



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:53 AM UTC

PDB ID : 1T0S / pdb_00001t0s
Title : Structure of the Toluene/o-Xylene Monooxygenase Hydroxylase with 4-bromophenol bound
Authors : Sazinsky, M.H.; Bard, J.; Di Donato, A.; Lippard, S.J.
Deposited on : 2004-04-12
Resolution : 2.20 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

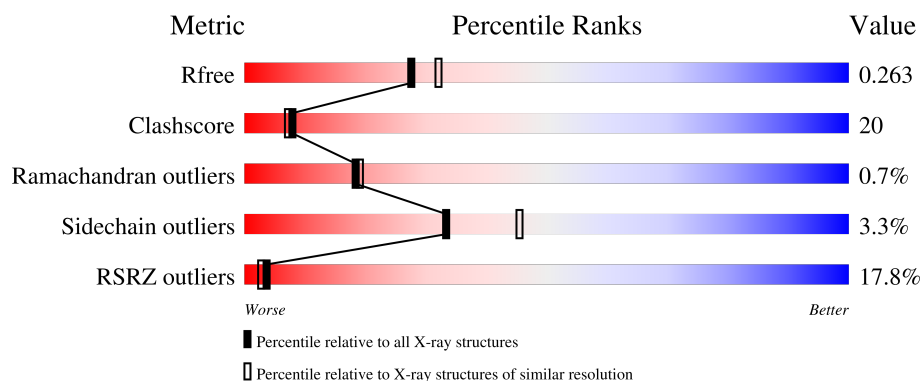
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	498	18% 59% 35% ..
2	B	330	2% 74% 20% ..
3	C	86	72% 37% 57% ..

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
7	BML	A	503	-	X	-	-
7	BML	A	504	-	X	-	-
7	BML	A	505	-	X	-	-
7	BML	A	506	-	X	-	-
7	BML	B	331	-	X	-	-
7	BML	B	332	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7667 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 toluene, o-xylene monooxygenase oxygenase subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			4018	2565	674	753	26			

- Molecule 2 is a protein called toluene, o-xylene monooxygenase oxygenase subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	323	Total	C	N	O	S	0	0	0
			2650	1680	468	492	10			

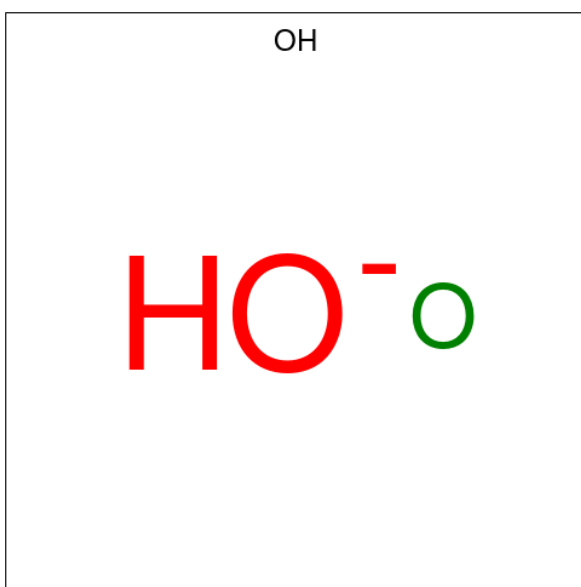
- Molecule 3 is a protein called touB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	83	Total	C	N	O	S	0	0	0
			676	425	120	126	5			

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

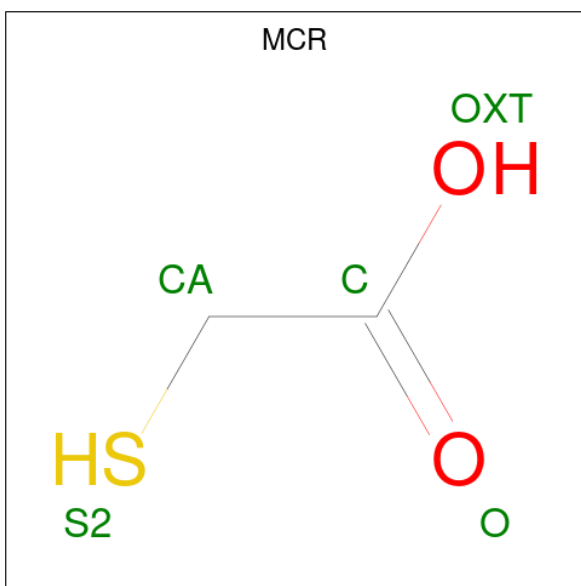
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Fe	0	0
			2	2		

- Molecule 5 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



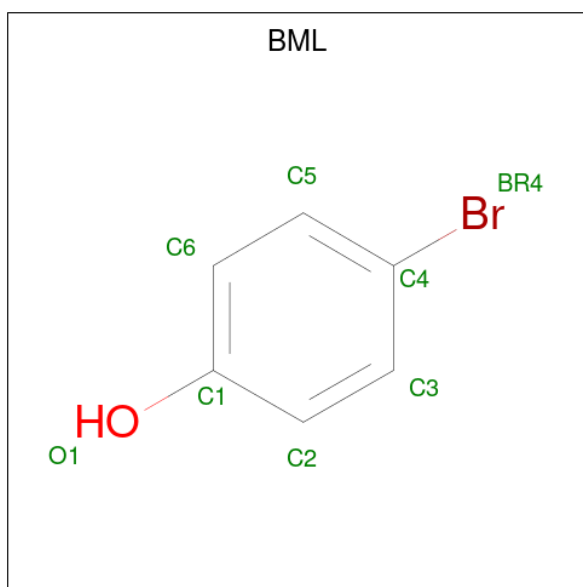
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O		0	0
			1	1			

- Molecule 6 is SULFANYLACETIC ACID (CCD ID: MCR) (formula: $C_2H_4O_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			5	2	2	1		

- Molecule 7 is 4-BROMOPHENOL (CCD ID: BML) (formula: C_6H_5BrO).

