



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:49 PM UTC

PDB ID : 3G4D / pdb_00003g4d
Title : Crystal Structure of (+)-delta-Cadinene Synthase from *Gossypium arboreum* and Evolutionary Divergence of Metal Binding Motifs for Catalysis
Authors : Gennadios, H.A.; Di Costanzo, L.; Miller, D.J.; Allemann, R.K.; Christianson, D.W.
Deposited on : 2009-02-03
Resolution : 2.40 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

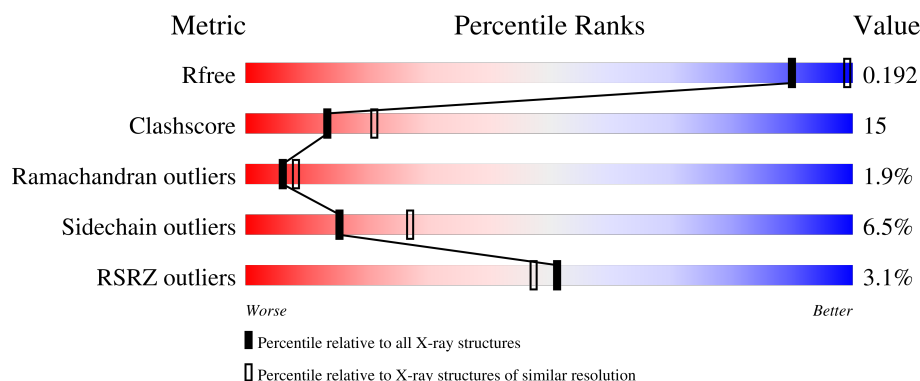
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	554	% 71% 18% • 7%
1	B	554	4% 63% 24% 5% • 8%

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
3	GOL	B	2431	-	X	-	-
3	GOL	B	2432	-	X	-	-
3	GOL	B	2433	-	X	-	-
3	GOL	B	2434	-	X	-	-

2 Entry composition [i](#)

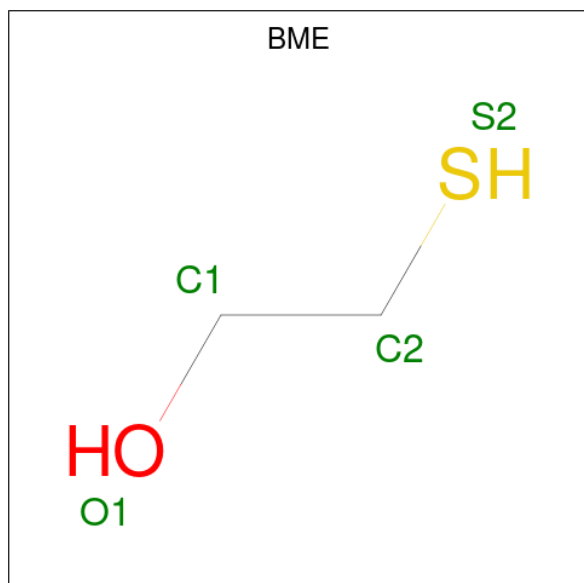
There are 4 unique types of molecules in this entry. The entry contains 8813 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (+)-delta-cadinene synthase isozyme XC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	15	0	0
			4217	2694	702	799	22			
1	B	512	Total	C	N	O	S	8	0	0
			4178	2670	699	787	22			

- Molecule 2 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

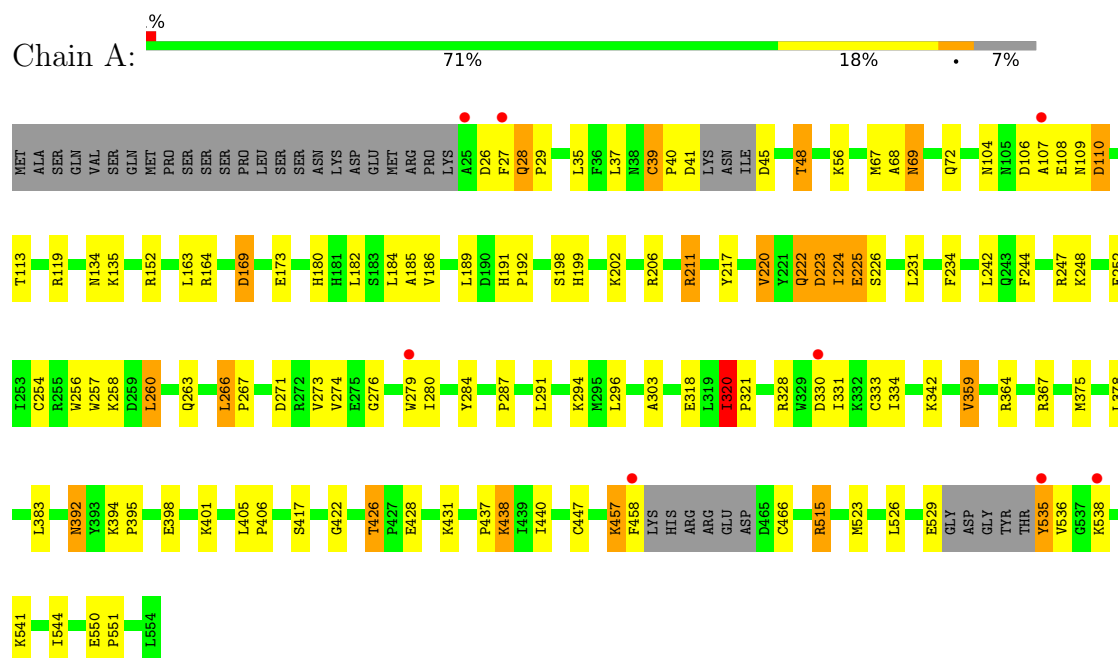
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	278	Total	O	0	0
			278	278		
4	B	104	Total	O	0	0
			104	104		

