



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:50 PM UTC

PDB ID : 8ZHS / pdb_00008zhs
Title : Structure of Mbp-Bte1 fusion protein
Authors : Xu, J.H.; Chen, Z.; Gao, X.
Deposited on : 2024-05-11
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

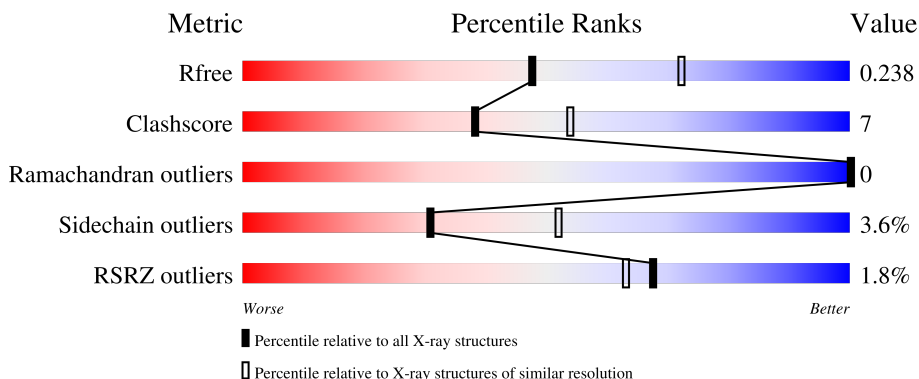
1 Overall quality at a glance

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	504	88% 11% .
1	B	504	88% 11% .
2	C	113	3% 73% 23% ..
2	D	113	11% 54% 24% 5% 16%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10039 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 Maltose/maltodextrin-binding periplasmic protein,N-terminal Bte1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			3955	2568	635	742	10			
1	B	503	Total	C	N	O	S	0	0	0
			3947	2563	634	741	9			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP P0AEX9
A	102	ALA	ASP	engineered mutation	UNP P0AEX9
A	103	ALA	LYS	engineered mutation	UNP P0AEX9
A	192	ALA	GLU	engineered mutation	UNP P0AEX9
A	193	ALA	ASN	engineered mutation	UNP P0AEX9
A	259	ALA	LYS	engineered mutation	UNP P0AEX9
A	387	ALA	-	linker	UNP P0AEX9
A	388	ALA	-	linker	UNP P0AEX9
A	389	ARG	-	linker	UNP P0AEX9
A	390	ALA	-	linker	UNP P0AEX9
A	391	PHE	-	linker	UNP P0AEX9
A	392	ALA	-	linker	UNP P0AEX9
A	393	ALA	-	linker	UNP P0AEX9
A	394	ALA	-	linker	UNP P0AEX9
B	20	MET	-	initiating methionine	UNP P0AEX9
B	102	ALA	ASP	engineered mutation	UNP P0AEX9
B	103	ALA	LYS	engineered mutation	UNP P0AEX9
B	192	ALA	GLU	engineered mutation	UNP P0AEX9
B	193	ALA	ASN	engineered mutation	UNP P0AEX9
B	259	ALA	LYS	engineered mutation	UNP P0AEX9
B	387	ALA	-	linker	UNP P0AEX9
B	388	ALA	-	linker	UNP P0AEX9
B	389	ARG	-	linker	UNP P0AEX9
B	390	ALA	-	linker	UNP P0AEX9

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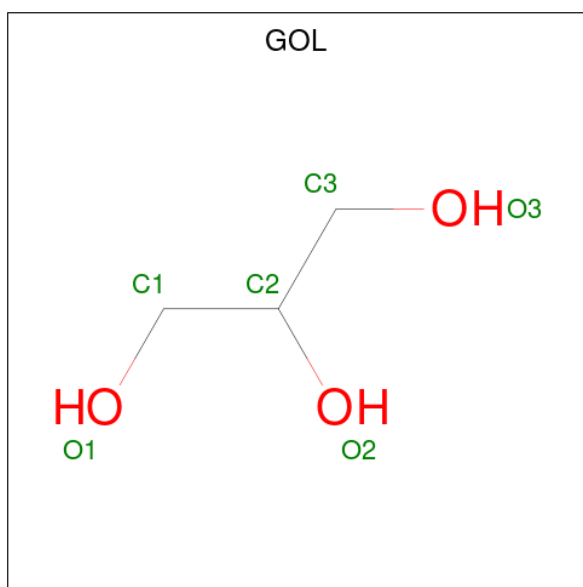
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Chain	Residue	Modelled	Actual	Comment	Reference
B	391	PHE	-	linker	UNP P0AEX9
B	392	ALA	-	linker	UNP P0AEX9
B	393	ALA	-	linker	UNP P0AEX9
B	394	ALA	-	linker	UNP P0AEX9