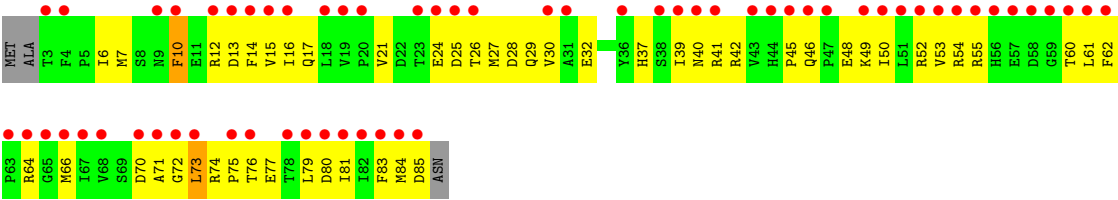


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	Br	C	O	0	0
			8	1	6	1		
7	A	1	Total	Br	C	O	0	0
			8	1	6	1		
7	A	1	Total	Br	C	O	0	0
			8	1	6	1		
7	A	1	Total	Br	C	O	0	0
			8	1	6	1		
7	B	1	Total	Br	C	O	0	0
			8	1	6	1		
7	B	1	Total	Br	C	O	0	0
			8	1	6	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	123	Total	O	0	0
			123	123		
8	B	141	Total	O	0	0
			141	141		
8	C	3	Total	O	0	0
			3	3		

● Molecule 3: touB



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.24Å 183.24Å 67.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.47 – 2.20 29.47 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.47-2.20) 95.8 (29.47-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.236 , 0.273 0.229 , 0.263	Depositor DCC
R_{free} test set	2301 reflections (3.17%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7667	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: OH, FE, BML, MCR

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	0.58	7/4142 (0.2%)	0.93	22/5629 (0.4%)
2	B	0.60	4/2722 (0.1%)	0.92	8/3699 (0.2%)
3	C	0.38	0/690	0.88	0/934
All	All	0.57	11/7554 (0.1%)	0.92	30/10262 (0.3%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	MET	SD-CE	-12.56	1.48	1.79
2	B	54	MET	SD-CE	-12.51	1.48	1.79
2	B	137	MET	SD-CE	-11.34	1.51	1.79
1	A	181	MET	SD-CE	-10.39	1.53	1.79
1	A	180	MET	SD-CE	-10.17	1.54	1.79
1	A	471	MET	SD-CE	-10.10	1.54	1.79
1	A	132	MET	SD-CE	-8.94	1.57	1.79
2	B	274	MET	SD-CE	-7.20	1.61	1.79
1	A	114	MET	SD-CE	-6.95	1.62	1.79
1	A	191	MET	SD-CE	-6.59	1.63	1.79
2	B	328	MET	SD-CE	-6.17	1.64	1.79

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ILE	N-CA-C	12.06	121.67	111.90
1	A	142	LEU	N-CA-C	-8.74	102.42	113.43
1	A	117	PHE	N-CA-C	6.81	121.75	113.17
2	B	33	THR	N-CA-C	6.62	121.08	109.96
2	B	195	ASN	N-CA-C	6.62	123.32	114.12
2	B	55	GLN	N-CA-C	-6.35	103.65	111.40
2	B	104	LEU	N-CA-C	-6.16	104.47	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ASN	N-CA-C	-6.11	104.62	111.28
1	A	166	GLU	N-CA-C	-6.04	101.33	110.28
1	A	257	MET	N-CA-C	-5.96	104.78	111.28
1	A	440	ASP	CA-C-N	5.89	125.09	118.97
1	A	440	ASP	C-N-CA	5.89	125.09	118.97
1	A	237	GLN	N-CA-C	5.82	119.48	112.38
1	A	191	MET	N-CA-C	5.77	117.65	111.36
1	A	180	MET	N-CA-C	5.76	120.96	113.88
1	A	79	ASP	N-CA-C	-5.74	106.91	114.31
2	B	213	TRP	N-CA-C	5.64	119.42	112.54
2	B	68	LYS	N-CA-C	5.63	118.87	110.14
1	A	120	ALA	CA-C-N	5.49	125.58	119.32
1	A	120	ALA	C-N-CA	5.49	125.58	119.32
1	A	231	GLU	N-CA-C	5.45	117.64	111.11
1	A	167	TRP	N-CA-C	5.43	117.91	111.33
1	A	384	LYS	CA-C-N	5.29	124.96	119.56
1	A	384	LYS	C-N-CA	5.29	124.96	119.56
1	A	104	GLU	N-CA-C	-5.23	105.47	111.07
1	A	160	LYS	N-CA-C	5.18	119.69	112.90
2	B	222	ILE	N-CA-C	5.17	116.26	111.45
2	B	292	TRP	N-CA-C	5.15	119.62	113.23
1	A	276	ILE	N-CA-C	5.12	115.26	110.30
1	A	40	SER	N-CA-C	5.10	117.26	110.53

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	4018	0	3773	177	0
2	B	2650	0	2548	78	0
3	C	676	0	667	58	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	32	0	16	3	0
7	B	16	0	8	1	0
8	A	123	0	0	3	0
8	B	141	0	0	8	0
8	C	3	0	0	0	0
All	All	7667	0	7012	284	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 20.

