



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:02 AM UTC

PDB ID : 3A3D / pdb_00003a3d
Title : Crystal structure of penicillin binding protein 4 (dacB) from Haemophilus influenzae
Authors : Kawai, F.; Roper, D.I.; Park, S.-Y.; Tame, J.R.H.
Deposited on : 2009-06-12
Resolution : 1.60 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

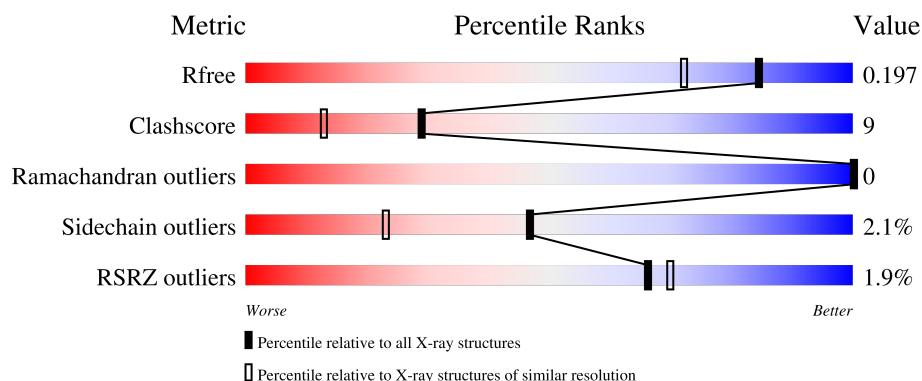
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	453	81% 17% .
1	B	453	3% 79% 18% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7960 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 Penicillin-binding protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3506	2237	605	652	12			
1	B	453	Total	C	N	O	S	4	0	0
			3506	2237	605	652	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	expression tag	UNP A8E0K8
B	27	MET	-	expression tag	UNP A8E0K8

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

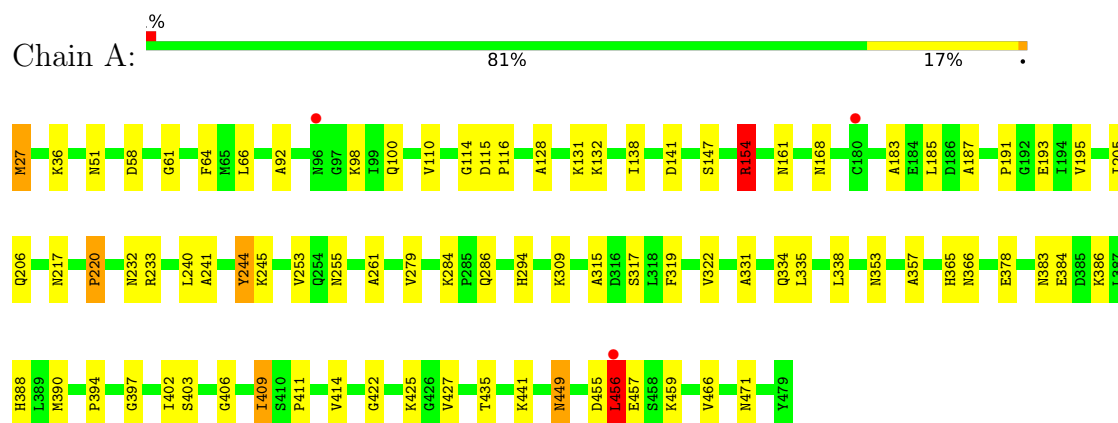
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	512	Total	O	0	0
			512	512		
3	B	412	Total	O	0	0
			412	412		

