

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	8IE4
Title	:	Crystal structure of GcCGT
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Deposited on	:	2023-02-15
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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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 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	485	78%	14%	• 7%
1	В	485	7% 76%	15%	• 8%
1	С	485	8%	13%	• 8%
1	D	485	7%	15%	11%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14531 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	Δ	450	Total	С	Ν	0	\mathbf{S}	0	0	0	
1	A	400	3543	2281	594	655	13	0	0	U	
1	р	445	Total	С	Ν	0	S	0	0	0	
1	D	440	3515	2265	586	650	14	0	0	0	
1	C	444	Total	С	Ν	0	S	0	0	0	
1		444	3496	2252	587	643	14	0	0	0	
1	П	424	Total	С	Ν	0	S	0	0	0	
	D	404	3441	2221	574	633	13	0	0	0	

• Molecule 1 is a protein called GcCGT.

• Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
2	А	1	Total 12	С 6	N 1	0 4	S 1	0	0

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	200	Total O 200 200	0	0
3	В	145	Total O 145 145	0	0
3	С	104	Total O 104 104	0	0
3	D	75	Total O 75 75	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: GcCGT





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	79.18Å 95.93Å 132.22Å	Depositor
a, b, c, α , β , γ	90.00° 103.54° 90.00°	Depositor
Bosolution(A)	39.50 - 2.10	Depositor
Resolution (A)	39.50 - 2.10	EDS
% Data completeness	99.6 (39.50-2.10)	Depositor
(in resolution range)	99.8 (39.50-2.10)	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.07 (at 2.10 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
P. P.	0.202 , 0.250	Depositor
n, n_{free}	0.199 , 0.247	DCC
R_{free} test set	5780 reflections (5.16%)	wwPDB-VP
Wilson B-factor $(Å^2)$	37.3	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, 46.1	EDS
L-test for twinning ²	$ < L >=0.46, < L^2>=0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14531	wwPDB-VP
Average B, all atoms $(Å^2)$	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.43% 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: MES

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

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.45	0/3635	0.58	0/4944	
1	В	0.41	0/3606	0.56	0/4901	
1	С	0.39	0/3586	0.55	0/4875	
1	D	0.37	0/3532	0.52	0/4801	
All	All	0.41	0/14359	0.55	0/19521	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3543	0	3500	34	0
1	В	3515	0	3482	41	0
1	С	3496	0	3462	32	0
1	D	3441	0	3415	38	0
2	А	12	0	12	0	0
3	А	200	0	0	5	0
3	В	145	0	0	1	0
3	С	104	0	0	1	0
3	D	75	0	0	2	0
All	All	14531	0	13871	144	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 (144)	close	contacts	within	the s	same	$\operatorname{asymmetric}$	unit	are	listed	below,	sorted	$\mathbf{b}\mathbf{y}$	their	clash
magnituo	le.													