- Molecule 2 is a protein called C-terminal Bte1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	112	Total	C	N	O	S	0	0	0
			899	575	145	172	7			
2	D	95	Total	C	N	O	S	0	0	0
			760	491	122	141	6			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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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	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

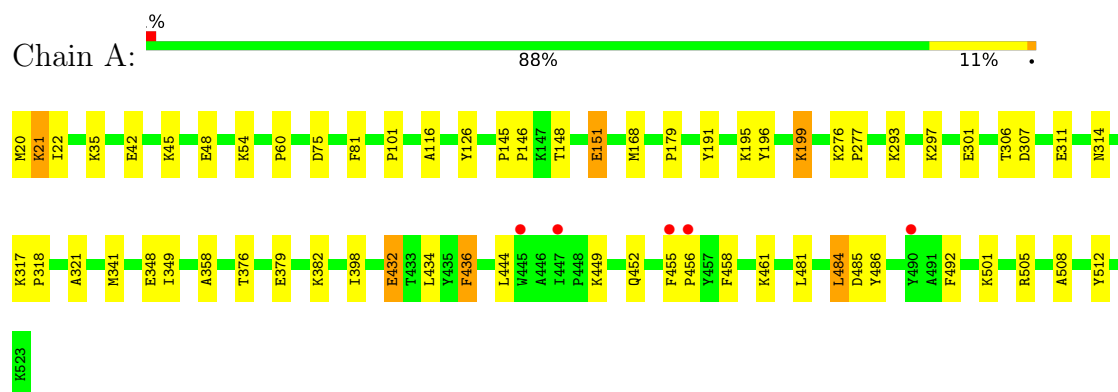
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		
4	B	199	Total	O	0	0
			199	199		
4	C	14	Total	O	0	0
			14	14		
4	D	12	Total	O	0	0
			12	12		

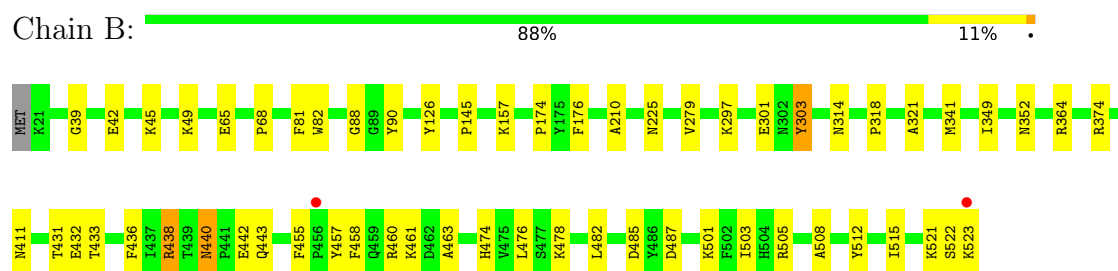
3 Residue-property plots

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.

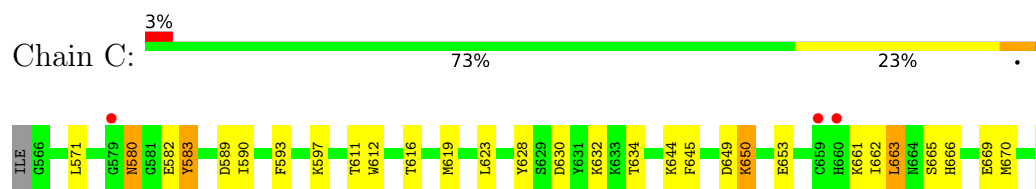
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein,N-terminal Bte1



