

Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 - 11:07 AM BST

PDB ID	:	1Z1N
Title	:	Crystal Structure of the sixteen heme cytochrome from Desulfovibrio gigas
Authors	:	Santos-Silva, T.; Dias, J.M.; Romao, M.J.
Deposited on	:	2005-03-04
Resolution	:	2.10 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	$7.0.044 \ (Gargrove)$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	5197(2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647(2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain						
1	Х	560	6%	21%	•	8%			
2	А	2	50%	50%					

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	NAG	А	1	X	-	-	-
5	GOL	Х	803	-	-	Х	-



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4998 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 sixteen heme cytochrome.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	X	516	Total 3837	$ m C \ 2355$	N 703	O 739	S 40	0	0	0

• Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-allopyranose-(1-3)-2-ace tamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	А	2	Total C N O 28 16 2 10	0	0	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Х	3	Total Zn 3 3	0	0

• Molecule 4 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).





Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	
4	v	1	Total	С	Fe	Ν	Ο	0	0	
4	A	1	43	34	1	4	4	0	0	
4	v	1	Total	С	Fe	Ν	Ο	0	0	
4	Λ	1	43	34	1	4	4	0	0	
4	v	1	Total	С	Fe	Ν	Ο	0	0	
4	Λ	1	43	34	1	4	4	0	0	
4	v	1	Total	С	Fe	Ν	Ο	0	0	
4	Λ	1	43	34	1	4	4	0	0	
4	v	1	Total	С	Fe	Ν	Ο	0	0	
4	Λ	L	43	34	1	4	4	0	0	
4	v	1	Total	С	Fe	Ν	Ο	0	0	
4	Λ	I	43	34	1	4	4	0	0	
4	X	x	1	Total	С	Fe	Ν	Ο	0	0
4		I	43	34	1	4	4	0	0	
4	v	1	Total	С	Fe	Ν	Ο	0	0	
4	Λ	I	43	34	1	4	4	0	0	
4	v	v	1	Total	С	Fe	Ν	Ο	0	0
4	Λ	I	43	34	1	4	4	0	0	
4	v	1	Total	С	Fe	Ν	Ο	0	0	
4	Λ	I	43	34	1	4	4	0	0	
4	v	1	Total	С	Fe	Ν	Ο	0	0	
-1	Δ	L	43	34	1	4	4	0	0	
4	v	1	Total	С	Fe	Ν	Ο	0	0	
-1	Δ	L	43	34	1	4	4	0	0	
	x	1	Total	C	Fe	N	0		0	
		L	43	34	1	4	4		U	
	x	1	Total	$\overline{\mathrm{C}}$	Fe	N	0	0	0	
- T		L L	43	34	1	4	4		U	



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Mol	Chain	Residues		\mathbf{At}	\mathbf{oms}			ZeroOcc	AltConf
4	v	1	Total	С	Fe	Ν	Ο	0	0
4	Λ	L	43	34	1	4	4	0	0
4	v	1	Total	С	Fe	Ν	Ο	0	0
4	Λ		43	34	1	4	4	0	0

• Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Х	412	Total O 412 412	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: sixteen heme cytochrome

• Molecule 2: 2-acetamido-2-deoxy-beta-D-allopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucop yranose

Chain A: 50% 50%

NAG1 NAA2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	88.89Å 90.80Å 83.93 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	25.00 - 2.10	Depositor
Resolution (A)	24.81 - 2.10	EDS
% Data completeness	98.2 (25.00-2.10)	Depositor
(in resolution range)	98.2(24.81-2.10)	EDS
R _{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.46 (at 2.10 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
D D	0.194 , 0.260	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.204 , 0.264	DCC
R_{free} test set	1979 reflections (5.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	44.3	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 56.1	EDS
L-test for twinning ²	$< L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4998	wwPDB-VP
Average B, all atoms $(Å^2)$	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.19% 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.



 $^{^1 {\}rm Intensities}$ 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: GOL, ZN, NAA, NAG, HEC

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	nd lengths	Bond angles	
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	Х	1.00	6/3925~(0.2%)	0.98	8/5326~(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	Х	0	1

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Х	479	CYS	CB-SG	6.77	1.93	1.82
1	Х	276	VAL	CB-CG2	6.29	1.66	1.52
1	Х	53	CYS	CB-SG	-5.78	1.72	1.81
1	Х	340	CYS	CB-SG	5.38	1.91	1.82
1	Х	455	PHE	CE1-CZ	5.08	1.47	1.37
1	Х	521	CYS	CB-SG	-5.08	1.73	1.81

All (6) bond length outliers are listed below:

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	389	ARG	NE-CZ-NH2	-11.92	114.34	120.30
1	Х	389	ARG	NE-CZ-NH1	10.31	125.45	120.30
1	Х	448	LYS	CD-CE-NZ	-7.46	94.53	111.70
1	Х	291	VAL	CG1-CB-CG2	7.42	122.77	110.90
1	Х	291	VAL	CB-CA-C	-7.21	97.70	111.40
1	Х	126	ASP	CB-CG-OD1	6.43	124.09	118.30
1	Х	457	GLY	N-CA-C	-5.93	98.27	113.10



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Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	254	VAL	CB-CA-C	-5.54	100.87	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Х	424	LYS	Peptide

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	Х	3837	0	3662	154	2
2	А	28	0	25	1	0
3	Х	3	0	0	0	0
4	Х	688	0	495	112	2
5	Х	30	0	40	6	0
6	Х	412	0	0	20	2
All	All	4998	0	4222	182	3

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 22.

All (182) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:50:CYS:SG	4:X:601:HEC:HAB	1.37	1.63
1:X:152:CYS:SG	4:X:604:HEC:HAC	1.54	1.44
1:X:524:CYS:SG	4:X:616:HEC:CAC	2.12	1.36
1:X:85:CYS:SG	4:X:602:HEC:CAB	2.14	1.35
1:X:88:CYS:SG	4:X:602:HEC:HAC	1.67	1.33
1:X:203:CYS:SG	4:X:606:HEC:HAB	1.69	1.33
1:X:293:CYS:SG	4:X:608:HEC:CAC	2.15	1.32
1:X:152:CYS:SG	4:X:604:HEC:CAC	2.24	1.25
1:X:50:CYS:SG	4:X:601:HEC:CAB	2.24	1.24