Atom 1	Atom 2	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:B:371:THR:HG23	1:B:397:LEU:HD21	1.66	0.78		
1:A:306:LEU:HD11	1:A:334:PHE:HA	1.66	0.76		
1:A:327:PRO:HB2	1:A:329:VAL:HG23	1.71	0.73		
1:B:327:PRO:HB2	1:B:329:VAL:HG23	1.72	0.70		
1:D:371:THR:HG23	1:D:397:LEU:HD21	1.75	0.69		
1:D:458:ASN:N	1:D:458:ASN:OD1	2.26	0.68		
1:A:447:LYS:NZ	3:A:604:HOH:O	2.27	0.66		
1:D:278:PRO:HG2	1:D:281:THR:HG21	1.78	0.65		
1:A:78:ASP:O	1:A:97:HIS:NE2	2.31	0.62		
1:D:237:THR:HG22	1:D:242:ILE:HB	1.81	0.62		
1:D:290:VAL:HG21	1:D:390:GLN:HE22	1.64	0.62		
1:B:318:PRO:HD3	1:B:346:GLN:HB3	1.81	0.61		
1:B:287:VAL:HG11	1:B:384:PHE:HD2	1.66	0.61		
1:C:371:THR:HG23	1:C:397:LEU:HD21	1.82	0.61		
1:C:290:VAL:HG21	1:C:390:GLN:HE22	1.65	0.60		
1:D:269:ASP:N	1:D:271:LYS:HZ3	1.99	0.60		
1:A:454:ALA:O	1:A:460:GLU:HG2	2.02	0.59		
1:D:81:GLU:H	1:D:81:GLU:CD	2.06	0.59		
1:D:279:PRO:HA	1:D:358:ALA:HA	1.85	0.57		
1:D:297:GLN:O	1:D:301:MET:HG3	2.04	0.57		
1:D:250:LYS:HE2	1:D:376:SER:HB3	1.87	0.57		
1:B:306:LEU:HD12	1:B:341:ARG:HH22	1.70	0.57		
1:B:437:GLU:O	1:B:440:GLU:HG2	2.05	0.57		
1:C:250:LYS:HG2	1:C:453:VAL:HG21	1.86	0.57		
1:A:56:ASN:N	1:A:56:ASN:OD1	2.38	0.57		
1:C:343:LYS:NZ	3:C:506:HOH:O	2.38	0.57		
1:C:375:ILE:HG23	1:C:445:TRP:HB3	1.85	0.57		
1:A:58:LEU:HB3	1:A:62:GLN:HA	1.86	0.56		
1:B:290:VAL:HG21	1:B:390:GLN:HE22	1.69	0.56		
1:B:233:ILE:O	1:B:237:THR:HG23	2.05	0.56		
1:B:375:ILE:HG23	1:B:445:TRP:HB3	1.88	0.56		
1:B:289:SER:HB3	1:B:365:HIS:NE2	2.20	0.56		
1:C:289:SER:HG	1:C:365:HIS:HE2	1.53	0.55		
1:B:405:VAL:HG21	1:B:428:GLU:HG2	1.89	0.54		
1:B:14:LEU:HB3	1:B:26:MET:HE3	1.88	0.54		
1:A:338:ALA:O	1:A:341:ARG:HG2	2.08	0.54		
1:A:287:VAL:HG11	1:A:384:PHE:HD2	1.71	0.54		



