR:O	1:C:228:TYR:CG	2.59	0.55
1:B:313:ASN:HB2	1:B:315:ASP:H	1.73	0.54
2:B:401:CNC:H531	2:B:401:CNC:C55	2.38	0.54



	lo uo pugom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:79:ASP:OD2	1:A:97:ASN:ND2	2.38	0.53	
1:D:195:THR:HG22	1:D:196:THR:HG23	1.92	0.52	
1:A:252:LYS:HG2	1:A:254:PHE:CZ	2.44	0.52	
2:D:401:CNC:H601	2:D:401:CNC:H252	1.91	0.51	
1:C:297:LEU:HD11	1:C:333:TYR:CE1	2.45	0.51	
2:B:401:CNC:H412	2:B:401:CNC:C4B	2.41	0.51	
1:C:228:TYR:O	1:C:228:TYR:CD2	2.63	0.51	
1:C:140:TYR:HA	1:C:161:MET:HE2	1.91	0.50	
1:C:183:TRP:CH2	2:C:401:CNC:H352	2.47	0.50	
1:D:101:ILE:HD12	1:D:134:ILE:HD13	1.93	0.50	
2:D:401:CNC:H531	2:D:401:CNC:C55	2.42	0.50	
1:D:87:ARG:HH11	1:D:87:ARG:HG3	1.77	0.50	
1:C:312:LYS:HA	1:C:312:LYS:HE2	1.94	0.49	
1:B:94:VAL:HG22	1:B:101:ILE:HG12	1.95	0.49	
1:A:122:ARG:NH2	2:A:401:CNC:H292	2.07	0.49	
1:D:203:LEU:HD11	1:D:250:ILE:HD11	1.95	0.49	
1:C:229:LYS:HD3	1:C:235:TYR:CE1	2.47	0.48	
1:C:140:TYR:HA	1:C:161:MET:CE	2.44	0.48	
1:C:281:ILE:HD12	1:C:304:TYR:CD2	2.49	0.48	
1:A:242:ARG:NH1	1:A:252:LYS:HB2	2.29	0.47	
1:D:211:SER:HB2	1:D:265:VAL:HG22	1.97	0.47	
1:A:242:ARG:HH11	1:A:252:LYS:HB2	1.79	0.47	
1:A:39:LEU:HD11	1:A:352:PHE:HB3	1.96	0.46	
1:A:61:THR:OG1	1:A:63:LYS:HB3	2.14	0.46	
1:B:188:ARG:HH21	1:B:188:ARG:HG3	1.81	0.46	
2:B:401:CNC:H351	2:B:401:CNC:C36	2.37	0.46	
2:B:401:CNC:H533	2:B:401:CNC:H482	1.98	0.45	
1:C:297:LEU:HD23	1:C:298:LYS:N	2.32	0.45	
1:B:34:ALA:HB2	1:B:109:PHE:CZ	2.52	0.45	
1:C:183:TRP:CZ3	2:C:401:CNC:H352	2.51	0.44	
1:A:101:ILE:HD12	1:A:134:ILE:HD13	1.99	0.44	
1:B:83:SER:OG	3:B:501:HOH:O	2.21	0.44	
1:C:46:ASN:ND2	1:C:51:ASN:HD21	2.16	0.44	
1:C:284:MET:HE2	1:C:291:VAL:HA	2.00	0.44	
1:D:279:LYS:HG2	1:D:299:TYR:CD1	2.53	0.44	
1:A:275:TYR:HB3	1:A:307:LEU:HD21	1.99	0.43	
1:D:43:ASN:HA	1:D:349:PRO:HA	2.01	0.43	
2:D:401:CNC:H252	2:D:401:CNC:C61	2.49	0.43	
1:C:242:ARG:NH1	1:C:251:GLU:OE2	2.52	0.43	
1:C:275:TYR:HB3	1:C:307:LEU:HD21	2.01	0.43	
2:D:401:CNC:H531	2:D:401:CNC:H552	1.98	0.43	