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:225:CYS:SG	4:X:607:HEC:CAC	2.27	1.23
1:X:53:CYS:SG	4:X:601:HEC:CAC	2.27	1.21
1:X:421:MET:O	6:X:1312:HOH:O	1.61	1.19
1:X:521:CYS:SG	4:X:616:HEC:HAB	1.73	1.16
1:X:108:CYS:SG	4:X:603:HEC:CAC	2.37	1.11
1:X:85:CYS:SG	4:X:602:HEC:HAB	1.93	1.07
1:X:340:CYS:SG	4:X:610:HEC:HAC	1.90	1.06
1:X:482:CYS:SG	4:X:614:HEC:HAC	1.91	1.05
1:X:261:ASN:OD1	6:X:1190:HOH:O	1.73	1.04
1:X:337:CYS:SG	4:X:610:HEC:HAB	2.00	1.00
1:X:108:CYS:SG	4:X:603:HEC:HAC	2.03	0.95
4:X:614:HEC:O1D	5:X:803:GOL:H32	1.65	0.95
1:X:53:CYS:SG	4:X:601:HEC:HAC	2.04	0.95
1:X:524:CYS:SG	4:X:616:HEC:CBC	2.55	0.94
1:X:120:THR:HG21	1:X:226:HIS:O	1.68	0.94
1:X:225:CYS:SG	4:X:607:HEC:HAC	2.13	0.89
1:X:186:VAL:HG22	1:X:189:ASP:HA	1.55	0.85
4:X:616:HEC:O2D	6:X:1046:HOH:O	1.94	0.85
1:X:359:GLN:HE22	1:X:362:ALA:H	1.21	0.84
1:X:344:GLN:OE1	1:X:348:ARG:NH2	2.10	0.84
1:X:337:CYS:SG	4:X:610:HEC:CBB	2.67	0.82
1:X:84:ASN:O	6:X:1230:HOH:O	1.99	0.80
4:X:602:HEC:HMC1	4:X:602:HEC:HBC3	1.63	0.80
1:X:253:LEU:HD21	4:X:608:HEC:HBD2	1.64	0.79
1:X:268:TRP:HE1	1:X:382:GLN:HE21	1.30	0.78
1:X:524:CYS:SG	4:X:616:HEC:C3C	2.71	0.78
1:X:293:CYS:SG	4:X:608:HEC:CBC	2.73	0.77
1:X:293:CYS:SG	4:X:608:HEC:HAC	2.23	0.77
1:X:524:CYS:SG	4:X:616:HEC:HBC3	2.26	0.76
1:X:310:CYS:SG	4:X:609:HEC:CAC	2.73	0.76
1:X:120:THR:CG2	1:X:226:HIS:O	2.34	0.76
1:X:37:GLU:OE2	6:X:1114:HOH:O	2.03	0.76
1:X:115:GLU:O	1:X:118:THR:HG22	1.86	0.75
1:X:173:CYS:SG	4:X:605:HEC:CBB	2.77	0.73
1:X:340:CYS:SG	4:X:610:HEC:C3C	2.77	0.72
1:X:225:CYS:SG	4:X:607:HEC:C3C	2.77	0.71
1:X:293:CYS:SG	4:X:608:HEC:C3C	2.79	0.70
4:X:606:HEC:CBC	4:X:606:HEC:HMC1	2.22	0.69
1:X:181:PRO:HB3	1:X:192:VAL:O	1.93	0.68
1:X:482:CYS:SG	4:X:614:HEC:C3C	2.81	0.68
1:X:482:CYS:SG	4:X:614:HEC:CBC	2.82	0.68



	• • • • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:53:CYS:SG	4:X:601:HEC:C3C	2.82	0.68
1:X:14:ASP:CB	1:X:37:GLU:HG3	2.24	0.67
1:X:386:LYS:NZ	4:X:608:HEC:O2A	2.22	0.67
1:X:426:ASP:HB2	1:X:528:LYS:NZ	2.11	0.66
1:X:37:GLU:CD	6:X:1114:HOH:O	2.34	0.66
1:X:490:ARG:NH2	6:X:1261:HOH:O	2.28	0.66
1:X:405:LYS:HB2	6:X:1142:HOH:O	1.96	0.65
1:X:521:CYS:SG	4:X:616:HEC:C3B	2.84	0.65
4:X:605:HEC:HMB1	4:X:605:HEC:HBB3	1.79	0.64
1:X:173:CYS:SG	4:X:605:HEC:C3B	2.84	0.63
1:X:85:CYS:SG	4:X:602:HEC:C3B	2.87	0.63
1:X:337:CYS:SG	4:X:610:HEC:C3B	2.86	0.62
4:X:612:HEC:O1D	5:X:804:GOL:O2	2.17	0.62
4:X:615:HEC:CGA	6:X:1231:HOH:O	2.47	0.62
4:X:614:HEC:HMC1	4:X:614:HEC:HBC3	1.80	0.62
1:X:359:GLN:NE2	1:X:362:ALA:H	1.93	0.62
1:X:524:CYS:SG	4:X:616:HEC:HAC	2.31	0.60
4:X:602:HEC:HMC1	4:X:602:HEC:CBC	2.30	0.60
1:X:101:GLN:O	1:X:102:ALA:HB2	2.02	0.60
1:X:104:GLU:HB3	1:X:107:ARG:HG3	1.83	0.60
1:X:36:HIS:HE1	4:X:601:HEC:NB	1.99	0.59
1:X:152:CYS:SG	4:X:604:HEC:C3C	2.91	0.59
1:X:198:ALA:O	1:X:202:SER:HB2	2.03	0.58
1:X:201:GLU:O	1:X:205:ASN:HB2	2.03	0.58
1:X:14:ASP:HB3	1:X:37:GLU:HG3	1.85	0.58
1:X:349:LYS:HE3	1:X:513:GLN:NE2	2.18	0.58
4:X:601:HEC:C3A	4:X:607:HEC:HBB2	2.34	0.58
1:X:261:ASN:N	6:X:1190:HOH:O	2.37	0.57
1:X:88:CYS:HG	4:X:602:HEC:HAC	1.65	0.57
1:X:458:ASP:O	1:X:461:THR:HG23	2.04	0.57
1:X:50:CYS:HG	4:X:601:HEC:CAB	2.14	0.57
1:X:152:CYS:HG	4:X:604:HEC:CAC	2.17	0.57
1:X:337:CYS:HG	4:X:610:HEC:HAB	1.67	0.57
1:X:437:LYS:HE3	4:X:615:HEC:O1D	2.04	0.57
1:X:207:HIS:O	1:X:211:ARG:HG3	2.05	0.57
4:X:610:HEC:HBD2	4:X:610:HEC:HMD1	1.86	0.57
1:X:437:LYS:HZ1	4:X:615:HEC:CGA	2.04	0.56
1:X:335:THR:HB	4:X:609:HEC:HMA2	1.88	0.56
4:X:606:HEC:HMB1	4:X:606:HEC:HBB3	1.87	0.56
1:X:421:MET:HE3	4:X:616:HEC:HAA2	1.87	0.56
4:X:613:HEC:HMB1	4:X:613:HEC:HBB3	1.87	0.55