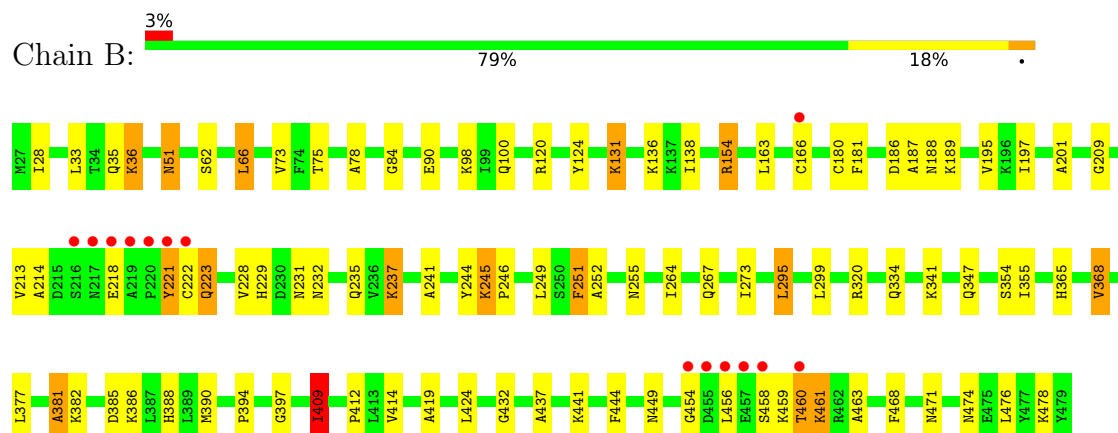
3 Residue-property plots [i](#)

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: Penicillin-binding protein 4



• Molecule 1: Penicillin-binding protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.55Å 92.59Å 104.88Å 90.00° 107.75° 90.00°	Depositor
Resolution (Å)	19.98 – 1.60 19.98 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-1.60) 94.8 (19.98-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.171 , 0.204 0.165 , 0.197	Depositor DCC
R_{free} test set	7346 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7960	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.72	28/3572 (0.8%)	1.51	14/4830 (0.3%)
1	B	1.70	32/3572 (0.9%)	1.50	21/4830 (0.4%)
All	All	1.71	60/7144 (0.8%)	1.50	35/9660 (0.4%)