A + 1	A + a	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:C:327:GLN:NE2	1:C:344:TYR:HB3	2.33	0.43	
2:D:401:CNC:H252	2:D:401:CNC:C60	2.48	0.43	
1:C:228:TYR:CD1	1:C:231:SER:HB2	2.54	0.43	
1:D:253:GLN:HE21	1:D:255:LYS:HG2	1.83	0.43	
2:C:401:CNC:H411	2:C:401:CNC:H363	1.79	0.43	
1:B:43:ASN:HA	1:B:349:PRO:HA	2.01	0.43	
1:B:39:LEU:HD11	1:B:352:PHE:HB3	2.00	0.42	
2:C:401:CNC:H601	2:C:401:CNC:H262	2.00	0.42	
1:C:228:TYR:HA	1:C:229:LYS:HE3	2.02	0.42	
1:B:84:MET:HA	1:B:92:TRP:O	2.19	0.42	
1:C:94:VAL:HG22	1:C:101:ILE:HG12	2.02	0.42	
1:C:228:TYR:O	1:C:229:LYS:C	2.58	0.42	
1:D:203:LEU:HD11	1:D:250:ILE:CD1	2.49	0.42	
1:C:228:TYR:O	1:C:229:LYS:O	2.38	0.42	
1:C:228:TYR:CD2	2:C:401:CNC:H472	2.55	0.42	
1:C:43:ASN:HA	1:C:349:PRO:HA	2.02	0.41	
1:A:195:THR:HG22	1:A:196:THR:HG23	2.03	0.41	
2:C:401:CNC:H481	2:C:401:CNC:H473	1.49	0.41	
1:D:39:LEU:HD11	1:D:352:PHE:HB3	2.02	0.41	
1:D:84:MET:HA	1:D:92:TRP:O	2.21	0.41	
1:D:253:GLN:HE21	1:D:255:LYS:CG	2.34	0.41	
1:A:84:MET:HA	1:A:92:TRP:O	2.21	0.40	
1:B:211:SER:HB2	$1:B:\overline{265:VAL:HG22}$	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	Percentiles
1	А	319/333~(96%)	292 (92%)	23~(7%)	4 (1%)	12 24
1	В	328/333~(98%)	299 (91%)	26 (8%)	3 (1%)	17 35



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	С	325/333~(98%)	301 (93%)	20 (6%)	4 (1%)	13 27
1	D	320/333~(96%)	297~(93%)	19 (6%)	4 (1%)	12 24
All	All	1292/1332~(97%)	1189 (92%)	88 (7%)	15 (1%)	13 27

All (15) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	С	229	LYS
1	D	229	LYS
1	А	322	ILE
1	С	322	ILE
1	D	322	ILE
1	В	322	ILE
1	А	345	VAL
1	А	37	ASP
1	D	345	VAL
1	С	345	VAL
1	В	345	VAL
1	В	30	HIS
1	А	80	VAL
1	С	80	VAL
1	D	80	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	284/294~(97%)	280~(99%)	4 (1%)	67 85		
1	В	292/294~(99%)	284~(97%)	8(3%)	44 71		
1	С	289/294~(98%)	281 (97%)	8 (3%)	43 69		
1	D	284/294~(97%)	279~(98%)	5 (2%)	59 80		
All	All	1149/1176~(98%)	1124 (98%)	25~(2%)	52 76		

All (25) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	В	27	HIS
1	В	65	GLU
1	В	89	THR
1	В	106	THR
1	В	195	THR
1	В	257	GLN
1	В	298	LYS
1	В	322	ILE
1	А	89	THR
1	А	163	MET
1	А	195	THR
1	А	326	GLN
1	С	89	THR
1	С	106	THR
1	С	184	SER
1	С	224	THR
1	С	229	LYS
1	С	248	PHE
1	С	274	LEU
1	С	338	GLU
1	D	89	THR
1	D	148	LYS
1	D	195	THR
1	D	240	LEU
1	D	294	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	173	GLN
1	А	96	ASN
1	А	208	GLN
1	А	326	GLN
1	А	327	GLN
1	С	46	ASN
1	С	96	ASN
1	С	313	ASN
1	С	327	GLN
1	D	96	ASN
1	D	97	ASN
1	D	253	GLN
1	D	325	GLN



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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).