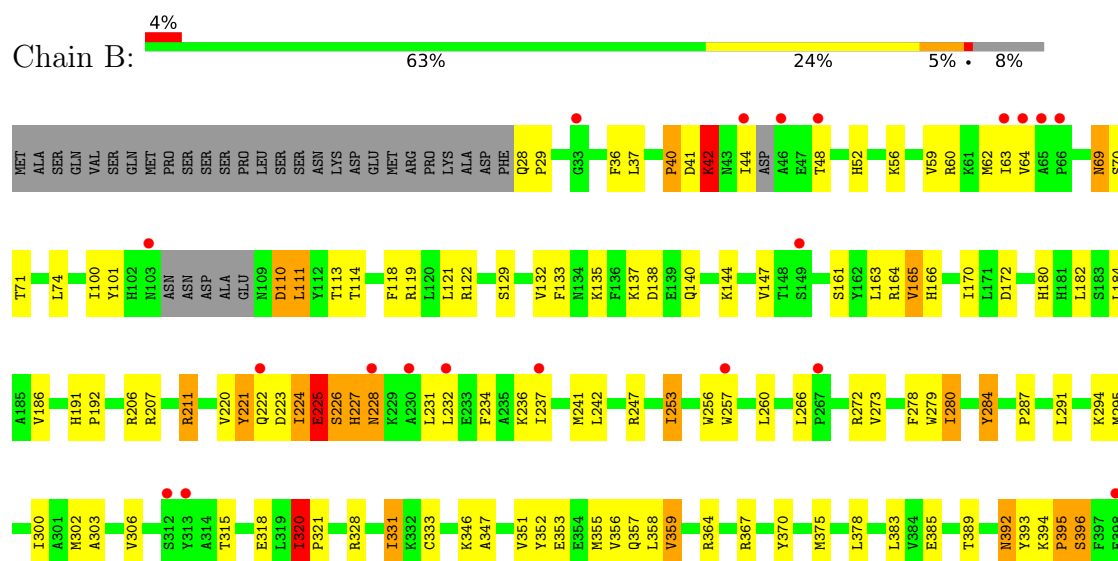
3 Residue-property plots

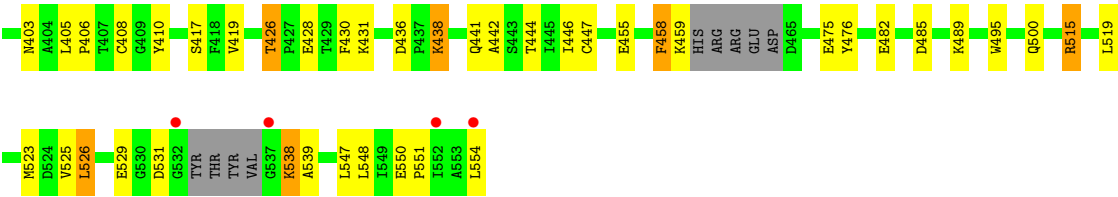
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: (+)-delta-cadinene synthase isozyme XC1



- Molecule 1: (+)-delta-cadinene synthase isozyme XC1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	158.19Å 158.19Å 158.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.70 – 2.40 47.70 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.70-2.40) 99.3 (47.70-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.192 , 0.238 0.192 , 0.192	Depositor DCC
R_{free} test set	2608 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8813	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BME, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	1/4313 (0.0%)	0.74	4/5835 (0.1%)
1	B	0.33	1/4271 (0.0%)	0.73	4/5772 (0.1%)
All	All	0.37	2/8584 (0.0%)	0.74	8/11607 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	ILE	CA-CB	6.26	1.57	1.54
1	B	320	ILE	CA-CB	5.71	1.57	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	320	ILE	N-CA-CB	5.94	114.24	110.50
1	A	39	CYS	CA-C-N	5.77	125.72	119.78
1	A	39	CYS	C-N-CA	5.77	125.72	119.78
1	B	266	LEU	CA-C-N	5.33	124.51	118.97
1	B	266	LEU	C-N-CA	5.33	124.51	118.97
1	A	266	LEU	CA-C-N	5.22	125.02	119.28
1	A	266	LEU	C-N-CA	5.22	125.02	119.28
1	B	111	LEU	N-CA-C	-5.20	105.53	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	4217	0	4103	105	0
1	B	4178	0	4088	141	0
2	A	12	0	18	5	0
3	B	24	0	24	0	0
4	A	278	0	0	7	0
4	B	104	0	0	7	0
All	All	8813	0	8233	244	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 15.

