



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:16 PM UTC

PDB ID : 2J5C / pdb_00002j5c
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	:	4-5-2 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

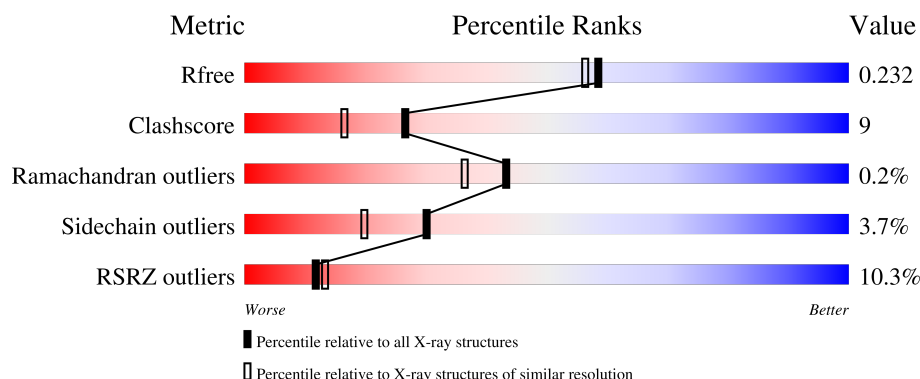
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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% 63% 18% • 15%
1	B	569	10% 65% 19% • 14%

2 Entry composition [i](#)

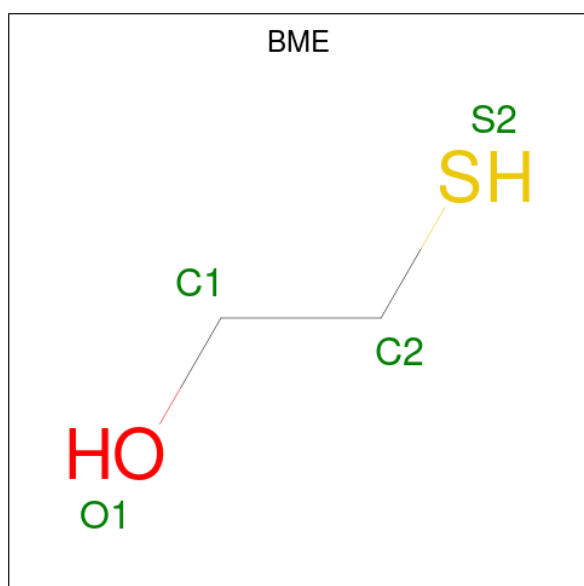
There are 3 unique types of molecules in this entry. The entry contains 8468 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	485	Total	C	N	O	S	0	0	0
			3959	2523	673	738	25			
1	B	491	Total	C	N	O	S	0	0	0
			4034	2575	682	751	26			

- 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	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		

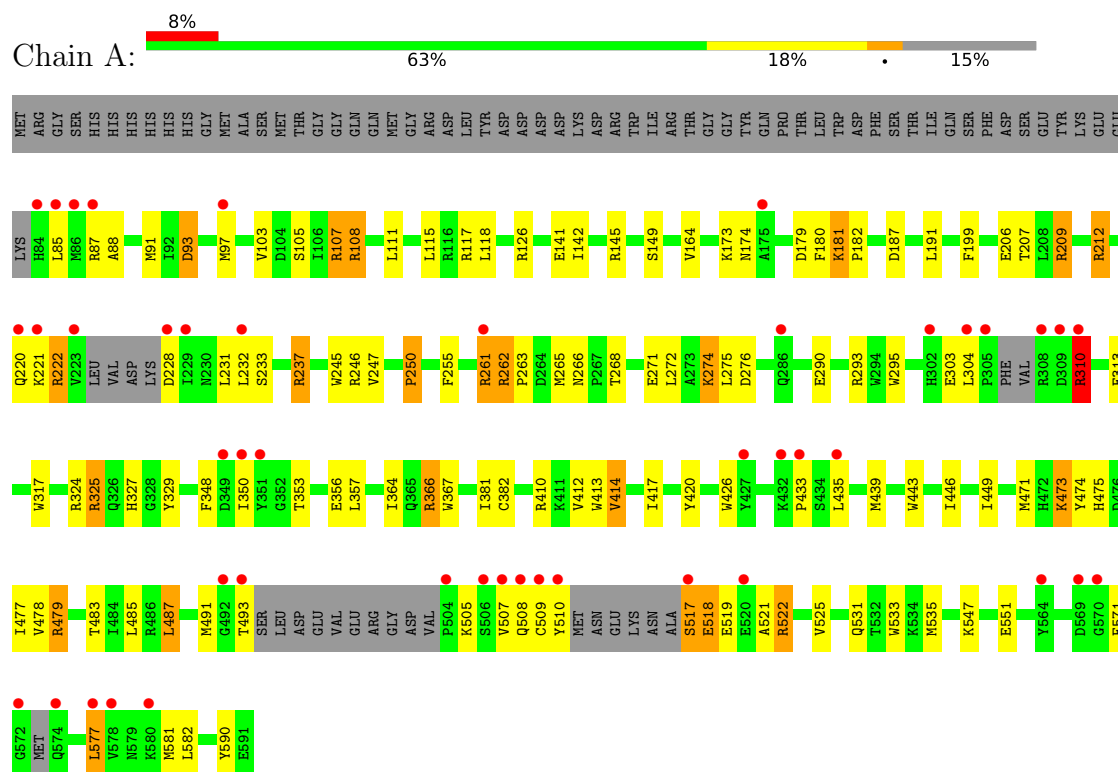
- Molecule 3 is water.

