

Full wwPDB X-ray Structure Validation Report (i)

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:	7QBG
:	TC:CD320 in complex with nanobody TC-Nb4
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:	2021-11-19
:	2.69 Å(reported)
	: : : :

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.69 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	2808 (2.70-2.70)				
Clashscore	141614	3122 (2.70-2.70)				
Ramachandran outliers	138981	3069 (2.70-2.70)				
Sidechain outliers	138945	3069 (2.70-2.70)				
RSRZ outliers	127900	2737 (2.70-2.70)				

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			\mathbf{Q}_{1}	uality o	of ch	ain			
1	А	409	2%		69%				22%	•	7%
1	С	409	4%		69%				24%		5%
2	В	147	4%	38%		17%	•		42%		
2	D	147	5%	39%		16%	•		45%	_	
3	Е	135	12%		60%			299	%	•	7%



Mol	Chain	Length		Quality of	chain	
			22%			
3	G	135		56%	30%	•• 10%

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
4	CNC	А	501	X	-	-	-
4	CNC	С	501	Х	-	-	-
5	GOL	А	502	-	-	-	Х



$7 \mathrm{QBG}$

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9349 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 Transcobalamin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	291	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	301	2972	1899	517	538	18	0	0	0	
1	С	200	Total	С	Ν	0	S	0	0	0
	300	3020	1932	525	545	18	0	U		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	209	GLN	ARG	conflict	UNP P20062
С	209	GLN	ARG	conflict	UNP P20062

• Molecule 2 is a protein called CD320 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	85	Total 628	C 371	N 110	0 135	S 12	0	0	0
2	D	81	Total 604	C 359	N 103	0 130	S 12	0	0	0

• Molecule 3 is a protein called Anti-TC:CD320 nanobody TC-Nb4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	195	Total	С	Ν	0	S	0	0	0
D E	125	944	590	164	185	5	0	0	0	
2	C	191	Total	С	Ν	0	S	0	0	0
3 G	121	924	579	161	179	5	0	0	0	

• Molecule 4 is CYANOCOBALAMIN (three-letter code: CNC) (formula: $C_{63}H_{89}CoN_{14}O_{14}P$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	Δ	1	Total	С	Со	Ν	Ο	Р	2	0
4 A	L	93	63	1	14	14	1	2	0	
4	C	1	Total	С	Co	Ν	Ο	Р	1	0
4 0	1	93	63	1	14	14	1	T	0	



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



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
5	С	1	Total 6	${ m C} { m 3}$	O 3	0	0

• Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	2	Total Ca 2 2	0	0
6	D	2	Total Ca 2 2	0	0
6	Е	1	Total Ca 1 1	0	0
6	G	1	Total Ca 1 1	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	21	Total O 21 21	0	0
7	В	2	Total O 2 2	0	0
7	С	16	Total O 16 16	0	0
7	D	1	Total O 1 1	0	0
7	Ε	5	$\begin{array}{cc} \text{Total} & \text{O} \\ 5 & 5 \end{array}$	0	0
7	G	2	Total O 2 2	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: Transcobalamin-2





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	105.34Å 116.42Å 125.50Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	48.92 - 2.69	Depositor
Resolution (A)	48.92 - 2.69	EDS
% Data completeness	97.4 (48.92-2.69)	Depositor
(in resolution range)	97.4(48.92-2.69)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.98 (at 2.69 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
B B.	0.227 , 0.285	Depositor
II, II, <i>free</i>	0.226 , 0.283	DCC
R_{free} test set	2111 reflections (5.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	56.3	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	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	0.93	EDS
Total number of atoms	9349	wwPDB-VP
Average B, all atoms $(Å^2)$	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.50% 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, CA, GOL

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	
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.52	0/3031	0.75	2/4101~(0.0%)
1	С	0.48	0/3082	0.70	1/4174~(0.0%)
2	В	0.55	0/638	0.89	1/866~(0.1%)
2	D	0.49	0/614	0.77	1/834~(0.1%)
3	Е	0.54	0/966	0.86	1/1311~(0.1%)
3	G	0.50	0/944	0.75	1/1279~(0.1%)
All	All	0.51	0/9275	0.76	7/12565~(0.1%)

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	С	0	1
2	В	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	81	LYS	CB-CA-C	5.70	121.80	110.40
2	В	93	PRO	N-CA-CB	5.63	110.06	103.30
1	А	224	ASN	CB-CA-C	5.46	121.31	110.40
1	А	226	TYR	CB-CA-C	5.38	121.16	110.40
2	D	53	SER	C-N-CA	5.33	135.02	121.70
3	Е	125	ASN	CB-CA-C	5.22	120.85	110.40
3	G	25	LEU	CA-CB-CG	5.00	126.81	115.30



There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	В	168	GLY	Peptide
1	С	102	ARG	Sidechain

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	2972	0	3004	67	0
1	С	3020	0	3044	64	0
2	В	628	0	545	18	0
2	D	604	0	533	17	0
3	Е	944	0	901	37	0
3	G	924	0	891	25	0
4	А	93	0	87	13	0
4	С	93	0	87	10	0
5	А	12	0	16	5	0
5	С	6	0	8	0	0
6	В	2	0	0	0	0
6	D	2	0	0	0	0
6	Е	1	0	0	0	0
6	G	1	0	0	0	0
7	А	21	0	0	4	0
7	В	2	0	0	0	0
7	С	16	0	0	0	0
7	D	1	0	0	0	0
7	Е	5	0	0	0	0
7	G	2	0	0	0	0
All	All	9349	0	9116	236	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 13.