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	ALA	CA-CB	-10.24	1.35	1.53
1	B	195	VAL	CA-CB	7.87	1.62	1.54
1	A	64	PHE	N-CA	7.07	1.54	1.46
1	B	73	VAL	N-CA	6.86	1.54	1.46
1	B	414	VAL	CA-CB	6.78	1.61	1.54
1	B	295	LEU	C-O	6.76	1.32	1.24
1	B	78	ALA	CA-CB	6.54	1.63	1.53
1	A	353	ASN	N-CA	-6.51	1.39	1.46
1	B	432	GLY	N-CA	6.50	1.52	1.45
1	B	444	PHE	N-CA	6.40	1.53	1.45
1	B	84	GLY	N-CA	6.37	1.52	1.45
1	B	320	ARG	CZ-NH1	6.37	1.41	1.32
1	A	279	VAL	CA-CB	6.25	1.61	1.54
1	B	197	ILE	C-O	6.20	1.31	1.24
1	B	209	GLY	C-O	-6.16	1.17	1.24
1	B	138	ILE	CA-CB	6.13	1.61	1.54
1	B	273	ILE	CA-CB	6.10	1.60	1.53
1	B	368	VAL	N-CA	5.99	1.53	1.46
1	A	58	ASP	C-O	5.98	1.29	1.23
1	B	51	ASN	N-CA	5.98	1.53	1.46
1	A	378	GLU	N-CA	5.97	1.53	1.46
1	A	411	PRO	CA-C	5.95	1.55	1.51
1	B	252	ALA	N-CA	-5.87	1.38	1.46
1	A	414	VAL	CA-CB	5.86	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	PRO	CA-C	-5.85	1.47	1.52
1	A	138	ILE	CA-CB	5.85	1.61	1.54
1	A	187	ALA	CA-CB	5.80	1.61	1.53
1	B	264	ILE	CA-CB	-5.80	1.48	1.54
1	A	322	VAL	CA-CB	5.76	1.60	1.54
1	B	347	GLN	C-O	-5.75	1.16	1.24
1	B	228	VAL	C-O	5.73	1.30	1.24
1	A	220	PRO	C-O	-5.70	1.16	1.24
1	B	187	ALA	CA-CB	5.69	1.61	1.53
1	B	251	PHE	CA-C	-5.68	1.45	1.52
1	B	424	LEU	N-CA	5.66	1.53	1.45
1	B	66	LEU	CA-C	5.63	1.58	1.52
1	A	456	LEU	CG-CD1	5.46	1.70	1.52
1	A	128	ALA	N-CA	5.41	1.53	1.46
1	A	331	ALA	C-O	5.38	1.30	1.24
1	A	466	VAL	C-O	5.36	1.30	1.24
1	A	244	TYR	N-CA	5.35	1.52	1.46
1	A	406	GLY	C-O	5.34	1.30	1.23
1	A	253	VAL	CA-CB	5.32	1.60	1.54
1	A	449	ASN	CG-OD1	5.31	1.33	1.23
1	A	61	GLY	C-O	5.30	1.30	1.24
1	A	110	VAL	CA-CB	-5.30	1.47	1.54
1	B	244	TYR	CA-C	-5.26	1.45	1.52
1	B	186	ASP	CA-C	-5.24	1.46	1.53
1	A	435	THR	CA-CB	5.21	1.60	1.53
1	B	381	ALA	C-O	5.18	1.30	1.24
1	A	183	ALA	N-CA	5.17	1.52	1.45
1	A	427	VAL	N-CA	5.17	1.52	1.46
1	B	354	SER	N-CA	5.14	1.52	1.46
1	A	319	PHE	C-O	5.10	1.29	1.24
1	B	419	ALA	N-CA	5.09	1.51	1.46
1	B	295	LEU	CA-C	-5.08	1.46	1.52
1	B	454	GLY	N-CA	5.07	1.50	1.45
1	A	92	ALA	N-CA	5.07	1.52	1.45
1	B	299	LEU	CA-CB	-5.06	1.49	1.54
1	B	409	ILE	CA-CB	5.05	1.61	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ARG	CB-CG-CD	7.81	129.26	111.30
1	A	27	MET	CB-CG-SD	-7.71	89.56	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	320	ARG	NE-CZ-NH2	-7.54	112.41	119.20
1	B	66	LEU	O-C-N	7.24	127.46	121.31
1	A	317	SER	CB-CA-C	-6.86	99.18	110.85
1	B	245	LYS	CA-C-N	6.72	126.68	119.76
1	B	245	LYS	C-N-CA	6.72	126.68	119.76
1	A	317	SER	CA-CB-OG	-6.67	97.77	111.10
1	B	201	ALA	N-CA-C	6.63	119.33	111.71
1	A	131	LYS	CB-CG-CD	-6.51	96.33	111.30
1	A	261	ALA	N-CA-C	-6.37	104.41	111.36
1	B	394	PRO	CB-CA-C	-6.22	103.43	111.39
1	A	147	SER	N-CA-C	6.08	119.80	112.38
1	A	161	ASN	N-CA-C	-6.02	105.90	113.18
1	B	136	LYS	N-CA-C	-6.01	106.28	113.97
1	B	437	ALA	N-CA-C	-5.94	105.29	112.54
1	B	252	ALA	N-CA-C	5.88	119.11	109.76
1	A	471	ASN	N-CA-C	5.72	117.19	111.07
1	B	241	ALA	N-CA-C	-5.69	102.06	110.48
1	A	241	ALA	CA-C-N	-5.56	113.06	120.90
1	A	241	ALA	C-N-CA	-5.56	113.06	120.90
1	B	131	LYS	N-CA-C	-5.51	105.36	111.36
1	B	377	LEU	N-CA-C	-5.51	105.28	111.28
1	B	35	GLN	CA-C-N	-5.47	113.90	122.65
1	B	35	GLN	C-N-CA	-5.47	113.90	122.65
1	B	397	GLY	N-CA-C	-5.41	107.51	115.30
1	A	422	GLY	N-CA-C	-5.38	100.44	113.18
1	B	124	TYR	N-CA-C	-5.36	105.34	111.07
1	A	456	LEU	CB-CG-CD1	5.35	126.76	110.70
1	B	154	ARG	CB-CG-CD	5.33	123.57	111.30
1	B	221	TYR	CB-CA-C	-5.25	99.64	109.72
1	B	75	THR	O-C-N	5.21	127.64	122.12
1	B	166	CYS	CB-CA-C	5.11	120.08	110.63
1	A	315	ALA	N-CA-C	5.03	116.45	111.07
1	B	62	SER	O-C-N	5.02	128.31	122.24