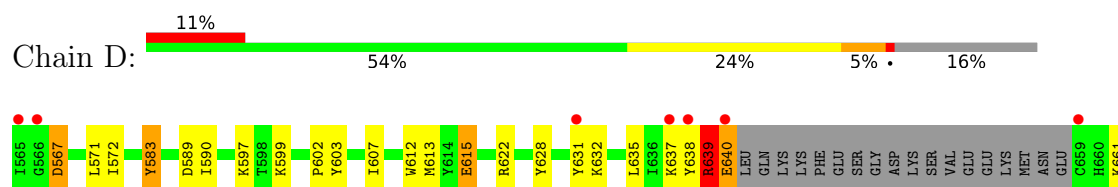
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein,N-terminal Bte1



- Molecule 2: C-terminal Bte1



- Molecule 2: C-terminal Bte1



L662	L663	S664	S665	H666	Y667	L668	E669	H670	Q671	K672	H673	L674	G675	H676	L677
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.17Å 253.87Å 56.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.13 – 2.40 42.13 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.2 (42.13-2.40) 93.2 (42.13-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.188 , 0.238 0.188 , 0.238	Depositor DCC
R_{free} test set	2000 reflections (3.37%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.785	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10039	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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: 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	0.39	2/4056 (0.0%)	0.65	2/5510 (0.0%)
1	B	0.35	1/4048 (0.0%)	0.65	0/5500
2	C	0.46	0/916	0.76	1/1231 (0.1%)
2	D	0.44	0/775	0.85	2/1045 (0.2%)
All	All	0.39	3/9795 (0.0%)	0.68	5/13286 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	145	PRO	CA-C	5.35	1.54	1.51
1	A	146	PRO	C-O	-5.23	1.17	1.23
1	A	145	PRO	C-O	-5.22	1.18	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	567	ASP	CA-CB-CG	5.58	118.18	112.60
2	C	662	ILE	N-CA-C	-5.56	104.94	111.00
1	A	151	GLU	CA-C-N	5.47	123.69	120.24
1	A	151	GLU	C-N-CA	5.47	123.69	120.24
2	D	639	ARG	N-CA-C	-5.29	106.01	113.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3955	0	3932	53	0
1	B	3947	0	3923	40	0
2	C	899	0	893	26	0
2	D	760	0	758	29	0
3	A	24	0	32	1	0
3	B	24	0	32	2	0
3	C	12	0	16	0	0
4	A	193	0	0	6	0
4	B	199	0	0	4	0
4	C	14	0	0	1	0
4	D	12	0	0	0	0
All	All	10039	0	9586	133	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 7.