Mol Tuno	Chain	e Chain Res	Chain	Chain	Chain	Chain	Chain	Chain	Dec	Deg Link	Bo	Bond lengths			Bond angles		
IVIOI	туре		nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2							
2	CNC	А	401	-	90,103,103	1.80	17 (18%)	139,171,171	2.10	44 (31%)							
2	CNC	В	401	-	90,103,103	1.60	8 (8%)	139,171,171	2.05	37 (26%)							
2	CNC	С	401	-	90,103,103	1.61	8 (8%)	139,171,171	2.36	41 (29%)							
2	CNC	D	401	-	90,103,103	1.77	18 (20%)	139,171,171	2.34	46 (33%)							

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CNC	А	401	-	1/1/38/38	8/52/235/235	0/3/11/11
2	CNC	В	401	-	2/2/38/38	15/52/235/235	0/3/11/11
2	CNC	С	401	-	2/2/38/38	12/52/235/235	0/3/11/11
2	CNC	D	401	-	1/1/38/38	12/52/235/235	0/3/11/11



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	401	CNC	C19-N24	-11.15	1.25	1.49
2	С	401	CNC	C19-N24	-9.71	1.28	1.49
2	А	401	CNC	C19-N24	-8.55	1.31	1.49
2	D	401	CNC	C19-N24	-8.10	1.32	1.49
2	А	401	CNC	C8B-C9B	5.62	1.52	1.40
2	С	401	CNC	C6B-C5B	5.35	1.54	1.40
2	С	401	CNC	C8B-C9B	4.76	1.50	1.40
2	D	401	CNC	C1-C2	-4.13	1.49	1.58
2	D	401	CNC	C53-C15	4.02	1.59	1.50
2	D	401	CNC	C8B-C9B	3.86	1.48	1.40
2	В	401	CNC	C4B-C9B	-3.70	1.36	1.41
2	А	401	CNC	C4B-C9B	-3.63	1.36	1.41
2	D	401	CNC	C35-C5	3.61	1.58	1.50
2	А	401	CNC	C7B-C6B	3.52	1.46	1.37
2	А	401	CNC	C35-C5	3.29	1.57	1.50
2	D	401	CNC	C7-C6	3.19	1.62	1.54
2	С	401	CNC	C10-C9	3.11	1.48	1.39
2	В	401	CNC	C6B-C5B	2.88	1.48	1.40
2	А	401	CNC	C16-C15	-2.86	1.30	1.42
2	D	401	CNC	C6B-C5B	2.86	1.48	1.40
2	С	401	CNC	C2R-C1R	-2.82	1.49	1.53
2	А	401	CNC	O6R-C4R	-2.74	1.38	1.45
2	D	401	CNC	C8-C9	-2.73	1.45	1.51
2	А	401	CNC	C53-C15	2.68	1.56	1.50
2	D	401	CNC	C1P-C2P	2.68	1.58	1.51
2	D	401	CNC	C55-C56	2.67	1.59	1.53
2	А	401	CNC	C1P-C2P	2.65	1.58	1.51
2	А	401	CNC	O3-C2P	2.64	1.52	1.45
2	D	401	CNC	P-O2	2.58	1.67	1.60
2	А	401	CNC	C9B-N3B	-2.51	1.30	1.38
2	D	401	CNC	C43-N45	2.50	1.40	1.32
2	С	401	CNC	C4-C5	2.47	1.53	1.43
2	А	401	CNC	C6B-C5B	2.45	1.47	1.40
2	D	401	CNC	C16-C15	-2.42	1.32	1.42
2	А	401	CNC	C56-C57	2.41	1.55	1.51
2	В	401	CNC	C8B-C9B	2.41	1.45	1.40
2	A	401	$CN\overline{C}$	C2B-N3B	2.41	1.39	1.34
2	D	401	CNC	C5M-C5B	2.38	1.55	1.51
2	A	401	CNC	C18-C19	-2.34	1.49	1.54
2	A	401	CNC	C10-C9	2.32	1.45	1.39
2	С	401	CNC	C56-C57	2.32	1.55	1.51
2	В	401	CNC	C10-C9	2.29	1.45	1.39