All (236) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom 1	Atom 2	Interatomic	\mathbf{Clash}
Atom-1	Atom-2	distance (\AA)	overlap (Å)
4:A:501:CNC:C19	4:A:501:CNC:C1	1.75	1.55
3:E:82:ALA:O	3:E:83:ASP:OD1	1.65	1.14
2:B:137:LEU:HD23	2:B:148:LEU:HD23	1.42	1.01
4:A:501:CNC:C19	4:A:501:CNC:H262	1.91	0.98
4:A:501:CNC:C19	4:A:501:CNC:C26	2.52	0.88
3:G:112:THR:HG23	3:G:143:THR:HA	1.59	0.85
3:E:82:ALA:O	3:E:83:ASP:CG	2.17	0.82
4:C:501:CNC:C14	4:C:501:CNC:H2B	2.11	0.80
2:B:129:ARG:HD2	2:B:143:ASP:OD2	1.81	0.80
1:A:185:PHE:HB3	1:A:201:ILE:HG23	1.65	0.77
1:C:84:MET:HE2	3:E:123:PRO:HG2	1.64	0.77
1:C:84:MET:CE	3:E:123:PRO:HG2	2.16	0.74
2:B:167:CYS:C	2:B:169:THR:HG23	2.09	0.73
4:A:501:CNC:C1	4:A:501:CNC:C18	2.67	0.73
1:A:154:HIS:CG	2:D:149:THR:HG21	2.24	0.72
1:C:244:GLU:O	1:C:247:THR:OG1	2.07	0.71
3:E:104:MET:HB3	3:E:107:LEU:HD21	1.72	0.70
1:C:322:LEU:HD23	1:C:323:PRO:HA	1.74	0.70
2:D:146:ILE:HD13	2:D:150:TRP:HB2	1.74	0.69
2:B:137:LEU:HD23	2:B:148:LEU:CD2	2.18	0.69
1:A:366:VAL:HG12	1:A:367:MET:HG3	1.75	0.68
1:C:33:ASN:HB3	1:C:36:ILE:HG13	1.76	0.68
2:D:89:CYS:SG	2:D:90:ARG:N	2.66	0.68
3:E:33:VAL:HG11	3:E:107:LEU:HD12	1.76	0.67
2:B:131:ALA:HA	2:B:138:ARG:HH22	1.61	0.66
1:A:6:PRO:HD2	1:A:253:ARG:HD2	1.78	0.65
3:E:109:PRO:HA	3:E:144:VAL:HG13	1.77	0.65
1:A:84:MET:HG3	1:A:116:PHE:HB2	1.79	0.65
1:A:197:ARG:HD2	1:A:200:ARG:HD3	1.78	0.65
1:C:341:LEU:HD23	1:C:352:TYR:CD2	2.32	0.64
1:C:312:ILE:HD11	1:C:398:ASP:HB2	1.78	0.64
1:A:289:PRO:HA	5:A:502:GOL:H11	1.80	0.63
1:C:66:LEU:HA	3:E:124:SER:HB3	1.80	0.63
4:A:501:CNC:C20	4:A:501:CNC:H18	2.28	0.63
2:B:167:CYS:O	2:B:169:THR:HG23	1.99	0.63
3:E:89:PHE:O	3:E:90:ILE:HD13	1.99	0.63
1:A:130:GLY:N	7:A:603:HOH:O	2.30	0.62
1:C:339:ASP:HA	1:C:342:LYS:HG3	1.81	0.62
1:C:155:ASP:HB3	1:C:197:ARG:HE	1.66	0.61
3:G:89:PHE:O	3:G:90:ILE:HD13	2.00	0.61
1:C:305:ILE:HD12	1:C:306:PRO:HD2	1.83	0.60
2:D:138:ARG:NH2	2:D:143:ASP:OD2	2.34	0.60



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:81:LYS:HB3	1:A:82:PRO:HA	1.82	0.60
4:A:501:CNC:C19	4:A:501:CNC:C20	2.75	0.60
3:E:70:SER:HG	3:E:81:TYR:HD1	1.48	0.60
3:G:88:ARG:NH1	3:G:111:ASP:OD2	2.34	0.60
1:C:84:MET:HE1	1:C:112:GLN:HB3	1.84	0.59
2:D:146:ILE:HD12	2:D:147:PRO:O	2.01	0.59
3:E:121:TYR:CZ	3:E:123:PRO:HG3	2.37	0.59
1:A:226:TYR:O	1:A:270:MET:HE1	2.03	0.58
2:B:129:ARG:HD2	2:B:143:ASP:CG	2.23	0.57
1:C:139:TYR:HD2	1:C:161:LEU:HD13	1.69	0.57
2:B:149:THR:HB	1:C:154:HIS:CD2	2.39	0.56
3:G:49:THR:HB	3:G:52:ILE:HD11	1.87	0.56
2:D:85:ASP:N	2:D:85:ASP:OD1	2.39	0.56
3:G:97:LYS:HB3	3:G:99:THR:HG23	1.86	0.56
4:A:501:CNC:H4B	4:A:501:CNC:C4	2.36	0.56
3:E:44:ALA:HA	3:E:99:THR:HG22	1.87	0.56
3:E:97:LYS:HB3	3:E:99:THR:HG23	1.87	0.56
1:A:246:GLY:O	1:A:250:LEU:HG	2.06	0.55
1:A:13:VAL:HG12	1:A:45:LEU:HD21	1.89	0.55
1:C:84:MET:HG3	1:C:116:PHE:HB2	1.90	0.54
1:C:9:ASP:OD2	1:C:11:HIS:N	2.37	0.54
4:C:501:CNC:N23	4:C:501:CNC:C2B	2.70	0.54
3:G:119:ALA:HB3	3:G:135:TYR:HB2	1.89	0.54
1:C:318:VAL:HG22	1:C:404:LEU:HB2	1.89	0.54
1:C:155:ASP:HB3	1:C:197:ARG:NE	2.23	0.54
3:E:83:ASP:HA	3:E:86:LYS:HB2	1.89	0.54
1:A:353:GLU:HB2	1:A:365:SER:HB3	1.88	0.53
1:A:357:SER:HB2	4:A:501:CNC:H2R	1.88	0.53
1:C:247:THR:O	1:C:251:LYS:HG3	2.07	0.53
3:G:94:ASP:HB3	3:G:97:LYS:HB2	1.89	0.53
1:A:294:PRO:HB2	2:B:171:GLU:HB2	1.91	0.53
3:E:65:GLU:HG2	3:E:66:ARG:N	2.24	0.53
3:G:44:ALA:HA	3:G:99:THR:HG22	1.90	0.53
3:G:130:ARG:HH12	3:G:132:GLU:CD	2.11	0.53
1:C:21:LEU:O	1:C:24:MET:HB2	2.09	0.53
1:A:1:GLU:HB2	1:A:245:LEU:HB3	1.90	0.52
3:G:79:THR:HB	3:G:91:ILE:HD11	1.90	0.52
1:C:382:ASP:OD2	1:C:383:PRO:HA	2.09	0.52
3:E:108:GLU:O	3:E:144:VAL:HG11	2.09	0.52
1:A:197:ARG:O	1:A:200:ARG:N	2.42	0.52
1:C:197:ARG:O	1:C:201:ILE:HG13	2.09	0.52