All (284) 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:131:MET:HE1	2:B:140:VAL:HG23	1.41	1.01
3:C:66:MET:HE3	3:C:71:ALA:HB2	1.58	0.84
1:A:2:SER:N	2:B:105:ASN:HD22	1.76	0.84
1:A:33:MET:SD	2:B:54:MET:HE1	2.18	0.83
1:A:139:GLN:HE22	2:B:83:TYR:H	1.25	0.82
1:A:106:ALA:HB1	1:A:181:MET:HE3	1.63	0.79
1:A:106:ALA:O	1:A:181:MET:HE1	1.83	0.79
3:C:27:MET:HE3	3:C:66:MET:CE	2.13	0.78
3:C:13:ASP:OD1	3:C:42:ARG:HD2	1.84	0.77
1:A:180:MET:HE2	1:A:192:LEU:HD13	1.66	0.77
1:A:37:ARG:NH2	1:A:257:MET:HE1	2.00	0.76
1:A:7:GLU:CD	1:A:7:GLU:H	1.93	0.76
1:A:176:PHE:HD1	1:A:180:MET:HE3	1.51	0.75
2:B:168:HIS:HD2	2:B:257:GLN:HE21	1.35	0.74
3:C:7:MET:HE3	3:C:76:THR:HG23	1.70	0.74
2:B:111:GLN:HE21	2:B:111:GLN:H	1.37	0.71
1:A:366:ASN:HA	1:A:370:GLY:HA3	1.71	0.71
2:B:134:ALA:HA	2:B:137:MET:HE2	1.72	0.71
1:A:140:ILE:HG21	1:A:227:ILE:HD11	1.72	0.71
1:A:170:ILE:HD13	1:A:173:ARG:NH2	2.06	0.71
2:B:309:ASP:HB3	8:B:426:HOH:O	1.91	0.70
1:A:9:TRP:HB3	2:B:174:ARG:HG3	1.73	0.70
1:A:68:GLY:O	1:A:72:ILE:HG12	1.90	0.70
3:C:66:MET:CE	3:C:71:ALA:HB2	2.22	0.70
1:A:377:THR:O	1:A:381:VAL:HG23	1.92	0.69
1:A:131:MET:HE1	2:B:140:VAL:CG2	2.20	0.68
2:B:224:LEU:HD22	2:B:328:MET:HE1	1.76	0.68
1:A:399:MET:HE1	1:A:444:TYR:CE2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ILE:O	1:A:281:THR:HG23	1.94	0.67
3:C:10:PHE:CE1	3:C:81:ILE:HG21	2.31	0.66
1:A:353:GLU:O	1:A:356:GLU:HG2	1.95	0.66
2:B:329:GLY:O	2:B:330:LEU:HB2	1.95	0.66
1:A:176:PHE:CD1	1:A:180:MET:HE3	2.30	0.66
1:A:377:THR:HG21	1:A:491:TYR:CD1	2.31	0.66
1:A:367:ASP:HB3	1:A:410:ASN:HD22	1.62	0.65
3:C:62:PHE:CD1	3:C:66:MET:HE1	2.32	0.65
1:A:405:ALA:HB1	3:C:14:PHE:O	1.97	0.64
1:A:405:ALA:HB2	3:C:15:VAL:HB	1.78	0.64
2:B:162:HIS:HE1	2:B:227:LYS:NZ	1.95	0.64
1:A:398:ASN:ND2	1:A:449:ASN:ND2	2.45	0.64
1:A:460:GLN:HA	1:A:461:PRO:C	2.21	0.64
2:B:168:HIS:CD2	2:B:257:GLN:HE21	2.16	0.64
1:A:131:MET:CE	2:B:140:VAL:HG23	2.23	0.64
1:A:240:PRO:O	1:A:244:ILE:HG12	1.98	0.64
1:A:39:ILE:HB	1:A:44:TRP:NE1	2.13	0.64
1:A:314:PRO:HD2	1:A:317:TRP:CE3	2.33	0.64
2:B:162:HIS:HE1	2:B:227:LYS:HZ2	1.45	0.63
1:A:464:LEU:HD23	1:A:465:ALA:N	2.13	0.63
1:A:468:LEU:HD22	1:A:478:MET:HE3	1.80	0.63
1:A:491:TYR:O	1:A:492:GLN:HB2	1.99	0.63
2:B:192:VAL:HG13	8:B:432:HOH:O	1.98	0.63
2:B:182:ASP:HB3	8:B:462:HOH:O	1.97	0.62
1:A:113:ARG:HH11	2:B:144:GLN:HE21	1.48	0.62
1:A:253:GLU:CD	1:A:253:GLU:H	2.09	0.61
1:A:295:LEU:HD23	1:A:299:VAL:HG21	1.82	0.61
2:B:258:LYS:O	2:B:262:GLU:HG3	2.00	0.61
1:A:382:ASN:O	1:A:384:LYS:HG3	2.00	0.61
1:A:383:GLY:C	1:A:385:PRO:HD3	2.26	0.61
2:B:33:THR:HB	2:B:34:ASN:HD22	1.65	0.61
2:B:41:ASN:HB3	2:B:43:GLU:OE2	2.00	0.60
2:B:111:GLN:H	2:B:111:GLN:NE2	1.99	0.60
2:B:196:ASP:HB2	8:B:432:HOH:O	1.99	0.60
2:B:322:ARG:O	2:B:326:GLN:HG3	2.02	0.60
2:B:134:ALA:CB	2:B:206:ILE:HD12	2.32	0.60
1:A:289:SER:OG	1:A:292:GLU:HG3	2.02	0.59
1:A:189:SER:O	1:A:193:THR:OG1	2.19	0.59
3:C:27:MET:HE3	3:C:66:MET:HE3	1.84	0.59
1:A:57:GLU:O	1:A:61:ILE:HG12	2.02	0.59
3:C:28:ASP:OD2	3:C:64:ARG:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ASN:ND2	1:A:449:ASN:HD22	2.00	0.59
1:A:344:TRP:O	1:A:346:PRO:HD3	2.02	0.59
2:B:43:GLU:CD	2:B:43:GLU:H	2.09	0.59
1:A:384:LYS:N	1:A:385:PRO:HD3	2.17	0.58
3:C:6:ILE:C	3:C:6:ILE:HD12	2.28	0.58
1:A:106:ALA:C	1:A:181:MET:HE1	2.29	0.58
1:A:95:LEU:HD23	1:A:276:ILE:HD11	1.84	0.58
1:A:422:GLU:OE1	1:A:445:LYS:HE3	2.04	0.57
2:B:325:ARG:HA	2:B:328:MET:HE2	1.85	0.57
1:A:137:HIS:CD2	1:A:227:ILE:HG23	2.39	0.57
1:A:336:TRP:O	1:A:339:ARG:HB3	2.04	0.57
3:C:27:MET:HE3	3:C:66:MET:HE2	1.85	0.57
1:A:271:VAL:HG13	1:A:272:LEU:HG	1.86	0.57
1:A:46:LYS:HD2	8:A:617:HOH:O	2.03	0.56
1:A:37:ARG:HH21	1:A:257:MET:HE1	1.68	0.56
1:A:265:SER:O	1:A:269:PHE:HB2	2.04	0.56
1:A:416:ASP:HB2	3:C:16:ILE:CD1	2.36	0.56
2:B:287:LYS:HB2	2:B:287:LYS:NZ	2.21	0.56
3:C:74:ARG:O	3:C:77:GLU:HB2	2.06	0.56
1:A:197:GLU:HA	1:A:201:THR:OG1	2.06	0.56
3:C:62:PHE:CG	3:C:66:MET:HE1	2.41	0.56
1:A:339:ARG:HH12	1:A:389:VAL:CG1	2.19	0.55
1:A:39:ILE:HB	1:A:44:TRP:HE1	1.72	0.55
3:C:80:ASP:C	3:C:81:ILE:HD12	2.31	0.55
1:A:345:ASP:HB3	1:A:482:ALA:HA	1.89	0.55
1:A:47:TYR:CE1	1:A:240:PRO:HB2	2.42	0.55
3:C:54:ARG:HB3	3:C:61:LEU:HA	1.89	0.55
1:A:338:TRP:C	1:A:340:PRO:HD2	2.32	0.54