All (51) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	CNC	C18-C19	-2.28	1.49	1.54
2	В	401	CNC	P-O3	2.20	1.66	1.60
2	С	401	CNC	P-O3	2.14	1.66	1.60
2	D	401	CNC	C10-C11	-2.13	1.31	1.37
2	А	401	CNC	C25-C2	2.12	1.58	1.54
2	D	401	CNC	C50-N52	2.10	1.39	1.32
2	В	401	CNC	C16-C15	-2.09	1.33	1.42
2	В	401	CNC	O6R-C1R	2.03	1.43	1.41
2	D	401	CNC	C38-N40	2.03	1.39	1.32

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	401	CNC	C13-C12-C11	-12.43	83.95	100.90
2	D	401	CNC	O3-C2P-C1P	7.55	121.98	106.92
2	А	401	CNC	C18-C19-N24	7.53	113.84	101.88
2	В	401	CNC	C20-C1-C19	-7.19	95.81	110.23
2	С	401	CNC	C1-C19-C18	6.98	132.13	121.81
2	А	401	CNC	C7B-C8B-C9B	-6.82	113.80	120.54
2	В	401	CNC	C18-C19-N24	6.81	112.69	101.88
2	С	401	CNC	C12-C11-N23	6.51	118.53	111.48
2	D	401	CNC	C1-C19-N24	5.97	115.78	106.33
2	С	401	CNC	C18-C19-N24	5.96	111.34	101.88
2	D	401	CNC	C2P-C1P-N59	5.95	121.71	112.93
2	D	401	CNC	C13-C12-C11	-5.90	92.86	100.90
2	В	401	CNC	C1-C19-N24	5.83	115.56	106.33
2	С	401	CNC	C1-C19-N24	5.70	115.36	106.33
2	D	401	CNC	C2-C1-C19	5.69	128.47	118.72
2	С	401	CNC	C47-C12-C11	5.68	129.95	110.29
2	А	401	CNC	C1-C19-N24	5.58	115.17	106.33
2	D	401	CNC	C7B-C8B-C9B	-5.50	115.10	120.54
2	D	401	CNC	C1-C19-C18	5.49	129.92	121.81
2	В	401	CNC	C1-C19-C18	5.12	129.38	121.81
2	В	401	CNC	C20-C1-C2	4.88	121.43	113.28
2	А	401	CNC	C60-C18-C19	4.83	125.60	114.09
2	В	401	CNC	O58-C57-C56	-4.80	113.25	122.02
2	С	401	CNC	O5-P-O3	4.79	125.70	106.78
2	D	401	CNC	C10-C9-N22	4.67	131.09	125.73
2	D	401	CNC	O6R-C4R-C5R	-4.66	99.13	109.21
2	A	401	CNC	O6R-C1R-C2R	-4.60	100.20	106.93
2	С	401	CNC	C37-C7-C8	4.57	120.64	108.39
2	D	401	CNC	C18-C19-N24	4.51	109.05	101.88