	A	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:C:81:LYS:HE3	3:E:123:PRO:HD2	1.90	0.52	
1:C:310:GLU:CD	1:C:310:GLU:H	2.13	0.52	
1:C:141:LEU:HD13	1:C:180:MET:HE2	1.92	0.52	
1:C:226:TYR:HB3	1:C:270:MET:SD	2.50	0.52	
1:C:250:LEU:O	1:C:254:VAL:HG23	2.10	0.52	
2:B:141:LEU:HD12	2:B:160:ASP:OD2	2.10	0.51	
4:C:501:CNC:H8	4:C:501:CNC:O39	2.10	0.51	
2:D:157:ASP:N	2:D:163:ASP:OD1	2.39	0.51	
2:B:58:LYS:HD3	2:B:67:CYS:HB3	1.91	0.51	
3:G:43:CYS:HB2	3:G:57:TRP:CZ2	2.45	0.51	
1:A:98:CYS:SG	1:A:289:PRO:HB2	2.50	0.51	
2:B:59:PHE:HE2	2:B:73:ARG:HH11	1.57	0.50	
2:D:163:ASP:OD2	2:D:163:ASP:N	2.42	0.50	
1:A:154:HIS:ND1	2:D:149:THR:HG21	2.25	0.50	
4:A:501:CNC:O39	4:A:501:CNC:H8	2.11	0.50	
1:C:101:VAL:HG12	1:C:149:HIS:ND1	2.27	0.50	
1:A:338:GLU:N	1:A:391:ILE:O	2.41	0.50	
1:C:382:ASP:HB2	1:C:401:THR:HB	1.93	0.50	
1:A:236:MET:HE2	1:A:282:THR:HG22	1.93	0.50	
3:E:33:VAL:HG22	3:E:37:GLY:HA3	1.93	0.50	
3:G:64:LYS:HG2	3:G:65:GLU:N	2.27	0.50	
1:C:270:MET:HA	1:C:270:MET:HE2	1.94	0.49	
3:E:121:TYR:CE2	3:E:123:PRO:HG3	2.48	0.49	
1:C:62:TYR:HA	1:C:82:PRO:HG2	1.94	0.49	
1:C:99:GLU:HG2	1:C:102:ARG:NH2	2.28	0.49	
2:D:130:LEU:HG	3:G:95:ASN:O	2.13	0.49	
1:A:101:VAL:HG12	1:A:149:HIS:ND1	2.28	0.49	
4:C:501:CNC:C6	4:C:501:CNC:C1A	2.80	0.49	
1:C:178:ALA:HB1	1:C:208:VAL:HG13	1.94	0.48	
3:G:58:PHE:CD2	3:G:68:GLY:HA2	2.47	0.48	
4:A:501:CNC:C18	4:A:501:CNC:C20	2.92	0.48	
1:A:198:ARG:O	1:A:202:THR:HG23	2.13	0.48	
1:A:342:LYS:HD3	1:A:352:TYR:OH	2.14	0.48	
1:C:366:VAL:HG12	1:C:367:MET:HG2	1.96	0.48	
1:A:59:LYS:O	1:A:63:GLN:HB2	2.13	0.48	
3:E:88:ARG:NH2	3:E:111:ASP:OD2	2.47	0.48	
1:A:151:LYS:HE2	2:D:155:HIS:CD2	2.49	0.47	
4:A:501:CNC:H2B	4:A:501:CNC:C14	2.43	0.47	
1:A:197:ARG:NH2	7:A:605:HOH:O	2.46	0.47	
3:E:84:SER:O	3:E:88:ARG:NH1	2.48	0.47	
2:B:130:LEU:HD21	3:E:98:ASN:HB2	1.97	0.47	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:226:TYR:O	1:A:229:PRO:HD2	2.14	0.47	
2:B:135:GLY:O	2:B:148:LEU:HG	2.14	0.47	
1:A:33:ASN:HB3	1:A:36:ILE:HD12	1.96	0.47	
1:C:216:GLN:HA	1:C:221:HIS:O	2.15	0.47	
3:E:82:ALA:C	3:E:83:ASP:OD1	2.47	0.47	
4:C:501:CNC:N21	4:C:501:CNC:N3B	2.62	0.47	
4:C:501:CNC:N23	4:C:501:CNC:N3B	2.63	0.47	
1:A:315:THR:HG22	7:A:604:HOH:O	2.15	0.46	
1:A:374:ARG:HD2	1:A:374:ARG:HA	1.45	0.46	
1:A:381:ARG:HB3	1:A:387:LEU:HD21	1.96	0.46	
1:C:146:LEU:HA	1:C:146:LEU:HD23	1.58	0.46	
3:E:89:PHE:C	3:E:90:ILE:HD13	2.36	0.46	
1:A:250:LEU:HA	1:A:253:ARG:HG2	1.97	0.46	
1:A:366:VAL:HG12	1:A:367:MET:CG	2.46	0.46	
2:B:129:ARG:HD2	2:B:143:ASP:OD1	2.15	0.46	
1:A:120:GLU:O	1:A:124:ILE:HG13	2.16	0.46	
1:C:36:ILE:HD11	1:C:268:ALA:HB1	1.97	0.46	
1:C:244:GLU:HB3	1:C:247:THR:HG23	1.97	0.46	
2:D:58:LYS:HG3	2:D:69:PRO:HA	1.98	0.46	
1:A:32:LEU:HD11	1:A:57:SER:HB3	1.98	0.46	
1:A:63:GLN:HE22	5:A:503:GOL:C3	2.29	0.46	
4:C:501:CNC:C14	4:C:501:CNC:C2B	2.89	0.46	
1:A:44:SER:O	1:A:296:VAL:HG12	2.16	0.45	
1:C:33:ASN:CB	1:C:36:ILE:HG13	2.45	0.45	
1:A:307:GLN:HG2	1:A:308:THR:H	1.82	0.45	
1:A:316:LEU:HD12	1:A:317:GLN:H	1.81	0.45	
1:C:124:ILE:HD13	1:C:136:TYR:OH	2.17	0.45	
3:E:65:GLU:HG2	3:E:66:ARG:H	1.80	0.45	
1:A:256:LEU:O	1:A:260:LEU:HD12	2.16	0.45	
1:C:27:LEU:HD11	1:C:53:LEU:HD21	1.98	0.45	
3:E:61:ALA:HB3	3:E:64:LYS:HB3	1.98	0.45	
3:G:27:GLU:CD	3:G:139:GLY:H	2.20	0.45	
1:A:154:HIS:CD2	1:A:155:ASP:H	2.35	0.45	
1:C:84:MET:HE3	3:E:123:PRO:HG2	1.98	0.45	
4:C:501:CNC:H422	4:C:501:CNC:H361	1.99	0.45	
3:G:86:LYS:O	3:G:86:LYS:HG3	2.16	0.45	
1:C:312:ILE:HG22	1:C:331:VAL:O	2.17	0.45	
4:C:501:CNC:H552	4:C:501:CNC:H531	1.99	0.45	
1:C:40:LEU:HD12	1:C:40:LEU:HA	1.74	0.44	
1:C:240:MET:HG3	1:C:243:ALA:N	2.33	0.44	
1:A:290:ASP:H	5:A:502:GOL:C1	2.30	0.44	