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	3506	0	3554	66	0
1	B	3506	0	3554	59	0
2	A	18	0	24	6	0
2	B	6	0	8	3	0
3	A	512	0	0	22	0
3	B	412	0	0	18	0
All	All	7960	0	7140	123	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 (123) 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:335:LEU:HD12	3:A:877:HOH:O	1.22	1.32
1:A:441:LYS:HE2	2:A:482:GOL:O1	1.29	1.28
1:A:141:ASP:OD1	2:A:480:GOL:H11	1.46	1.14
1:B:98:LYS:HE2	1:B:100:GLN:CD	1.71	1.13
1:A:441:LYS:HE2	2:A:482:GOL:HO1	1.21	0.95
1:B:66:LEU:H	1:B:449:ASN:HD21	1.13	0.95
1:A:66:LEU:H	1:A:449:ASN:HD21	1.13	0.94
1:A:456:LEU:CD1	1:A:456:LEU:H	1.81	0.93
1:A:232:ASN:HD21	1:A:255:ASN:H	1.16	0.90
1:A:441:LYS:CE	2:A:482:GOL:O1	2.20	0.87
1:A:456:LEU:H	1:A:456:LEU:HD12	1.38	0.86
1:B:368:VAL:HG23	3:B:835:HOH:O	1.75	0.86
1:B:98:LYS:HE2	1:B:100:GLN:NE2	1.92	0.83
1:A:193:GLU:HG3	3:A:829:HOH:O	1.79	0.83
1:B:460:THR:HG23	3:B:708:HOH:O	1.79	0.83
1:A:98:LYS:NZ	1:A:100:GLN:OE1	2.14	0.81
1:B:232:ASN:HD21	1:B:255:ASN:H	1.29	0.80
1:B:154:ARG:HD3	3:B:669:HOH:O	1.81	0.79
1:B:36:LYS:HD3	1:B:468:PHE:HA	1.65	0.77
1:B:33:LEU:O	1:B:36:LYS:HD2	1.86	0.76
1:B:267:GLN:HE21	2:B:1:GOL:H32	1.51	0.76
1:A:98:LYS:NZ	1:A:98:LYS:HB2	2.01	0.75
1:B:368:VAL:CG2	3:B:835:HOH:O	2.33	0.75
1:A:357:ALA:H	1:A:366:ASN:ND2	1.84	0.74
1:A:335:LEU:CD1	3:A:877:HOH:O	1.97	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:HD13	3:A:936:HOH:O	1.91	0.71
1:A:98:LYS:HB2	1:A:98:LYS:HZ2	1.56	0.70
1:A:244:TYR:C	1:A:245:LYS:HG3	2.14	0.70
1:B:131:LYS:HE3	3:B:808:HOH:O	1.91	0.69
1:B:36:LYS:NZ	1:B:471:ASN:HD22	1.92	0.67
1:A:141:ASP:CG	2:A:480:GOL:H11	2.18	0.66
1:B:154:ARG:HD2	1:B:163:LEU:HD22	1.76	0.66
1:B:461:LYS:HD2	1:B:463:ALA:H	1.61	0.64
1:A:357:ALA:H	1:A:366:ASN:HD21	1.44	0.63
1:A:232:ASN:ND2	1:A:255:ASN:H	1.93	0.63
1:A:66:LEU:H	1:A:449:ASN:ND2	1.93	0.62
1:B:232:ASN:ND2	1:B:255:ASN:H	1.98	0.62
1:B:66:LEU:H	1:B:449:ASN:ND2	1.93	0.61
1:A:309:LYS:NZ	3:A:648:HOH:O	2.34	0.60