2:B:133:HIS:O	2:B:136:GLN:HB3	2.07	0.54
1:A:413:ASN:O	1:A:415:LYS:HG3	2.06	0.54
2:B:114:THR:O	2:B:118:VAL:HG23	2.07	0.54
1:A:136:ARG:NH1	1:A:230:ASP:OD2	2.40	0.54
1:A:281:THR:HG22	7:A:505:BML:C4	2.38	0.54
1:A:251:LYS:NZ	1:A:251:LYS:HB3	2.23	0.54
2:B:276:LEU:HD22	2:B:282:ARG:HB2	1.89	0.54
3:C:7:MET:HE3	3:C:76:THR:CG2	2.38	0.54
1:A:371:GLN:O	1:A:374:ASP:HB2	2.08	0.53
1:A:427:HIS:CE1	3:C:76:THR:HG22	2.43	0.53
1:A:277:MET:HA	1:A:281:THR:CG2	2.39	0.53
3:C:53:VAL:HG22	3:C:81:ILE:HG13	1.90	0.53
1:A:180:MET:HB3	1:A:192:LEU:HD22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:GLN:HB2	3:C:83:PHE:CE1	2.43	0.53
3:C:73:LEU:HD22	3:C:77:GLU:HG2	1.91	0.53
2:B:250:LEU:HG	8:B:440:HOH:O	2.08	0.53
1:A:37:ARG:HH21	1:A:257:MET:CE	2.22	0.53
1:A:338:TRP:CD1	1:A:390:PRO:HG3	2.43	0.53
1:A:474:GLU:O	1:A:478:MET:HG3	2.09	0.53
1:A:416:ASP:OD2	1:A:418:GLN:HG3	2.09	0.52
1:A:339:ARG:HG2	1:A:340:PRO:HD3	1.90	0.52
1:A:353:GLU:CD	1:A:353:GLU:H	2.18	0.52
1:A:409:GLY:O	3:C:12:ARG:HG2	2.09	0.52
1:A:211:ASP:OD2	7:A:504:BML:H6	2.09	0.52
1:A:266:TRP:CZ3	1:A:294:MET:HE2	2.45	0.52
2:B:193:TRP:CZ2	2:B:206:ILE:HD11	2.46	0.51
1:A:282:PRO:O	1:A:286:ARG:HG3	2.11	0.51
3:C:39:ILE:CG2	3:C:45:PRO:HG3	2.40	0.51
3:C:75:PRO:O	3:C:76:THR:CB	2.57	0.51
1:A:267:LYS:NZ	1:A:433:ASP:OD2	2.44	0.51
1:A:351:SER:O	1:A:355:ARG:HG3	2.10	0.51
1:A:399:MET:HE1	1:A:444:TYR:CZ	2.46	0.50
2:B:54:MET:CE	2:B:54:MET:HA	2.41	0.50
3:C:52:ARG:HG3	3:C:52:ARG:HH11	1.76	0.50
1:A:491:TYR:CD2	1:A:491:TYR:N	2.79	0.50
1:A:166:GLU:HA	1:A:471:MET:HB3	1.92	0.50
1:A:18:TRP:CH2	2:B:137:MET:HE1	2.47	0.50
1:A:24:THR:OG1	1:A:27:GLU:HG3	2.12	0.49
1:A:468:LEU:HD13	1:A:478:MET:HE1	1.94	0.49
1:A:270:SER:O	1:A:275:PRO:HD3	2.12	0.49
1:A:384:LYS:HA	1:A:386:GLU:OE2	2.11	0.49
2:B:39:THR:HG22	2:B:63:PHE:HE1	1.78	0.49
2:B:134:ALA:HB1	2:B:206:ILE:HD12	1.93	0.49
1:A:277:MET:HA	1:A:281:THR:HG21	1.94	0.49
1:A:301:GLN:CD	1:A:301:GLN:H	2.20	0.49
1:A:399:MET:HE1	1:A:444:TYR:CD2	2.47	0.49
1:A:190:ILE:HD12	1:A:242:LEU:CD2	2.43	0.49
2:B:101:PHE:HE2	2:B:249:LEU:HD21	1.78	0.49
8:A:623:HOH:O	3:C:13:ASP:HB3	2.11	0.49
1:A:153:ARG:NH1	2:B:12:LEU:HD21	2.27	0.49
1:A:491:TYR:N	1:A:491:TYR:HD2	2.10	0.49
2:B:143:HIS:C	2:B:143:HIS:CD2	2.91	0.49
1:A:263:TRP:CE2	1:A:432:ALA:HB3	2.48	0.48
1:A:400:CYS:O	1:A:402:LEU:HG	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:SER:N	2:B:105:ASN:ND2	2.54	0.48
1:A:131:MET:CE	2:B:140:VAL:CG2	2.87	0.48
2:B:111:GLN:NE2	2:B:111:GLN:N	2.62	0.48
1:A:76:LEU:O	1:A:79:ASP:HB3	2.14	0.48
1:A:295:LEU:HA	1:A:299:VAL:CG2	2.43	0.48
2:B:117:TRP:CE3	2:B:245:GLU:HG3	2.49	0.48
1:A:7:GLU:CD	1:A:7:GLU:N	2.69	0.48
1:A:243:LYS:O	1:A:247:GLU:HB2	2.14	0.48
1:A:175:PHE:CE1	1:A:179:MET:HG3	2.48	0.48
3:C:55:ARG:HA	3:C:79:LEU:HD23	1.95	0.48
3:C:10:PHE:HE2	3:C:39:ILE:HD11	1.78	0.48
1:A:153:ARG:CZ	2:B:12:LEU:HD21	2.43	0.48
1:A:339:ARG:NH1	1:A:389:VAL:HG12	2.28	0.48
3:C:49:LYS:C	3:C:50:ILE:HD12	2.38	0.48
1:A:377:THR:HG21	1:A:491:TYR:CE1	2.49	0.47
3:C:81:ILE:HD12	3:C:81:ILE:N	2.29	0.47
2:B:192:VAL:HA	8:B:432:HOH:O	2.14	0.47
3:C:39:ILE:HG22	3:C:40:ASN:ND2	2.28	0.47
1:A:339:ARG:O	1:A:479:GLY:HA3	2.14	0.47
1:A:355:ARG:HA	1:A:358:LEU:HD12	1.96	0.47
1:A:404:ILE:O	3:C:15:VAL:HG23	2.15	0.47
1:A:37:ARG:HG3	1:A:37:ARG:HH11	1.79	0.47
1:A:317:TRP:O	1:A:321:MET:HG2	2.15	0.47
1:A:337:TYR:CE2	3:C:42:ARG:NH2	2.82	0.47
1:A:367:ASP:HB3	1:A:410:ASN:ND2	2.28	0.47
3:C:39:ILE:HG23	3:C:45:PRO:HG3	1.96	0.47
1:A:294:MET:O	1:A:299:VAL:HG23	2.15	0.47
2:B:54:MET:HA	2:B:54:MET:HE3	1.97	0.47
3:C:25:ASP:HB3	3:C:29:GLN:HB2	1.97	0.47
2:B:201:GLY:HA3	2:B:299:ALA:HA	1.97	0.46
2:B:154:CYS:HB3	2:B:267:TRP:CE2	2.50	0.46
1:A:162:ILE:HG22	1:A:162:ILE:O	2.15	0.46
1:A:400:CYS:SG	1:A:402:LEU:HB2	2.56	0.46
1:A:339:ARG:CD	1:A:480:ASP:HA	2.45	0.46
1:A:186:VAL:O	1:A:190:ILE:HG12	2.16	0.45
2:B:206:ILE:HG13	2:B:207:GLU:N	2.31	0.45
1:A:450:LEU:HD12	1:A:450:LEU:HA	1.74	0.45
1:A:488:VAL:C	1:A:490:ALA:N	2.74	0.45
1:A:104:GLU:HG3	1:A:141:GLN:NE2	2.32	0.45
1:A:165:ASN:OD1	1:A:170:ILE:HD11	2.17	0.45
1:A:287:ASN:N	1:A:287:ASN:HD22	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:N	1:A:309:LEU:HD12	2.31	0.45
2:B:23:ARG:HD2	2:B:23:ARG:O	2.17	0.45