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

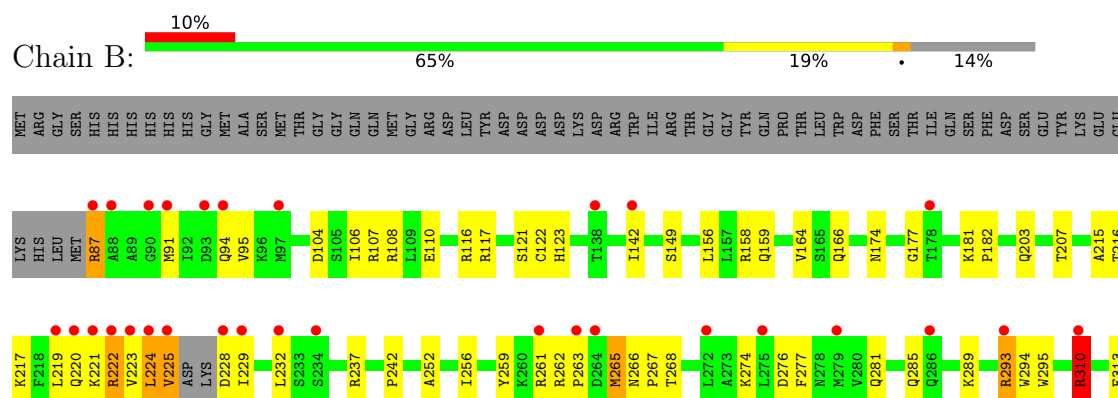
3 Residue-property plots [i](#)

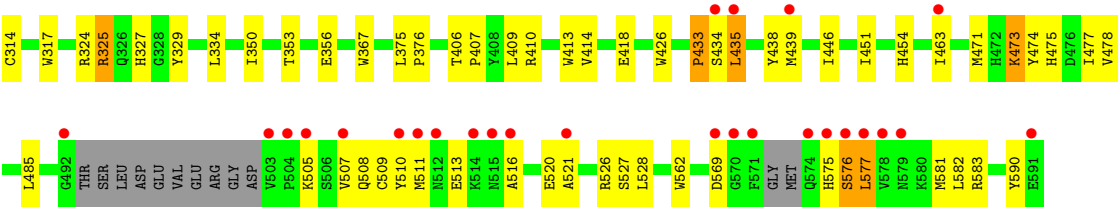
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 1,8-CINEOLE SYNTHASE



• Molecule 1: 1,8-CINEOLE SYNTHASE





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) 99.5 (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)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.235 0.214 , 0.232	Depositor DCC
R_{free} test set	4786 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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	0.90	7/4042 (0.2%)	1.19	20/5458 (0.4%)
1	B	0.91	6/4121 (0.1%)	1.22	19/5568 (0.3%)
All	All	0.91	13/8163 (0.2%)	1.21	39/11026 (0.4%)