All (133) 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)
2:D:661:LYS:O	2:D:665:SER:HB3	1.75	0.85
1:A:21:LYS:HB2	1:A:21:LYS:NZ	1.97	0.79
1:A:21:LYS:HB2	1:A:21:LYS:HZ2	1.50	0.75
1:A:20:MET:HE2	1:A:20:MET:HA	1.68	0.75
1:B:438:ARG:HG3	1:B:440:ASN:H	1.52	0.75
1:A:432:GLU:OE2	1:A:505:ARG:NH1	2.21	0.73
2:C:628:TYR:CE2	2:C:632:LYS:HE2	2.28	0.68
1:A:116:ALA:HB2	1:A:349:ILE:HD12	1.75	0.66
1:B:157:LYS:NZ	4:B:802:HOH:O	2.30	0.65
1:A:199:LYS:HE3	1:A:484:LEU:O	1.97	0.64
1:B:321:ALA:HB1	1:B:341:MET:HE2	1.80	0.64
1:A:455:PHE:H	1:A:508:ALA:HB1	1.63	0.64
1:A:321:ALA:HB1	1:A:341:MET:HE2	1.80	0.63
1:A:306:THR:HB	4:A:813:HOH:O	1.99	0.63
1:B:438:ARG:HH11	1:B:440:ASN:HB3	1.62	0.63
1:A:42:GLU:HG2	4:A:808:HOH:O	2.00	0.62
1:B:455:PHE:H	1:B:508:ALA:HB1	1.66	0.61
1:A:376:THR:OG1	1:A:379:GLU:HG2	1.99	0.61
1:A:484:LEU:HD13	2:C:619:MET:HE3	1.83	0.60
1:B:521:LYS:HG2	2:C:611:THR:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:638:TYR:C	2:D:640:GLU:H	2.09	0.59
2:C:650:LYS:HD2	2:C:650:LYS:H	1.67	0.58
1:A:45:LYS:HG2	4:A:851:HOH:O	2.03	0.57
2:D:597:LYS:HE2	2:D:599:LYS:O	2.04	0.57
2:D:571:LEU:HD21	2:D:612:TRP:CE2	2.40	0.57
1:A:20:MET:HA	1:A:20:MET:CE	2.35	0.57
1:B:88:GLY:HA3	1:B:352:ASN:O	2.05	0.56
1:A:45:LYS:NZ	4:A:808:HOH:O	2.38	0.56
1:A:293:LYS:O	1:A:297:LYS:HG3	2.05	0.56
1:A:436:PHE:CE2	2:C:583:TYR:HB3	2.40	0.56
1:A:148:THR:OG1	1:A:151:GLU:HG2	2.06	0.56
1:B:174:PRO:HG3	1:B:364:ARG:HA	1.86	0.56
2:D:635:LEU:HD21	2:D:639:ARG:CZ	2.37	0.55
1:A:455:PHE:CG	1:A:505:ARG:HG3	2.42	0.55
1:A:21:LYS:HD2	1:A:75:ASP:HB3	1.89	0.54
1:A:307:ASP:N	4:A:813:HOH:O	2.41	0.54
1:A:358:ALA:HA	1:A:398:ILE:HD11	1.90	0.54
1:B:411:ASN:OD1	2:D:599:LYS:NZ	2.40	0.53
2:D:628:TYR:CE2	2:D:632:LYS:HE2	2.43	0.53
1:B:68:PRO:HG3	1:B:90:TYR:CE1	2.44	0.52
2:D:672:LYS:O	2:D:676:ASN:ND2	2.42	0.52
1:B:314:ASN:OD1	1:B:318:PRO:HA	2.10	0.52
1:B:82:TRP:CE3	3:B:704:GOL:H12	2.46	0.51
2:D:572:ILE:HG22	2:D:602:PRO:HD3	1.91	0.51
1:B:476:LEU:HD21	2:D:615:GLU:HG3	1.93	0.51
2:D:667:TYR:HE1	2:D:671:GLN:HG2	1.75	0.51
1:A:48:GLU:OE2	1:A:54:LYS:HG2	2.12	0.50
1:B:442:GLU:HG2	4:B:973:HOH:O	2.10	0.50
1:A:195:LYS:HE2	4:A:818:HOH:O	2.11	0.50
1:B:460:ARG:NH2	2:C:630:ASP:OD2	2.39	0.50
1:A:461:LYS:HE3	2:D:622:ARG:NH2	2.26	0.50
1:B:522:SER:O	1:B:523:LYS:HB2	2.11	0.50
2:C:645:PHE:CE1	2:C:653:GLU:HB2	2.47	0.49
1:B:279:VAL:HB	1:B:349:ILE:HD13	1.93	0.49
1:A:314:ASN:OD1	1:A:318:PRO:HA	2.12	0.49
1:B:39:GLY:O	1:B:42:GLU:HG2	2.13	0.49
2:C:628:TYR:O	2:C:632:LYS:HG3	2.13	0.48
1:A:484:LEU:HD13	2:C:619:MET:CE	2.43	0.48
1:B:210:ALA:O	4:B:801:HOH:O	2.20	0.48
2:C:634:THR:HG22	2:C:663:LEU:HD12	1.94	0.48
1:A:484:LEU:HD12	1:A:492:PHE:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:HG2	1:A:486:TYR:CE1	2.50	0.47
1:B:474:HIS:CE1	2:D:612:TRP:CZ2	3.02	0.47
1:B:515:ILE:HD13	2:C:674:LEU:HD21	1.96	0.47
1:A:485:ASP:H	2:C:619:MET:HE3	1.80	0.47
2:D:635:LEU:HD21	2:D:639:ARG:HG3	1.97	0.47
1:B:478:LYS:O	1:B:482:LEU:HG	2.15	0.47
2:C:645:PHE:HA	2:C:649:ASP:O	2.15	0.47
2:D:667:TYR:HD1	2:D:667:TYR:O	1.98	0.47
1:A:484:LEU:HD12	1:A:492:PHE:CE2	2.49	0.46
1:B:455:PHE:HA	1:B:457:TYR:CE1	2.50	0.46
2:D:667:TYR:O	2:D:667:TYR:CD1	2.69	0.46