All (244) 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:A:320:ILE:HG13	1:A:321:PRO:HD3	1.37	1.06
1:A:28:GLN:HB3	1:A:29:PRO:HA	1.41	1.02
1:B:222:GLN:HB3	1:B:223:ASP:CA	1.90	1.01
1:B:222:GLN:HB2	1:B:232:LEU:HD22	1.44	0.97
1:B:222:GLN:HB3	1:B:223:ASP:HA	1.49	0.95
1:A:392:ASN:HB2	1:B:140:GLN:HG3	1.50	0.93
1:A:28:GLN:HB3	1:A:29:PRO:CA	2.01	0.91
1:B:222:GLN:CB	1:B:223:ASP:HA	2.01	0.91
1:B:222:GLN:HB3	1:B:223:ASP:C	1.94	0.91
1:B:211:ARG:HG2	1:B:211:ARG:HH11	1.38	0.89
1:A:438:LYS:HE3	1:A:438:LYS:H	1.39	0.87
1:B:320:ILE:HG13	1:B:321:PRO:HD3	1.58	0.85
1:B:438:LYS:HE3	1:B:438:LYS:H	1.42	0.85
1:B:525:VAL:HG12	1:B:526:LEU:HD13	1.58	0.84
1:A:27:PHE:HD2	1:A:267:PRO:HA	1.43	0.83
1:A:276:GLY:HA2	1:A:279:TRP:CE3	2.13	0.83
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.44	0.81
1:A:438:LYS:HE3	1:A:438:LYS:N	1.94	0.81
1:B:211:ARG:HH11	1:B:211:ARG:CG	1.93	0.81
1:B:455:GLU:HG3	1:B:531:ASP:OD2	1.80	0.81
1:B:359:VAL:HG13	1:B:364:ARG:HB2	1.62	0.81
1:B:438:LYS:HE3	1:B:438:LYS:N	1.98	0.78
1:B:222:GLN:CB	1:B:223:ASP:CA	2.60	0.78
1:A:426:THR:HG23	1:A:428:GLU:H	1.48	0.77
1:A:27:PHE:HB2	1:A:28:GLN:HE21	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLU:HB2	1:A:135:LYS:HZ2	1.54	0.73
1:A:320:ILE:HG13	1:A:321:PRO:CD	2.17	0.73
1:B:222:GLN:H	1:B:232:LEU:HD13	1.53	0.72
1:A:28:GLN:CB	1:A:29:PRO:HA	2.19	0.71
1:A:211:ARG:HG2	1:A:211:ARG:NH1	2.04	0.71
1:A:27:PHE:HB2	1:A:28:GLN:NE2	2.05	0.71
1:A:106:ASP:C	1:A:108:GLU:HA	2.16	0.70
1:B:438:LYS:H	1:B:438:LYS:CE	2.05	0.70
1:A:359:VAL:HG13	1:A:364:ARG:HB2	1.73	0.69
1:B:458:PHE:O	1:B:459:LYS:HG3	1.93	0.69
1:B:114:THR:HG23	1:B:132:VAL:HG12	1.74	0.69
1:A:438:LYS:H	1:A:438:LYS:CE	2.06	0.68
1:B:135:LYS:HG2	4:B:645:HOH:O	1.93	0.67
1:A:211:ARG:HH11	1:A:211:ARG:CG	2.06	0.67
1:A:108:GLU:HB2	1:A:135:LYS:NZ	2.10	0.67
1:B:284:TYR:HB3	1:B:515:ARG:NH2	2.09	0.67
1:B:211:ARG:HG2	1:B:211:ARG:NH1	2.03	0.67
1:B:475:GLU:HG3	1:B:476:TYR:CD2	2.29	0.66
1:A:28:GLN:HG3	1:A:271:ASP:HB2	1.76	0.66
1:A:69:ASN:ND2	1:A:72:GLN:H	1.94	0.66
1:A:328:ARG:NH2	1:A:333:CYS:SG	2.68	0.65
1:A:40:PRO:O	1:A:41:ASP:HB2	1.95	0.65
1:A:364:ARG:HD2	1:A:367:ARG:CZ	2.27	0.65
1:B:164:ARG:HD2	1:B:172:ASP:OD1	1.97	0.65
1:B:428:GLU:HA	1:B:431:LYS:HD3	1.79	0.65
1:A:254:CYS:SG	4:A:623:HOH:O	2.55	0.64
1:B:426:THR:HG22	1:B:428:GLU:H	1.62	0.64
1:B:60:ARG:O	1:B:64:VAL:HG23	1.98	0.64
1:B:226:SER:O	1:B:227:HIS:HB2	1.96	0.64
1:A:39:CYS:SG	2:A:1275:BME:S2	2.90	0.63
1:A:106:ASP:O	1:A:108:GLU:HA	1.97	0.63
1:B:364:ARG:HD3	4:B:635:HOH:O	1.99	0.63
1:A:276:GLY:HA2	1:A:279:TRP:HE3	1.63	0.62
1:A:303:ALA:HB2	1:A:375:MET:HE1	1.82	0.62
1:A:27:PHE:CD2	1:A:267:PRO:HA	2.29	0.62
1:B:426:THR:CG2	1:B:428:GLU:H	2.13	0.62