	las page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:421:MET:CE	4:X:616:HEC:HAA2	2.37	0.55
1:X:434:PRO:HG3	4:X:615:HEC:HBA1	1.89	0.55
1:X:359:GLN:HE22	1:X:362:ALA:N	2.00	0.55
1:X:43:LEU:HD12	4:X:601:HEC:HMC1	1.89	0.54
1:X:486:PRO:HD2	1:X:489:GLU:HG3	1.89	0.54
1:X:400:LYS:O	1:X:402:GLU:N	2.40	0.54
1:X:117:ALA:HA	1:X:120:THR:HG22	1.89	0.54
1:X:120:THR:HG23	6:X:976:HOH:O	2.08	0.53
1:X:426:ASP:HB2	1:X:528:LYS:HZ2	1.73	0.53
4:X:606:HEC:HBC3	4:X:606:HEC:HMC1	1.88	0.53
4:X:615:HEC:O1A	6:X:1231:HOH:O	2.19	0.53
1:X:437:LYS:CE	4:X:615:HEC:O1A	2.56	0.53
1:X:340:CYS:SG	4:X:610:HEC:CBC	2.93	0.53
4:X:608:HEC:HMB1	4:X:608:HEC:HBB3	1.89	0.52
1:X:348:ARG:NH1	6:X:1010:HOH:O	2.29	0.52
1:X:120:THR:CG2	6:X:976:HOH:O	2.57	0.52
1:X:456:HIS:O	1:X:461:THR:HG21	2.08	0.51
4:X:614:HEC:O1D	5:X:803:GOL:C2	2.55	0.51
1:X:140:ARG:HD3	6:X:1148:HOH:O	2.11	0.51
1:X:143:VAL:HG21	1:X:147:GLU:HG2	1.92	0.50
1:X:150:LYS:O	6:X:1194:HOH:O	2.19	0.50
1:X:40:THR:HG22	4:X:601:HEC:HBB2	1.93	0.50
1:X:509:HIS:CE1	1:X:516:PRO:HD2	2.47	0.50
1:X:88:CYS:SG	4:X:602:HEC:C3C	2.95	0.50
1:X:79:GLU:HG3	6:X:1161:HOH:O	2.12	0.49
4:X:614:HEC:O2D	5:X:803:GOL:H2	2.12	0.49
1:X:143:VAL:CG1	1:X:147:GLU:HB3	2.42	0.49
1:X:101:GLN:O	1:X:102:ALA:CB	2.61	0.49
1:X:329:HIS:HE1	4:X:612:HEC:C4A	2.26	0.49
1:X:174:VAL:HG12	1:X:174:VAL:O	2.11	0.49
1:X:396:ILE:HG22	1:X:400:LYS:HE2	1.94	0.49
1:X:491:THR:H	1:X:494:GLN:HE21	1.61	0.49
4:X:606:HEC:HBC2	4:X:606:HEC:HMC1	1.92	0.49
1:X:329:HIS:HE1	4:X:612:HEC:NA	2.07	0.48
1:X:482:CYS:HG	4:X:614:HEC:HAC	1.74	0.48
1:X:456:HIS:O	1:X:461:THR:CG2	2.62	0.48
1:X:293:CYS:SG	4:X:608:HEC:HBC3	2.52	0.48
4:X:615:HEC:HBB3	4:X:615:HEC:HMB1	1.96	0.48
1:X:14:ASP:CG	1:X:37:GLU:HG3	2.33	0.47
1:X:203:CYS:SG	4:X:606:HEC:C3B	2.98	0.47
1:X:509:HIS:HE1	1:X:516:PRO:HD2	1.80	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:X:609:HEC:HBC2	4:X:609:HEC:HMC1	1.97	0.46
4:X:616:HEC:HMB1	4:X:616:HEC:HBB3	1.97	0.46
1:X:444:GLU:HG3	1:X:445:GLU:N	2.30	0.46
1:X:143:VAL:HG11	1:X:147:GLU:HB3	1.97	0.46
1:X:143:VAL:HG22	1:X:144:LYS:H	1.81	0.46
1:X:345:ALA:O	1:X:351:CYS:HB2	2.16	0.45
1:X:247:GLN:HB3	4:X:608:HEC:CHB	2.46	0.45
4:X:614:HEC:O1A	5:X:803:GOL:C3	2.61	0.45
1:X:221:LEU:HD21	4:X:601:HEC:HBB3	1.97	0.45
1:X:133:HIS:HB3	4:X:604:HEC:HBC3	1.97	0.45
1:X:369:ILE:HG23	6:X:1004:HOH:O	2.17	0.45
1:X:185:PRO:HA	1:X:186:VAL:HB	1.98	0.45
1:X:426:ASP:HB2	1:X:528:LYS:HZ1	1.78	0.45
1:X:203:CYS:HB2	4:X:607:HEC:HBC2	1.99	0.45
1:X:133:HIS:HB3	4:X:604:HEC:CBC	2.47	0.44
1:X:346:ASN:ND2	1:X:356:ALA:HA	2.33	0.44
1:X:203:CYS:SG	4:X:606:HEC:CBB	2.96	0.43
1:X:283:HIS:HB3	4:X:608:HEC:HBC2	2.00	0.43
4:X:610:HEC:HBC3	4:X:610:HEC:HMC1	2.01	0.43
1:X:454:HIS:CD2	4:X:610:HEC:HMA3	2.53	0.43
1:X:512:MET:O	1:X:513:GLN:HB2	2.18	0.43
4:X:610:HEC:HMC1	4:X:610:HEC:CBC	2.48	0.43
1:X:53:CYS:CB	4:X:601:HEC:C3C	2.97	0.43
1:X:85:CYS:SG	4:X:602:HEC:CBB	3.02	0.43
1:X:268:TRP:HB3	1:X:377:PRO:O	2.19	0.43
1:X:199:SER:O	1:X:203:CYS:SG	2.76	0.43
1:X:524:CYS:HG	4:X:616:HEC:CAC	2.22	0.43
1:X:45:LYS:C	1:X:47:ALA:H	2.22	0.42
1:X:360:LYS:NZ	6:X:1043:HOH:O	2.21	0.42
1:X:43:LEU:CD1	4:X:601:HEC:HMC1	2.48	0.42
1:X:468:HIS:HD1	5:X:803:GOL:C1	2.32	0.42
1:X:17:VAL:HG22	1:X:33:VAL:HG22	2.02	0.41
4:X:602:HEC:HMB1	4:X:602:HEC:HBB3	2.01	0.41
1:X:261:ASN:HD22	2:A:1:NAG:C7	2.34	0.41
1:X:491:THR:H	1:X:494:GLN:NE2	2.17	0.41
1:X:88:CYS:HG	4:X:602:HEC:CAC	2.21	0.41
1:X:50:CYS:HB2	1:X:61:LEU:HD21	2.01	0.41
1:X:40:THR:CG2	4:X:601:HEC:HBB2	2.50	0.41
1:X:37:GLU:HG2	6:X:1114:HOH:O	2.21	0.41
1:X:320:ASN:HD22	1:X:320:ASN:HA	1.64	0.41
4:X:608:HEC:HBC3	4:X:608:HEC:HMC1	2.01	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:504:GLN:CB	4:X:614:HEC:HMB2	2.50	0.41
1:X:33:VAL:HG12	1:X:33:VAL:O	2.21	0.41
1:X:461:THR:O	4:X:611:HEC:HMD2	2.21	0.41
4:X:610:HEC:HHB	4:X:610:HEC:HMA1	1.85	0.41
1:X:337:CYS:SG	4:X:610:HEC:HBB3	2.58	0.41
1:X:368:CYS:HA	4:X:612:HEC:CHC	2.51	0.40
1:X:310:CYS:SG	4:X:609:HEC:C3C	3.09	0.40
1:X:225:CYS:HG	4:X:607:HEC:HAC	1.83	0.40
1:X:88:CYS:SG	4:X:602:HEC:CBC	3.01	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:401:ASP:O	6:X:1234:HOH:O[3_546]	1.75	0.45
4:X:613:HEC:O2A	6:X:1304:HOH:O[3_556]	2.14	0.06
1:X:437:LYS:NZ	4:X:615:HEC:O2D[2_565]	2.15	0.05

