



Full wwPDB X-ray Structure Validation Report

Dec 2, 2023 – 03:24 pm GMT

PDB ID : 2J5C
Title : Rational conversion of substrate and product specificity in a monoterpene synthase. Structural insights into the molecular basis of rapid evolution.
Authors : Kampranis, S.C.; Ioannidis, D.; Purvis, A.; Mahrez, W.; Ninga, E.; Katerelos, N.A.; Anssour, S.; Dunwell, J.M.; Makris, A.M.; Goodenough, P.W.; Johnson, C.B.
Deposited on : 2006-09-14
Resolution : 1.95 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (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

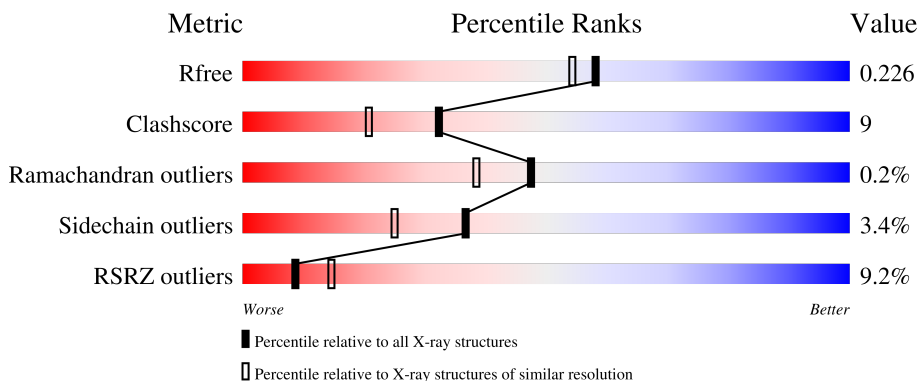
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	569	 8% 65% 19% 15%
1	B	569	 8% 68% 17% 14%

2 Entry composition [i](#)

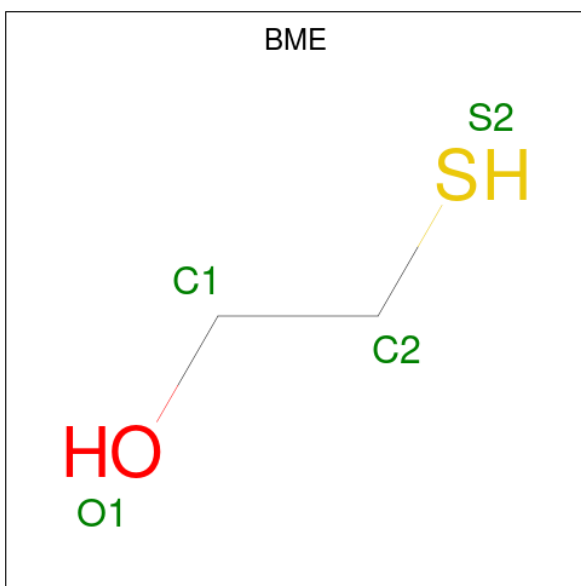
There are 3 unique types of molecules in this entry. The entry contains 8468 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1,8-CINEOLE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	485	Total 3959	C 2523	N 673	O 738	S 25	0	0	0
1	B	491	Total 4034	C 2575	N 682	O 751	S 26	0	0	0

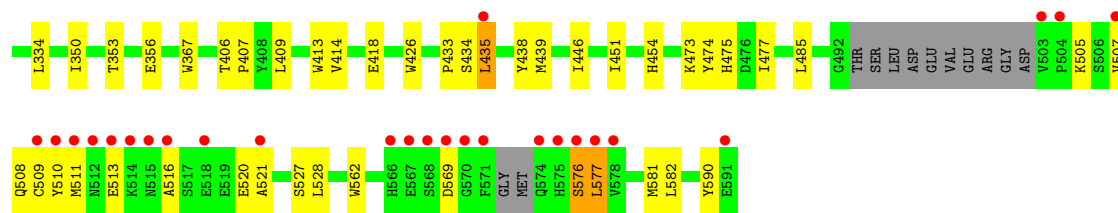
- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	221	Total 221	O 221	0	0
3	B	238	Total 238	O 238	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	124.55Å 171.15Å 123.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.70 – 1.95 29.70 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.70-1.95) 99.6 (29.70-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 1.95Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.235 0.207 , 0.226	Depositor DCC
R_{free} test set	4786 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtrriage
Anisotropy	0.678	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8468	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: BME