2:B:81:LEU:HD11	2:B:263:ARG:HD3	1.98	0.45
1:A:177:ASP:HA	1:A:181:MET:HB2	1.98	0.45
1:A:316:TYR:CD1	1:A:316:TYR:C	2.95	0.45
1:A:281:THR:HG22	7:A:505:BML:BR4	2.72	0.45
1:A:350:VAL:HG11	1:A:373:TRP:CD2	2.51	0.45
1:A:405:ALA:CB	3:C:15:VAL:HB	2.46	0.45
1:A:474:GLU:O	1:A:477:VAL:HG22	2.16	0.45
2:B:45:PRO:HG2	2:B:55:GLN:OE1	2.17	0.45
3:C:75:PRO:O	3:C:76:THR:HB	2.17	0.45
2:B:12:LEU:N	2:B:12:LEU:HD22	2.33	0.44
3:C:12:ARG:HG3	3:C:12:ARG:HH11	1.81	0.44
1:A:2:SER:HB2	2:B:105:ASN:HD21	1.83	0.44
3:C:41:ARG:HH11	3:C:41:ARG:HG2	1.82	0.44
1:A:137:HIS:CD2	1:A:227:ILE:HD12	2.52	0.44
3:C:17:GLN:NE2	3:C:37:HIS:HB3	2.33	0.44
1:A:21:LYS:HB3	2:B:203:ARG:NH2	2.32	0.44
1:A:299:VAL:O	1:A:303:GLU:HG3	2.18	0.44
1:A:368:THR:C	1:A:408:PRO:HG2	2.42	0.44
1:A:136:ARG:HB2	2:B:83:TYR:CE2	2.51	0.44
1:A:113:ARG:HH11	2:B:144:GLN:NE2	2.14	0.44
1:A:326:GLU:O	1:A:329:HIS:HB2	2.17	0.44
3:C:7:MET:CE	3:C:76:THR:HG23	2.44	0.44
2:B:68:LYS:HB2	2:B:278:LYS:HE2	2.00	0.44
1:A:287:ASN:N	1:A:287:ASN:ND2	2.66	0.44
1:A:386:GLU:H	1:A:386:GLU:CD	2.26	0.44
3:C:53:VAL:O	3:C:62:PHE:HB2	2.17	0.44
1:A:179:MET:HE2	1:A:179:MET:HA	1.99	0.43
1:A:203:MET:HG2	1:A:297:TRP:HB3	1.99	0.43
2:B:249:LEU:C	2:B:249:LEU:HD23	2.43	0.43
2:B:308:PRO:O	2:B:309:ASP:HB2	2.17	0.43
3:C:25:ASP:HA	3:C:29:GLN:OE1	2.17	0.43
1:A:95:LEU:HD13	1:A:344:TRP:CZ3	2.53	0.43
3:C:54:ARG:HB2	3:C:60:THR:O	2.18	0.43
1:A:263:TRP:O	1:A:266:TRP:HB3	2.19	0.43
3:C:7:MET:HB3	3:C:16:ILE:CG2	2.49	0.43
1:A:340:PRO:HA	1:A:479:GLY:O	2.19	0.43
2:B:162:HIS:CE1	2:B:227:LYS:NZ	2.82	0.43
2:B:174:ARG:HG2	2:B:174:ARG:NH2	2.34	0.43
1:A:178:ASP:HA	2:B:48:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:HD12	1:A:242:LEU:HG	2.00	0.42
1:A:314:PRO:O	1:A:317:TRP:HB2	2.19	0.42
1:A:31:GLU:OE2	1:A:35:GLY:HA2	2.20	0.42
1:A:166:GLU:OE1	1:A:168:ALA:HB3	2.20	0.42
1:A:380:LEU:HD21	1:A:388:THR:HG21	2.01	0.42
2:B:23:ARG:HD2	2:B:23:ARG:C	2.45	0.42
2:B:36:HIS:HE1	2:B:152:THR:OG1	2.01	0.42
3:C:6:ILE:HD12	3:C:6:ILE:O	2.19	0.42
3:C:24:GLU:OE2	3:C:24:GLU:HA	2.20	0.42
1:A:79:ASP:HB3	8:A:553:HOH:O	2.18	0.42
1:A:368:THR:HA	1:A:409:GLY:HA3	2.02	0.42
2:B:59:LYS:HA	2:B:63:PHE:HD2	1.85	0.42
1:A:223:LEU:O	1:A:227:ILE:HG12	2.20	0.42
2:B:293:GLU:N	2:B:294:PRO:CD	2.83	0.42
1:A:448:THR:HB	1:A:452:ASP:HB2	2.02	0.42
3:C:21:VAL:HG11	3:C:30:VAL:HG13	2.01	0.42
1:A:323:ASP:C	1:A:325:ASP:N	2.75	0.42
1:A:180:MET:CB	1:A:192:LEU:HD22	2.50	0.41
1:A:333:LEU:HD23	3:C:14:PHE:CG	2.54	0.41
3:C:54:ARG:CB	3:C:61:LEU:HA	2.50	0.41
1:A:301:GLN:CD	1:A:301:GLN:N	2.78	0.41
1:A:449:ASN:ND2	1:A:452:ASP:OD2	2.53	0.41
2:B:145:ILE:HG23	2:B:215:TRP:HB2	2.02	0.41
2:B:258:LYS:HE2	7:B:332:BML:BR4	2.76	0.41
3:C:39:ILE:O	3:C:40:ASN:HB2	2.20	0.41
3:C:17:GLN:HE22	3:C:37:HIS:HB3	1.85	0.41
3:C:52:ARG:HG3	3:C:52:ARG:NH1	2.35	0.41
3:C:84:MET:HB3	3:C:85:ASP:H	1.67	0.41
1:A:19:THR:HA	1:A:20:PRO:HD2	1.89	0.41
1:A:301:GLN:O	1:A:305:GLN:HG2	2.20	0.41
1:A:109:THR:HG23	2:B:144:GLN:HB2	2.03	0.41
2:B:193:TRP:CZ2	2:B:203:ARG:HG3	2.56	0.41
3:C:70:ASP:C	3:C:72:GLY:H	2.28	0.41
1:A:2:SER:HB2	2:B:105:ASN:ND2	2.35	0.41
1:A:159:HIS:ND1	1:A:159:HIS:C	2.78	0.41
1:A:323:ASP:C	1:A:325:ASP:H	2.28	0.41
2:B:154:CYS:HB3	2:B:267:TRP:CD2	2.56	0.41
1:A:5:LYS:HB3	1:A:7:GLU:OE1	2.20	0.41
1:A:305:GLN:O	1:A:309:LEU:HD13	2.20	0.41
2:B:192:VAL:HG22	8:B:432:HOH:O	2.21	0.41
1:A:100:ILE:CG2	1:A:104:GLU:HG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:LEU:HD23	1:A:464:LEU:C	2.45	0.41
1:A:253:GLU:CD	1:A:253:GLU:N	2.75	0.40
1:A:280:TYR:N	1:A:280:TYR:CD2	2.89	0.40
2:B:145:ILE:HG13	2:B:145:ILE:O	2.21	0.40
1:A:89:TRP:O	1:A:92:THR:HB	2.20	0.40
1:A:266:TRP:CD2	1:A:320:PHE:HE1	2.39	0.40
1:A:376:ILE:HG23	1:A:388:THR:HG22	2.02	0.40
3:C:26:THR:O	3:C:29:GLN:N	2.54	0.40
2:B:115:ARG:HD3	8:B:472:HOH:O	2.21	0.40
1:A:468:LEU:HD13	1:A:478:MET:CE	2.51	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	489/498 (98%)	443 (91%)	41 (8%)	5 (1%)	12	11
2	B	321/330 (97%)	315 (98%)	6 (2%)	0	100	100
3	C	81/86 (94%)	70 (86%)	10 (12%)	1 (1%)	10	8
All	All	891/914 (98%)	828 (93%)	57 (6%)	6 (1%)	18	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	GLU
1	A	445	LYS
3	C	73	LEU
1	A	287	ASN
1	A	408	PRO
1	A	383	GLY