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	X	510/560 (91%)	484 (95%)	21 (4%)	5 (1%)	15 11	

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Х	102	ALA
1	Х	160	GLN
1	Х	150	LYS
1	Х	161	LYS
1	Х	185	PRO



5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Х	410/450 (91%)	382~(93%)	28 (7%)	16 13	

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Х	18	ILE
1	Х	26	LYS
1	Х	43	LEU
1	Х	48	LYS
1	Х	72	THR
1	Х	93	VAL
1	Х	120	THR
1	Х	146	ASP
1	Х	190	ARG
1	Х	202	SER
1	Х	217	SER
1	Х	245	ARG
1	Х	254	VAL
1	Х	291	VAL
1	Х	299	THR
1	Х	320	ASN
1	Х	359	GLN
1	Х	405	LYS
1	Х	415	LYS
1	Х	421	MET
1	Х	458	ASP
1	Х	461	THR
1	Х	468	HIS
1	Х	472	PRO
1	Х	478	LYS
1	Х	488	GLN
1	Х	489	GLU
1	Х	522	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such



Mol	Chain	Res	Type
1	Х	80	GLN
1	Х	231	GLN
1	Х	320	ASN
1	Х	330	GLN
1	Х	346	ASN
1	Х	359	GLN
1	Х	382	GLN
1	Х	494	GLN
1	Х	513	GLN

sidechains are listed below:

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)

2 monosaccharides are modelled in this entry.

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

Mal	Tuno	Chain	Dog	Tink	Bo	ond leng	ths	B	ond ang	les
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	А	1	1,2	14,14,15	0.77	1 (7%)	17,19,21	2.82	<u>6 (35%)</u>
2	NAA	А	2	2	14,14,15	0.87	1 (7%)	17,19,21	1.17	1 (5%)

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	NAG	А	1	1,2	1/1/5/7	2/6/23/26	0/1/1/1
2	NAA	А	2	2	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(\operatorname{\AA})$
2	А	2	NAA	C8-C7	2.72	1.56	1.50
2	А	1	NAG	C3-C2	2.30	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	1	NAG	O3-C3-C2	6.75	123.43	109.47
2	А	1	NAG	C1-O5-C5	5.51	119.66	112.19
2	А	1	NAG	C3-C4-C5	-4.69	101.87	110.24
2	А	1	NAG	O4-C4-C5	2.94	116.59	109.30
2	А	2	NAA	C3-C4-C5	2.78	115.21	110.24
2	А	1	NAG	C1-C2-N2	-2.70	105.88	110.49
2	А	1	NAG	O4-C4-C3	2.33	115.74	110.35

All (1) chirality outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atom
2	А	1	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	1	NAG	O5-C5-C6-O6
2	А	1	NAG	C4-C5-C6-O6
2	А	2	NAA	C8-C7-N2-C2
2	А	2	NAA	O7-C7-N2-C2
2	А	2	NAA	O5-C5-C6-O6
2	А	2	NAA	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	1	NAG	1	0



5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 for Mogul analysis.

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

Mal	Tuno	Chain	Dog	Tink	B	Bond lengths			Bond angles		
WIOI	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
4	HEC	Х	612	1	$26,\!50,\!50$	1.90	7 (26%)	18,82,82	4.01	11 (61%)	
4	HEC	Х	602	1	26,50,50	2.47	10 (38%)	18,82,82	2.31	<mark>6 (33%)</mark>	
4	HEC	Х	608	1	26,50,50	<mark>2.26</mark>	9 (34%)	18,82,82	3.72	<mark>9 (50%)</mark>	
4	HEC	Х	609	1	26,50,50	1.99	6 (23%)	18,82,82	2.46	7 (38%)	
4	HEC	Х	611	1	26,50,50	1.91	8 (30%)	18,82,82	3.53	<mark>11 (61%)</mark>	
4	HEC	Х	613	1	26,50,50	2.29	8 (30%)	18,82,82	3.41	10(55%)	
4	HEC	Х	605	1	26,50,50	2.06	5 (19%)	18,82,82	2.60	<mark>9 (50%)</mark>	
5	GOL	Х	805	-	$5,\!5,\!5$	0.51	0	5, 5, 5	1.99	2(40%)	
5	GOL	Х	804	-	$5,\!5,\!5$	0.43	0	5, 5, 5	0.50	0	
4	HEC	Х	601	1	26,50,50	1.95	5 (19%)	18,82,82	2.71	8 (44%)	
4	HEC	Х	606	1	26,50,50	2.36	5 (19%)	18,82,82	2.36	8 (44%)	
4	HEC	Х	610	1	26,50,50	2.21	10 (38%)	18,82,82	3.50	10 (55%)	
4	HEC	Х	604	1	26,50,50	2.22	8 (30%)	18,82,82	2.57	<mark>6 (33%)</mark>	
5	GOL	Х	801	-	$5,\!5,\!5$	0.47	0	5, 5, 5	0.27	0	
4	HEC	Х	614	1,5	26,50,50	2.80	9 (34%)	18,82,82	3.65	10(55%)	
5	GOL	Х	802	-	$5,\!5,\!5$	0.35	0	5, 5, 5	0.33	0	
4	HEC	Х	607	1	26,50,50	2.10	3 (11%)	18,82,82	2.26	<mark>9 (50%)</mark>	
5	GOL	Х	803	4	$5,\!5,\!5$	0.62	0	5, 5, 5	0.46	0	
4	HEC	X	616	1,3	26,50,50	2.57	11 (42%)	18,82,82	3.63	7 (38%)	
4	HEC	X	615	1	$2\overline{6,50,50}$	2.15	9(34%)	18,82,82	3.94	8 (44%)	
4	HEC	X	603	1	26,50,50	2.18	4 (15%)	18,82,82	2.47	8 (44%)	