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	0.72	7/4042 (0.2%)	0.92	1/5458 (0.0%)
1	B	0.72	6/4121 (0.1%)	0.92	2/5568 (0.0%)
All	All	0.72	13/8163 (0.2%)	0.92	3/11026 (0.0%)

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	A	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	TRP	NE1-CE2	8.92	1.49	1.37
1	A	413	TRP	NE1-CE2	8.78	1.49	1.37
1	B	294	TRP	NE1-CE2	8.75	1.49	1.37
1	A	443	TRP	NE1-CE2	8.71	1.48	1.37
1	A	367	TRP	NE1-CE2	8.70	1.48	1.37
1	B	413	TRP	NE1-CE2	8.54	1.48	1.37
1	B	317	TRP	NE1-CE2	8.53	1.48	1.37
1	B	562	TRP	NE1-CE2	8.48	1.48	1.37
1	B	367	TRP	NE1-CE2	8.48	1.48	1.37
1	A	533	TRP	NE1-CE2	8.44	1.48	1.37
1	B	295	TRP	NE1-CE2	8.42	1.48	1.37
1	A	317	TRP	NE1-CE2	8.18	1.48	1.37
1	A	295	TRP	NE1-CE2	7.46	1.47	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	B	87	ARG	CD-NE-CZ	-5.22	116.29	123.60
1	A	325	ARG	CD-NE-CZ	-5.19	116.34	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	518	GLU	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	A	3959	0	3816	70	0
1	B	4034	0	3914	69	0
2	A	8	0	10	3	0
2	B	8	0	10	3	0
3	A	221	0	0	1	0
3	B	238	0	0	1	0
All	All	8468	0	7750	139	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 9.