1:B:455:PHE:CD1	1:B:505:ARG:HG2	2.51	0.46
2:C:650:LYS:H	2:C:650:LYS:CD	2.28	0.45
2:D:667:TYR:CD1	2:D:667:TYR:C	2.94	0.45
1:A:501:LYS:O	1:A:505:ARG:HD3	2.16	0.45
1:A:179:PRO:HG3	1:A:277:PRO:HA	1.98	0.45
1:B:458:PHE:HB2	1:B:512:TYR:OH	2.16	0.45
1:A:60:PRO:HA	3:A:701:GOL:H32	1.98	0.45
2:C:644:LYS:HB3	2:C:649:ASP:HB3	1.98	0.45
2:D:583:TYR:N	2:D:583:TYR:CD1	2.85	0.45
1:A:148:THR:HG1	1:A:151:GLU:HG2	1.82	0.45
1:A:195:LYS:HE3	1:B:463:ALA:O	2.17	0.45
2:C:593:PHE:HA	2:C:597:LYS:HE3	1.98	0.45
1:A:455:PHE:CD2	1:A:505:ARG:HG3	2.51	0.44
2:C:580:ASN:OD1	2:C:580:ASN:N	2.38	0.44
2:D:638:TYR:C	2:D:640:GLU:N	2.73	0.44
1:A:481:LEU:O	1:A:484:LEU:HB2	2.17	0.44
1:B:225:ASN:ND2	4:B:819:HOH:O	2.50	0.44
2:D:674:LEU:HA	2:D:677:LEU:CD2	2.48	0.44
2:C:628:TYR:HB2	2:C:670:MET:SD	2.58	0.44
2:C:630:ASP:HB3	2:C:666:HIS:CE1	2.52	0.44
1:B:461:LYS:HE2	1:B:461:LYS:HB2	1.87	0.44
1:A:348:GLU:HA	1:A:348:GLU:OE1	2.18	0.44
1:A:434:LEU:HD22	1:A:452:GLN:NE2	2.33	0.44
1:B:503:ILE:HD13	2:D:613:MET:HE3	1.99	0.44
1:A:432:GLU:HA	1:A:432:GLU:OE1	2.18	0.43
1:A:456:PRO:HG2	1:A:512:TYR:CD2	2.53	0.43
2:D:589:ASP:OD1	2:D:590:ILE:HD12	2.18	0.43
2:D:671:GLN:OE1	2:D:674:LEU:HD12	2.18	0.43
2:D:613:MET:HE3	2:D:613:MET:HB2	1.90	0.43
1:B:42:GLU:HA	1:B:45:LYS:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:665:SER:O	2:C:669:GLU:HG2	2.19	0.43
1:A:101:PRO:HB3	1:A:301:GLU:OE2	2.19	0.43
2:C:645:PHE:HE1	2:C:653:GLU:HB2	1.84	0.43
1:A:449:LYS:HE3	2:C:582:GLU:OE1	2.19	0.42
2:C:589:ASP:CG	2:C:590:ILE:HD12	2.43	0.42
1:A:455:PHE:CD1	1:A:505:ARG:HG3	2.53	0.42
1:A:432:GLU:CD	1:A:505:ARG:HH12	2.25	0.42
2:D:669:GLU:HA	2:D:672:LYS:HD3	2.02	0.42
2:D:668:ILE:HG22	2:D:672:LYS:HD2	2.02	0.42
1:A:35:LYS:C	1:A:317:LYS:HD2	2.43	0.42
2:D:668:ILE:HD12	2:D:668:ILE:HA	1.90	0.42
1:A:21:LYS:HD2	1:A:75:ASP:CB	2.49	0.42
1:B:487:ASP:OD1	1:B:487:ASP:C	2.63	0.42
1:B:82:TRP:CD2	3:B:704:GOL:H12	2.55	0.42
1:B:432:GLU:HG3	1:B:433:THR:N	2.35	0.42
1:A:436:PHE:CD1	1:A:436:PHE:N	2.88	0.41
1:A:458:PHE:CG	2:D:622:ARG:HG3	2.55	0.41
1:B:431:THR:O	1:B:501:LYS:HE3	2.20	0.41
1:B:297:LYS:HE3	1:B:301:GLU:OE2	2.20	0.41
1:B:65:GLU:O	1:B:68:PRO:HD2	2.20	0.41
1:A:191:TYR:HB2	1:A:196:TYR:CE1	2.56	0.41
1:B:303:TYR:CD1	1:B:303:TYR:N	2.89	0.41
1:A:276:LYS:HE2	1:A:348:GLU:HG2	2.03	0.41
1:B:440:ASN:ND2	1:B:443:GLN:OE1	2.37	0.41
2:C:583:TYR:CD1	2:C:583:TYR:N	2.88	0.41
2:C:616:THR:HG23	4:C:1204:HOH:O	2.20	0.41
2:D:603:TYR:CZ	2:D:607:ILE:HD11	2.55	0.41
1:B:374:ARG:HH11	1:B:374:ARG:HD2	1.67	0.41
1:B:455:PHE:O	1:B:457:TYR:CE2	2.74	0.41
1:A:168:MET:HE2	1:A:168:MET:HB3	1.98	0.40
2:C:571:LEU:HD21	2:C:612:TRP:CZ2	2.57	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	502/504 (100%)	494 (98%)	8 (2%)	0	100	100
1	B	501/504 (99%)	491 (98%)	10 (2%)	0	100	100
2	C	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
2	D	91/113 (80%)	90 (99%)	1 (1%)	0	100	100
All	All	1204/1234 (98%)	1182 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/406 (100%)	395 (97%)	11 (3%)	39	62
1	B	405/406 (100%)	396 (98%)	9 (2%)	45	67
2	C	98/99 (99%)	92 (94%)	6 (6%)	17	30
2	D	82/99 (83%)	72 (88%)	10 (12%)	5	7
All	All	991/1010 (98%)	955 (96%)	36 (4%)	31	52

