



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:21 AM UTC

PDB ID : 8IE4 / pdb_00008ie4
Title : Crystal structure of GcCGT
Authors : Zhang, M.; Bao, Y.; He, C.; Ye, M.
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

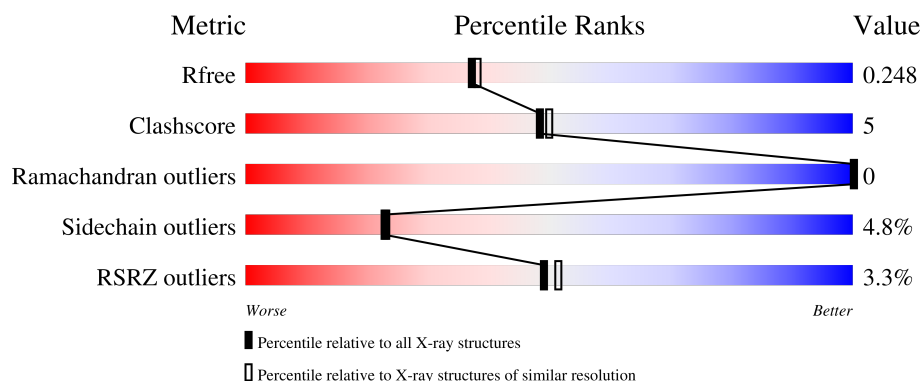
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	A	485	0% 78% 13% 7%
1	B	485	3% 75% 15% 8%
1	C	485	4% 77% 14% 8%
1	D	485	4% 74% 15% 11%

2 Entry composition [i](#)

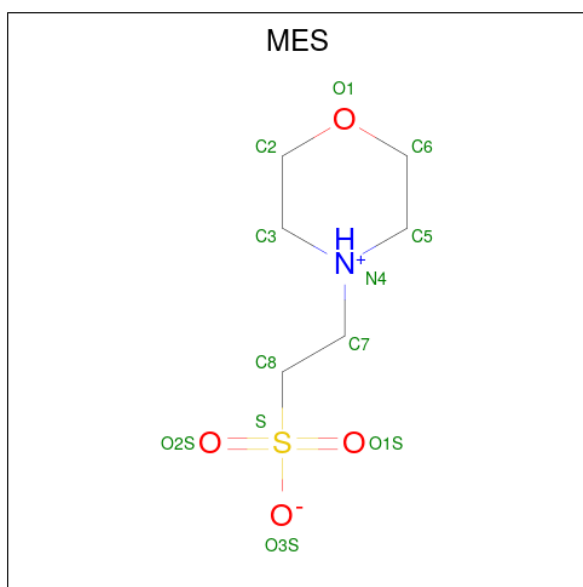
There are 3 unique types of molecules in this entry. The entry contains 14531 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

- Molecule 1 is a protein called GcCGT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3543	2281	594	655	13			
1	B	445	Total	C	N	O	S	0	0	0
			3515	2265	586	650	14			
1	C	444	Total	C	N	O	S	0	0	0
			3496	2252	587	643	14			
1	D	434	Total	C	N	O	S	0	0	0
			3441	2221	574	633	13			