	A h C	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:C:13:VAL:HG12	1:C:45:LEU:HD21	1.99	0.44	
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.88	0.44	
2:B:137:LEU:HB3	2:B:148:LEU:HD21	2.00	0.44	
1:C:203:MET:O	1:C:207:THR:HG23	2.17	0.44	
2:D:71:THR:HG22	2:D:72:TRP:HD1	1.83	0.44	
3:E:40:ARG:HG3	3:E:103:GLN:OE1	2.18	0.44	
1:A:16:LEU:HD21	1:A:274:LEU:HD23	1.99	0.44	
1:A:80:GLY:O	1:A:81:LYS:HB2	2.18	0.43	
1:A:95:ARG:HD2	1:A:95:ARG:HA	1.70	0.43	
4:A:501:CNC:H541	4:A:501:CNC:H602	1.54	0.43	
1:A:5:ILE:HD13	1:A:253:ARG:HB3	1.99	0.43	
1:C:55:LEU:O	1:C:58:LEU:HB2	2.18	0.43	
3:E:59:ARG:HB3	3:E:115:TYR:CE2	2.53	0.43	
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.84	0.43	
2:B:78:LEU:HD12	2:B:86:GLU:HG3	2.01	0.43	
1:A:110:VAL:HG13	1:A:146:LEU:CD2	2.49	0.43	
1:C:161:LEU:HD23	1:C:185:PHE:CZ	2.54	0.43	
3:E:89:PHE:CD2	3:E:89:PHE:N	2.86	0.43	
1:A:39:GLY:O	1:A:43:SER:HB3	2.18	0.43	
3:G:27:GLU:N	3:G:27:GLU:OE1	2.52	0.43	
1:A:2:MET:HE3	1:A:2:MET:HB3	1.92	0.42	
1:C:60:LEU:O	1:C:64:GLN:HB2	2.18	0.42	
1:C:141:LEU:HA	1:C:180:MET:CE	2.50	0.42	
3:G:69:VAL:HG13	3:G:85:VAL:HG21	2.01	0.42	
1:A:290:ASP:H	5:A:502:GOL:H2	1.83	0.42	
3:E:89:PHE:HA	3:E:103:GLN:O	2.18	0.42	
1:A:1:GLU:HB2	1:A:245:LEU:CB	2.49	0.42	
1:A:81:LYS:O	3:G:124:SER:OG	2.37	0.42	
1:A:154:HIS:HD2	7:A:618:HOH:O	2.01	0.42	
1:A:307:GLN:HG2	1:A:308:THR:N	2.35	0.42	
1:C:230:LEU:HA	1:C:230:LEU:HD12	1.81	0.42	
1:A:267:ASN:HB3	1:A:270:MET:HB2	2.00	0.42	
1:C:62:TYR:O	1:C:66:LEU:HB2	2.20	0.42	
1:C:361:PRO:HG2	1:C:392:ALA:HB2	2.01	0.42	
1:A:377:TRP:CZ3	1:A:406:LEU:HB2	2.55	0.42	
4:A:501:CNC:H18	4:A:501:CNC:H201	1.98	0.42	
3:E:91:ILE:H	3:E:91:ILE:HG13	1.67	0.42	
1:A:63:GLN:HE22	5:A:503:GOL:H31	1.85	0.42	
1:A:334:GLY:O	1:A:395:ARG:HD3	2.19	0.41	
3:E:85:VAL:HA	3:E:88:ARG:HH11	1.84	0.41	
1:C:20:LEU:HD22	1:C:36:ILE:HD13	2.02	0.41	



A tom 1	A.t.a.m. 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:G:107:LEU:HD12	3:G:144:VAL:HG21	2.02	0.41
1:C:45:LEU:HG	1:C:298:LEU:HD21	2.01	0.41
1:A:111:SER:HA	1:A:114:LYS:HD3	2.02	0.41
3:G:57:TRP:CD1	3:G:102:LEU:HB2	2.55	0.41
1:C:4:GLU:O	1:C:5:ILE:HD13	2.20	0.41
2:D:59:PHE:HE2	2:D:85:ASP:HA	1.86	0.41
3:G:74:SER:HB3	3:G:75:ARG:HG3	2.03	0.41
1:A:78:CYS:HB3	1:A:79:GLN:H	1.75	0.41
1:C:81:LYS:HD2	3:E:124:SER:O	2.21	0.41
3:E:85:VAL:HA	3:E:88:ARG:NH1	2.35	0.41
1:A:86:GLN:HG2	1:A:358:LEU:HD11	2.01	0.41
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.90	0.41
1:A:335:SER:HB3	1:A:339:ASP:HB2	2.01	0.41
1:C:139:TYR:HD2	1:C:161:LEU:CD1	2.32	0.41
1:C:176:ASP:OD1	1:C:176:ASP:N	2.50	0.41
1:C:338:GLU:N	1:C:391:ILE:O	2.50	0.41
2:D:137:LEU:HD12	2:D:138:ARG:H	1.86	0.41
1:A:16:LEU:HD12	1:A:16:LEU:HA	1.95	0.41
1:C:41:ARG:HA	1:C:41:ARG:HD2	1.80	0.40
3:E:34:GLN:O	3:E:37:GLY:N	2.53	0.40
1:C:46:GLN:NE2	1:C:297:MET:HG2	2.36	0.40
2:D:155:HIS:CD2	2:D:156:PRO:HD2	2.56	0.40
3:E:130:ARG:HD2	3:E:132:GLU:OE2	2.21	0.40
4:C:501:CNC:H562	4:C:501:CNC:H18	1.95	0.40
3:G:54:ASP:OD1	3:G:74:SER:HB2	2.21	0.40
1:A:314:VAL:HG13	1:A:400:GLU:O	2.22	0.40
2:D:137:LEU:HD12	2:D:138:ARG:N	2.36	0.40
3:G:102:LEU:HD12	3:G:102:LEU:HA	1.85	0.40
2:B:147:PRO:HD2	2:B:150:TRP:CD2	2.57	0.40
3:G:25:LEU:HD23	3:G:25:LEU:H	1.87	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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	369/409~(90%)	357~(97%)	11 (3%)	1 (0%)	41 66
1	С	376/409~(92%)	360~(96%)	14 (4%)	2~(0%)	29 54
2	В	81/147~(55%)	77~(95%)	3~(4%)	1 (1%)	13 32
2	D	77/147~(52%)	70~(91%)	7~(9%)	0	100 100
3	Ε	123/135~(91%)	111 (90%)	10 (8%)	2(2%)	9 24
3	G	117/135~(87%)	111 (95%)	5~(4%)	1 (1%)	17 40
All	All	1143/1382~(83%)	1086 (95%)	50 (4%)	7 (1%)	25 50

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

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Е	83	ASP
2	В	71	THR
1	С	81	LYS
3	Е	50	PRO
3	G	46	SER
1	А	81	LYS
1	С	383	PRO