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	22	ILE
1	A	81	PHE
1	A	126	TYR
1	A	199	LYS
1	A	311	GLU
1	A	382	LYS
1	A	432	GLU
1	A	436	PHE
1	A	444	LEU

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Mol	Chain	Res	Type
1	A	484	LEU
1	B	49	LYS
1	B	81	PHE
1	B	126	TYR
1	B	176	PHE
1	B	303	TYR
1	B	436	PHE
1	B	438	ARG
1	B	440	ASN
1	B	485	ASP
2	C	580	ASN
2	C	583	TYR
2	C	623	LEU
2	C	650	LYS
2	C	661	LYS
2	C	663	LEU
2	D	567	ASP
2	D	583	TYR
2	D	615	GLU
2	D	631	TYR
2	D	637	LYS
2	D	639	ARG
2	D	640	GLU
2	D	664	ASN
2	D	668	ILE
2	D	677	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	273	GLN
1	A	375	GLN
1	B	261	ASN
1	B	440	ASN
1	B	443	GLN
2	C	660	HIS
2	C	664	ASN
2	D	676	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 ⓘ

10 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	A	702	-	5,5,5	0.68	0	5,5,5	1.13	0
3	GOL	A	701	-	5,5,5	1.16	0	5,5,5	1.23	0
3	GOL	B	703	-	5,5,5	0.99	0	5,5,5	0.99	0
3	GOL	B	704	-	5,5,5	0.88	0	5,5,5	1.21	1 (20%)
3	GOL	B	701	-	5,5,5	1.05	0	5,5,5	1.32	1 (20%)
3	GOL	A	703	-	5,5,5	1.31	1 (20%)	5,5,5	0.94	0
3	GOL	C	1101	-	5,5,5	0.99	0	5,5,5	0.97	0
3	GOL	B	702	-	5,5,5	1.06	0	5,5,5	0.99	0
3	GOL	C	1102	-	5,5,5	1.01	0	5,5,5	1.00	0
3	GOL	A	704	-	5,5,5	0.99	0	5,5,5	1.05	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
3	GOL	A	702	-	-	0/4/4/4	-
3	GOL	A	701	-	-	4/4/4/4	-
3	GOL	B	703	-	-	4/4/4/4	-
3	GOL	B	704	-	-	4/4/4/4	-
3	GOL	B	701	-	-	4/4/4/4	-
3	GOL	A	703	-	-	4/4/4/4	-
3	GOL	C	1101	-	-	0/4/4/4	-
3	GOL	B	702	-	-	0/4/4/4	-
3	GOL	C	1102	-	-	2/4/4/4	-
3	GOL	A	704	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	GOL	C3-C2	2.53	1.61	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	704	GOL	C3-C2-C1	-2.11	104.06	111.80
3	B	701	GOL	C3-C2-C1	-2.07	104.19	111.80