1:A:40:PRO:HG3	1:A:247:ARG:HB3	1.82	0.62
1:A:426:THR:HG23	1:A:428:GLU:N	2.15	0.61
1:A:110:ASP:HB2	1:A:113:THR:H	1.64	0.61
1:B:62:MET:HE1	1:B:228:ASN:HD21	1.66	0.61
1:B:221:TYR:CD1	1:B:221:TYR:C	2.79	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ILE:HG13	1:B:321:PRO:CD	2.31	0.60
1:B:211:ARG:NH2	1:B:242:LEU:HD12	2.16	0.60
1:A:538:LYS:H	1:A:538:LYS:HD2	1.67	0.60
1:B:110:ASP:HB3	1:B:113:THR:H	1.66	0.60
1:A:107:ALA:HA	1:A:108:GLU:HB3	1.84	0.60
1:B:192:PRO:HG3	1:B:224:ILE:CG2	2.32	0.60
1:B:278:PHE:HE1	1:B:547:LEU:HD12	1.66	0.59
1:A:328:ARG:CZ	1:A:333:CYS:SG	2.91	0.59
1:A:535:TYR:N	1:A:536:VAL:HA	2.16	0.59
1:B:232:LEU:HD11	1:B:236:LYS:HE2	1.85	0.59
1:A:69:ASN:C	1:A:69:ASN:HD22	2.09	0.59
1:A:541:LYS:HE3	1:B:482:GLU:OE1	2.01	0.59
1:A:422:GLY:CA	2:A:1274:BME:H11	2.33	0.58
1:A:67:MET:HE2	1:A:72:GLN:HB3	1.86	0.58
1:A:199:HIS:HA	1:A:202:LYS:NZ	2.19	0.57
1:B:165:VAL:CG1	1:B:166:HIS:N	2.68	0.57
1:A:274:VAL:HG12	1:A:544:ILE:HD13	1.87	0.57
1:B:180:HIS:CE1	1:B:184:LEU:HD11	2.39	0.57
1:A:169:ASP:O	1:A:173:GLU:HG3	2.04	0.56
1:B:222:GLN:NE2	1:B:227:HIS:O	2.39	0.56
1:B:364:ARG:HD2	1:B:367:ARG:CZ	2.35	0.56
1:A:417:SER:OG	1:A:515:ARG:HG2	2.04	0.56
1:A:280:ILE:HD12	1:A:296:LEU:HG	1.87	0.55
1:B:396:SER:HB3	4:B:648:HOH:O	2.05	0.55
1:A:294:LYS:HG2	4:A:817:HOH:O	2.07	0.55
1:B:295:MET:HE1	1:B:359:VAL:HG23	1.87	0.55
1:B:426:THR:HG22	1:B:428:GLU:N	2.21	0.55
1:B:221:TYR:C	1:B:221:TYR:HD1	2.15	0.55
1:A:198:SER:O	1:A:202:LYS:HG3	2.07	0.55
1:A:106:ASP:HB3	4:A:761:HOH:O	2.07	0.55
1:A:169:ASP:OD1	1:A:169:ASP:N	2.38	0.55
1:B:225:GLU:O	1:B:225:GLU:HG2	2.06	0.55
1:B:538:LYS:HE3	1:B:538:LYS:HA	1.89	0.55
1:B:137:LYS:HE3	1:B:170:ILE:HG13	1.89	0.54
1:A:242:LEU:HD21	1:A:287:PRO:HG3	1.90	0.54
1:B:225:GLU:O	1:B:225:GLU:CG	2.56	0.54
1:B:69:ASN:HD22	1:B:69:ASN:N	2.05	0.54
1:A:110:ASP:HB3	4:A:788:HOH:O	2.06	0.53
1:A:69:ASN:HD22	1:A:72:GLN:H	1.56	0.53
1:B:59:VAL:O	1:B:63:ILE:HG13	2.09	0.53
1:B:295:MET:HE2	1:B:355:MET:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:PRO:O	1:B:396:SER:HB3	2.09	0.53
1:B:182:LEU:O	1:B:186:VAL:HG23	2.09	0.53
1:B:303:ALA:HB2	1:B:375:MET:HE1	1.91	0.53
1:A:222:GLN:C	1:A:223:ASP:O	2.51	0.52
1:B:247:ARG:HD3	1:B:548:LEU:O	2.09	0.52
1:B:44:ILE:HD11	1:B:554:LEU:HD11	1.92	0.52
1:A:422:GLY:HA3	2:A:1274:BME:H11	1.92	0.52
1:B:191:HIS:CG	1:B:192:PRO:HA	2.45	0.52
1:A:334:ILE:O	1:A:342:LYS:HE2	2.09	0.52
1:B:222:GLN:HB2	1:B:223:ASP:HA	1.86	0.52
1:B:315:THR:OG1	1:B:318:GLU:HG3	2.09	0.52
1:A:185:ALA:O	1:A:189:LEU:HG	2.11	0.51
1:A:180:HIS:CE1	1:A:184:LEU:HD11	2.46	0.51
1:A:252:GLU:OE1	1:A:294:LYS:HE3	2.10	0.51
1:A:330:ASP:OD1	1:A:331:ILE:N	2.44	0.51
1:B:165:VAL:HG13	4:B:597:HOH:O	2.10	0.50