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	322/348~(92%)	305~(95%)	17 (5%)	22 48
1	С	326/348~(94%)	303~(93%)	23 (7%)	14 34
2	В	73/129~(57%)	65~(89%)	8 (11%)	6 14
2	D	72/129~(56%)	68~(94%)	4 (6%)	21 45
3	Е	102/112~(91%)	93~(91%)	9 (9%)	10 23
3	G	100/112~(89%)	90 (90%)	10 (10%)	7 18
All	All	995/1178~(84%)	924 (93%)	71 (7%)	14 34



All	(71)	residues	with a	non-rotar	neric	sidechain	are listed	l below:
	(· - /	100101000			110110	or or o or router	0110 110000	

$\begin{array}{c ccccccccccccccccccccccccccccccccccc$
1 A 78 CYS 1 A 83 SER 1 A 176 ASP 1 A 202 THR 1 A 206 ARG 1 A 224 ASN 1 A 225 VAL 1 A 269 LEU 1 A 311 ILE 1 A 315 THR 1 A 320 SER 1 A 367 MET
1 A 83 SER 1 A 176 ASP 1 A 202 THR 1 A 206 ARG 1 A 206 ARG 1 A 224 ASN 1 A 225 VAL 1 A 269 LEU 1 A 311 ILE 1 A 315 THR 1 A 320 SER 1 A 367 MET
1 A 176 ASP 1 A 202 THR 1 A 206 ARG 1 A 224 ASN 1 A 225 VAL 1 A 253 ARG 1 A 269 LEU 1 A 311 ILE 1 A 315 THR 1 A 320 SER 1 A 367 MET
1 A 202 THR 1 A 206 ARG 1 A 224 ASN 1 A 225 VAL 1 A 253 ARG 1 A 269 LEU 1 A 311 ILE 1 A 315 THR 1 A 320 SER 1 A 367 MET
1 A 206 ARG 1 A 224 ASN 1 A 225 VAL 1 A 253 ARG 1 A 269 LEU 1 A 311 ILE 1 A 315 THR 1 A 320 SER 1 A 367 MET
1 A 224 ASN 1 A 225 VAL 1 A 253 ARG 1 A 269 LEU 1 A 311 ILE 1 A 315 THR 1 A 320 SER 1 A 367 MET
1 A 225 VAL 1 A 253 ARG 1 A 269 LEU 1 A 311 ILE 1 A 315 THR 1 A 320 SER 1 A 367 MET
1 A 253 ARG 1 A 269 LEU 1 A 311 ILE 1 A 315 THR 1 A 320 SER 1 A 367 MET
1 A 269 LEU 1 A 311 ILE 1 A 315 THR 1 A 320 SER 1 A 367 MET
1 A 311 ILE 1 A 315 THR 1 A 320 SER 1 A 367 MET
1 A 315 THR 1 A 320 SER 1 A 367 MET
1 A 320 SER 1 A 367 MET
1 A 367 MET
1 A 374 ARG
1 A 401 THR
1 A 406 LEU
2 B 64 SER
2 B 71 THR
2 B 73 ARG
2 B 128 SER
2 B 138 ARG
2 B 143 ASP
2 B 151 ARG
2 B 170 ASN
1 C 36 ILE
1 C 52 ASP
1 C 81 LYS
1 C 83 SER
1 C 108 ARG
1 C 127 ASP
1 C 129 LYS
1 C 172 HIS
1 C 176 ASP
1 C 206 ARG
1 C 209 GLN
1 C 235 LEU
1 C 238 SER
1 C 245 LEU
1 C 253 ARG
1 C 269 LEU
1 C 272 SER



Mol	Chain	Res	Type
1	С	297	MET
1	С	311	ILE
1	С	322	LEU
1	С	327	GLN
1	С	359	SER
1	С	400	GLU
2	D	54	CYS
2	D	141	LEU
2	D	149	THR
2	D	151	ARG
3	Е	25	LEU
3	Е	73	SER
3	Е	75	ARG
3	Е	89	PHE
3	Е	91	ILE
3	Е	97	LYS
3	Е	124	SER
3	Е	134	SER
3	Е	146	SER
3	G	24	GLN
3	G	25	LEU
3	G	28	SER
3	G	67	GLU
3	G	74	SER
3	G	89	PHE
3	G	91	ILE
3	G	93	ARG
3	G	96	VAL
3	G	106	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	63	GLN
1	А	261	GLN
2	В	155	HIS
2	D	60	GLN
3	Е	34	GLN
3	G	60	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)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	Bog Link Bond lengths		Bond angles				
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
5	GOL	А	503	-	$5,\!5,\!5$	0.91	0	5,5,5	1.13	0
4	CNC	А	501	-	90,103,103	<mark>3.59</mark>	42 (46%)	139,171,171	4.97	59 (42%)
5	GOL	С	502	-	$5,\!5,\!5$	1.28	1 (20%)	5,5,5	1.23	1 (20%)
4	CNC	С	501	-	90,103,103	3.62	38 (42%)	139,171,171	4.48	55 (39%)
5	GOL	А	502	-	$5,\!5,\!5$	1.28	1 (20%)	5,5,5	1.00	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
5	GOL	А	503	-	-	2/4/4/4	-
4	CNC	А	501	-	1/1/36/38	7/52/235/235	0/3/11/11
5	GOL	С	502	-	-	2/4/4/4	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CNC	С	501	-	1/1/36/38	2/52/235/235	0/3/11/11
5	GOL	А	502	-	-	2/4/4/4	-