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	417/422 (99%)	406 (97%)	11 (3%)	40	55
2	B	275/282 (98%)	264 (96%)	11 (4%)	28	38
3	C	77/79 (98%)	74 (96%)	3 (4%)	28	39
All	All	769/783 (98%)	744 (97%)	25 (3%)	33	45

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	228	GLN
1	A	251	LYS
1	A	280	TYR
1	A	304	ARG
1	A	386	GLU
1	A	408	PRO
1	A	430	SER
1	A	450	LEU
1	A	469	MET
1	A	491	TYR
2	B	32	SER
2	B	34	ASN
2	B	43	GLU
2	B	54	MET
2	B	82	VAL
2	B	111	GLN
2	B	140	VAL
2	B	166	LEU
2	B	174	ARG
2	B	287	LYS
2	B	309	ASP
3	C	10	PHE
3	C	32	GLU
3	C	48	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	202	ASN
1	A	204	GLN
1	A	228	GLN
1	A	287	ASN
1	A	305	GLN
1	A	322	GLN
1	A	332	HIS
1	A	379	ASN
1	A	398	ASN
1	A	410	ASN
1	A	418	GLN
1	A	427	HIS
2	B	34	ASN
2	B	36	HIS
2	B	87	ASN
2	B	93	GLN
2	B	98	GLN
2	B	111	GLN
2	B	144	GLN
2	B	153	ASN
2	B	162	HIS
2	B	168	HIS
2	B	223	ASN
2	B	286	GLN
2	B	326	GLN
3	C	40	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - leaving 7 for Mogul analysis.