	le us pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:290:VAL:HG21	1:A:390:GLN:HE22	1.73	0.54
1:B:383:THR:OG1	1:B:406:ARG:HA	2.08	0.54
1:C:10:LEU:HB2	1:C:38:LEU:HD22	1.89	0.53
1:A:278:PRO:HG3	1:C:108:ILE:HD11	1.90	0.53
1:D:271:LYS:NZ	3:D:507:HOH:O	2.42	0.53
1:C:279:PRO:HA	1:C:358:ALA:HA	1.91	0.53
1:D:473:LYS:NZ	3:D:506:HOH:O	2.41	0.53
1:A:7:ASN:N	3:A:619:HOH:O	2.43	0.52
1:B:70:MET:SD	1:B:72:ARG:NH2	2.82	0.52
1:A:221:LEU:HD22	1:A:245:ILE:HD13	1.90	0.52
1:A:247:PRO:HG2	1:A:250:LYS:HB2	1.91	0.52
1:C:437:GLU:O	1:C:440:GLU:HG3	2.11	0.51
1:B:454:ALA:O	1:B:460:GLU:HG2	2.11	0.51
1:D:424:ARG:O	1:D:428:GLU:HB2	2.11	0.51
1:B:279:PRO:HA	1:B:358:ALA:HA	1.93	0.50
1:A:110:LEU:HD12	1:A:139:LEU:HD12	1.93	0.50
1:D:410:GLY:O	1:D:413:GLU:HB2	2.11	0.50
1:C:14:LEU:HB3	1:C:26:MET:HE3	1.94	0.49
1:B:281:THR:O	1:B:311:SER:HB3	2.12	0.49
1:A:43:SER:HA	1:A:74:GLU:O	2.11	0.49
1:D:233:ILE:O	1:D:237:THR:HG23	2.13	0.49
1:C:179:LEU:HB2	1:C:182:MET:HE3	1.95	0.48
1:C:195:HIS:CE1	1:C:197:ARG:HD2	2.48	0.48
1:A:50:ARG:NH1	1:A:54:LYS:HD2	2.28	0.48
1:A:222:MET:HG2	1:A:224:THR:HG22	1.95	0.48
1:B:333:GLU:OE1	1:B:333:GLU:N	2.36	0.47
1:B:49:GLY:O	1:B:53:ARG:HG3	2.15	0.47
1:D:161:HIS:HB2	1:D:208:LEU:HD22	1.96	0.47
1:D:306:LEU:HD13	1:D:334:PHE:CD2	2.50	0.47
1:C:12:ILE:HG21	1:C:33:PHE:CE2	2.50	0.47
1:D:316:LEU:HD12	1:D:316:LEU:HA	1.80	0.47
1:A:381:VAL:HG21	1:A:397:LEU:HD13	1.97	0.47
1:D:136:ALA:HB1	1:D:141:ILE:O	2.15	0.47
1:D:290:VAL:HG21	1:D:390:GLN:NE2	2.29	0.47
1:A:326:GLU:HA	1:A:327:PRO:HD3	1.76	0.46
1:B:333:GLU:H	1:B:333:GLU:CD	2.19	0.46
1:D:28:ARG:HD2	1:D:249:PHE:HA	1.96	0.46
1:B:287:VAL:HG11	1:B:384:PHE:CD2	2.50	0.46
1:B:456:GLY:N	1:B:460:GLU:OE2	2.28	0.46
1:C:177:VAL:HG12	1:C:179:LEU:HD13	1.97	0.46
1:D:249:PHE:HZ	1:D:376:SER:HB2	1.80	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:33:PHE:HB3	1:C:38:LEU:HD12	1.97	0.46
1:D:381:VAL:O	1:D:404:GLY:HA2	2.15	0.46
1:A:333:GLU:HB2	1:A:337:LYS:HD3	1.96	0.46
1:A:28:ARG:NE	3:A:608:HOH:O	2.33	0.45
1:D:14:LEU:HB3	1:D:26:MET:HE3	1.98	0.45
1:B:362:PHE:HB3	1:B:381:VAL:HG12	1.98	0.45
1:C:306:LEU:HD11	1:C:337:LYS:HD3	1.98	0.45
1:C:381:VAL:HG21	1:C:397:LEU:HD13	1.98	0.45
1:B:182:MET:HE3	1:B:182:MET:HB2	1.66	0.45
1:A:476:SER:O	3:A:601:HOH:O	2.21	0.45
1:C:31:LYS:HG2	1:C:66:VAL:HG21	1.97	0.45
1:A:165:VAL:HG11	1:A:179:LEU:HD23	1.99	0.44
1:A:412:LEU:HD23	1:A:412:LEU:HA	1.69	0.44
1:D:18:ILE:HG23	1:D:48:VAL:HG13	1.99	0.44
1:D:356:HIS:CG	1:D:357:PRO:HD2	2.52	0.44
1:A:17:PHE:CG	1:A:18:ILE:N	2.86	0.44
1:D:365:HIS:HD1	1:D:367:GLY:H	1.66	0.44
1:A:371:THR:HG23	1:A:397:LEU:HD21	2.00	0.44
1:A:279:PRO:HA	1:A:358:ALA:HA	2.00	0.43
1:B:251:ILE:HG12	1:B:453:VAL:CG2	2.48	0.43
1:D:385:PRO:O	1:D:410:GLY:HA2	2.18	0.43
1:A:77:ASP:O	1:A:105:LYS:HE2	2.18	0.43
1:B:311:SER:HA	1:B:341:ARG:O	2.19	0.43
1:B:113:HIS:HB3	1:B:118:THR:O	2.18	0.43
1:C:56:ASN:OD1	1:C:56:ASN:N	2.51	0.43
1:B:306:LEU:HD11	1:B:337:LYS:HB2	2.00	0.43
1:D:105:LYS:O	1:D:109:MET:HG3	2.19	0.43
1:B:102:GLY:HA3	1:B:131:TRP:CH2	2.53	0.43
1:B:289:SER:HA	1:B:317:ARG:NH1	2.34	0.42
1:C:14:LEU:HG	1:C:124:ILE:HB	2.00	0.42
1:A:326:GLU:HG3	3:A:606:HOH:O	2.20	0.42
1:A:280:SER:C	1:A:360:ALA:HB2	2.40	0.42
1:D:7:ASN:O	1:D:9:ASN:N	2.52	0.42
1:D:27:LEU:HD12	1:D:27:LEU:HA	1.83	0.42
1:C:399:GLU:O	1:C:402:LYS:NZ	2.46	0.42
1:D:13:PHE:HE1	1:D:43:SER:HG	1.66	0.42
1:D:415:ARG:HH22	1:D:421:GLU:CD	2.22	0.42
1:C:105:LYS:HA	1:C:108:ILE:HD12	2.00	0.42
1:A:318:PRO:HB3	1:A:346:GLN:OE1	2.19	0.42
1:C:413:GLU:HG3	1:C:415:ARG:HG2	2.00	0.42
1:C:250:LYS:HE2	1:C:250:LYS:HB2	1.87	0.42