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

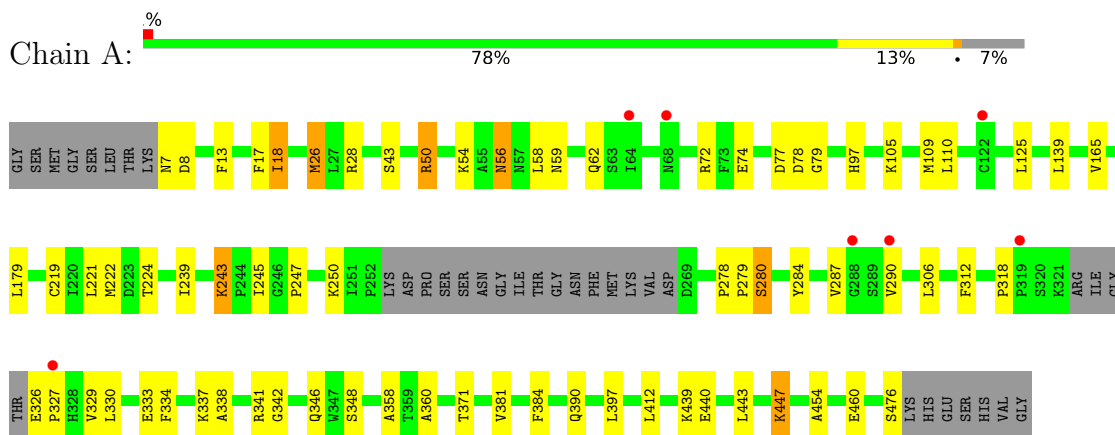
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	200	Total 200	O 200	0	0
3	B	145	Total 145	O 145	0	0
3	C	104	Total 104	O 104	0	0
3	D	75	Total 75	O 75	0	0

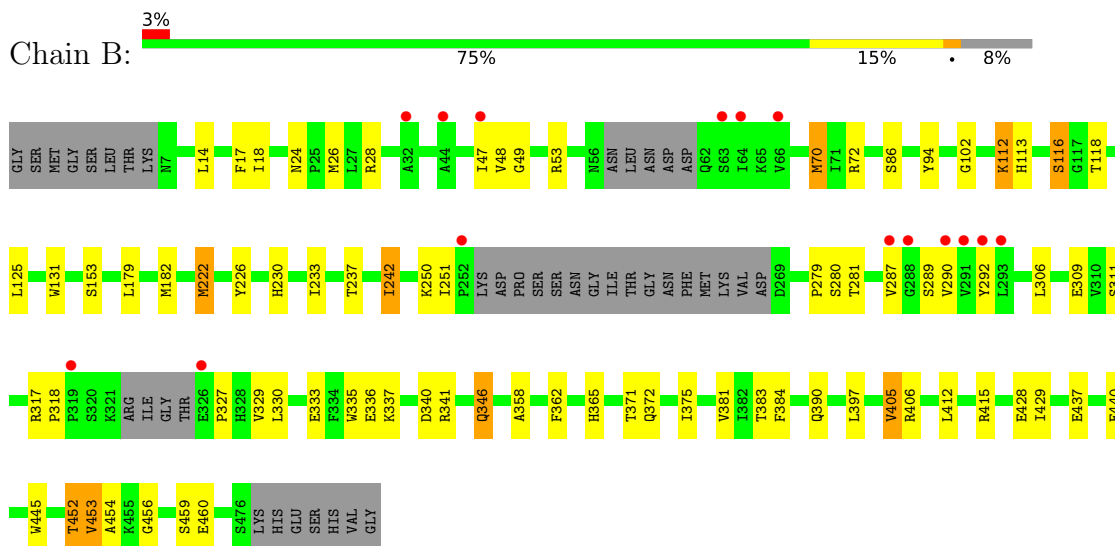
3 Residue-property plots [i](#)

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.