All (139) 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:225:VAL:HG12	1:B:225:VAL:O	1.62	0.99
1:B:225:VAL:O	1:B:225:VAL:CG1	2.11	0.98
1:B:475:HIS:HD2	1:B:477:ILE:H	1.28	0.82
1:B:142:ILE:HG23	1:B:149:SER:HB3	1.65	0.77
1:B:310:ARG:O	1:B:310:ARG:HG2	1.86	0.76
1:A:88:ALA:HB2	1:A:275:LEU:HD21	1.70	0.74
1:A:310:ARG:HG2	2:A:1593:BME:C1	2.17	0.74
1:A:577:LEU:O	1:A:581:MET:HG3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:O	1:A:276:ASP:HB2	1.90	0.72
1:A:142:ILE:HG23	1:A:149:SER:HB3	1.74	0.70
1:A:475:HIS:HD2	1:A:477:ILE:H	1.41	0.69
1:A:310:ARG:HG2	2:A:1593:BME:H11	1.73	0.68
1:B:156:LEU:HD23	1:B:159:GLN:NE2	2.08	0.68
1:A:247:VAL:HG21	1:A:250:PRO:HG2	1.79	0.65
1:A:505:LYS:HG2	1:A:508:GLN:CB	2.27	0.65
1:A:446:ILE:HG12	1:A:485:LEU:HG	1.81	0.63
1:B:310:ARG:O	1:B:310:ARG:CG	2.46	0.63
1:A:93:ASP:O	1:A:97:MET:HG3	1.99	0.62
1:B:281:GLN:O	1:B:285:GLN:HG3	2.00	0.62
1:B:325:ARG:HD2	2:B:1592:BME:H12	1.80	0.62
1:B:510:TYR:CD2	1:B:521:ALA:HA	2.36	0.61
1:B:221:LYS:O	1:B:222:ARG:HG3	2.00	0.60
1:A:232:LEU:C	1:A:232:LEU:HD13	2.22	0.60
1:B:289:LYS:HE3	1:B:293:ARG:NH2	2.16	0.60
1:B:156:LEU:HD23	1:B:159:GLN:HE22	1.65	0.60
1:B:224:LEU:HD13	1:B:232:LEU:HD12	1.83	0.60
1:A:221:LYS:O	1:A:222:ARG:HG3	2.02	0.59
1:A:304:LEU:HD11	1:A:382:CYS:SG	2.44	0.58
1:B:353:THR:OG1	1:B:356:GLU:HG3	2.04	0.58
1:A:435:LEU:HD23	1:A:439:MET:HG2	1.86	0.57
1:A:303:GLU:HG3	1:A:381:ILE:HD13	1.87	0.57
1:B:516:ALA:HB1	1:B:520:GLU:OE1	2.04	0.57
1:A:531:GLN:O	1:A:535:MET:HG3	2.05	0.56
1:A:410:ARG:O	1:A:414:VAL:HG13	2.05	0.56
1:B:225:VAL:O	1:B:225:VAL:HG13	2.02	0.56
1:A:199:PHE:HA	1:A:212:ARG:HH21	1.71	0.56
1:B:334:LEU:HD13	1:B:451:ILE:HG23	1.88	0.55
1:B:224:LEU:HD13	1:B:232:LEU:CD1	2.36	0.54
1:A:199:PHE:HA	1:A:212:ARG:NH2	2.23	0.54
1:A:473:LYS:N	1:A:474:TYR:HA	2.22	0.54
1:B:252:ALA:O	1:B:256:ILE:HG13	2.07	0.54
1:B:438:TYR:CE2	1:B:439:MET:HE2	2.42	0.54
1:B:324:ARG:HB2	1:B:327:HIS:ND1	2.22	0.54
1:A:547:LYS:O	1:A:551:GLU:HG3	2.08	0.54
1:B:216:THR:O	1:B:220:GLN:HG3	2.08	0.53
1:A:310:ARG:O	1:A:313:GLU:HB2	2.08	0.53
1:B:473:LYS:N	1:B:474:TYR:HA	2.23	0.53