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:330:LEU:HD12	1:B:335:TRP:CZ2	2.55	0.42
1:D:174:GLU:HA	1:D:187:TYR:CG	2.55	0.42
1:A:219:CYS:SG	1:A:243:LYS:HG3	2.60	0.41
1:D:274:LEU:HB3	1:D:356:HIS:CE1	2.55	0.41
1:C:223:ASP:HB2	1:C:248:LEU:HD22	2.03	0.41
1:B:47:ILE:HD11	1:B:94:TYR:CE1	2.56	0.41
1:B:290:VAL:HG21	1:B:390:GLN:NE2	2.34	0.41
1:D:45:PRO:HG3	1:D:98:LEU:HD11	2.01	0.41
1:B:226:TYR:O	1:B:230:HIS:HB3	2.21	0.41
1:C:24:ASN:O	1:C:28:ARG:HG3	2.21	0.41
1:B:24:ASN:O	1:B:28:ARG:HG3	2.20	0.41
1:C:111:LYS:HB3	1:C:111:LYS:HE3	1.67	0.41
1:C:410:GLY:O	1:C:413:GLU:HG2	2.21	0.41
1:D:127:PRO:HA	1:D:210:GLN:OE1	2.21	0.41
1:B:17:PHE:CG	1:B:18:ILE:N	2.86	0.41
1:B:238:LYS:NZ	3:B:518:HOH:O	2.52	0.41
1:C:369:ASN:O	1:C:373:GLU:HG3	2.20	0.41
1:D:225:PHE:HB3	1:D:246:GLY:O	2.21	0.41
1:B:412:LEU:HA	1:B:412:LEU:HD23	1.77	0.41
1:B:112:LYS:O	1:B:116:SER:OG	2.25	0.40
1:B:452:THR:HG23	1:B:459:SER:HB2	2.02	0.40
1:C:340:ASP:H	1:C:341:ARG:HH12	1.68	0.40
1:C:381:VAL:O	1:C:404:GLY:HA2	2.21	0.40
1:A:312:PHE:CZ	1:A:342:GLY:HA3	2.56	0.40
1:B:336:GLU:OE2	1:B:337:LYS:HE3	2.21	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	444/485~(92%)	433 (98%)	11 (2%)	0	100 100	



Mol	Chain	Analysed Favoured Allowed		Outliers	Perce	ntiles	
1	В	437/485~(90%)	422 (97%)	15 (3%)	0	100	100
1	С	436/485~(90%)	417 (96%)	19 (4%)	0	100	100
1	D	426/485 (88%)	415 (97%)	11 (3%)	0	100	100
All	All	1743/1940~(90%)	1687 (97%)	56(3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	389/424~(92%)	369~(95%)	20~(5%)	24	22	
1	В	388/424~(92%)	370~(95%)	18 (5%)	27	26	
1	С	384/424~(91%)	363 (94%)	21 (6%)	21	19	
1	D	380/424~(90%)	367~(97%)	13 (3%)	37	39	
All	All	1541/1696~(91%)	1469~(95%)	72 (5%)	26	25	