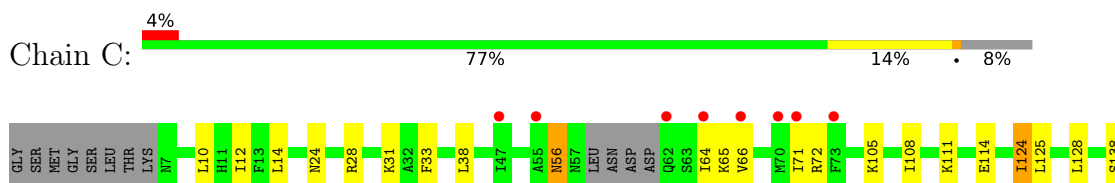
• Molecule 1: GcCGT

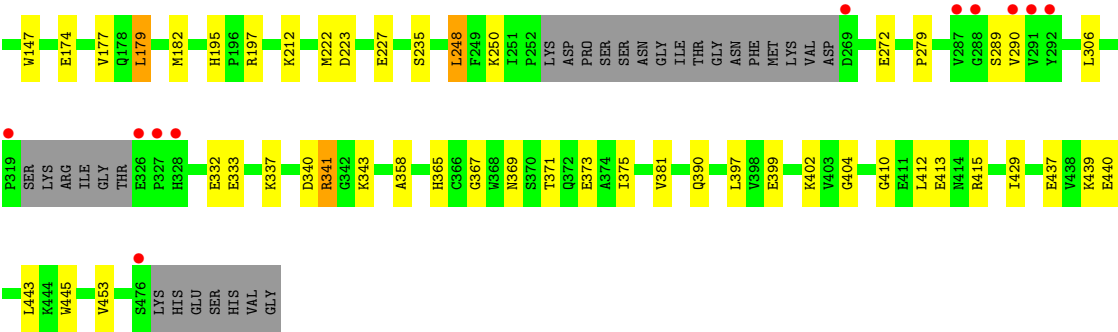


• Molecule 1: GcCGT

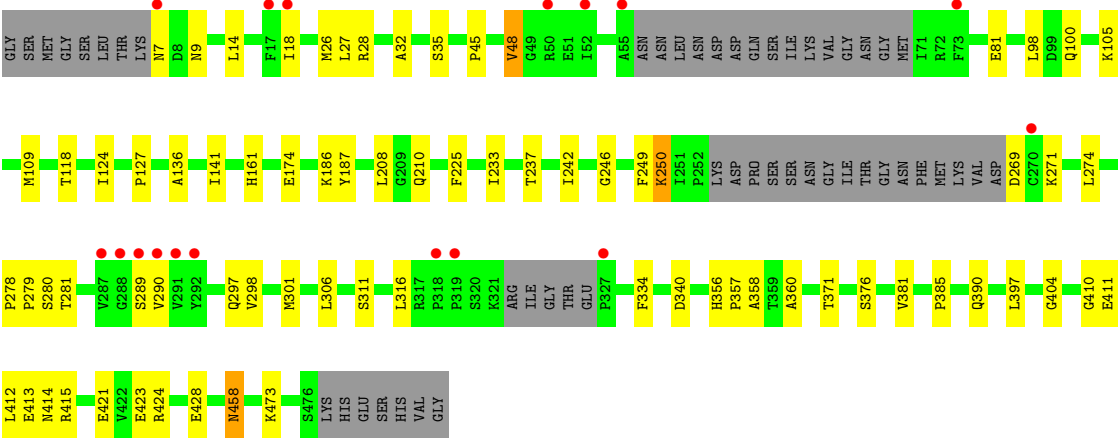


• Molecule 1: GcCGT





• Molecule 1: GcCGT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.18Å 95.93Å 132.22Å 90.00° 103.54° 90.00°	Depositor
Resolution (Å)	39.50 – 2.10 39.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.50-2.10) 99.8 (39.50-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.202 , 0.250 0.199 , 0.248	Depositor DCC
R_{free} test set	5781 reflections (4.94%)	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 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.*

¹Intensities estimated from amplitudes.

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.