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		i previ	ous page		7	$\mathbf{O}\mathbf{h}$ a survey $\mathbf{d}(0)$	$\mathbf{I}_{\mathbf{J}_{\mathbf{a}}} = \mathbf{I}(0)$
NIO	Chain	Res	Type	Atoms		Observed(°)	Ideal(°)
2	C	401	CNC	C4B-C9B-C8B	-4.41	116.58	121.10
2	A	401	CNC	<u>C36-C7-C37</u>	-4.40	103.55	110.80
2	B	401	CNC	C4B-C9B-C8B	-4.40	116.59	121.10
2	C	401	CNC	C47-C12-C13	-4.38	94.87	112.72
2	D	401	CNC	C9-C10-C11	-4.26	119.59	125.88
2	A	401	CNC	C2-C1-C19	4.12	125.78	118.72
2	D	401	CNC	C8-C7-C6	-4.05	93.96	100.92
2	C	401	CNC	C56-C55-C17	4.05	123.32	115.52
2	В	401	CNC	C48-C49-C50	-4.05	98.86	112.59
2	A	401	CNC	O3-C2P-C1P	4.04	114.98	106.92
2	В	401	CNC	C7-C8-C9	-4.02	95.76	100.90
2	D	401	CNC	C8B-C9B-N3B	-4.00	99.39	107.83
2	В	401	CNC	C13-C12-C11	-4.00	95.46	100.90
2	С	401	CNC	C20-C1-C19	-3.96	102.29	110.23
2	D	401	CNC	C20-C1-C19	-3.96	102.29	110.23
2	D	401	CNC	O2-C3R-C4R	3.93	124.31	110.08
2	С	401	CNC	C13-C14-C15	3.89	130.36	123.81
2	D	401	CNC	C60-C61-N62	-3.83	106.99	116.21
2	D	401	CNC	C48-C13-C14	3.82	118.52	109.63
2	В	401	CNC	O58-C57-N59	3.80	130.19	123.01
2	А	401	CNC	C1-C19-C18	3.77	127.38	121.81
2	В	401	CNC	C5M-C5B-C4B	-3.77	111.32	120.34
2	А	401	CNC	C56-C55-C17	3.73	122.70	115.52
2	А	401	CNC	C20-C1-C19	-3.71	102.79	110.23
2	D	401	CNC	C36-C7-C37	-3.70	104.71	110.80
2	В	401	CNC	O5-P-O2	3.69	121.33	106.78
2	D	401	CNC	O5-P-O2	3.60	120.98	106.78
2	В	401	CNC	C60-C18-C19	3.57	122.60	114.09
2	D	401	CNC	O63-C61-C60	3.57	128.38	120.87
2	А	401	CNC	C48-C49-C50	-3.48	100.78	112.59
2	А	401	CNC	C2-C1-N21	3.43	106.55	101.77
2	В	401	CNC	C1-N21-C4	3.39	114.74	109.37
2	В	401	CNC	C8-C9-N22	3.37	117.47	110.77
2	А	401	CNC	O8R-C5R-C4R	-3.36	99.75	111.29
2	В	401	CNC	C2-C1-C19	3.33	124.43	118.72
2	В	401	CNC	02-P-04	-3.32	97.00	109.47
2	D	401	CNC	C54-C17-C18	-3.29	108.12	112.98
2	С	401	CNC	C2-C1-C19	3.26	124.32	118.72
2	С	401	CNC	C12-C11-C10	-3.25	120.58	123.54
2	D	401	CNC	C8-C9-C10	-3.24	116.32	123.32
2	A	401	CNC	C6M-C6B-C5B	-3.23	114.11	120.74
2	В	401	CNC	C26-C2-C1	3.21	115.01	110.01