1:B:40:PRO:HG3	1:B:247:ARG:HB3	1.91	0.50
1:A:40:PRO:O	1:A:41:ASP:CB	2.59	0.50
1:A:458:PHE:HB2	1:A:529:GLU:O	2.12	0.50
1:B:526:LEU:HD12	1:B:539:ALA:HB1	1.93	0.50
1:B:346:LYS:HG3	1:B:347:ALA:N	2.26	0.49
1:B:458:PHE:CD2	1:B:459:LYS:N	2.80	0.49
1:B:74:LEU:HD21	1:B:100:ILE:HG21	1.95	0.49
1:B:295:MET:HE3	1:B:358:LEU:CB	2.42	0.49
1:A:39:CYS:CB	2:A:1275:BME:HS2	2.25	0.49
1:B:118:PHE:O	1:B:122:ARG:HB2	2.13	0.49
1:B:279:TRP:HE3	1:B:300:ILE:HD11	1.78	0.49
1:B:256:TRP:O	1:B:260:LEU:HD23	2.12	0.49
1:B:287:PRO:HD2	4:B:619:HOH:O	2.12	0.49
1:A:191:HIS:CG	1:A:192:PRO:HA	2.48	0.48
1:A:109:ASN:HB3	1:A:113:THR:HB	1.94	0.48
1:B:114:THR:HG23	1:B:132:VAL:CG1	2.40	0.48
1:B:222:GLN:C	1:B:224:ILE:H	2.20	0.48
1:B:119:ARG:HG3	1:B:163:LEU:HD13	1.95	0.48
1:A:318:GLU:C	1:A:321:PRO:HD2	2.39	0.47
1:B:122:ARG:HD2	4:B:577:HOH:O	2.13	0.47
1:A:225:GLU:O	1:A:226:SER:CB	2.62	0.47
1:B:133:PHE:HB2	1:B:170:ILE:HD13	1.96	0.47
1:A:199:HIS:HA	1:A:202:LYS:HZ3	1.79	0.47
1:B:207:ARG:HG2	1:B:495:TRP:CH2	2.49	0.47
1:A:182:LEU:O	1:A:186:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:VAL:HG11	1:B:500:GLN:OE1	2.14	0.46
1:B:221:TYR:HD1	1:B:221:TYR:O	1.98	0.46
1:B:302:MET:O	1:B:306:VAL:HG23	2.16	0.46
1:B:302:MET:HG3	1:B:351:VAL:HG21	1.97	0.46
1:A:447:CYS:HA	1:A:523:MET:HG3	1.98	0.46
1:B:359:VAL:CG1	1:B:364:ARG:HB2	2.39	0.46
1:B:393:TYR:CE2	1:B:395:PRO:HA	2.50	0.46
1:B:417:SER:OG	1:B:515:ARG:HG2	2.15	0.46
1:A:398:GLU:HA	1:A:401:LYS:HB3	1.98	0.46
1:B:447:CYS:HA	1:B:523:MET:HG3	1.97	0.46
1:B:42:LYS:HD2	1:B:44:ILE:H	1.81	0.46
1:B:41:ASP:O	1:B:42:LYS:HB3	2.16	0.46
1:B:129:SER:O	1:B:132:VAL:HG23	2.15	0.46
1:B:328:ARG:CZ	1:B:333:CYS:SG	3.04	0.46
1:A:68:ALA:HB3	1:A:72:GLN:CD	2.42	0.45
1:B:52:HIS:HB2	1:B:237:ILE:HG21	1.97	0.45
1:B:436:ASP:OD2	1:B:441:GLN:HG3	2.16	0.45
1:B:253:ILE:CG2	1:B:294:LYS:HG2	2.46	0.45
1:B:257:TRP:CD2	1:B:273:VAL:HG21	2.51	0.45
1:B:475:GLU:HG3	1:B:476:TYR:HD2	1.79	0.45
1:B:426:THR:CG2	1:B:428:GLU:OE1	2.65	0.45
1:A:223:ASP:O	1:A:224:ILE:C	2.55	0.45
1:A:266:LEU:HA	1:A:267:PRO:HD2	1.80	0.45
1:B:111:LEU:HD22	1:B:147:VAL:HG13	1.99	0.45
1:B:191:HIS:CD2	1:B:224:ILE:HD13	2.52	0.45
1:A:257:TRP:CG	1:A:273:VAL:HG21	2.52	0.44
1:A:318:GLU:O	1:A:321:PRO:HD2	2.17	0.44
1:A:252:GLU:HB2	1:A:294:LYS:HE3	1.98	0.44
1:B:56:LYS:HG3	1:B:234:PHE:CZ	2.52	0.44
1:B:280:ILE:C	1:B:280:ILE:HD12	2.43	0.44
1:B:331:ILE:H	1:B:331:ILE:HG13	1.58	0.44
1:A:104:ASN:ND2	4:A:761:HOH:O	2.50	0.44
1:B:28:GLN:HB3	1:B:29:PRO:HD3	2.00	0.44
1:A:45:ASP:HB3	1:A:48:THR:CG2	2.47	0.44
1:B:138:ASP:HB3	1:B:144:LYS:HG2	2.00	0.44
1:B:485:ASP:O	1:B:489:LYS:HG3	2.18	0.44
1:B:253:ILE:HD11	1:B:273:VAL:HG13	2.00	0.44
1:A:152:ARG:NH2	4:A:735:HOH:O	2.37	0.44
1:A:191:HIS:NE2	1:A:223:ASP:OD1	2.47	0.44