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	0/3635	0.54	0/4944
1	B	0.33	0/3606	0.50	0/4901
1	C	0.30	0/3586	0.47	0/4875
1	D	0.27	0/3532	0.44	0/4801
All	All	0.32	0/14359	0.49	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	A	3543	0	3500	38	0
1	B	3515	0	3482	43	0
1	C	3496	0	3462	35	0
1	D	3441	0	3415	38	0
2	A	12	0	12	0	0
3	A	200	0	0	5	0
3	B	145	0	0	0	0
3	C	104	0	0	2	0
3	D	75	0	0	2	0
All	All	14531	0	13871	153	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 (153) 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: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:14:LEU:HB3	1:B:26:MET:HE3	1.73	0.71
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:D:81:GLU:H	1:D:81:GLU:CD	2.06	0.64
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:A:454:ALA:O	1:A:460:GLU:HG2	2.02	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:C:212:LYS:NZ	3:C:503:HOH:O	2.35	0.56
1:D:269:ASP:N	1:D:271:LYS:HZ3	2.03	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:B:405:VAL:HG21	1:B:428:GLU:HG2	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:B:179:LEU:HB2	1:B:182:MET:HE3	1.88	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:13:PHE:HZ	1:A:109:MET:HE2	1.74	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:D:14:LEU:HB3	1:D:26:MET:HE3	1.91	0.51
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:B:333:GLU:H	1:B:333:GLU:CD	2.19	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: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: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:C:179:LEU:HB2	1:C:182:MET:HE3	1.96	0.47
1:B:333:GLU:OE1	1:B:333:GLU:N	2.36	0.47
1:A:280:SER:C	1:A:360:ALA:HB2	2.40	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:D:415:ARG:HH22	1:D:421:GLU:CD	2.22	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:C:147:TRP:CD1	1:C:222:MET:HE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:399:GLU:O	1:C:402:LYS:NZ	2.46	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:C:289:SER:OG	1:C:365:HIS:NE2	2.47	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: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:C:365:HIS:HD1	1:C:367:GLY:H	1.64	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: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:A:77:ASP:CG	1:A:79:GLY:H	2.26	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:D:280:SER:C	1:D:360:ALA:HB2	2.43	0.43
1:A:284:TYR:OH	1:A:348:SER:OG	2.37	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:MET:HB3	1:B:70:MET:HE2	1.75	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:B:222:MET:HE3	1:B:242:ILE:HG12	2.02	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
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:26:MET:HE1	1:A:125:LEU:O	2.20	0.41
1:A:219:CYS:SG	1:A:243:LYS:HG3	2.60	0.41
1:B:182:MET:HE3	1:B:182:MET:HB2	1.81	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: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
1:C:179:LEU:CB	1:C:182:MET:HE3	2.51	0.40
1:D:32:ALA:O	1:D:35:SER:OG	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	A	444/485 (92%)	433 (98%)	11 (2%)	0	100	100
1	B	437/485 (90%)	422 (97%)	15 (3%)	0	100	100
1	C	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

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	A	389/424 (92%)	374 (96%)	15 (4%)	28	31
1	B	388/424 (92%)	367 (95%)	21 (5%)	20	18
1	C	384/424 (91%)	361 (94%)	23 (6%)	17	15
1	D	380/424 (90%)	365 (96%)	15 (4%)	28	31
All	All	1541/1696 (91%)	1467 (95%)	74 (5%)	23	23

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	18	ILE

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Mol	Chain	Res	Type
1	A	26	MET
1	A	50	ARG
1	A	56	ASN
1	A	59	ASN
1	A	72	ARG
1	A	239	ILE
1	A	243	LYS
1	A	280	SER
1	A	330	LEU
1	A	439	LYS
1	A	440	GLU
1	A	443	LEU
1	A	447	LYS
1	B	48	VAL
1	B	70	MET
1	B	86	SER
1	B	112	LYS
1	B	116	SER
1	B	125	LEU
1	B	153	SER
1	B	222	MET
1	B	242	ILE
1	B	250	LYS
1	B	280	SER
1	B	292	TYR
1	B	309	GLU
1	B	340	ASP
1	B	346	GLN
1	B	372	GLN
1	B	405	VAL
1	B	415	ARG
1	B	429	ILE
1	B	452	THR
1	B	453	VAL
1	C	56	ASN
1	C	64	ILE
1	C	65	LYS
1	C	71	ILE
1	C	72	ARG
1	C	114	GLU
1	C	124	ILE
1	C	125	LEU