1:B:51:ASN:ND2	1:B:441:LYS:H	1.99	0.60
1:A:51:ASN:ND2	1:A:441:LYS:H	1.99	0.60
1:A:98:LYS:NZ	1:A:98:LYS:CB	2.65	0.60
1:B:98:LYS:HE2	1:B:100:GLN:OE1	2.03	0.59
1:B:36:LYS:HD3	1:B:468:PHE:CA	2.33	0.59
1:A:284:LYS:HG3	1:A:286:GLN:NE2	2.20	0.57
1:B:341:LYS:CE	3:B:859:HOH:O	2.52	0.57
1:B:36:LYS:HZ1	1:B:471:ASN:HD22	1.51	0.57
1:B:386:LYS:HG2	3:B:585:HOH:O	2.05	0.56
1:B:66:LEU:N	1:B:449:ASN:HD21	1.93	0.56
1:A:425:LYS:NZ	1:A:456:LEU:HB3	2.20	0.56
1:A:456:LEU:HD12	1:A:456:LEU:N	2.15	0.55
1:A:141:ASP:OD1	2:A:480:GOL:C1	2.36	0.55
1:A:334:GLN:NE2	1:B:223:GLN:OE1	2.41	0.54
1:A:98:LYS:CE	1:A:100:GLN:OE1	2.56	0.54
1:B:388:HIS:HE1	3:B:769:HOH:O	1.91	0.53
1:A:245:LYS:HE2	3:A:975:HOH:O	2.07	0.53
1:A:193:GLU:HG3	3:A:901:HOH:O	2.09	0.53
1:A:233:ARG:HD3	3:A:674:HOH:O	2.09	0.52
3:A:531:HOH:O	1:B:365:HIS:HE1	1.93	0.51
1:A:132:LYS:NZ	3:A:886:HOH:O	2.43	0.51
1:A:397:GLY:HA2	1:A:403:SER:O	2.11	0.50
3:A:548:HOH:O	1:B:334:GLN:HG3	2.10	0.50
1:B:120:ARG:HE	2:B:1:GOL:C2	2.24	0.50
1:A:168:ASN:ND2	3:A:757:HOH:O	2.26	0.49
1:A:338:LEU:HG	3:A:860:HOH:O	2.12	0.49
1:A:240:LEU:HD23	1:A:240:LEU:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:TYR:O	1:A:245:LYS:HG3	2.11	0.49
1:B:180:CYS:SG	3:B:509:HOH:O	2.60	0.49
1:A:425:LYS:HZ1	1:A:456:LEU:HB3	1.75	0.49
1:A:386:LYS:HE3	3:A:806:HOH:O	2.13	0.48
1:B:51:ASN:HD21	1:B:441:LYS:H	1.59	0.48
1:A:206:GLN:OE1	3:A:910:HOH:O	2.20	0.48
1:A:294:HIS:HE1	3:A:4:HOH:O	1.96	0.48
1:B:237:LYS:HE2	3:B:704:HOH:O	2.12	0.48
1:A:456:LEU:HD11	3:B:724:HOH:O	2.14	0.47
1:A:66:LEU:N	1:A:449:ASN:HD21	1.97	0.47
1:A:205:ILE:C	1:A:205:ILE:HD12	2.40	0.47
1:A:409:ILE:C	1:A:409:ILE:CD1	2.88	0.46
1:B:231:ASN:ND2	3:B:888:HOH:O	2.48	0.46
1:A:456:LEU:HG	1:B:355:ILE:HD12	1.97	0.46
1:A:456:LEU:HD22	3:B:749:HOH:O	2.16	0.45
1:B:478:LYS:HB2	1:B:478:LYS:HE2	1.56	0.45
1:A:154:ARG:CD	3:A:825:HOH:O	2.64	0.45
1:A:394:PRO:HB2	1:A:402:ILE:HG12	1.98	0.45
1:B:267:GLN:NE2	2:B:1:GOL:H32	2.24	0.45
1:A:388:HIS:HE1	3:A:960:HOH:O	1.99	0.45