1:B:62:MET:HE1	1:B:228:ASN:ND2	2.32	0.44
1:B:320:ILE:C	1:B:320:ILE:HD12	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:TYR:O	1:B:356:VAL:HG23	2.18	0.43
1:B:442:ALA:O	1:B:446:ILE:HG13	2.18	0.43
1:B:101:TYR:HD1	1:B:121:LEU:HD13	1.82	0.43
1:B:295:MET:HE3	1:B:358:LEU:HB2	1.99	0.43
1:B:475:GLU:HG3	1:B:476:TYR:N	2.33	0.43
1:B:165:VAL:HG13	1:B:166:HIS:N	2.33	0.43
1:A:107:ALA:N	1:A:108:GLU:HA	2.29	0.43
1:B:295:MET:CE	1:B:355:MET:HA	2.48	0.43
1:B:410:TYR:CE2	1:B:519:LEU:HB3	2.53	0.43
1:B:278:PHE:CE1	1:B:547:LEU:HD12	2.52	0.43
1:B:44:ILE:HD13	1:B:237:ILE:HG23	1.99	0.42
1:B:70:SER:O	1:B:74:LEU:HG	2.19	0.42
1:A:256:TRP:CE2	1:A:260:LEU:HD21	2.53	0.42
1:A:437:PRO:HD2	1:A:440:ILE:HB	2.00	0.42
1:B:100:ILE:O	1:B:100:ILE:HG22	2.20	0.42
1:A:27:PHE:HB3	1:A:266:LEU:O	2.19	0.42
1:A:28:GLN:NE2	1:A:263:GLN:HA	2.35	0.42
1:A:191:HIS:ND1	1:A:192:PRO:HA	2.34	0.42
1:A:244:PHE:O	1:A:248:LYS:HG3	2.19	0.42
1:A:405:LEU:N	1:A:406:PRO:CD	2.82	0.42
1:B:395:PRO:HB2	1:B:396:SER:H	1.54	0.42
1:A:256:TRP:O	1:A:260:LEU:HD22	2.20	0.42
1:B:69:ASN:OD1	1:B:71:THR:HG22	2.19	0.42
1:B:526:LEU:HD12	1:B:526:LEU:HA	1.87	0.42
1:B:405:LEU:HD22	1:B:444:THR:HG22	2.02	0.42
1:A:398:GLU:HA	1:A:401:LYS:CB	2.49	0.42
1:B:165:VAL:HG13	1:B:166:HIS:H	1.85	0.42
1:B:355:MET:CE	1:B:419:VAL:HG11	2.50	0.42
1:A:394:LYS:HA	1:A:395:PRO:HD3	1.89	0.41
1:A:134:ASN:HD22	1:A:134:ASN:HA	1.69	0.41
1:B:140:GLN:H	1:B:140:GLN:NE2	2.19	0.41
1:B:161:SER:O	1:B:164:ARG:HB3	2.21	0.41
1:A:39:CYS:HA	1:A:40:PRO:HD3	1.80	0.41
1:B:458:PHE:CG	1:B:459:LYS:N	2.84	0.41
1:B:550:GLU:HA	1:B:551:PRO:HD2	1.77	0.41
1:A:364:ARG:HD3	4:A:683:HOH:O	2.20	0.41
1:B:257:TRP:CG	1:B:273:VAL:HG21	2.56	0.41
1:B:353:GLU:HG3	4:B:620:HOH:O	2.21	0.41
1:B:385:GLU:O	1:B:389:THR:HG23	2.21	0.41
1:A:217:TYR:HA	1:A:220:VAL:HG13	2.03	0.41
1:A:550:GLU:HA	1:A:551:PRO:HD2	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:TYR:CD2	1:B:430:PHE:HB3	2.55	0.41
1:B:114:THR:CG2	1:B:132:VAL:HG12	2.46	0.40
1:B:328:ARG:NH2	1:B:333:CYS:SG	2.93	0.40
1:A:192:PRO:HG3	1:A:223:ASP:CB	2.50	0.40
1:B:241:MET:HE2	1:B:241:MET:HB3	1.96	0.40
1:A:27:PHE:CG	1:A:263:GLN:O	2.75	0.40
1:A:39:CYS:HG	2:A:1275:BME:HS2	1.39	0.40
1:A:56:LYS:HB2	1:A:234:PHE:CE1	2.56	0.40
1:A:109:ASN:HB3	1:A:113:THR:CG2	2.52	0.40
1:B:295:MET:HE2	1:B:355:MET:HG2	2.02	0.40
1:B:320:ILE:N	1:B:321:PRO:CD	2.85	0.40
1:A:119:ARG:HG3	1:A:163:LEU:HD13	2.03	0.40
1:B:272:ARG:O	1:B:273:VAL:C	2.63	0.40
1:B:403:ASN:C	1:B:406:PRO:HD2	2.47	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	A	508/554 (92%)	489 (96%)	12 (2%)	7 (1%)	9	13
1	B	502/554 (91%)	467 (93%)	23 (5%)	12 (2%)	4	5
All	All	1010/1108 (91%)	956 (95%)	35 (4%)	19 (2%)	6	8