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Mol	Chain	Res	Type
1	C	128	LEU
1	C	138	SER
1	C	174	GLU
1	C	179	LEU
1	C	227	GLU
1	C	235	SER
1	C	248	LEU
1	C	272	GLU
1	C	332	GLU
1	C	333	GLU
1	C	341	ARG
1	C	412	LEU
1	C	429	ILE
1	C	439	LYS
1	C	443	LEU
1	D	48	VAL
1	D	100	GLN
1	D	118	THR
1	D	124	ILE
1	D	186	LYS
1	D	250	LYS
1	D	289	SER
1	D	298	VAL
1	D	311	SER
1	D	340	ASP
1	D	411	GLU
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. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	104	GLN
1	A	350	GLN
1	A	352	GLN
1	A	386	GLN
1	B	56	ASN
1	B	346	GLN
1	B	458	ASN

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Mol	Chain	Res	Type
1	C	162	HIS
1	C	210	GLN
1	D	7	ASN

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 oligosaccharides 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MES	A	501	-	12,12,12	1.41	1 (8%)	15,16,16	1.91	4 (26%)

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	A	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	A	501	MES	C8-S	-4.36	1.71	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	MES	C5-N4-C3	4.13	117.73	108.84
2	A	501	MES	C6-C5-N4	-3.40	104.96	110.12
2	A	501	MES	C7-N4-C5	2.60	118.17	111.24
2	A	501	MES	C7-N4-C3	2.60	118.17	111.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

6.1 Protein, DNA and RNA chains

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, 95th 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	A	450/485 (92%)	0.14	7 (1%) 70 73	30, 43, 80, 128	0
1	B	445/485 (91%)	0.41	15 (3%) 48 50	35, 51, 97, 144	0
1	C	444/485 (91%)	0.42	19 (4%) 40 41	39, 55, 100, 132	0
1	D	434/485 (89%)	0.60	17 (3%) 43 45	43, 62, 99, 169	0
All	All	1773/1940 (91%)	0.39	58 (3%) 49 51	30, 53, 95, 169	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	291	VAL	5.2
1	D	327	PRO	4.4
1	B	319	PRO	4.2
1	D	319	PRO	4.0
1	D	55	ALA	3.8
1	D	292	TYR	3.5
1	C	66	VAL	3.5
1	C	64	ILE	3.4
1	B	290	VAL	3.4
1	D	291	VAL	3.4
1	C	327	PRO	3.3
1	A	319	PRO	3.3
1	D	52	ILE	3.3
1	D	290	VAL	3.2
1	D	288	GLY	3.2
1	C	291	VAL	3.1
1	B	64	ILE	3.1
1	B	293	LEU	2.9
1	B	288	GLY	2.9
1	C	70	MET	2.8
1	D	73	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	32	ALA	2.8
1	B	292	TYR	2.7
1	D	18	ILE	2.7
1	C	319	PRO	2.7
1	B	287	VAL	2.7
1	A	68	ASN	2.6
1	B	44	ALA	2.5
1	D	270	CYS	2.5
1	C	47	ILE	2.5
1	B	252	PRO	2.4
1	C	55	ALA	2.4
1	B	66	VAL	2.4
1	C	476	SER	2.4
1	C	290	VAL	2.4
1	D	289	SER	2.4
1	D	50	ARG	2.3
1	B	63	SER	2.3
1	D	287	VAL	2.3
1	D	17	PHE	2.3
1	C	292	TYR	2.3
1	B	47	ILE	2.2
1	A	290	VAL	2.2
1	A	327	PRO	2.2
1	C	62	GLN	2.2
1	D	318	PRO	2.1
1	C	287	VAL	2.1
1	C	269	ASP	2.1
1	A	64	ILE	2.1
1	C	73	PHE	2.1
1	C	288	GLY	2.1
1	B	326	GLU	2.1
1	C	326	GLU	2.1
1	C	328	HIS	2.1
1	C	71	ILE	2.1
1	D	7	ASN	2.0
1	A	122	CYS	2.0
1	A	288	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
2	MES	A	501	12/12	0.92	0.11	32,41,47,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.