1:A:111:LEU:O	1:A:115:LEU:HG	2.08	0.52
1:A:521:ALA:O	1:A:525:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:ASP:OD1	1:B:569:ASP:C	2.47	0.52
1:B:117:ARG:HD3	3:B:2068:HOH:O	2.09	0.52
1:B:406:THR:N	1:B:407:PRO:HD2	2.25	0.52
1:A:266:ASN:OD1	1:A:266:ASN:C	2.49	0.51
1:A:353:THR:OG1	1:A:356:GLU:HG3	2.11	0.51
1:B:223:VAL:HG22	1:B:224:LEU:H	1.76	0.51
1:A:366:ARG:NE	1:A:366:ARG:HA	2.26	0.50
1:A:582:LEU:C	1:A:582:LEU:HD23	2.31	0.50
1:A:228:ASP:HB2	1:A:231:LEU:HB2	1.92	0.50
1:A:348:PHE:CD2	1:A:420:TYR:HB3	2.47	0.50
1:B:266:ASN:OD1	1:B:266:ASN:C	2.50	0.49
1:B:475:HIS:CD2	1:B:477:ILE:H	2.18	0.49
1:A:91:MET:SD	1:A:271:GLU:HB3	2.52	0.49
1:A:412:VAL:HB	1:A:449:ILE:HG22	1.93	0.49
1:B:406:THR:OG1	1:B:407:PRO:HD3	2.13	0.49
1:B:329:TYR:C	1:B:329:TYR:CD1	2.86	0.48
1:B:507:VAL:HG12	1:B:511:MET:HE2	1.95	0.48
1:A:187:ASP:O	1:A:191:LEU:HG	2.13	0.48
1:A:87:ARG:O	1:A:91:MET:HG3	2.13	0.48
1:A:505:LYS:CG	1:A:508:GLN:H	2.27	0.48
1:B:215:ALA:O	1:B:219:LEU:HG	2.14	0.48
1:B:289:LYS:HE3	1:B:293:ARG:HH21	1.77	0.48
1:B:314:CYS:HA	2:B:1593:BME:H22	1.96	0.48
1:B:91:MET:O	1:B:95:VAL:HG23	2.14	0.47
1:B:334:LEU:CD1	1:B:451:ILE:HG23	2.44	0.47
1:B:582:LEU:HD23	1:B:582:LEU:C	2.35	0.47
1:B:123:HIS:NE2	1:B:276:ASP:OD2	2.48	0.47
1:B:505:LYS:O	1:B:509:CYS:HB2	2.14	0.47
1:A:483:THR:HG22	1:A:487:LEU:HD22	1.97	0.47
1:A:173:LYS:HA	1:A:180:PHE:HA	1.97	0.47
1:B:507:VAL:HG12	1:B:511:MET:CE	2.45	0.47
1:B:435:LEU:O	1:B:435:LEU:HD22	2.15	0.46
1:B:426:TRP:CE3	1:B:433:PRO:HG3	2.50	0.46
1:A:329:TYR:C	1:A:329:TYR:CD1	2.88	0.46
1:B:508:GLN:HA	1:B:511:MET:HE2	1.97	0.46
1:B:174:ASN:OD1	1:B:177:GLY:N	2.49	0.46
1:A:117:ARG:HD2	1:A:255:PHE:CE1	2.51	0.46
1:B:266:ASN:OD1	1:B:268:THR:N	2.49	0.46
1:A:290:GLU:HA	1:A:293:ARG:NH1	2.31	0.45
1:A:232:LEU:HD13	1:A:232:LEU:O	2.17	0.45
1:B:106:ILE:O	1:B:110:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LYS:HG2	1:B:590:TYR:CD1	2.52	0.45
1:B:116:ARG:HA	1:B:121:SER:HB3	1.96	0.45
1:A:233:SER:OG	1:A:237:ARG:NH1	2.50	0.45
1:A:364:ILE:HG22	1:A:414:VAL:HG12	1.99	0.45
1:B:576:SER:OG	1:B:577:LEU:N	2.50	0.45
1:B:122:CYS:HB2	2:B:1592:BME:H22	1.84	0.45