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	501	CNC	C2R-C1R	-13.39	1.33	1.53
4	С	501	CNC	C2R-C1R	-13.29	1.33	1.53
4	С	501	CNC	C10-C9	9.85	1.67	1.39
4	А	501	CNC	C10-C9	9.57	1.66	1.39
4	А	501	CNC	C3R-C4R	-9.35	1.27	1.52
4	С	501	CNC	C10-C11	9.25	1.64	1.37
4	А	501	CNC	C10-C11	8.84	1.63	1.37
4	С	501	CNC	O6R-C1R	8.26	1.52	1.41
4	С	501	CNC	C3R-C4R	-8.20	1.30	1.52
4	А	501	CNC	C1-C19	7.78	1.75	1.54
4	А	501	CNC	O6R-C1R	7.53	1.51	1.41
4	А	501	CNC	C57-N59	7.33	1.50	1.33
4	С	501	CNC	C1-C19	7.10	1.74	1.54
4	С	501	CNC	C6-C5	6.97	1.56	1.36
4	А	501	CNC	C4-C5	6.81	1.71	1.43
4	С	501	CNC	C57-N59	6.80	1.48	1.33
4	С	501	CNC	C4-C5	6.67	1.70	1.43
4	А	501	CNC	C6-C5	6.61	1.55	1.36
4	С	501	CNC	O6R-C4R	5.88	1.58	1.45
4	С	501	CNC	C1-C2	-5.78	1.45	1.58
4	А	501	CNC	C19-N24	-5.52	1.37	1.49
4	А	501	CNC	O6R-C4R	5.45	1.57	1.45
4	С	501	CNC	C19-N24	-5.26	1.38	1.49
4	А	501	CNC	C3-C4	-5.20	1.38	1.51
4	А	501	CNC	C54-C17	-4.88	1.46	1.54
4	С	501	CNC	C50-N52	4.68	1.48	1.32
4	С	501	CNC	C38-N40	4.63	1.47	1.32
4	С	501	CNC	C54-C17	-4.48	1.46	1.54
4	С	501	CNC	C61-N62	4.45	1.47	1.32
4	С	501	CNC	C36-C7	-4.43	1.47	1.54
4	С	501	CNC	C43-N45	4.32	1.46	1.32
4	А	501	CNC	C7-C6	4.32	1.64	1.54
4	С	501	CNC	C3-C4	-4.30	1.41	1.51
4	С	501	CNC	C27-N29	4.22	1.46	1.32
4	А	501	CNC	C38-N40	4.20	1.46	1.32
4	А	501	CNC	C14-C15	4.12	1.60	1.43



7QBG

Conti	Continued from previous page								
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$		
4	С	501	CNC	C32-N33	4.10	1.46	1.32		
4	А	501	CNC	C2R-C3R	4.09	1.62	1.52		
4	С	501	CNC	C14-C15	4.05	1.59	1.43		
4	А	501	CNC	C50-N52	4.03	1.45	1.32		
4	А	501	CNC	C43-N45	4.01	1.45	1.32		
4	А	501	CNC	C27-N29	3.98	1.45	1.32		
4	А	501	CNC	C61-N62	3.96	1.45	1.32		
4	А	501	CNC	C32-N33	3.78	1.45	1.32		
4	А	501	CNC	C9-N22	3.70	1.41	1.30		
4	С	501	CNC	C2R-C3R	3.68	1.61	1.52		
4	С	501	CNC	C16-C15	3.56	1.58	1.42		
4	С	501	CNC	C9-N22	3.53	1.40	1.30		
4	С	501	CNC	C7-C6	3.52	1.62	1.54		
4	С	501	CNC	C56-C57	3.37	1.57	1.51		
4	А	501	CNC	C16-C15	3.28	1.57	1.42		
4	С	501	CNC	C17-C16	3.18	1.61	1.54		
4	С	501	CNC	C35-C5	3.08	1.57	1.50		
4	А	501	CNC	C56-C57	3.06	1.57	1.51		
4	А	501	CNC	C2-C3	3.01	1.66	1.57		
4	С	501	CNC	C12-C11	2.93	1.61	1.51		
4	А	501	CNC	C1-C2	-2.91	1.52	1.58		
4	А	501	CNC	C26-C2	2.90	1.62	1.55		
4	С	501	CNC	P-O2	2.87	1.68	1.60		
4	С	501	CNC	C14-N23	2.84	1.39	1.30		
4	А	501	CNC	C9B-N3B	-2.83	1.29	1.38		
4	А	501	CNC	C35-C5	2.76	1.56	1.50		
5	С	502	GOL	C3-C2	2.69	1.62	1.51		
4	А	501	CNC	O3-C2P	-2.69	1.38	1.45		
4	А	501	CNC	C55-C56	2.57	1.59	1.53		
4	А	501	CNC	C14-N23	2.50	1.38	1.30		
4	А	501	CNC	C8B-C9B	-2.46	1.35	1.40		
4	А	501	CNC	O63-C61	-2.45	1.16	1.24		
4	С	501	CNC	C55-C56	2.44	1.58	1.53		
4	А	501	CNC	P-O2	2.39	1.66	1.60		
4	А	501	CNC	C26-C27	2.37	1.59	1.51		
4	А	501	CNC	O58-C57	-2.32	1.18	1.23		
4	А	501	CNC	C12-C11	2.28	1.59	1.51		
4	С	501	CNC	O28-C27	-2.22	1.17	1.24		
4	С	501	CNC	C37-C38	2.15	1.58	1.51		
4	С	501	CNC	P-O3	2.14	1.66	1.60		
4	А	501	CNC	C36-C7	-2.14	1.50	1.54		
4	С	501	CNC	C26-C2	2.13	1.60	1.55		

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
5	А	502	GOL	C3-C2	2.09	1.60	1.51
4	А	501	CNC	C37-C38	2.07	1.58	1.51
4	С	501	CNC	C25-C2	-2.07	1.50	1.54
4	А	501	CNC	O44-C43	-2.03	1.17	1.24

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	С	501	CNC	C3-C4-C5	-24.20	83.04	123.81
4	А	501	CNC	C36-C7-C37	-20.48	77.04	110.80
4	А	501	CNC	C3-C4-C5	-19.46	91.02	123.81
4	А	501	CNC	C25-C2-C26	-19.29	70.71	109.71
4	С	501	CNC	C36-C7-C37	-16.29	83.96	110.80
4	А	501	CNC	C26-C2-C3	-15.35	80.27	107.41
4	А	501	CNC	C26-C2-C1	-14.35	87.65	110.01
4	С	501	CNC	C8-C9-C10	-13.43	94.32	123.32
4	С	501	CNC	C25-C2-C26	-13.21	83.00	109.71
4	А	501	CNC	C7-C6-C5	-12.84	107.87	128.07
4	А	501	CNC	C8-C9-C10	-12.79	95.70	123.32
4	С	501	CNC	C26-C2-C1	-11.43	92.20	110.01
4	С	501	CNC	C1-C19-C18	-11.37	104.99	121.81
4	А	501	CNC	C13-C14-C15	-11.32	104.74	123.81
4	А	501	CNC	C12-C11-N23	-10.71	99.88	111.48
4	А	501	CNC	C37-C7-C8	-10.19	81.08	108.39
4	А	501	CNC	C37-C7-C6	-10.18	75.12	107.12
4	С	501	CNC	C26-C2-C3	-9.76	90.15	107.41
4	С	501	CNC	C13-C14-C15	-9.72	107.44	123.81
4	С	501	CNC	C12-C11-N23	-9.38	101.32	111.48
4	А	501	CNC	C17-C16-C15	-8.97	113.09	126.73
4	С	501	CNC	C7-C6-C5	-8.97	113.96	128.07
4	А	501	CNC	C1-C19-C18	-8.93	108.60	121.81
4	С	501	CNC	C25-C2-C1	8.36	126.38	113.78
4	С	501	CNC	C30-C3-C2	-7.72	102.75	119.09
4	С	501	CNC	C18-C19-N24	7.60	113.95	101.88
4	А	501	CNC	C35-C5-C4	7.53	132.15	116.79
4	А	501	CNC	C9-C10-C11	-7.41	114.94	125.88
4	С	501	CNC	C37-C7-C8	-7.14	89.26	108.39
4	С	501	CNC	C37-C7-C6	-7.03	85.01	107.12
4	С	501	CNC	C9-C10-C11	-6.96	115.61	125.88
4	С	501	CNC	C5-C4-N21	-6.45	113.72	124.19
4	А	501	CNC	C6-C5-C4	-6.42	110.04	121.54
4	А	501	CNC	C12-C11-C10	-6.31	117.78	123.54