1:B:218:GLU:O	1:B:221:TYR:HB2	2.16	0.45
1:A:51:ASN:H	1:A:51:ASN:HD22	1.65	0.45
1:A:384:GLU:OE1	1:A:390:MET:HG2	2.17	0.45
1:A:284:LYS:NZ	1:A:286:GLN:HE22	2.15	0.44
1:B:341:LYS:HE2	3:B:698:HOH:O	2.17	0.44
1:B:385:ASP:HB3	3:B:585:HOH:O	2.17	0.44
1:B:90:GLU:HG2	1:B:295:LEU:CD2	2.48	0.43
1:B:412:PRO:HD2	1:B:474:ASN:HD21	1.82	0.43
1:A:409:ILE:C	1:A:409:ILE:HD12	2.44	0.43
1:B:249:LEU:HD23	1:B:249:LEU:HA	1.79	0.43
3:A:548:HOH:O	1:B:334:GLN:CG	2.67	0.42
1:B:223:GLN:NE2	3:B:771:HOH:O	2.52	0.42
1:A:383:ASN:HD22	1:A:386:LYS:NZ	2.17	0.42
1:B:28:ILE:CD1	1:B:476:LEU:HD23	2.49	0.42
1:B:51:ASN:H	1:B:51:ASN:HD22	1.67	0.42
1:A:154:ARG:HD3	3:A:825:HOH:O	2.18	0.42
1:B:381:ALA:HA	1:B:390:MET:HE2	2.02	0.42
1:A:365:HIS:HE1	3:B:613:HOH:O	2.02	0.42
1:A:455:ASP:OD1	1:A:455:ASP:C	2.63	0.42
1:B:382:LYS:HB2	1:B:382:LYS:HE3	1.88	0.41
1:B:229:HIS:HE1	1:B:235:GLN:OE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ALA:CB	1:B:222:CYS:SG	3.08	0.41
1:B:461:LYS:HD3	1:B:461:LYS:HA	1.21	0.41
1:A:334:GLN:HG2	3:B:923:HOH:O	2.21	0.41
1:B:245:LYS:HA	1:B:246:PRO:HD2	1.85	0.41
1:B:188:ASN:C	1:B:189:LYS:HG2	2.46	0.41
1:A:114:GLY:O	1:A:115:ASP:C	2.64	0.41
1:A:185:LEU:HB3	1:A:195:VAL:CG1	2.51	0.41
1:A:217:ASN:O	1:A:220:PRO:HD2	2.21	0.41
1:B:98:LYS:CE	1:B:100:GLN:NE2	2.74	0.40
1:A:284:LYS:HG3	1:A:286:GLN:HE21	1.86	0.40
3:A:826:HOH:O	1:B:456:LEU:HD13	2.20	0.40
1:B:189:LYS:HB2	1:B:213:VAL:HG21	2.03	0.40
1:A:193:GLU:CG	3:A:829:HOH:O	2.53	0.40
1:B:181:PHE:CZ	1:B:251:PHE:HB2	2.57	0.40
1:B:214:ALA:HB2	1:B:222:CYS:SG	2.61	0.40
1:B:409:ILE:C	1:B:409:ILE:CD1	2.94	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	451/453 (100%)	442 (98%)	9 (2%)	0	100	100
1	B	451/453 (100%)	441 (98%)	10 (2%)	0	100	100
All	All	902/906 (100%)	883 (98%)	19 (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	378/378 (100%)	370 (98%)	8 (2%)	47	23
1	B	378/378 (100%)	370 (98%)	8 (2%)	47	23
All	All	756/756 (100%)	740 (98%)	16 (2%)	47	23