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	10.63	1.49	1.37
1	A	413	TRP	NE1-CE2	10.46	1.49	1.37
1	B	294	TRP	NE1-CE2	10.43	1.49	1.37
1	A	443	TRP	NE1-CE2	10.39	1.48	1.37
1	A	367	TRP	NE1-CE2	10.37	1.48	1.37
1	B	413	TRP	NE1-CE2	10.19	1.48	1.37
1	B	317	TRP	NE1-CE2	10.17	1.48	1.37
1	B	562	TRP	NE1-CE2	10.12	1.48	1.37
1	B	367	TRP	NE1-CE2	10.12	1.48	1.37
1	A	533	TRP	NE1-CE2	10.06	1.48	1.37
1	B	295	TRP	NE1-CE2	10.04	1.48	1.37
1	A	317	TRP	NE1-CE2	9.75	1.48	1.37
1	A	295	TRP	NE1-CE2	8.91	1.47	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	LYS	N-CA-C	7.56	119.16	111.07
1	B	473	LYS	N-CA-C	6.92	119.42	111.11
1	B	433	PRO	N-CA-CB	6.03	108.67	103.31
1	B	375	LEU	N-CA-C	5.95	118.13	110.39
1	B	376	PRO	CB-CA-C	-5.88	105.64	111.17
1	B	87	ARG	CD-NE-CZ	-5.79	116.29	124.40
1	A	325	ARG	CD-NE-CZ	-5.76	116.34	124.40
1	B	228	ASP	CA-CB-CG	-5.51	107.09	112.60
1	B	376	PRO	N-CA-CB	5.48	106.07	103.22
1	B	242	PRO	N-CA-CB	5.46	108.10	103.35
1	A	222	ARG	N-CA-C	5.45	116.69	108.46
1	B	325	ARG	CD-NE-CZ	-5.44	116.79	124.40
1	B	310	ARG	CD-NE-CZ	-5.36	116.90	124.40
1	A	212	ARG	CD-NE-CZ	-5.32	116.95	124.40
1	A	246	ARG	CD-NE-CZ	-5.27	117.03	124.40
1	A	310	ARG	O-C-N	5.24	128.38	122.20
1	A	366	ARG	CD-NE-CZ	-5.22	117.09	124.40
1	A	181	LYS	O-C-N	5.19	125.64	121.38
1	A	222	ARG	CD-NE-CZ	-5.17	117.16	124.40
1	A	108	ARG	CD-NE-CZ	-5.17	117.17	124.40
1	B	410	ARG	CD-NE-CZ	-5.13	117.22	124.40
1	B	293	ARG	CD-NE-CZ	-5.11	117.25	124.40
1	A	261	ARG	CD-NE-CZ	-5.10	117.25	124.40
1	B	575	HIS	CA-CB-CG	-5.10	108.70	113.80
1	B	237	ARG	CD-NE-CZ	-5.10	117.26	124.40
1	B	222	ARG	CD-NE-CZ	-5.09	117.28	124.40
1	A	479	ARG	CD-NE-CZ	-5.08	117.28	124.40
1	A	107	ARG	CD-NE-CZ	-5.08	117.28	124.40
1	A	145	ARG	CD-NE-CZ	-5.08	117.28	124.40
1	A	209	ARG	CD-NE-CZ	-5.08	117.28	124.40
1	A	310	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	A	262	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	B	526	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	A	126	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	B	261	ARG	CD-NE-CZ	-5.06	117.32	124.40
1	B	107	ARG	CD-NE-CZ	-5.05	117.33	124.40
1	A	250	PRO	N-CA-CB	5.02	108.13	103.41
1	B	583	ARG	CD-NE-CZ	-5.02	117.37	124.40
1	A	237	ARG	CD-NE-CZ	-5.01	117.39	124.40