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
4	HEC	Х	612	1	-	0/6/54/54	-
4	HEC	Х	602	1	-	0/6/54/54	-
4	HEC	Х	608	1	-	0/6/54/54	-
4	HEC	Х	609	1	-	1/6/54/54	-
4	HEC	Х	611	1	-	0/6/54/54	-
4	HEC	Х	613	1	_	0/6/54/54	-
4	HEC	Х	605	1	-	0/6/54/54	-
5	GOL	Х	805	-	-	2/4/4/4	-
5	GOL	Х	804	-	-	2/4/4/4	-
4	HEC	Х	601	1	-	1/6/54/54	-
4	HEC	Х	606	1	-	0/6/54/54	-
4	HEC	Х	610	1	-	3/6/54/54	-
4	HEC	Х	604	1	-	0/6/54/54	-
5	GOL	Х	801	-	-	2/4/4/4	-
4	HEC	Х	614	1,5	-	1/6/54/54	-
5	GOL	Х	802	-	-	3/4/4/4	-
4	HEC	Х	607	1	-	0/6/54/54	-
5	GOL	X	803	4	-	4/4/4/4	-
4	HEC	Х	616	1,3	-	0/6/54/54	-
4	HEC	Х	615	1	-	0/6/54/54	-
4	HEC	Х	603	1	-	0/6/54/54	-

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
4	Х	614	HEC	CAD-C3D	7.30	1.62	1.52
4	Х	607	HEC	C3B-C2B	-6.90	1.33	1.40
4	Х	602	HEC	C3B-C2B	-6.65	1.33	1.40
4	Х	608	HEC	C3B-C2B	-6.37	1.34	1.40
4	Х	614	HEC	C3C-C2C	-6.26	1.34	1.40
4	Х	613	HEC	C3B-C2B	-6.03	1.34	1.40
4	Х	606	HEC	C3C-C2C	-6.01	1.34	1.40
4	Х	616	HEC	C3B-C2B	-5.96	1.34	1.40
4	Х	604	HEC	C3B-C2B	-5.82	1.34	1.40
4	Х	606	HEC	C3D-C2D	5.77	1.54	1.37
4	Х	616	HEC	C3D-C2D	5.72	1.54	1.37
4	Х	614	HEC	C3B-C2B	-5.56	1.35	1.40
4	Х	603	HEC	C3D-C2D	5.54	1.54	1.37
4	Х	609	HEC	C3D-C2D	5.53	1.54	1.37
4	X	603	HEC	C3B-C2B	-5.53	1.35	1.40
4	X	606	HEC	C3B-C2B	-5.44	1.35	1.40
4	Х	602	HEC	C3C-C2C	-5.41	1.35	1.40



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	602	HEC	C3D-C2D	5.36	1.53	1.37
4	X	605	HEC	C3D-C2D	5.28	1.53	1.37
4	X	614	HEC	C3D-C2D	5.22	1.53	1.37
4	X	610	HEC	C3C-C2C	-5.15	1.35	1.40
4	X	607	HEC	C3D-C2D	5.04	1.52	1.37
4	X	608	HEC	C3D-C2D	4.99	1.52	1.37
4	X	605	HEC	C3C-C2C	-4.98	1.35	1.40
4	X	609	HEC	C3B-C2B	-4.98	1.35	1.40
4	X	601	HEC	C3B-C2B	-4.97	1.35	1.40
4	Х	601	HEC	C3D-C2D	4.94	1.52	1.37
4	Х	603	HEC	C3C-C2C	-4.89	1.35	1.40
4	Х	604	HEC	C3D-C2D	4.81	1.51	1.37
4	Х	612	HEC	C3D-C2D	4.70	1.51	1.37
4	Х	616	HEC	C3C-C2C	-4.62	1.35	1.40
4	Х	610	HEC	C3B-C2B	-4.46	1.36	1.40
4	Х	611	HEC	C3B-C4B	4.46	1.51	1.43
4	Х	604	HEC	C3C-C2C	-4.45	1.36	1.40
4	Х	615	HEC	C3B-C4B	4.37	1.51	1.43
4	Х	615	HEC	C3D-C2D	4.27	1.50	1.37
4	Х	611	HEC	C3D-C2D	4.24	1.50	1.37
4	Х	613	HEC	CAD-C3D	4.24	1.58	1.52
4	Х	615	HEC	C4A-C3A	3.85	1.51	1.42
4	Х	609	HEC	C3C-C2C	-3.79	1.36	1.40
4	Х	605	HEC	C3B-C2B	-3.77	1.36	1.40
4	Х	615	HEC	C1A-C2A	3.58	1.50	1.42
4	Х	613	HEC	C1C-NC	3.53	1.43	1.36
4	Х	610	HEC	C3D-C2D	3.47	1.47	1.37
4	Х	613	HEC	CMC-C2C	3.41	1.59	1.51
4	Х	612	HEC	C3B-C4B	3.38	1.49	1.43
4	X	612	HEC	C3C-C2C	-3.38	1.37	1.40
4	X	608	HEC	C3C-C4C	3.25	1.49	1.43
4	Х	616	HEC	C1A-C2A	3.25	1.49	1.42
4	Х	605	HEC	CAA-C2A	3.22	1.57	1.52
4	Х	610	HEC	C1C-NC	3.20	1.42	1.36
4	Х	608	HEC	CMA-C3A	3.20	1.59	1.51
4	Х	616	HEC	C4A-C3A	3.19	1.49	1.42
4	X	612	HEC	C3C-C4C	3.18	1.48	1.43
4	X	616	HEC	C1D-ND	3.18	1.42	1.36
4	X	615	HEC	CAD-C3D	3.11	1.56	1.52
4	X	607	HEC	C3C-C2C	-3.09	1.37	1.40
4	X	610	HEC	CAD-C3D	3.07	1.56	1.52
4	Х	616	HEC	C3C-C4C	2.98	1.48	1.43



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Х	614	HEC	CBB-CAB	2.93	1.60	1.49
4	X	614	HEC	CAA-C2A	2.90	1.57	1.52
4	Х	611	HEC	C1A-C2A	2.89	1.49	1.42
4	X	613	HEC	C3D-C2D	2.85	1.46	1.37
4	Х	615	HEC	CBB-CAB	2.85	1.60	1.49
4	Х	611	HEC	C4A-C3A	2.79	1.48	1.42
4	Х	611	HEC	C1D-CHD	-2.70	1.33	1.41
4	Х	614	HEC	CMD-C2D	2.68	1.57	1.51
4	Х	601	HEC	CAD-C3D	2.66	1.55	1.52
4	Х	615	HEC	CMB-C2B	2.65	1.57	1.51
4	Х	613	HEC	CMA-C3A	2.58	1.57	1.51
4	Х	615	HEC	C3C-C4C	2.55	1.47	1.43
4	Х	614	HEC	CBD-CAD	2.55	1.71	1.53
4	Х	612	HEC	C3B-C2B	-2.54	1.38	1.40
4	Х	604	HEC	C1D-ND	2.53	1.41	1.36
4	Х	610	HEC	C3B-C4B	2.51	1.47	1.43
4	Х	602	HEC	CAA-C2A	2.48	1.56	1.52
4	Х	602	HEC	C1B-CHB	-2.47	1.34	1.41
4	Х	608	HEC	C1A-C2A	2.45	1.48	1.42
4	Х	608	HEC	C3B-C4B	2.45	1.47	1.43
4	Х	602	HEC	C1C-CHC	-2.44	1.34	1.41
4	Х	616	HEC	CMD-C2D	2.41	1.56	1.51
4	Х	610	HEC	CAA-C2A	2.40	1.56	1.52
4	Х	616	HEC	CAD-C3D	2.36	1.55	1.52
4	Х	611	HEC	CBB-CAB	2.34	1.58	1.49
4	Х	609	HEC	CBB-CAB	2.32	1.58	1.49
4	Х	601	HEC	C3C-C2C	-2.30	1.38	1.40
4	Х	611	HEC	C1D-ND	2.30	1.40	1.36
4	Х	613	HEC	CAA-C2A	2.28	1.56	1.52
4	X	612	HEC	C4A-C3A	2.27	1.47	1.42
4	Х	615	HEC	CAA-C2A	2.22	1.56	1.52
4	Х	613	HEC	C1B-NB	2.21	1.40	1.36
4	Х	616	HEC	C4D-ND	2.21	1.40	1.36
4	Х	606	HEC	CMD-C2D	2.21	1.56	1.51
4	Х	602	HEC	C3B-C4B	2.16	1.47	1.43
4	X	614	HEC	CMB-C2B	2.16	1.56	1.51
4	X	604	HEC	C1A-C2A	2.15	1.47	1.42
4	X	608	HEC	C1D-CHD	-2.14	1.35	1.41
4	X	604	HEC	C3C-C4C	2.14	1.46	1.43
4	X	601	HEC	C4A-C3A	2.13	1.47	1.42
4	X	616	HEC	CMB-C2B	2.12	1.56	1.51
4	X	611	HEC	C3C-C4C	2.12	1.46	1.43



Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
4	Х	602	HEC	C4D-CHA	-2.11	1.35	1.41
4	Х	602	HEC	CMD-C2D	2.09	1.56	1.51
4	Х	612	HEC	CBB-CAB	2.08	1.57	1.49
4	Х	602	HEC	CBB-CAB	2.08	1.57	1.49
4	Х	610	HEC	CMC-C2C	2.08	1.56	1.51
4	Х	609	HEC	CAA-C2A	2.07	1.55	1.52
4	Х	608	HEC	CAD-C3D	2.07	1.55	1.52
4	Х	610	HEC	C3C-C4C	2.06	1.46	1.43
4	Х	604	HEC	CBB-CAB	2.05	1.57	1.49
4	Х	609	HEC	C3B-C4B	2.04	1.46	1.43
4	Х	604	HEC	CMD-C2D	2.04	1.55	1.51
4	Х	605	HEC	C1A-C2A	2.03	1.47	1.42
4	Х	608	HEC	C4A-C3A	2.03	1.47	1.42
4	Х	606	HEC	C2A-C3A	-2.01	1.31	1.37
4	X	610	HEC	C4D-ND	-2.00	1.32	1.36
4	X	603	HEC	CMB-C2B	2.00	1.56	1.51

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	Х	614	HEC	CAD-CBD-CGD	11.90	132.64	112.67
4	Х	611	HEC	CMC-C2C-C1C	-9.31	114.15	128.46
4	Х	612	HEC	CAD-CBD-CGD	-9.07	97.45	112.67
4	Х	608	HEC	CMC-C2C-C1C	-9.03	114.58	128.46
4	Х	616	HEC	CMC-C2C-C1C	-8.41	115.54	128.46
4	Х	615	HEC	CMC-C2C-C3C	7.72	134.90	125.82
4	Х	608	HEC	CAD-CBD-CGD	-7.60	99.91	112.67
4	Х	615	HEC	CMC-C2C-C1C	-7.51	116.92	128.46
4	Х	616	HEC	CBD-CAD-C3D	-7.32	98.98	112.49
4	Х	613	HEC	CMB-C2B-C1B	-7.11	117.53	128.46
4	Х	612	HEC	CMC-C2C-C3C	6.99	134.03	125.82
4	Х	616	HEC	CAD-CBD-CGD	6.94	124.31	112.67
4	Х	613	HEC	CMB-C2B-C3B	6.91	133.95	125.82
4	Х	615	HEC	CBD-CAD-C3D	-6.65	100.22	112.49
4	Х	609	HEC	CMC-C2C-C1C	-6.61	118.30	128.46
4	Х	601	HEC	CMC-C2C-C1C	-6.54	118.41	128.46
4	Х	608	HEC	CMC-C2C-C3C	6.42	133.36	125.82
4	Х	612	HEC	CMC-C2C-C1C	-6.34	118.72	128.46
4	Х	610	HEC	CMB-C2B-C1B	-6.12	119.06	128.46
4	Х	616	HEC	CMC-C2C-C3C	5.92	132.78	125.82
4	Х	604	HEC	CBA-CAA-C2A	-5.89	101.63	112.48
4	Х	602	HEC	CMB-C2B-C3B	5.84	132.69	125.82



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	Х	612	HEC	CAA-CBA-CGA	-5.80	102.94	112.67
4	Х	603	HEC	CBD-CAD-C3D	-5.72	101.94	112.49
4	Х	610	HEC	CMB-C2B-C3B	5.69	132.50	125.82
4	Х	615	HEC	CMB-C2B-C1B	-5.68	119.74	128.46
4	Х	610	HEC	CMD-C2D-C3D	5.60	135.50	124.94
4	Х	613	HEC	CBD-CAD-C3D	-5.60	102.17	112.49
4	Х	610	HEC	CAD-CBD-CGD	-5.52	103.40	112.67
4	Х	610	HEC	CMD-C2D-C1D	-5.35	120.24	128.46
4	Х	615	HEC	CMB-C2B-C3B	5.24	131.98	125.82
4	Х	605	HEC	CBA-CAA-C2A	5.22	122.09	112.48
4	Х	611	HEC	CBA-CAA-C2A	-4.86	103.52	112.48
4	Х	612	HEC	CBD-CAD-C3D	-4.82	103.60	112.49
4	X	615	HEC	CAD-CBD-CGD	-4.79	104.63	112.67
4	X	611	HEC	CMC-C2C-C3C	4.78	131.44	125.82
4	X	604	HEC	CMC-C2C-C1C	-4.69	121.25	128.46
4	Х	605	HEC	CMB-C2B-C1B	-4.58	121.43	128.46
4	X	611	HEC	C4C-C3C-C2C	-4.52	101.47	106.35
4	Х	603	HEC	CBA-CAA-C2A	-4.52	104.15	112.48
4	Х	601	HEC	CAA-CBA-CGA	-4.47	105.17	112.67
4	Х	605	HEC	CMC-C2C-C1C	-4.43	121.65	128.46
4	Х	614	HEC	CMB-C2B-C1B	-4.24	121.95	128.46
4	Х	608	HEC	CBD-CAD-C3D	4.22	120.28	112.49
4	Х	606	HEC	CAA-CBA-CGA	-4.20	105.63	112.67
4	Х	601	HEC	CBD-CAD-C3D	-4.16	104.81	112.49
4	Х	614	HEC	CMC-C2C-C1C	-4.04	122.25	128.46
4	Х	613	HEC	C1D-C2D-C3D	-4.02	104.20	107.00
4	Х	604	HEC	C1D-C2D-C3D	-3.99	104.22	107.00
4	X	610	HEC	C1D-C2D-C3D	-3.97	104.23	107.00
4	X	607	HEC	CBD-CAD-C3D	-3.95	105.20	112.49
4	X	613	HEC	CMC-C2C-C3C	3.92	130.43	125.82
4	X	603	HEC	CMC-C2C-C1C	-3.79	122.64	128.46
4	X	611	HEC	C1D-C2D-C3D	-3.78	104.37	107.00
4	X	609	HEC	CAA-CBA-CGA	3.77	118.99	112.67
4	X	607	HEC	CMC-C2C-C1C	-3.75	122.70	128.46
4	X	608	HEC	CAA-CBA-CGA	-3.74	106.39	112.67
4	X	610	HEC	CAA-CBA-CGA	-3.74	106.40	112.67
4	X	607	HEC	CAD-CBD-CGD	-3.74	106.40	112.67
4	X	604	HEC	CAA-CBA-CGA	-3.68	106.49	112.67
4	Х	614	HEC	CMB-C2B-C3B	3.68	130.15	125.82
4	X	611	HEC	CMB-C2B-C1B	-3.65	122.85	128.46
4	Х	602	HEC	CMB-C2B-C1B	-3.64	122.86	128.46
4	Х	615	HEC	CBA-CAA-C2A	-3.60	105.85	112.48