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	GOL	O1-C1-C2-C3
3	A	701	GOL	C1-C2-C3-O3
3	A	703	GOL	O1-C1-C2-C3
3	A	704	GOL	O1-C1-C2-C3
3	B	703	GOL	C1-C2-C3-O3
3	B	704	GOL	O1-C1-C2-O2
3	B	704	GOL	O1-C1-C2-C3
3	B	704	GOL	C1-C2-C3-O3
3	A	704	GOL	O1-C1-C2-O2
3	A	703	GOL	C1-C2-C3-O3
3	A	704	GOL	C1-C2-C3-O3
3	B	701	GOL	O1-C1-C2-C3
3	B	701	GOL	C1-C2-C3-O3
3	B	703	GOL	O1-C1-C2-C3
3	C	1102	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	701	GOL	O2-C2-C3-O3
3	A	703	GOL	O2-C2-C3-O3
3	A	701	GOL	O1-C1-C2-O2
3	B	703	GOL	O2-C2-C3-O3
3	C	1102	GOL	O1-C1-C2-O2
3	A	703	GOL	O1-C1-C2-O2
3	B	701	GOL	O2-C2-C3-O3
3	B	704	GOL	O2-C2-C3-O3
3	A	704	GOL	O2-C2-C3-O3
3	B	703	GOL	O1-C1-C2-O2
3	B	701	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	GOL	1	0
3	B	704	GOL	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	504/504 (100%)	-0.32	5 (0%) 79 76	26, 41, 67, 107	0
1	B	503/504 (99%)	-0.34	2 (0%) 88 86	30, 42, 61, 84	0
2	C	112/113 (99%)	0.25	3 (2%) 56 52	41, 60, 82, 98	0
2	D	95/113 (84%)	0.53	12 (12%) 8 6	41, 56, 113, 142	0
All	All	1214/1234 (98%)	-0.21	22 (1%) 67 63	26, 44, 74, 142	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	565	ILE	4.3
2	D	664	ASN	3.6
2	D	638	TYR	3.4
1	A	455	PHE	3.2
1	A	445	TRP	3.1
1	A	447	ILE	3.1
1	A	490	TYR	3.0
2	D	640	GLU	2.9
1	A	456	PRO	2.7
2	D	631	TYR	2.5
2	D	637	LYS	2.4
2	D	566	GLY	2.4
2	D	668	ILE	2.3
2	D	677	LEU	2.3
2	D	667	TYR	2.2
2	C	659	CYS	2.1
2	D	659	CYS	2.1
2	D	662	ILE	2.1
1	B	456	PRO	2.1
1	B	523	LYS	2.1
2	C	660	HIS	2.1
2	C	579	GLY	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	C	1102	6/6	0.59	0.13	68,80,83,89	0
3	GOL	C	1101	6/6	0.61	0.16	82,83,86,86	0
3	GOL	A	702	6/6	0.74	0.12	49,55,57,58	0
3	GOL	A	703	6/6	0.77	0.17	44,47,53,59	0
3	GOL	A	704	6/6	0.78	0.15	54,56,65,66	0
3	GOL	B	702	6/6	0.80	0.14	44,57,58,62	0
3	GOL	B	703	6/6	0.85	0.14	44,59,69,71	0
3	GOL	B	704	6/6	0.87	0.15	42,48,52,61	0
3	GOL	B	701	6/6	0.90	0.11	45,49,58,62	0
3	GOL	A	701	6/6	0.91	0.12	44,46,56,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.