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	Chain	$\frac{1}{\mathbf{P}}$	Type	Atoms	7	Observed(0)	Ideal(0)
	Cliain	401	CNC		2.00	$\frac{00.67}{00.67}$	110 70
	D	401	CNC	C40-C12-C13	-3.20	99.07	
2	D	401	CNC	$C_{2}C_{1}N_{2}$	-3.18	104.99	111.10
		401	CNC	$\frac{\text{O2-O1-N21}}{\text{O2-O1-N21}}$	0.10 2.10	100.21	101.77
	A	401	CNC	C7D $C6D$ $C5D$	-3.12	110.59	123.32
2	В	401	CNC	$C_1B-C_0B-C_0B$	-3.12	114.00	119.91
2	A	401	CNC	044 049 049	3.09	105.14	101.03
2	D	401	CNC	044-C43-C42	-3.09	111.99	121.07
2	C	401	CNC	C15-C16-N24	-3.07	119.26	122.38
2	B	401	CNC	05-P-03	3.07	118.90	106.78
2	C	401	CNC	O5-P-O2	3.06	118.86	106.78
2	A	401	CNC	O5-P-O2	-3.05	94.74	106.78
2	C	401	CNC	C8-C7-C6	-3.03	95.73	100.92
2	С	401	CNC	O2-C3R-C4R	-3.02	99.17	110.08
2	A	401	CNC	C1-C2-C3	-3.00	97.77	101.60
2	С	401	CNC	C5M-C5B-C4B	-2.99	113.20	120.34
2	С	401	CNC	O63-C61-C60	2.99	127.16	120.87
2	D	401	CNC	C55-C17-C18	2.97	116.89	111.15
2	D	401	CNC	C41-C8-C9	-2.97	105.96	111.19
2	В	401	CNC	O63-C61-C60	2.96	127.11	120.87
2	С	401	CNC	C17-C16-C15	2.93	131.18	126.73
2	А	401	CNC	O34-C32-C31	-2.91	112.51	121.07
2	А	401	CNC	C8-C9-N22	2.91	116.56	110.77
2	С	401	CNC	C36-C7-C8	-2.90	106.71	112.08
2	В	401	CNC	C8-C9-C10	-2.90	117.06	123.32
2	D	401	CNC	C20-C1-C2	-2.89	108.46	113.28
2	D	401	CNC	C25-C2-C3	2.89	120.35	112.96
2	А	401	CNC	O51-C50-C49	-2.87	112.64	121.07
2	С	401	CNC	C9-C10-C11	-2.86	121.65	125.88
2	D	401	CNC	O7R-C2R-C1R	2.86	121.43	110.85
2	В	401	CNC	C37-C38-N40	2.81	125.44	116.52
2	А	401	CNC	O63-C61-C60	2.81	126.79	120.87
2	С	401	CNC	O2-C3R-C2R	2.79	121.80	111.68
2	D	401	CNC	C4B-C5B-C6B	-2.77	115.24	119.91
2	А	401	CNC	O28-C27-N29	-2.77	114.95	122.50
2	А	401	CNC	C3P-C2P-C1P	-2.75	106.05	111.39
2	А	401	CNC	C26-C2-C3	-2.74	102.57	107.41
2	А	401	CNC	C4B-C9B-C8B	2.72	123.89	121.10
2	С	401	CNC	C5M-C5B-C6B	2.70	126.27	120.74
2	D	401	CNC	C3P-C2P-C1P	-2.69	106.16	111.39
2	В	401	CNC	C41-C8-C7	2.69	121.55	114.14
2	D	401	CNC	O51-C50-N52	2.67	129.79	122.50
2	В	401	CNC	C9-C10-C11	-2.67	121.94	125.88