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	Х	601	HEC	CAD-CBD-CGD	3.54	118.62	112.67
4	Х	601	HEC	CMB-C2B-C1B	-3.54	123.02	128.46
4	Х	612	HEC	CMA-C3A-C2A	3.49	131.52	124.94
4	Х	606	HEC	CMB-C2B-C3B	3.44	129.86	125.82
4	Х	606	HEC	CMC-C2C-C1C	-3.40	123.24	128.46
4	Х	605	HEC	CMB-C2B-C3B	3.39	129.81	125.82
4	Х	612	HEC	C1D-C2D-C3D	-3.39	104.64	107.00
5	Х	805	GOL	C3-C2-C1	-3.36	98.64	111.70
4	Х	606	HEC	CBA-CAA-C2A	3.36	118.67	112.48
4	Х	608	HEC	CBA-CAA-C2A	3.36	118.66	112.48
4	Х	613	HEC	CMC-C2C-C1C	-3.35	123.32	128.46
4	Х	611	HEC	CBD-CAD-C3D	-3.31	106.38	112.49
4	Х	615	HEC	CAA-CBA-CGA	-3.31	107.12	112.67
4	Х	603	HEC	C1D-C2D-C3D	-3.26	104.73	107.00
4	Х	616	HEC	CMA-C3A-C2A	3.25	131.07	124.94
4	Х	613	HEC	C4C-C3C-C2C	3.25	109.86	106.35
4	Х	609	HEC	CMD-C2D-C1D	-3.23	123.50	128.46
4	Х	610	HEC	CBA-CAA-C2A	-3.21	106.57	112.48
4	Х	602	HEC	CAA-CBA-CGA	3.18	118.01	112.67
4	Х	609	HEC	CMD-C2D-C3D	3.17	130.92	124.94
4	Х	606	HEC	C1D-C2D-C3D	-3.16	104.80	107.00
4	Х	606	HEC	CMB-C2B-C1B	-3.14	123.64	128.46
4	Х	614	HEC	CBD-CAD-C3D	3.09	118.19	112.49
4	Х	612	HEC	CMD-C2D-C1D	3.04	133.13	128.46
4	Х	609	HEC	CAD-CBD-CGD	-3.03	107.58	112.67
4	Х	611	HEC	CAA-CBA-CGA	-3.00	107.63	112.67
4	Х	602	HEC	C1D-C2D-C3D	-3.00	104.91	107.00
4	Х	613	HEC	CMD-C2D-C3D	2.98	130.56	124.94
4	Х	612	HEC	CMB-C2B-C1B	-2.96	123.91	128.46
4	Х	604	HEC	CMC-C2C-C3C	2.93	129.27	125.82
4	Х	614	HEC	CMD-C2D-C1D	-2.92	123.98	128.46
4	Х	607	HEC	CBA-CAA-C2A	-2.91	107.11	112.48
4	Х	606	HEC	CBD-CAD-C3D	-2.91	107.13	112.49
4	X	611	HEC	CMB-C2B-C3B	2.87	129.20	125.82
4	X	605	HEC	C1D-C2D-C3D	-2.85	105.01	107.00
4	X	607	HEC	CMC-C2C-C3C	2.84	129.16	125.82
4	X	605	HEC	CAD-CBD-CGD	-2.71	108.13	112.67
4	X	607	HEC	CMD-C2D-C3D	2.70	$1\overline{30.03}$	124.94
4	X	610	HEC	CMC-C2C-C1C	-2.70	124.32	128.46
5	X	805	GOL	O1-C1-C2	-2.68	97.33	110.20
4	X	608	HEC	$CMA-C\overline{3}A-C\overline{2}A$	2.67	129.97	124.94
4	X	607	HEC	CMD-C2D-C1D	-2.63	124.42	128.46



Mol	Chain	Res	Type	$\begin{tabular}{ c c c c c } Atoms & Z & Observed(^{o}) \\ \hline \end{tabular}$		$Ideal(^{o})$	
4	Х	604	HEC	CBD-CAD-C3D	-2.57	107.75	112.49
4	Х	609	HEC	CMB-C2B-C1B	-2.55	124.54	128.46
4	Х	608	HEC	C1D-C2D-C3D	-2.54	105.23	107.00
4	Х	611	HEC	CMA-C3A-C2A	2.53	129.71	124.94
4	Х	603	HEC	CMB-C2B-C1B	-2.51	124.61	128.46
4	Х	616	HEC	C1D-C2D-C3D	-2.45	105.29	107.00
4	Х	614	HEC	CAA-CBA-CGA	-2.42	108.62	112.67
4	Х	602	HEC	C4B-C3B-C2B	2.38	108.92	106.35
4	Х	602	HEC	CBA-CAA-C2A	2.37	116.85	112.48
4	Х	614	HEC	C1D-C2D-C3D	2.36	108.64	107.00
4	Х	603	HEC	CMC-C2C-C3C	2.36	128.59	125.82
4	Х	605	HEC	CMC-C2C-C3C	2.36	128.59	125.82
4	Х	605	HEC	C3B-C4B-NB	-2.29	106.63	110.94
4	Х	601	HEC	CBA-CAA-C2A	-2.24	108.35	112.48
4	Х	610	HEC	C3B-C4B-NB	-2.23	106.73	110.94
4	Х	612	HEC	CAA-C2A-C3A	2.22	133.63	127.25
4	Х	612	HEC	CMB-C2B-C3B	2.22	128.43	125.82
4	Х	613	HEC	CAD-CBD-CGD	-2.20	108.98	112.67
4	Х	607	HEC	C1D-C2D-C3D	-2.14	105.50	107.00
4	Х	607	HEC	C3B-C4B-NB	-2.14	106.90	110.94
4	Х	606	HEC	CAD-CBD-CGD	-2.14	109.08	112.67
4	Х	603	HEC	C4B-C3B-C2B	2.13	108.65	106.35
4	Х	603	HEC	CMB-C2B-C3B	2.13	128.32	125.82
4	Х	609	HEC	C1D-C2D-C3D	-2.12	105.52	107.00
4	Х	608	HEC	C3C-C4C-NC	-2.12	106.95	110.94
4	Х	613	HEC	CMD-C2D-C1D	-2.09	125.25	128.46
4	Х	601	HEC	C1D-C2D-C3D	-2.09	105.54	107.00
4	Х	601	HEC	C3B-C4B-NB	-2.08	107.01	110.94
4	X	605	HEC	CAA-CBA-CGA	-2.06	109.22	112.67
4	X	614	HEC	CAD-C3D-C2D	2.05	133.14	127.25
4	X	614	HEC	C3B-C4B-NB	-2.05	107.08	110.94
4	X	611	HEC	CAD-CBD-CGD	-2.03	109.26	112.67
4	X	616	HEC	C3C-C4C-NC	-2.01	107.14	110.94