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 ⓘ

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	74	0
1	B	4034	0	3914	73	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	147	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 (147) 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:507:VAL:HG12	1:B:511:MET:HE2	1.49	0.94
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:B:508:GLN:HA	1:B:511:MET:HE3	1.69	0.75
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
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:491:MET:HE1	1:A:522:ARG:HG2	1.77	0.66
1:A:471:MET:HE2	1:A:478:VAL:HG21	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LEU:C	1:A:232:LEU:HD13	2.22	0.65
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:471:MET:HE2	1:B:478:VAL:HG21	1.80	0.61
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: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:491:MET:HE1	1:A:522:ARG:CG	2.33	0.59
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:569:ASP:OD1	1:B:569:ASP:C	2.47	0.57
1:B:516:ALA:HB1	1:B:520:GLU:OE1	2.04	0.57
1:B:438:TYR:CE2	1:B:439:MET:HE2	2.40	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:A:266:ASN:OD1	1:A:266:ASN:C	2.49	0.56
1:A:582:LEU:C	1:A:582:LEU:HD23	2.31	0.55
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:266:ASN:OD1	1:B:266:ASN:C	2.50	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:329:TYR:C	1:B:329:TYR:CD1	2.86	0.53
1:B:473:LYS:N	1:B:474:TYR:HA	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:582:LEU:HD23	1:B:582:LEU:C	2.35	0.52
1:A:329:TYR:C	1:A:329:TYR:CD1	2.88	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:B:471:MET:HE2	1:B:478:VAL:CG2	2.41	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: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: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:A:265:MET:C	1:A:265:MET:SD	2.97	0.47
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: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: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: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:B:106:ILE:O	1:B:110:GLU:HG3	2.17	0.45
1:B:274:LYS:HG2	1:B:590:TYR:CD1	2.52	0.45
1:A:232:LEU:HD13	1:A:232:LEU:O	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:SER:OG	1:B:577:LEU:N	2.50	0.45
1:A:206:GLU:CD	1:A:209:ARG:HE	2.24	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:B:104:ASP:C	1:B:104:ASP:OD1	2.61	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:B:310:ARG:HG3	1:B:313:GLU:CD	2.44	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: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:B:262:ARG:HA	1:B:263:PRO:HD3	1.94	0.41
1:A:232:LEU:C	1:A:232:LEU:CD1	2.90	0.41
1:B:277:PHE:CD1	1:B:277:PHE:C	2.97	0.41
1:A:310:ARG:HG2	2:A:1593:BME:H12	1.99	0.41
1:A:446:ILE:O	1:A:446:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:174:ASN:OD1	1:B:174:ASN:C	2.64	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%)	43	36
1	B	483/569 (85%)	466 (96%)	16 (3%)	1 (0%)	43	36
All	All	956/1138 (84%)	925 (97%)	29 (3%)	2 (0%)	43	36

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%)	407 (96%)	15 (4%)	31	21
1	B	435/515 (84%)	418 (96%)	17 (4%)	28	18
All	All	857/1030 (83%)	825 (96%)	32 (4%)	30	20

All (32) 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	220	GLN
1	A	274	LYS
1	A	310	ARG
1	A	325	ARG
1	A	350	ILE
1	A	414	VAL
1	A	487	LEU
1	A	493	THR
1	A	517	SER
1	A	518	GLU
1	A	522	ARG
1	A	577	LEU
1	B	87	ARG
1	B	94	GLN
1	B	203	GLN
1	B	217	LYS
1	B	224	LEU
1	B	225	VAL
1	B	229	ILE
1	B	265	MET
1	B	310	ARG
1	B	434	SER
1	B	435	LEU
1	B	463	ILE
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 (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	133	ASN
1	A	159	GLN
1	A	220	GLN
1	A	230	ASN
1	A	286	GLN
1	A	475	HIS
1	A	524	HIS
1	A	531	GLN
1	A	566	HIS
1	B	133	ASN
1	B	159	GLN
1	B	203	GLN
1	B	380	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 oligosaccharides 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	A	1592	1	3,3,3	0.37	0	2,2,2	0.31	0
2	BME	B	1592	1	3,3,3	0.36	0	2,2,2	0.32	0
2	BME	B	1593	1	3,3,3	0.36	0	2,2,2	0.32	0
2	BME	A	1593	1	3,3,3	0.36	0	2,2,2	0.32	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	A	1592	1	-	0/1/1/1	-
2	BME	B	1592	1	-	0/1/1/1	-
2	BME	B	1593	1	-	0/1/1/1	-
2	BME	A	1593	1	-	1/1/1/1	-