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Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$\overline{\text{Ideal}(^{o})}$
2	D	401	CNC	C26-C2-C3	-2.65	102.72	107.41
2	А	401	CNC	O39-C38-C37	-2.65	113.60	121.99
2	А	401	CNC	O2-C3R-C2R	2.65	121.27	111.68
2	С	401	CNC	O6R-C1R-C2R	-2.63	103.08	106.93
2	А	401	CNC	O39-C38-N40	2.62	129.65	122.50
2	D	401	CNC	C37-C7-C6	2.61	115.33	107.12
2	D	401	CNC	C46-C12-C11	2.61	119.31	110.29
2	С	401	CNC	C10-C11-N23	-2.58	120.68	124.93
2	D	401	CNC	C4B-C9B-N3B	2.57	137.77	130.88
2	D	401	CNC	C31-C32-N33	2.57	124.50	116.51
2	В	401	CNC	C12-C11-N23	2.55	114.24	111.48
2	А	401	CNC	C5M-C5B-C6B	2.53	125.91	120.74
2	С	401	CNC	C7-C8-C9	-2.49	97.72	100.90
2	А	401	CNC	C31-C32-N33	2.47	124.19	116.51
2	D	401	CNC	C60-C18-C17	2.45	121.69	115.74
2	D	401	CNC	C47-C12-C46	-2.42	105.27	109.35
2	С	401	CNC	C60-C18-C19	2.40	119.81	114.09
2	С	401	CNC	O6R-C4R-C5R	2.38	114.36	109.21
2	С	401	CNC	C15-C14-N23	-2.38	121.96	126.68
2	D	401	CNC	O34-C32-C31	-2.38	114.09	121.07
2	А	401	CNC	C13-C14-N23	2.37	114.49	109.39
2	С	401	CNC	C6M-C6B-C5B	2.35	125.56	120.74
2	А	401	CNC	C36-C7-C6	2.35	124.59	112.40
2	С	401	CNC	C1-N21-C4	2.35	113.08	109.37
2	А	401	CNC	O7R-C2R-C1R	2.34	119.51	110.85
2	D	401	CNC	C56-C55-C17	2.33	120.01	115.52
2	А	401	CNC	O5-P-O3	2.30	115.86	106.78
2	В	401	CNC	O39-C38-N40	-2.28	116.27	122.50
2	С	401	CNC	C25-C2-C1	2.25	117.18	113.78
2	С	401	CNC	C41-C8-C7	2.25	120.32	114.14
2	В	401	CNC	C12-C13-C14	2.23	104.80	101.86
2	D	401	CNC	C42-C41-C8	2.22	121.15	114.73
2	А	401	CNC	O51-C50-N52	2.21	128.53	122.50
2	В	401	CNC	C12-C11-C10	-2.21	121.53	123.54
2	В	401	CNC	C37-C7-C8	2.19	114.26	108.39
2	А	401	CNC	O44-C43-C42	-2.19	114.65	121.07
2	А	401	CNC	C54-C17-C55	2.17	112.83	109.25
2	В	401	CNC	C5M-C5B-C6B	2.17	125.17	120.74
2	В	401	CNC	O2-C3R-C4R	2.16	117.90	110.08
2	А	401	CNC	C15-C16-N24	2.15	124.57	122.38
4							1
$\frac{2}{2}$	D	401	CNC	C5M-C5B-C4B	2.14	125.46	120.34



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	401	CNC	C55-C17-C18	-2.13	107.03	111.15
2	D	401	CNC	O8R-C5R-C4R	2.11	118.54	111.29
2	D	401	CNC	C17-C18-C19	2.11	105.19	102.66
2	С	401	CNC	C20-C1-N21	2.11	113.72	110.27
2	С	401	CNC	C7B-C8B-C9B	2.10	122.62	120.54
2	А	401	CNC	C25-C2-C3	2.10	118.33	112.96
2	А	401	CNC	O6R-C4R-C5R	-2.08	104.71	109.21
2	В	401	CNC	C54-C17-C55	2.08	112.68	109.25
2	А	401	CNC	O3-C2P-C3P	2.08	116.73	108.72
2	С	401	CNC	C35-C5-C6	-2.06	119.15	122.43
2	С	401	CNC	C46-C12-C11	2.03	117.33	110.29
2	D	401	CNC	C30-C3-C4	2.01	114.32	109.63
2	В	401	CNC	C2P-C1P-N59	-2.01	109.97	112.93

All (6) chirality outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atom
2	В	401	CNC	C19
2	В	401	CNC	N24
2	А	401	CNC	N24
2	С	401	CNC	C19
2	С	401	CNC	N24
2	D	401	CNC	N24

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	401	CNC	C3P-C2P-O3-P
2	В	401	CNC	C2P-O3-P-O5
2	А	401	CNC	C38-C37-C7-C6
2	А	401	CNC	C1P-C2P-O3-P
2	А	401	CNC	C3P-C2P-O3-P
2	С	401	CNC	C8-C41-C42-C43
2	D	401	CNC	C1P-C2P-O3-P
2	D	401	CNC	C3P-C2P-O3-P
2	С	401	CNC	C3R-C4R-C5R-O8R
2	С	401	CNC	O6R-C4R-C5R-O8R
2	С	401	CNC	C13-C48-C49-C50
2	С	401	CNC	C2R-C3R-O2-P
2	D	401	CNC	C13-C48-C49-C50
2	С	401	CNC	C3R-O2-P-O3
2	В	401	CNC	N59-C1P-C2P-C3P