1:B:166:GLN:OE1	1:B:207:THR:HB	2.17	0.44
1:A:173:LYS:HE3	1:A:207:THR:HG23	2.00	0.44
1:A:274:LYS:HD2	1:A:590:TYR:CE1	2.53	0.44
1:B:414:VAL:O	1:B:418:GLU:HG3	2.18	0.44
1:B:446:ILE:HG12	1:B:485:LEU:HG	1.99	0.44
1:A:107:ARG:HH11	1:A:107:ARG:HD3	1.64	0.44
1:A:426:TRP:CZ3	1:A:433:PRO:HG3	2.53	0.43
1:A:507:VAL:HG12	1:A:517:SER:HB2	2.00	0.43
1:B:266:ASN:HA	1:B:267:PRO:HD2	1.88	0.43
1:B:158:ARG:HG3	1:B:164:VAL:CG1	2.48	0.43
1:A:181:LYS:HA	1:A:182:PRO:HD3	1.89	0.43
1:B:108:ARG:HH11	1:B:108:ARG:HD2	1.63	0.43
1:A:417:ILE:O	1:A:420:TYR:HB2	2.18	0.43
1:A:103:VAL:HG22	3:A:2005:HOH:O	2.18	0.43
1:A:265:MET:C	1:A:265:MET:SD	2.97	0.43
1:A:266:ASN:OD1	1:A:268:THR:N	2.52	0.43
1:A:274:LYS:HD2	1:A:590:TYR:HE1	1.84	0.43
1:B:142:ILE:CG2	1:B:149:SER:HB3	2.43	0.43
1:B:259:TYR:HA	1:B:262:ARG:HD3	2.00	0.42
1:A:505:LYS:O	1:A:509:CYS:HB2	2.18	0.42
1:A:510:TYR:CD2	1:A:521:ALA:HA	2.54	0.42
1:B:293:ARG:HE	1:B:293:ARG:HB2	1.69	0.42
1:A:479:ARG:HH11	1:A:479:ARG:HD2	1.60	0.42
1:B:310:ARG:HG3	1:B:313:GLU:HB2	2.01	0.42
1:B:507:VAL:HG13	1:B:521:ALA:HB3	2.02	0.42
1:A:108:ARG:HH11	1:A:108:ARG:HD2	1.59	0.42
1:A:353:THR:O	1:A:357:LEU:HG	2.20	0.42
1:A:324:ARG:HB2	1:A:327:HIS:ND1	2.34	0.42
1:B:409:LEU:HD22	1:B:454:HIS:CE1	2.55	0.42
1:B:508:GLN:HA	1:B:511:MET:CE	2.50	0.42
1:A:313:GLU:HG2	1:A:571:PHE:CZ	2.55	0.42
1:B:577:LEU:O	1:B:581:MET:HG3	2.18	0.41
1:A:105:SER:HB3	1:A:141:GLU:OE1	2.19	0.41
1:A:324:ARG:HB2	1:A:327:HIS:HD1	1.86	0.41
1:B:262:ARG:HA	1:B:263:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ILE:O	1:A:446:ILE:HG13	2.21	0.41
1:A:310:ARG:HG2	2:A:1593:BME:H12	1.99	0.41
1:B:181:LYS:HA	1:B:182:PRO:HD3	1.93	0.41
1:A:261:ARG:HH11	1:A:261:ARG:HD3	1.68	0.40
1:A:262:ARG:HA	1:A:263:PRO:HD3	1.93	0.40
1:A:118:LEU:HD23	1:A:255:PHE:HD2	1.87	0.40
1:A:174:ASN:N	1:A:179:ASP:O	2.49	0.40
1:B:265:MET:O	1:B:265:MET:HG3	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	A	473/569 (83%)	459 (97%)	13 (3%)	1 (0%)	47	38
1	B	483/569 (85%)	466 (96%)	16 (3%)	1 (0%)	47	38
All	All	956/1138 (84%)	925 (97%)	29 (3%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	519	GLU
1	B	350	ILE