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	1592	BME	2	0
2	B	1593	BME	1	0
2	A	1593	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	485/569 (85%)	0.59	45 (9%)	14 16	16, 30, 56, 65	0
1	B	491/569 (86%)	0.58	56 (11%)	10 11	14, 30, 57, 73	0
All	All	976/1138 (85%)	0.58	101 (10%)	12 13	14, 30, 57, 73	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	503	VAL	5.5
1	A	223	VAL	5.2
1	A	84	HIS	5.2
1	B	504	PRO	5.2
1	A	85	LEU	5.0
1	A	305	PRO	4.9
1	A	510	TYR	4.8
1	B	224	LEU	4.8
1	B	225	VAL	4.7
1	A	229	ILE	4.7
1	A	493	THR	4.6
1	A	509	CYS	4.6
1	B	223	VAL	4.5
1	A	572	GLY	4.5
1	A	304	LEU	4.2
1	A	570	GLY	4.2
1	B	88	ALA	4.1
1	A	309	ASP	4.0
1	B	515	ASN	4.0
1	A	86	MET	4.0
1	A	574	GLN	3.9
1	B	507	VAL	3.9
1	B	219	LEU	3.9
1	B	492	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	577	LEU	3.7
1	B	570	GLY	3.7
1	B	516	ALA	3.6
1	B	229	ILE	3.6
1	B	571	PHE	3.5
1	A	517	SER	3.5
1	A	435	LEU	3.5
1	B	578	VAL	3.4
1	B	138	THR	3.3
1	A	508	GLN	3.3
1	B	220	GLN	3.2
1	A	228	ASP	3.2
1	B	569	ASP	3.2
1	B	435	LEU	3.2
1	B	514	LYS	3.2
1	B	310	ARG	3.2
1	A	578	VAL	3.2
1	A	520	GLU	3.2
1	B	97	MET	3.1
1	B	261	ARG	3.1
1	B	577	LEU	3.1
1	B	591	GLU	3.1
1	A	351	TYR	3.1
1	A	286	GLN	3.0
1	B	94	GLN	3.0
1	A	310	ARG	2.9
1	B	232	LEU	2.9
1	B	576	SER	2.9
1	B	510	TYR	2.8
1	B	264	ASP	2.8
1	B	434	SER	2.8
1	B	579	ASN	2.8
1	A	261	ARG	2.8
1	A	506	SER	2.7
1	A	87	ARG	2.7
1	A	232	LEU	2.7
1	A	569	ASP	2.7
1	B	505	LYS	2.7
1	A	427	TYR	2.6
1	A	308	ARG	2.6
1	B	222	ARG	2.6
1	A	220	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	507	VAL	2.6
1	B	279	MET	2.5
1	B	272	LEU	2.5
1	A	492	GLY	2.5
1	B	286	GLN	2.5
1	B	178	THR	2.4
1	B	93	ASP	2.4
1	B	263	PRO	2.4
1	A	504	PRO	2.4
1	A	97	MET	2.4
1	B	142	ILE	2.3
1	B	463	ILE	2.3
1	B	511	MET	2.3
1	B	228	ASP	2.3
1	B	275	LEU	2.3
1	B	90	GLY	2.3
1	A	432	LYS	2.3
1	B	521	ALA	2.2
1	B	221	LYS	2.2
1	A	302	HIS	2.2
1	B	439	MET	2.2
1	B	293	ARG	2.2
1	A	580	LYS	2.2
1	A	433	PRO	2.2
1	A	175	ALA	2.2
1	B	91	MET	2.1
1	B	512	ASN	2.1
1	B	574	GLN	2.1
1	A	349	ASP	2.1
1	A	221	LYS	2.1
1	B	87	ARG	2.1
1	B	234	SER	2.0
1	A	350	ILE	2.0
1	B	575	HIS	2.0
1	A	564	TYR	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	BME	B	1592	4/4	0.79	0.20	77,77,78,79	0
2	BME	A	1592	4/4	0.84	0.22	45,48,51,56	0
2	BME	B	1593	4/4	0.86	0.19	41,44,46,50	0
2	BME	A	1593	4/4	0.87	0.20	41,45,46,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.