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	A	457	LYS
1	B	395	PRO
1	B	396	SER

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Mol	Chain	Res	Type
1	B	458	PHE
1	A	28	GLN
1	A	110	ASP
1	B	110	ASP
1	B	225	GLU
1	B	226	SER
1	B	529	GLU
1	A	26	ASP
1	A	466	CYS
1	B	42	LYS
1	B	392	ASN
1	A	224	ILE
1	B	40	PRO
1	B	227	HIS
1	B	228	ASN

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	457/492 (93%)	429 (94%)	28 (6%)	17	30
1	B	453/492 (92%)	422 (93%)	31 (7%)	14	25
All	All	910/984 (92%)	851 (94%)	59 (6%)	15	27

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	37	LEU
1	A	48	THR
1	A	69	ASN
1	A	164	ARG
1	A	169	ASP
1	A	206	ARG
1	A	211	ARG

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Mol	Chain	Res	Type
1	A	220	VAL
1	A	222	GLN
1	A	225	GLU
1	A	231	LEU
1	A	258	LYS
1	A	260	LEU
1	A	284	TYR
1	A	291	LEU
1	A	320	ILE
1	A	359	VAL
1	A	378	LEU
1	A	383	LEU
1	A	392	ASN
1	A	426	THR
1	A	431	LYS
1	A	438	LYS
1	A	457	LYS
1	A	515	ARG
1	A	526	LEU
1	A	535	TYR
1	B	36	PHE
1	B	37	LEU
1	B	42	LYS
1	B	48	THR
1	B	69	ASN
1	B	165	VAL
1	B	206	ARG
1	B	211	ARG
1	B	220	VAL
1	B	221	TYR
1	B	224	ILE
1	B	225	GLU
1	B	231	LEU
1	B	253	ILE
1	B	280	ILE
1	B	284	TYR
1	B	291	LEU
1	B	320	ILE
1	B	331	ILE
1	B	357	GLN
1	B	359	VAL
1	B	378	LEU

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Mol	Chain	Res	Type
1	B	383	LEU
1	B	392	ASN
1	B	394	LYS
1	B	408	CYS
1	B	426	THR
1	B	438	LYS
1	B	515	ARG
1	B	526	LEU
1	B	538	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	69	ASN
1	A	81	GLN
1	A	104	ASN
1	A	109	ASN
1	A	134	ASN
1	A	180	HIS
1	A	181	HIS
1	A	357	GLN
1	A	362	HIS
1	A	441	GLN
1	A	490	HIS
1	B	28	GLN
1	B	72	GLN
1	B	134	ASN
1	B	180	HIS
1	B	222	GLN
1	B	324	ASN
1	B	357	GLN
1	B	441	GLN

5.3.3 RNA ⓘ

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](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	B	2431	-	5,5,5	4.90	3 (60%)	5,5,5	2.42	4 (80%)
3	GOL	B	2432	-	5,5,5	5.03	3 (60%)	5,5,5	2.32	4 (80%)
2	BME	A	1274	-	3,3,3	0.40	0	2,2,2	0.45	0
3	GOL	B	2434	-	5,5,5	4.97	3 (60%)	5,5,5	2.33	5 (100%)
2	BME	A	1275	-	3,3,3	0.23	0	2,2,2	0.41	0
2	BME	A	1273	-	3,3,3	0.27	0	2,2,2	0.38	0
3	GOL	B	2433	-	5,5,5	4.89	3 (60%)	5,5,5	2.40	5 (100%)