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
7	BML	A	505	-	8,8,8	3.82	6 (75%)	10,10,10	3.47	5 (50%)
7	BML	B	332	-	8,8,8	3.86	6 (75%)	10,10,10	3.47	5 (50%)
7	BML	A	504	-	8,8,8	3.91	6 (75%)	10,10,10	3.43	5 (50%)
7	BML	B	331	-	8,8,8	3.85	5 (62%)	10,10,10	3.53	5 (50%)
6	MCR	A	502	4	4,4,4	1.29	1 (25%)	3,4,4	1.30	0
7	BML	A	503	-	8,8,8	3.72	6 (75%)	10,10,10	3.61	5 (50%)
7	BML	A	506	-	8,8,8	3.82	5 (62%)	10,10,10	3.58	5 (50%)

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
7	BML	A	505	-	-	-	0/1/1/1
7	BML	B	332	-	-	-	0/1/1/1
7	BML	A	504	-	-	-	0/1/1/1
7	BML	B	331	-	-	-	0/1/1/1
6	MCR	A	502	4	-	0/0/2/2	-
7	BML	A	503	-	-	-	0/1/1/1
7	BML	A	506	-	-	-	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	331	BML	C2-C1	5.77	1.49	1.39
7	A	506	BML	C2-C1	5.73	1.49	1.39
7	A	504	BML	C2-C1	5.73	1.49	1.39
7	A	505	BML	C2-C1	5.72	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	503	BML	C2-C1	5.61	1.49	1.39
7	B	331	BML	C3-C2	5.59	1.47	1.38
7	B	332	BML	C2-C1	5.55	1.49	1.39
7	A	506	BML	C3-C2	5.54	1.47	1.38
7	A	504	BML	C3-C2	5.49	1.47	1.38
7	A	505	BML	C3-C2	5.44	1.47	1.38
7	A	503	BML	C3-C2	5.40	1.47	1.38
7	B	332	BML	C3-C2	5.39	1.47	1.38
7	A	504	BML	C6-C5	-5.29	1.30	1.38
7	B	332	BML	C6-C5	-4.79	1.31	1.38
7	B	331	BML	C6-C5	-4.76	1.31	1.38
7	A	505	BML	C6-C5	-4.68	1.31	1.38
7	A	506	BML	C6-C5	-4.67	1.31	1.38
7	A	503	BML	C6-C5	-4.58	1.31	1.38
7	A	506	BML	C6-C1	4.51	1.47	1.39
7	B	332	BML	C6-C1	4.49	1.47	1.39
7	B	331	BML	C6-C1	4.43	1.47	1.39
7	A	505	BML	C6-C1	4.39	1.47	1.39
7	A	503	BML	C6-C1	4.15	1.46	1.39
7	A	504	BML	C6-C1	4.00	1.46	1.39
7	B	331	BML	C3-C4	2.67	1.43	1.38
7	B	332	BML	BR4-C4	-2.58	1.85	1.90
7	A	504	BML	BR4-C4	-2.53	1.85	1.90
7	B	332	BML	C3-C4	2.53	1.43	1.38
7	A	504	BML	C3-C4	2.48	1.43	1.38
7	A	505	BML	C3-C4	2.43	1.43	1.38
7	A	506	BML	C3-C4	2.42	1.43	1.38
7	A	503	BML	C3-C4	2.29	1.42	1.38
7	A	505	BML	BR4-C4	-2.25	1.85	1.90
6	A	502	MCR	OXT-C	-2.21	1.23	1.30
7	A	503	BML	BR4-C4	-2.09	1.86	1.90