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	A	422/515 (82%)	408 (97%)	14 (3%)	38	26
1	B	435/515 (84%)	420 (97%)	15 (3%)	37	25
All	All	857/1030 (83%)	828 (97%)	29 (3%)	37	25

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	93	ASP
1	A	164	VAL
1	A	265	MET
1	A	274	LYS
1	A	310	ARG
1	A	325	ARG
1	A	350	ILE
1	A	471	MET
1	A	487	LEU
1	A	493	THR
1	A	517	SER
1	A	522	ARG
1	A	577	LEU
1	B	87	ARG
1	B	94	GLN
1	B	224	LEU
1	B	225	VAL
1	B	229	ILE
1	B	265	MET
1	B	276	ASP
1	B	310	ARG
1	B	434	SER
1	B	435	LEU
1	B	513	GLU
1	B	527	SER
1	B	528	LEU
1	B	576	SER
1	B	577	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	159	GLN
1	A	220	GLN
1	A	286	GLN
1	A	475	HIS
1	A	531	GLN
1	B	159	GLN
1	B	475	HIS
1	B	531	GLN
1	B	579	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
2	BME	B	1593	1	3,3,3	0.35	0	1,2,2	0.35	0
2	BME	A	1593	1	3,3,3	0.35	0	1,2,2	0.34	0
2	BME	A	1592	1	3,3,3	0.36	0	1,2,2	0.32	0
2	BME	B	1592	1	3,3,3	0.35	0	1,2,2	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BME	B	1593	1	-	0/1/1/1	-
2	BME	A	1593	1	-	1/1/1/1	-
2	BME	A	1592	1	-	0/1/1/1	-
2	BME	B	1592	1	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1593	BME	O1-C1-C2-S2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1593	BME	1	0
2	A	1593	BME	3	0
2	B	1592	BME	2	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	485/569 (85%)	0.53	43 (8%) 9 15	16, 30, 56, 65	0
1	B	491/569 (86%)	0.60	47 (9%) 8 13	14, 30, 57, 73	0
All	All	976/1138 (85%)	0.56	90 (9%) 9 14	14, 30, 57, 73	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	VAL	8.8
1	A	493	THR	6.6
1	B	229	ILE	6.3
1	B	223	VAL	6.2
1	B	224	LEU	5.9
1	B	503	VAL	5.5
1	A	229	ILE	4.9
1	B	515	ASN	4.8
1	B	507	VAL	4.8
1	B	569	ASP	4.6
1	A	84	HIS	4.6
1	B	88	ALA	4.5
1	A	517	SER	4.3
1	A	577	LEU	4.2
1	A	85	LEU	4.2
1	B	90	GLY	4.2
1	A	305	PRO	4.2
1	B	232	LEU	4.2
1	A	520	GLU	4.1
1	A	228	ASP	4.1
1	A	351	TYR	4.0
1	B	576	SER	4.0
1	A	308	ARG	4.0
1	A	232	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	509	CYS	3.9
1	A	175	ALA	3.9
1	B	511	MET	3.8
1	B	261	ARG	3.8
1	B	512	ASN	3.7
1	B	521	ALA	3.7
1	A	570	GLY	3.6
1	A	223	VAL	3.6
1	A	510	TYR	3.6
1	B	220	GLN	3.5
1	A	427	TYR	3.5
1	B	591	GLU	3.5
1	B	435	LEU	3.5
1	B	577	LEU	3.5
1	A	350	ILE	3.4
1	A	263	PRO	3.4
1	B	138	THR	3.4
1	B	570	GLY	3.3
1	A	435	LEU	3.3
1	B	504	PRO	3.3
1	A	569	ASP	3.0
1	A	521	ALA	3.0
1	B	310	ARG	2.9
1	A	230	ASN	2.9
1	A	304	LEU	2.8
1	B	175	ALA	2.8
1	B	510	TYR	2.8
1	B	516	ALA	2.8
1	B	93	ASP	2.8
1	B	566	HIS	2.8
1	B	571	PHE	2.8
1	B	230	ASN	2.7
1	A	507	VAL	2.7
1	B	513	GLU	2.6
1	B	575	HIS	2.6
1	A	504	PRO	2.6
1	B	567	GLU	2.6
1	B	578	VAL	2.6
1	A	261	ARG	2.6
1	B	568	SER	2.6
1	A	156	LEU	2.6
1	B	518	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	275	LEU	2.5
1	B	219	LEU	2.5
1	B	509	CYS	2.5
1	A	309	ASP	2.4
1	A	204	GLY	2.4
1	B	178	THR	2.4
1	A	574	GLN	2.4
1	A	578	VAL	2.3
1	A	580	LYS	2.3
1	A	126	ARG	2.3
1	A	86	MET	2.3
1	A	310	ARG	2.2
1	B	514	LYS	2.2
1	B	139	ASN	2.2
1	B	574	GLN	2.2
1	A	145	ARG	2.2
1	B	263	PRO	2.1
1	A	575	HIS	2.1
1	A	286	GLN	2.1
1	B	243	THR	2.1
1	A	566	HIS	2.0
1	B	302	HIS	2.0
1	A	220	GLN	2.0
1	B	203	GLN	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, 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(\AA^2)	Q<0.9
2	BME	B	1592	4/4	0.88	0.24	77,77,78,79	0
2	BME	A	1593	4/4	0.90	0.22	41,45,46,51	0
2	BME	A	1592	4/4	0.91	0.32	45,48,51,56	0
2	BME	B	1593	4/4	0.91	0.20	41,44,46,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.