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	8	ASP
1	А	18	ILE
1	А	26	MET
1	А	50	ARG
1	А	56	ASN
1	А	59	ASN
1	А	60	ASP
1	А	72	ARG
1	А	112	LYS
1	А	125	LEU
1	А	186	LYS
1	А	239	ILE
1	А	243	LYS



Mol	Chain	Res	Type
1	А	280	SER
1	А	317	ARG
1	А	330	LEU
1	А	340	ASP
1	А	387	PHE
1	А	440	GLU
1	А	443	LEU
1	В	48	VAL
1	В	70	MET
1	В	86	SER
1	В	112	LYS
1	В	116	SER
1	В	125	LEU
1	В	153	SER
1	В	280	SER
1	В	292	TYR
1	В	309	GLU
1	В	317	ARG
1	В	340	ASP
1	В	372	GLN
1	В	387	PHE
1	В	415	ARG
1	В	429	ILE
1	В	452	THR
1	В	453	VAL
1	С	64	ILE
1	С	65	LYS
1	С	72	ARG
1	С	111	LYS
1	С	114	GLU
1	C	125	LEU
1	C	128	LEU
1	C	138	SER
1	C	179	LEU
1	C	210	GLN
1	C	227	GLU
1	С	235	SER
1	C	248	LEU
1	C	332	GLU
1	C	341	ARG
1	C	348	SER
1	C	384	PHE



Mol Chain Bog Type								
IVIOI	Chain	nes	Type					
1	С	412	LEU					
1	С	415	ARG					
1	С	443	LEU					
1	С	447	LYS					
1	D	20	GLN					
1	D	48	VAL					
1	D	100	GLN					
1	D	118	THR					
1	D	125	LEU					
1	D	289	SER					
1	D	311	SER					
1	D	340	ASP					
1	D	395	LYS					
1	D	412	LEU					
1	D	414	ASN					
1	D	423	GLU					
1	D	458	ASN					

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	Type	Chain	Dog	Tink	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MES	А	501	-	12,12,12	1.37	1 (8%)	14,16,16	2.00	5 (35%)

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	MES	А	501	-	-	2/6/14/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	501	MES	C8-S	-4.24	1.71	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	501	MES	C5-N4-C3	3.96	117.73	108.83
2	А	501	MES	C6-C5-N4	-3.39	104.96	110.10
2	А	501	MES	C7-N4-C5	2.71	118.17	111.23
2	А	501	MES	C7-N4-C3	2.71	118.17	111.23
2	А	501	MES	O1S-S-C8	2.30	109.69	106.92

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	501	MES	C8-C7-N4-C5
2	А	501	MES	C8-C7-N4-C3

There are no ring outliers.

No monomer is involved in short contacts.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	450/485~(92%)	0.21	16 (3%) 42 49	30, 43, 80, 128	0
1	В	445/485~(91%)	0.49	33 (7%) 14 18	35, 51, 97, 144	0
1	С	444/485~(91%)	0.52	38 (8%) 10 13	39, 55, 100, 132	0
1	D	434/485~(89%)	0.57	34 (7%) 13 17	43, 62, 99, 169	0
All	All	1773/1940~(91%)	0.45	121 (6%) 17 21	30, 53, 95, 169	0

All (121) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	С	476	SER	10.1
1	С	66	VAL	8.7
1	С	70	MET	7.1
1	С	63	SER	6.3
1	D	319	PRO	6.2
1	В	292	TYR	5.8
1	В	54	LYS	5.3
1	В	52	ILE	5.2
1	А	60	ASP	5.1
1	D	50	ARG	5.1
1	С	64	ILE	5.0
1	В	47	ILE	5.0
1	В	50	ARG	4.7
1	С	326	GLU	4.5
1	D	7	ASN	4.5
1	В	55	ALA	4.4
1	С	46	GLU	4.1
1	В	53	ARG	4.1
1	В	319	PRO	3.9
1	С	57	ASN	3.9
1	В	66	VAL	3.8