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There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Х	610	HEC	C2D-C3D-CAD-CBD
4	Х	610	HEC	C4D-C3D-CAD-CBD
4	Х	610	HEC	C3D-CAD-CBD-CGD
5	Х	802	GOL	C1-C2-C3-O3



Mol	Chain	Res	Type	Atoms
5	Х	804	GOL	C1-C2-C3-O3
5	Х	801	GOL	O1-C1-C2-C3
4	Х	601	HEC	C3D-CAD-CBD-CGD
5	Х	803	GOL	C1-C2-C3-O3
5	Х	803	GOL	O2-C2-C3-O3
5	Х	802	GOL	O2-C2-C3-O3
5	Х	804	GOL	O2-C2-C3-O3
5	Х	801	GOL	O1-C1-C2-O2
5	Х	805	GOL	O1-C1-C2-O2
5	Х	805	GOL	O1-C1-C2-C3
5	Х	803	GOL	O1-C1-C2-C3
5	Х	803	GOL	O1-C1-C2-O2
4	Х	614	HEC	C3D-CAD-CBD-CGD
5	Х	802	GOL	O1-C1-C2-C3
4	Х	609	HEC	C2A-CAA-CBA-CGA

Continued from previous page...

There are no ring outliers.

18 monomers are in	volved in 115	short contacts:
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Х	612	HEC	4	0
4	Х	602	HEC	12	0
4	Х	608	HEC	11	0
4	Х	609	HEC	4	0
4	Х	611	HEC	1	0
4	Х	613	HEC	1	1
4	Х	605	HEC	3	0
5	Х	804	GOL	1	0
4	Х	601	HEC	14	0
4	Х	606	HEC	7	0
4	Х	610	HEC	13	0
4	Х	604	HEC	6	0
4	Х	614	HEC	10	0
4	Х	607	HEC	6	0
5	Х	803	GOL	5	0
4	Х	616	HEC	12	0
4	Х	615	HEC	7	1
4	X	603	HEC	2	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 similar 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	X	516/560~(92%)	0.37	35 (6%) 17 21	28, 55, 82, 91	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Х	530	SER	8.1
1	Х	159	ALA	5.4
1	Х	58	GLU	4.1
1	Х	529	ASN	4.0
1	Х	253	LEU	3.6
1	Х	119	VAL	3.4
1	Х	113	GLY	3.4
1	Х	182	LEU	3.1
1	Х	59	GLY	3.0
1	Х	152	CYS	2.8
1	Х	160	GLN	2.7
1	Х	180	GLU	2.7
1	Х	276	VAL	2.6
1	Х	221	LEU	2.5
1	Х	34	PHE	2.5
1	Х	298	GLN	2.5
1	Х	251	THR	2.4
1	Х	22	ALA	2.4
1	Х	215	THR	2.4
1	Х	44	GLU	2.3
1	Х	23	VAL	2.3
1	Х	252	LEU	2.3
1	Х	361	THR	2.3
1	Х	142	GLN	2.2
1	Х	24	PHE	2.2
1	Х	424	LYS	2.2
1	Х	116	GLY	2.2



Mol	Chain	Res	Type	RSRZ
1	Х	53	CYS	2.1
1	Х	85	CYS	2.1
1	Х	156	TYR	2.1
1	Х	158	GLU	2.1
1	Х	320	ASN	2.0
1	Х	259	THR	2.0
1	Х	260	ALA	2.0
1	Х	93	VAL	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)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	А	1	14/15	0.83	0.26	75,79,86,86	0
2	NAA	А	2	14/15	0.85	0.38	89,91,94,94	0

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	Х	802	6/6	0.81	0.15	62,69,71,73	0
5	GOL	Х	801	6/6	0.81	0.29	86,88,89,90	0
3	ZN	Х	702	1/1	0.83	0.11	72,72,72,72	0
3	ZN	Х	703	1/1	0.84	0.07	69,69,69,69	0
5	GOL	Х	804	6/6	0.88	0.37	$53,\!61,\!66,\!70$	0
5	GOL	Х	805	6/6	0.88	0.16	57,62,66,73	0
4	HEC	Х	605	43/43	0.90	0.17	48,58,73,78	0
5	GOL	Х	803	6/6	0.92	0.17	28,54,59,60	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
4	HEC	Х	602	43/43	0.93	0.19	$45,\!51,\!75,\!80$	0
4	HEC	Х	601	43/43	0.93	0.19	$52,\!59,\!63,\!65$	0
4	HEC	Х	614	43/43	0.93	0.14	20,31,41,50	0
4	HEC	Х	606	43/43	0.94	0.15	45,49,65,71	0
4	HEC	Х	603	43/43	0.94	0.15	$58,\!73,\!75,\!77$	0
4	HEC	Х	616	43/43	0.94	0.12	$29,\!38,\!50,\!64$	0
4	HEC	Х	611	43/43	0.95	0.15	$28,\!33,\!52,\!58$	0
4	HEC	Х	609	43/43	0.95	0.12	$40,\!50,\!61,\!67$	0
4	HEC	Х	607	43/43	0.95	0.14	$49,\!55,\!65,\!72$	0
4	HEC	Х	608	43/43	0.96	0.14	$27,\!37,\!52,\!61$	0
4	HEC	Х	610	43/43	0.97	0.10	$20,\!26,\!41,\!47$	0
4	HEC	Х	615	43/43	0.97	0.16	$25,\!31,\!49,\!56$	0
4	HEC	Х	604	43/43	0.97	0.16	$38,\!48,\!54,\!57$	0
4	HEC	Х	612	43/43	0.97	0.21	$30,\!38,\!56,\!65$	0
4	HEC	X	613	43/43	0.97	0.14	$28,\!31,\!43,\!53$	0
3	ZN	Х	701	1/1	0.99	0.08	42,42,42,42	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.

