



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:41 AM UTC

PDB ID : 2ZB2 / pdb_00002zb2
Title : Human liver glycogen phosphorylase a complexed with glucose and 5-chloro-N-[4-(1,2-dihydroxyethyl)phenyl]-1H-indole-2-carboxamide
Authors : Katayama, N.; Onda, K.
Deposited on : 2007-10-15
Resolution : 2.45 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

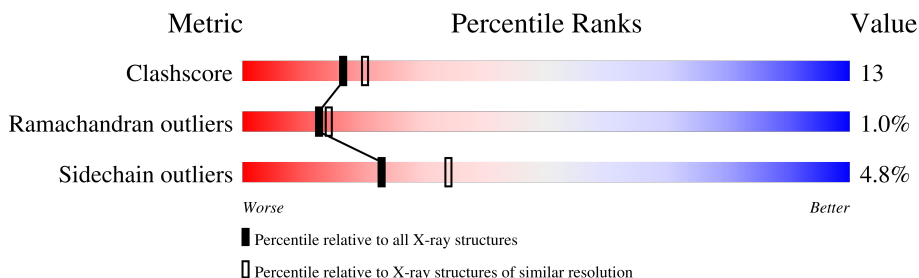
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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))
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	849	
1	B	849	

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
6	MPD	B	852	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13413 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.

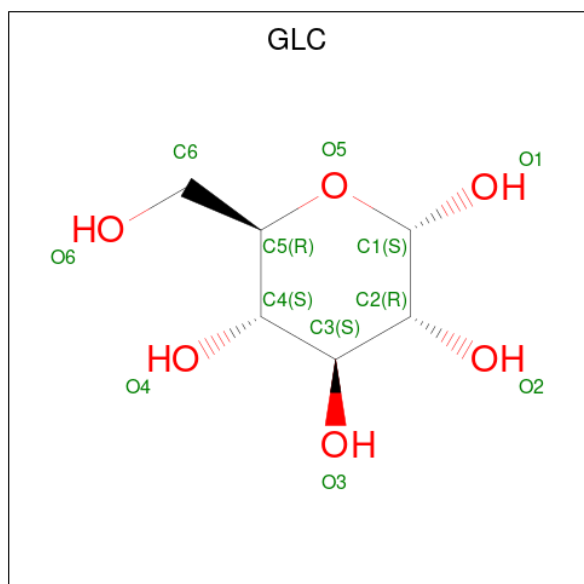
- Molecule 1 is a protein called Glycogen phosphorylase, liver form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	798	Total	C	N	O	S	0	0	0
			6466	4154	1097	1186	29			
1	B	791	Total	C	N	O	S	0	0	0
			6410	4116	1088	1177	29			

There are 4 discrepancies between the modelled and reference sequences:

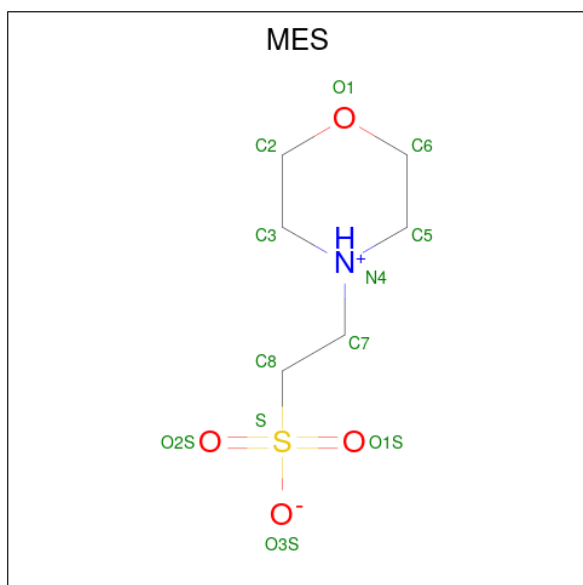
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P06737
A	-1	SER	-	expression tag	UNP P06737
B	-2	GLY	-	expression tag	UNP P06737
B	-1	SER	-	expression tag	UNP P06737

- Molecule 2 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



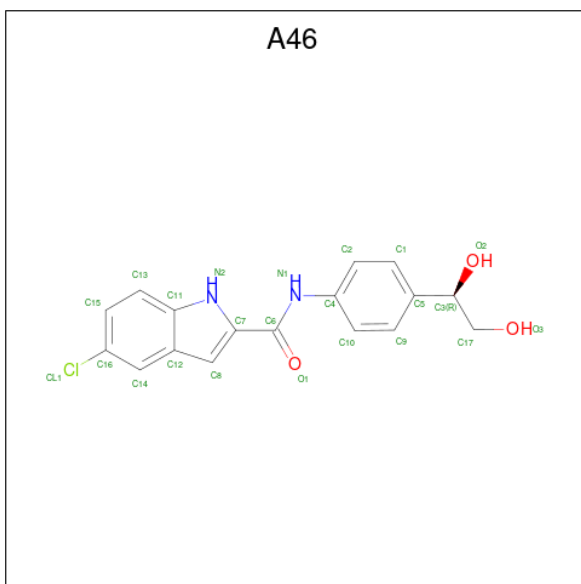
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 5 is 5-chloro-N-{4-[(1R)-1,2-dihydroxyethyl]phenyl}-1H-indole-2-carboxamide (CCD ID: A46) (formula: C₁₇H₁₅ClN₂O₃).