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	MET
1	A	36	LYS
1	A	154	ARG
1	A	191	PRO
1	A	409	ILE
1	A	456	LEU
1	A	457	GLU
1	A	459	LYS
1	B	36	LYS
1	B	223	GLN
1	B	237	LYS
1	B	409	ILE
1	B	458	SER
1	B	459	LYS
1	B	460	THR
1	B	461	LYS

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	42	ASN
1	A	51	ASN
1	A	178	ASN
1	A	232	ASN
1	A	286	GLN
1	A	294	HIS

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Mol	Chain	Res	Type
1	A	366	ASN
1	A	383	ASN
1	A	449	ASN
1	B	51	ASN
1	B	88	GLN
1	B	103	ASN
1	B	139	ASN
1	B	179	ASN
1	B	198	ASN
1	B	210	GLN
1	B	217	ASN
1	B	229	HIS
1	B	232	ASN
1	B	267	GLN
1	B	365	HIS
1	B	388	HIS
1	B	446	GLN
1	B	449	ASN
1	B	467	GLN
1	B	471	ASN
1	B	474	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	GOL	A	480	-	5,5,5	0.42	0	5,5,5	0.65	0
2	GOL	A	482	-	5,5,5	0.53	0	5,5,5	1.38	1 (20%)
2	GOL	B	1	-	5,5,5	0.79	0	5,5,5	1.48	1 (20%)
2	GOL	A	481	-	5,5,5	1.16	0	5,5,5	0.93	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	GOL	A	480	-	-	4/4/4/4	-
2	GOL	A	482	-	-	0/4/4/4	-
2	GOL	B	1	-	-	3/4/4/4	-
2	GOL	A	481	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GOL	O2-C2-C1	-3.19	95.96	109.18
2	A	482	GOL	O1-C1-C2	-2.49	99.18	110.38

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	480	GOL	O1-C1-C2-C3
2	A	480	GOL	C1-C2-C3-O3
2	B	1	GOL	C1-C2-C3-O3
2	A	480	GOL	O1-C1-C2-O2
2	A	480	GOL	O2-C2-C3-O3
2	B	1	GOL	O2-C2-C3-O3
2	B	1	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	480	GOL	3	0
2	A	482	GOL	3	0
2	B	1	GOL	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	453/453 (100%)	-0.54	3 (0%) 84 87	7, 14, 30, 46	0
1	B	453/453 (100%)	-0.21	14 (3%) 51 54	10, 18, 40, 64	1 (0%)
All	All	906/906 (100%)	-0.37	17 (1%) 66 70	7, 16, 34, 64	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	456	LEU	7.3
1	B	454	GLY	5.4
1	B	221	TYR	4.7
1	A	456	LEU	4.2
1	B	457	GLU	4.2
1	B	222	CYS	4.0
1	B	220	PRO	3.8
1	B	219	ALA	3.5
1	B	458	SER	3.4
1	B	460	THR	3.4
1	B	455	ASP	3.2
1	B	217	ASN	2.7
1	B	166	CYS	2.3
1	B	216	SER	2.3
1	A	96	ASN	2.2
1	B	218	GLU	2.1
1	A	180	CYS	2.1

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	GOL	A	480	6/6	0.76	0.15	50,51,52,53	0
2	GOL	B	1	6/6	0.81	0.14	34,39,44,44	0
2	GOL	A	482	6/6	0.89	0.12	20,29,35,45	0
2	GOL	A	481	6/6	0.95	0.08	19,23,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.