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
3	GOL	B	2431	-	-	2/4/4/4	-
3	GOL	B	2432	-	-	2/4/4/4	-
2	BME	A	1274	-	-	1/1/1/1	-
3	GOL	B	2434	-	-	2/4/4/4	-
2	BME	A	1275	-	-	1/1/1/1	-
2	BME	A	1273	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	2433	-	-	3/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2432	GOL	O2-C2	-8.52	1.18	1.43
3	B	2434	GOL	O2-C2	-8.45	1.18	1.43
3	B	2433	GOL	O2-C2	-8.39	1.19	1.43
3	B	2431	GOL	O2-C2	-8.27	1.19	1.43
3	B	2432	GOL	C3-C2	-5.23	1.31	1.51
3	B	2434	GOL	C3-C2	-5.17	1.32	1.51
3	B	2432	GOL	C1-C2	-5.13	1.32	1.51
3	B	2431	GOL	C3-C2	-5.12	1.32	1.51
3	B	2434	GOL	C1-C2	-5.04	1.32	1.51
3	B	2431	GOL	C1-C2	-5.03	1.32	1.51
3	B	2433	GOL	C3-C2	-4.97	1.32	1.51
3	B	2433	GOL	C1-C2	-4.94	1.32	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2431	GOL	O2-C2-C1	2.91	121.23	109.18
3	B	2432	GOL	O2-C2-C1	2.76	120.59	109.18
3	B	2434	GOL	O2-C2-C1	2.58	119.86	109.18
3	B	2433	GOL	C3-C2-C1	2.57	121.21	111.80
3	B	2431	GOL	O2-C2-C3	2.55	119.75	109.18
3	B	2432	GOL	O2-C2-C3	2.55	119.73	109.18
3	B	2434	GOL	O2-C2-C3	2.55	119.73	109.18
3	B	2433	GOL	O2-C2-C3	2.53	119.64	109.18
3	B	2433	GOL	O3-C3-C2	2.45	121.41	110.38
3	B	2431	GOL	O1-C1-C2	2.45	121.39	110.38
3	B	2433	GOL	O2-C2-C1	2.40	119.14	109.18
3	B	2432	GOL	O1-C1-C2	2.17	120.15	110.38
3	B	2434	GOL	O3-C3-C2	2.17	120.15	110.38
3	B	2434	GOL	C3-C2-C1	2.16	119.72	111.80
3	B	2434	GOL	O1-C1-C2	2.12	119.94	110.38
3	B	2431	GOL	O3-C3-C2	2.10	119.84	110.38
3	B	2432	GOL	C3-C2-C1	2.10	119.50	111.80
3	B	2433	GOL	O1-C1-C2	2.04	119.56	110.38

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2431	GOL	C1-C2-C3-O3
3	B	2432	GOL	O1-C1-C2-C3
3	B	2432	GOL	C1-C2-C3-O3
3	B	2434	GOL	C1-C2-C3-O3
3	B	2433	GOL	C1-C2-C3-O3
3	B	2431	GOL	O1-C1-C2-O2
3	B	2433	GOL	O1-C1-C2-O2
3	B	2434	GOL	O1-C1-C2-O2
3	B	2433	GOL	O2-C2-C3-O3
2	A	1274	BME	O1-C1-C2-S2
2	A	1275	BME	O1-C1-C2-S2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1274	BME	2	0
2	A	1275	BME	3	0

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	515/554 (92%)	-0.22	8 (1%) 70 66	31, 49, 84, 126	2 (0%)
1	B	511/554 (92%)	0.34	24 (4%) 36 32	42, 74, 120, 146	0
All	All	1026/1108 (92%)	0.06	32 (3%) 51 47	31, 60, 112, 146	2 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	458	PHE	6.1
1	A	27	PHE	4.2
1	A	279	TRP	4.2
1	B	228	ASN	4.0
1	B	103	ASN	3.8
1	B	66	PRO	3.5
1	B	232	LEU	3.4
1	A	25	ALA	3.3
1	B	537	GLY	3.2
1	B	48	THR	3.0
1	A	535	TYR	3.0
1	B	222	GLN	3.0
1	B	267	PRO	2.9
1	B	65	ALA	2.9
1	B	554	LEU	2.9
1	B	532	GLY	2.9
1	B	398	GLU	2.8
1	B	46	ALA	2.7
1	B	33	GLY	2.7
1	B	230	ALA	2.5
1	B	149	SER	2.5
1	B	44	ILE	2.4
1	B	64	VAL	2.4
1	B	313	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	538	LYS	2.3
1	A	330	ASP	2.2
1	A	107	ALA	2.2
1	B	312	SER	2.2
1	B	237	ILE	2.1
1	B	63	ILE	2.1
1	B	552	ILE	2.1
1	B	257	TRP	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 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
3	GOL	B	2433	6/6	0.65	0.15	70,90,98,98	0
2	BME	A	1274	4/4	0.74	0.17	75,76,78,88	0
3	GOL	B	2431	6/6	0.87	0.10	69,76,88,91	0
2	BME	A	1273	4/4	0.87	0.14	73,75,75,76	0
2	BME	A	1275	4/4	0.88	0.14	69,71,73,100	0
3	GOL	B	2432	6/6	0.92	0.09	67,76,81,82	0
3	GOL	B	2434	6/6	0.93	0.11	80,84,92,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.