8IE4

Mol	Chain	Res	Type	RSRZ
1	D	52	ILE	3.7
1	D	292	TYR	3.6
1	В	56	ASN	3.6
1	В	291	VAL	3.6
1	D	288	GLY	3.5
1	А	57	ASN	3.5
1	В	288	GLY	3.4
1	С	368	TRP	3.4
1	В	68	ASN	3.3
1	В	287	VAL	3.3
1	С	85	GLY	3.3
1	D	340	ASP	3.2
1	D	291	VAL	3.2
1	С	67	GLY	3.2
1	А	55	ALA	3.2
1	D	8	ASP	3.1
1	С	65	LYS	3.1
1	D	347	TRP	3.1
1	А	62	GLN	3.1
1	В	63	SER	3.0
1	А	58	LEU	3.0
1	D	476	SER	2.9
1	D	475	GLY	2.9
1	D	433	PRO	2.9
1	А	50	ARG	2.8
1	А	54	LYS	2.8
1	В	44	ALA	2.8
1	С	62	GLN	2.8
1	С	53	ARG	2.7
1	D	289	SER	2.7
1	D	25	PRO	2.7
1	С	69	GLY	2.7
1	D	140	GLN	2.7
1	D	327	PRO	2.6
1	В	69	GLY	2.6
1	D	117	GLY	2.6
1	В	293	LEU	2.6
1	В	48	VAL	2.5
1	A	59	ASN	2.5
1	С	54	LYS	2.5
1	D	271	LYS	2.5
1	А	66	VAL	2.5



Mol	Chain	Res	Type	RSRZ
1	D	73	PHE	2.5
1	С	68	ASN	2.5
1	С	291	VAL	2.4
1	В	46	GLU	2.4
1	С	49	GLY	2.4
1	С	112	LYS	2.4
1	А	319	PRO	2.4
1	С	47	ILE	2.4
1	А	366	CYS	2.4
1	D	55	ALA	2.4
1	В	272	GLU	2.3
1	В	368	TRP	2.3
1	С	114	GLU	2.3
1	D	336	GLU	2.3
1	А	337	LYS	2.3
1	В	70	MET	2.2
1	А	320	SER	2.2
1	D	116	SER	2.2
1	С	23	VAL	2.2
1	А	65	LYS	2.2
1	В	73	PHE	2.2
1	В	76	PHE	2.2
1	С	433	PRO	2.2
1	С	317	ARG	2.2
1	С	147	TRP	2.2
1	В	290	VAL	2.2
1	В	326	GLU	2.2
1	А	347	TRP	2.2
1	С	72	ARG	2.2
1	С	73	PHE	2.2
1	С	287	VAL	2.1
1	A	122	CYS	2.1
1	В	67	GLY	2.1
1	С	172	GLU	2.1
1	D	174	GLU	2.1
1	В	366	CYS	2.1
1	D	127	PRO	2.1
1	С	375	ILE	2.1
1	D	48	VAL	2.1
1	D	388	GLY	2.1
1	D	318	PRO	2.1
1	D	53	ARG	2.1



Mol	Chain	Res	Type	RSRZ
1	С	413	GLU	2.1
1	С	52	ILE	2.1
1	С	327	PRO	2.1
1	С	340	ASP	2.1
1	С	8	ASP	2.1
1	D	187	TYR	2.1
1	D	147	TRP	2.1
1	В	388	GLY	2.1
1	С	289	SER	2.0
1	D	269	ASP	2.0
1	С	86	SER	2.0
1	В	270	CYS	2.0
1	В	365	HIS	2.0
1	В	336	GLU	2.0
1	D	71	ILE	2.0
1	D	306	LEU	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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	MES	А	501	12/12	0.97	0.11	32,41,47,50	0

6.5 Other polymers (i)

There are no such residues in this entry.