Mol	Chain	Res	Type	Atoms
2	В	401	CNC	C1P-C2P-O3-P
2	В	401	CNC	C2P-O3-P-O2
2	D	401	CNC	C41-C42-C43-N45
2	В	401	CNC	C3-C30-C31-C32
2	В	401	CNC	C13-C48-C49-C50
2	А	401	CNC	C8-C41-C42-C43
2	С	401	CNC	C42-C41-C8-C9
2	В	401	CNC	C3R-O2-P-O3
2	А	401	CNC	C2P-O3-P-O2
2	В	401	CNC	C2P-O3-P-O4
2	D	401	CNC	C18-C17-C55-C56
2	В	401	CNC	C41-C42-C43-O44
2	В	401	CNC	N59-C1P-C2P-O3
2	А	401	CNC	C38-C37-C7-C8
2	D	401	CNC	C54-C17-C55-C56
2	В	401	CNC	C42-C41-C8-C9
2	D	401	CNC	C3R-O2-P-O3
2	D	401	CNC	C17-C18-C60-C61
2	А	401	CNC	C4-C3-C30-C31
2	С	401	CNC	C38-C37-C7-C8
2	В	401	CNC	C41-C42-C43-N45
2	D	401	CNC	C16-C17-C55-C56
2	D	401	CNC	C41-C42-C43-O44
2	В	401	CNC	C7-C37-C38-O39
2	С	401	CNC	C30-C31-C32-N33
2	С	401	CNC	C38-C37-C7-C36
2	С	401	CNC	C14-C13-C48-C49
2	D	401	CNC	C4-C3-C30-C31
2	В	401	CNC	C8-C41-C42-C43
2	С	401	CNC	C30-C31-C32-O34
2	А	401	CNC	C17-C18-C60-C61
2	D	401	CNC	C19-C18-C60-C61

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There are no ring outliers.

4 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	401	CNC	9	0
2	В	401	CNC	6	0
2	С	401	CNC	9	0
2	D	401	CNC	8	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 >	#RSR2	Z>2	$OWAB(Å^2)$	Q<0.9
1	А	321/333~(96%)	0.10	1 (0%) 94	93	43, 66, 96, 123	0
1	В	330/333~(99%)	0.21	1 (0%) 94	93	39, 69, 109, 130	0
1	С	327/333~(98%)	0.50	17 (5%) 2'	7 21	34, 75, 118, 146	0
1	D	322/333~(96%)	0.23	4 (1%) 79	9 76	44, 72, 104, 124	0
All	All	1300/1332~(97%)	0.26	23 (1%) 68	8 64	34, 70, 109, 146	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	293	VAL	3.7
1	С	294	ARG	3.6
1	С	235	TYR	3.0
1	А	261	ALA	2.9
1	С	29	HIS	2.9
1	С	271	GLY	2.9
1	С	59	PRO	2.6
1	В	235	TYR	2.5
1	С	279	LYS	2.5
1	С	286	VAL	2.5
1	С	309	VAL	2.4
1	D	325	GLN	2.4
1	С	277	ILE	2.4
1	С	258	LEU	2.3
1	D	262	PRO	2.3
1	С	230	GLY	2.2
1	D	333	TYR	2.2
1	С	223	ILE	2.2
1	С	274	LEU	2.2
1	С	228	TYR	2.1
1	С	68	ILE	2.1

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Mol	Chain	\mathbf{Res}	Type	RSRZ
1	С	240	LEU	2.1
1	D	241	TYR	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	CNC	С	401	93/93	0.94	0.22	$60,\!87,\!130,\!153$	0
2	CNC	А	401	93/93	0.96	0.23	$34,\!59,\!78,\!107$	0
2	CNC	D	401	93/93	0.96	0.23	37,59,87,95	0
2	CNC	В	401	93/93	0.97	0.21	49,77,123,138	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.