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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	CNC	C18-C19-N24	6.16	111.66	101.88
4	A	501	CNC	C2-C26-C27	6.12	132.43	115.22
4	A	501	CNC	C30-C3-C2	-5.99	106.40	119.09
4	С	501	CNC	C36-C7-C8	5.66	122.54	112.08
4	A	501	CNC	C36-C7-C8	5.59	122.42	112.08
4	С	501	CNC	C35-C5-C4	5.49	127.98	116.79
4	А	501	CNC	C7-C6-N22	-5.48	97.91	107.94
4	С	501	CNC	C12-C11-C10	-5.45	118.56	123.54
4	С	501	CNC	C6-C5-C4	-5.23	112.18	121.54
4	С	501	CNC	C25-C2-C3	5.18	126.22	112.96
4	С	501	CNC	C7-C6-N22	-5.17	98.49	107.94
4	А	501	CNC	C5M-C5B-C4B	-5.13	108.07	120.34
4	А	501	CNC	C5M-C5B-C6B	5.08	131.14	120.74
4	А	501	CNC	C25-C2-C3	4.89	125.47	112.96
4	С	501	CNC	C8-C7-C6	4.84	109.24	100.92
4	А	501	CNC	C16-C15-C14	-4.80	114.72	121.30
4	А	501	CNC	C5-C4-N21	-4.73	116.52	124.19
4	А	501	CNC	C7-C37-C38	4.72	128.45	114.25
4	С	501	CNC	C19-N24-C16	-4.66	104.42	111.96
4	А	501	CNC	C41-C8-C9	4.64	119.38	111.19
4	С	501	CNC	C16-C15-C14	-4.59	115.00	121.30
4	С	501	CNC	C17-C16-C15	-4.46	119.94	126.73
4	А	501	CNC	C5-C6-N22	-4.44	117.10	123.88
4	А	501	CNC	C19-C1-N21	-4.42	96.06	101.67
4	С	501	CNC	C1-C2-C3	4.29	107.08	101.60
4	А	501	CNC	C20-C1-C2	-4.27	106.15	113.28
4	А	501	CNC	C13-C12-C11	-4.10	95.31	100.90
4	С	501	CNC	C35-C5-C6	-3.93	116.18	122.43
4	С	501	CNC	C41-C8-C9	3.69	117.70	111.19
4	А	501	CNC	O28-C27-N29	-3.60	112.68	122.50
4	A	501	CNC	C60-C18-C17	-3.59	107.04	115.74
4	C	$50\overline{1}$	CNC	C60-C18-C17	-3.56	$107.1\overline{2}$	115.74
4	A	501	CNC	C25-C2-C1	3.55	119.14	113.78
4	C	501	CNC	C5M-C5B-C4B	-3.54	111.88	120.34
4	A	501	CNC	C15-C14-N23	-3.47	119.80	126.68
4	C	$50\overline{1}$	$CN\overline{C}$	O28-C27-N29	-3.45	113.09	122.50
4	С	501	CNC	C30-C31-C32	-3.42	100.98	112.59
4	C	501	CNC	C55-C17-C18	-3.41	104.56	111.15
4	A	501	$CN\overline{C}$	C17-C16-N24	-3.27	105.37	110.87
4	A	501	CNC	C18-C17-C16	3.25	105.55	100.33
4	С	501	CNC	C5M-C5B-C6B	3.25	127.39	120.74
4	C	501	CNC	C5-C6-N22	-3.12	119.11	123.88



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Mol	Chain	Res	Type	Atoms	Ζ	Observed(°)	$Ideal(^{o})$
4	А	501	CNC	C35-C5-C6	-2.98	117.69	122.43
4	С	501	CNC	C55-C17-C16	2.96	122.61	116.24
4	С	501	CNC	C26-C27-N29	2.90	125.71	116.52
4	С	501	CNC	C3R-C2R-C1R	2.84	106.19	99.89
4	А	501	CNC	C19-N24-C16	-2.81	107.41	111.96
4	А	501	CNC	C6M-C6B-C5B	-2.76	115.08	120.74
4	С	501	CNC	C36-C7-C6	2.75	126.71	112.40
4	А	501	CNC	C2-C1-C19	2.74	123.42	118.72
4	С	501	CNC	O2-C3R-C2R	-2.71	101.86	111.68
4	С	501	CNC	C2-C1-C19	-2.69	114.11	118.72
4	С	501	CNC	C10-C11-N23	-2.62	120.62	124.93
4	С	501	CNC	C13-C14-N23	2.61	115.00	109.39
4	А	501	CNC	C5R-C4R-C3R	-2.61	106.54	114.85
4	А	501	CNC	C20-C1-N21	2.58	114.50	110.27
4	А	501	CNC	C41-C8-C7	-2.55	107.12	114.14
4	С	501	CNC	C18-C60-C61	2.42	120.01	113.97
4	С	501	CNC	C53-C15-C16	2.41	125.56	120.37
4	А	501	CNC	C3R-C2R-C1R	2.38	105.17	99.89
4	А	501	CNC	C53-C15-C14	2.35	121.58	116.79
4	А	501	CNC	C2P-C1P-N59	2.34	116.39	112.93
4	А	501	CNC	O39-C38-N40	-2.32	116.17	122.50
4	С	501	CNC	C13-C12-C11	-2.30	97.76	100.90
4	С	501	CNC	O58-C57-N59	-2.22	118.82	123.01
4	А	501	CNC	C8-C7-C6	2.20	104.71	100.92
4	А	501	CNC	C60-C61-N62	2.20	121.51	116.21
4	А	501	CNC	C7B-C8B-C9B	-2.18	118.39	120.54
4	А	501	CNC	O63-C61-N62	-2.14	116.65	122.50
4	С	501	CNC	C2-C26-C27	2.14	121.23	115.22
4	А	501	CNC	C2R-C3R-C4R	2.13	107.00	103.22
4	А	501	CNC	C47-C12-C46	-2.12	105.77	109.35
4	А	501	CNC	C10-C11-N23	-2.11	121.46	124.93
5	С	502	GOL	O2-C2-C3	2.11	118.42	109.12
4	А	501	CNC	C15-C16-N24	-2.10	120.25	122.38
4	С	501	CNC	C20-C1-C19	2.05	114.34	110.23
4	С	501	CNC	C12-C13-C14	-2.02	99.18	101.86
4	А	501	CNC	C1-C2-C3	2.02	104.17	101.60
4	С	501	CNC	O3-C2P-C1P	2.02	110.94	106.92
4	С	501	CNC	C42-C41-C8	-2.01	108.92	114.73
4	С	501	CNC	O7R-C2R-C3R	-2.00	105.48	111.17