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	331	BML	C6-C5-C4	7.26	127.88	119.18
7	A	506	BML	C6-C5-C4	7.15	127.75	119.18
7	A	503	BML	C6-C5-C4	7.14	127.73	119.18
7	A	504	BML	C6-C5-C4	7.11	127.70	119.18
7	A	505	BML	C6-C5-C4	7.06	127.63	119.18
7	B	332	BML	C6-C5-C4	6.94	127.49	119.18
7	A	506	BML	C3-C2-C1	-5.16	114.42	119.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	504	BML	C3-C2-C1	-5.15	114.43	119.88
7	B	332	BML	C3-C2-C1	-5.13	114.45	119.88
7	A	503	BML	C3-C2-C1	-5.11	114.47	119.88
7	A	503	BML	BR4-C4-C5	5.00	126.11	119.30
7	B	331	BML	C3-C2-C1	-5.00	114.59	119.88
7	A	505	BML	C3-C2-C1	-4.98	114.61	119.88
7	A	506	BML	BR4-C4-C5	4.80	125.84	119.30
7	B	331	BML	BR4-C4-C5	4.74	125.75	119.30
7	B	332	BML	BR4-C4-C5	4.70	125.71	119.30
7	A	505	BML	BR4-C4-C5	4.66	125.65	119.30
7	A	504	BML	BR4-C4-C5	4.39	125.28	119.30
7	A	506	BML	C5-C4-C3	-3.26	116.39	121.33
7	A	506	BML	C2-C3-C4	3.25	123.07	119.18
7	A	503	BML	C5-C4-C3	-3.24	116.42	121.33
7	A	503	BML	C2-C3-C4	3.18	122.99	119.18
7	B	331	BML	C5-C4-C3	-3.17	116.52	121.33
7	A	505	BML	C5-C4-C3	-3.00	116.78	121.33
7	A	504	BML	C5-C4-C3	-2.94	116.87	121.33
7	B	332	BML	C5-C4-C3	-2.91	116.91	121.33
7	B	332	BML	C2-C3-C4	2.90	122.65	119.18
7	B	331	BML	C2-C3-C4	2.90	122.65	119.18
7	A	505	BML	C2-C3-C4	2.87	122.62	119.18
7	A	504	BML	C2-C3-C4	2.64	122.34	119.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	505	BML	2	0
7	B	332	BML	1	0
7	A	504	BML	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	491/498 (98%)	0.98	90 (18%) 3 2	23, 49, 84, 103	0
2	B	323/330 (97%)	0.09	8 (2%) 58 55	24, 35, 58, 90	0
3	C	83/86 (96%)	2.69	62 (74%) 0 0	44, 78, 94, 101	0
All	All	897/914 (98%)	0.82	160 (17%) 4 3	23, 43, 85, 103	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	43	VAL	4.5
3	C	82	ILE	4.3
3	C	76	THR	4.3
1	A	405	ALA	4.2
3	C	51	LEU	4.2
3	C	50	ILE	4.2
3	C	59	GLY	4.1
1	A	315	TRP	4.1
1	A	283	LEU	4.0
3	C	83	PHE	4.0
1	A	51	TYR	4.0
3	C	61	LEU	4.0
1	A	364	GLY	4.0
3	C	81	ILE	4.0
3	C	54	ARG	3.9
1	A	491	TYR	3.9
1	A	82	VAL	3.8
1	A	281	THR	3.8
3	C	62	PHE	3.8
1	A	365	TRP	3.8
1	A	366	ASN	3.7
3	C	66	MET	3.7
3	C	60	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	409	GLY	3.6
3	C	65	GLY	3.6
1	A	362	TYR	3.6
3	C	20	PRO	3.6
3	C	40	ASN	3.6
2	B	330	LEU	3.6
3	C	53	VAL	3.5
3	C	67	ILE	3.5
1	A	358	LEU	3.5
1	A	375	VAL	3.5
3	C	64	ARG	3.5
1	A	320	PHE	3.5
1	A	357	TRP	3.5
1	A	324	LEU	3.4
3	C	38	SER	3.4
3	C	16	ILE	3.4
3	C	63	PRO	3.4
1	A	349	GLY	3.4
1	A	421	TYR	3.3
3	C	39	ILE	3.3
1	A	406	HIS	3.2
3	C	84	MET	3.2
3	C	9	ASN	3.2
3	C	73	LEU	3.2
1	A	348	ALA	3.2
3	C	31	ALA	3.2
3	C	25	ASP	3.1
3	C	71	ALA	3.1
1	A	381	VAL	3.1
1	A	352	PRO	3.1
1	A	376	ILE	3.1
1	A	383	GLY	3.1
3	C	80	ASP	3.1
1	A	389	VAL	3.1
3	C	19	VAL	3.1
3	C	45	PRO	3.0
2	B	9	LEU	3.0
3	C	30	VAL	3.0
3	C	72	GLY	3.0
1	A	414	VAL	3.0
1	A	387	LEU	2.9
3	C	79	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	368	THR	2.9
1	A	380	LEU	2.9
3	C	14	PHE	2.9
3	C	68	VAL	2.9
3	C	78	THR	2.9
1	A	423	GLY	2.8
2	B	8	ALA	2.8
3	C	15	VAL	2.8
1	A	369	TRP	2.8
1	A	285	SER	2.8
1	A	350	VAL	2.8
1	A	309	LEU	2.8
1	A	277	MET	2.8
3	C	23	THR	2.7
1	A	286	ARG	2.7
1	A	304	ARG	2.7
1	A	290	PHE	2.7
1	A	410	ASN	2.7
1	A	413	ASN	2.7
1	A	279	TYR	2.7
1	A	317	TRP	2.7
3	C	56	HIS	2.7
3	C	10	PHE	2.7
1	A	388	THR	2.7
3	C	52	ARG	2.7
3	C	36	TYR	2.6
1	A	374	ASP	2.6
3	C	55	ARG	2.6
1	A	338	TRP	2.6
1	A	412	TRP	2.6
1	A	367	ASP	2.6
1	A	311	LEU	2.6
1	A	382	ASN	2.6
1	A	81	PHE	2.6
1	A	407	THR	2.6
1	A	408	PRO	2.6
3	C	47	PRO	2.6
1	A	417	TYR	2.6
3	C	44	HIS	2.6
1	A	373	TRP	2.5
1	A	485	TYR	2.5
1	A	442	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	85	ASP	2.5
1	A	363	PRO	2.5
2	B	107	ARG	2.5
3	C	3	THR	2.5
1	A	308	ASP	2.4
1	A	404	ILE	2.4
3	C	4	PHE	2.4
1	A	322	GLN	2.4
3	C	24	GLU	2.4
3	C	26	THR	2.3
3	C	18	LEU	2.3
1	A	296	GLU	2.3
1	A	287	ASN	2.3
3	C	58	ASP	2.3
1	A	361	LYS	2.3
2	B	11	PRO	2.3
1	A	293	PHE	2.3
1	A	336	TRP	2.3
1	A	488	VAL	2.3
1	A	263	TRP	2.3
1	A	298	ILE	2.2
1	A	325	ASP	2.2
1	A	314	PRO	2.2
1	A	326	GLU	2.2
1	A	487	TRP	2.2
2	B	112	MET	2.2
1	A	429	GLY	2.2
1	A	328	HIS	2.2
1	A	289	SER	2.2
1	A	280	TYR	2.2
2	B	12	LEU	2.2
3	C	70	ASP	2.2
3	C	41	ARG	2.1
1	A	306	LEU	2.1
1	A	386	GLU	2.1
1	A	334	GLY	2.1
1	A	378	ASP	2.1
3	C	13	ASP	2.1
3	C	75	PRO	2.1
1	A	78	ARG	2.1
1	A	85	ALA	2.1
1	A	482	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	419	LEU	2.1
3	C	57	GLU	2.1
3	C	12	ARG	2.1
3	C	49	LYS	2.1
1	A	323	ASP	2.1
1	A	439	ILE	2.1
3	C	46	GLN	2.1
1	A	355	ARG	2.1
2	B	41	ASN	2.0
1	A	337	TYR	2.0
1	A	291	LYS	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(Å ²)	Q<0.9
7	BML	A	503	8/8	0.89	0.19	75,78,80,87	0
6	MCR	A	502	5/5	0.91	0.13	48,50,52,53	0
7	BML	A	504	8/8	0.91	0.19	72,73,75,81	0
7	BML	A	505	8/8	0.92	0.15	70,70,70,74	0
7	BML	A	506	8/8	0.92	0.17	71,73,75,79	0
7	BML	B	332	8/8	0.94	0.14	63,64,65,66	0
7	BML	B	331	8/8	0.98	0.11	31,33,35,45	0
4	FE	A	500	1/1	0.99	0.02	37,37,37,37	0
4	FE	A	499	1/1	0.99	0.04	37,37,37,37	0
5	OH	A	501	1/1	1.00	0.02	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.