All (2) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
4	А	501	CNC	N24
4	С	501	CNC	N24

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	501	CNC	C2P-O3-P-O2
5	А	503	GOL	O1-C1-C2-C3
4	А	501	CNC	C3R-C4R-C5R-O8R
4	А	501	CNC	C18-C17-C55-C56
4	А	501	CNC	C16-C17-C55-C56
4	С	501	CNC	C13-C48-C49-C50
5	А	502	GOL	C1-C2-C3-O3
5	С	502	GOL	C1-C2-C3-O3
5	А	502	GOL	O2-C2-C3-O3
5	А	503	GOL	O1-C1-C2-O2
4	А	501	CNC	O6R-C4R-C5R-O8R
4	А	501	CNC	C2R-C3R-O2-P
5	С	502	GOL	O2-C2-C3-O3
4	А	501	CNC	C4R-C3R-O2-P
4	С	501	CNC	C17-C18-C60-C61

There are no ring outliers.

4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	503	GOL	2	0
4	А	501	CNC	13	0
4	С	501	CNC	10	0
5	А	502	GOL	3	0

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







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q < 0.9
1	А	381/409~(93%)	0.10	10 (2%) 56 57	32, 49, 76, 105	0
1	С	388/409~(94%)	0.23	17 (4%) 34 33	36, 58, 92, 122	0
2	В	85/147~(57%)	0.53	6 (7%) 16 14	44, 75, 96, 107	0
2	D	81/147~(55%)	0.55	8 (9%) 7 5	45, 76, 99, 112	0
3	Ε	125/135~(92%)	0.64	16 (12%) 3 3	49, 69, 96, 106	0
3	G	121/135~(89%)	1.25	30 (24%) 0 0	52, 90, 117, 213	0
All	All	1181/1382 (85%)	0.38	87 (7%) 14 12	32, 61, 100, 213	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Е	95	ASN	6.3
3	G	87	GLY	6.2
3	G	34	GLN	6.0
3	G	89	PHE	5.8
3	G	96	VAL	5.5
1	С	304	THR	5.3
2	D	172	ILE	4.5
2	D	168	GLY	4.4
2	D	171	GLU	4.3
3	Ε	96	VAL	3.9
1	С	243	ALA	3.8
3	G	97	LYS	3.8
3	Ε	146	SER	3.8
3	G	145	SER	3.8
3	Е	98	ASN	3.7
3	G	36	GLY	3.6
2	D	53	SER	3.6
3	G	31	GLY	3.6
3	Е	97	LYS	3.5



Mol	Chain	Res	Type	RSRZ	
1	А	78	CYS	3.5	
2	В	129	ARG	3.5	
3	G	39	LEU	3.4	
3	G	30	GLY	3.4	
2	В	128	SER	3.4	
2	В	62	ARG	3.3	
3	G	37	GLY	3.3	
2	В	76	ARG	3.2	
1	С	397	LYS	3.0	
3	G	115	TYR	3.0	
3	G	107	LEU	3.0	
2	D	73	ARG	3.0	
3	G	110	GLU	3.0	
3	G	82	ALA	3.0	
3	G	90	ILE	2.9	
3	G	140	THR	2.9	
1	С	321	LEU	2.9	
3	G	86	LYS	2.9	
2	D	88	GLU	2.8	
1	С	240	MET	2.8	
1	С	383	PRO	2.8	
3	G	59	ARG	2.8	
1	С	322	LEU	2.8	
3	G	144	VAL	2.7	
1	А	2	MET	2.7	
3	G	105	ASN	2.7	
1	С	303	GLU	2.7	
1	С	9	ASP	2.6	
3	Е	147	HIS	2.6	
3	G	78	SER	2.6	
3	G	94	ASP	2.5	
1	С	329	ILE	2.5	
3	G	58	PHE	2.5	
3	Е	145	SER	2.4	
1	С	305	ILE	2.4	
3	G	72	ILE	2.4	
1	A	163	TYR	2.4	
1	С	145	ALA	2.4	
3	Е	64	LYS	2.4	
1	A	244	GLU	2.4	
3	G	88	ARG	2.4	
3	Е	32	LEU	2.4	



Mol	Chain	Res	Type	RSRZ
3	G	32	LEU	2.3
1	С	306	PRO	2.3
3	Е	101	TYR	2.3
3	G	55	ILE	2.3
1	А	239	PRO	2.3
1	А	80	GLY	2.3
2	В	142	SER	2.3
1	С	331	VAL	2.3
2	D	71	THR	2.2
2	В	143	ASP	2.2
3	Е	89	PHE	2.2
3	Е	94	ASP	2.2
1	А	147	CYS	2.2
1	А	308	THR	2.2
1	С	398	ASP	2.2
2	D	62	ARG	2.2
1	А	300	PRO	2.2
3	Е	102	LEU	2.1
3	Е	100	VAL	2.1
3	G	95	ASN	2.1
1	А	149	HIS	2.1
1	С	316	LEU	2.1
1	С	246	GLY	2.1
3	G	102	LEU	2.0
3	Е	75	ARG	2.0
3	Е	141	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
5	GOL	А	502	6/6	0.72	0.47	$53,\!56,\!60,\!66$	0
5	GOL	С	502	6/6	0.88	0.26	59,63,67,70	0
4	CNC	А	501	93/93	0.93	0.25	$27,\!40,\!48,\!57$	7
5	GOL	А	503	6/6	0.94	0.13	58,66,67,70	0
4	CNC	С	501	93/93	0.94	0.21	$35,\!46,\!53,\!66$	11
6	CA	В	201	1/1	0.94	0.14	70,70,70,70	0
6	CA	Е	201	1/1	0.95	0.16	59, 59, 59, 59, 59	0
6	CA	D	202	1/1	0.97	0.10	75,75,75,75	0
6	CA	В	202	1/1	0.98	0.15	50,50,50,50	0
6	CA	G	201	1/1	0.98	0.12	56, 56, 56, 56	0
6	CA	D	201	1/1	0.99	0.23	47,47,47,47	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.