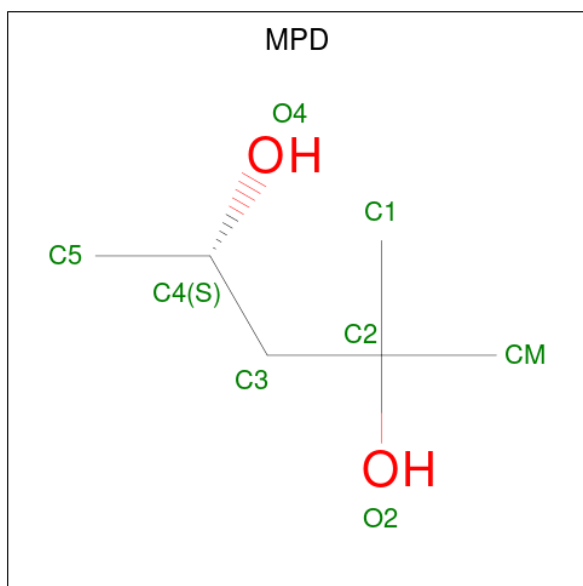
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	0
			23	17	1	2	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	Cl	N	O	
			23	17	1	2	3	
							0	0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O		
			8	6	2		
						0	0
6	B	1	Total	C	O		
			8	6	2		
						0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	199	Total	O		
			199	199		
					0	0
7	B	198	Total	O		
			198	198		
					0	0



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	123.82Å 123.82Å 123.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.18 – 2.45	Depositor
% Data completeness (in resolution range)	99.4 (49.18-2.45)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.37	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.261 , 0.307	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13413	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, A46, MES, GLC, PLP

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	0.74	2/6611 (0.0%)	0.93	23/8940 (0.3%)
1	B	0.73	2/6553 (0.0%)	0.92	19/8865 (0.2%)
All	All	0.73	4/13164 (0.0%)	0.92	42/17805 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	PRO	CA-CB	-6.76	1.45	1.53
1	B	181	ASP	CA-CB	6.37	1.61	1.52
1	B	225	PRO	CA-CB	-5.07	1.47	1.53
1	A	181	ASP	CA-CB	5.04	1.59	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	ILE	N-CA-C	8.04	120.37	108.96
1	A	216	ILE	N-CA-C	7.62	119.77	108.96
1	B	91	MET	N-CA-C	7.09	121.16	112.23
1	A	91	MET	N-CA-C	7.01	121.06	112.23
1	B	576	GLN	N-CA-C	-6.99	104.02	112.54
1	B	650	VAL	N-CA-C	6.42	116.53	110.30
1	A	650	VAL	N-CA-C	6.41	116.52	110.30
1	A	232	GLY	N-CA-C	-6.37	104.03	112.82
1	A	576	GLN	N-CA-C	-6.29	104.87	112.54
1	A	728	ALA	N-CA-C	6.18	118.81	111.71
1	A	565	VAL	N-CA-C	6.12	118.84	108.86
1	A	354	VAL	N-CA-C	6.11	116.75	110.82
1	A	454	GLY	N-CA-C	-6.10	102.94	112.58
1	B	575	ARG	N-CA-C	6.05	119.59	111.24
1	B	454	GLY	N-CA-C	-6.05	103.02	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	565	VAL	N-CA-C	5.99	118.63	108.86
1	B	728	ALA	N-CA-C	5.99	118.60	111.71
1	A	575	ARG	N-CA-C	5.97	119.48	111.24
1	B	232	GLY	N-CA-C	-5.94	104.62	112.82
1	A	754	GLN	CA-C-N	5.86	126.00	119.32
1	A	754	GLN	C-N-CA	5.86	126.00	119.32
1	B	666	ILE	N-CA-C	5.83	121.47	109.34
1	B	754	GLN	CA-C-N	5.75	125.88	119.32
1	B	754	GLN	C-N-CA	5.75	125.88	119.32
1	B	689	ILE	N-CA-C	-5.74	100.13	108.17
1	A	666	ILE	N-CA-C	5.72	121.23	109.34
1	A	646	GLU	N-CA-C	5.65	118.64	110.28
1	A	166	PHE	N-CA-C	5.58	117.93	110.35
1	A	105	GLN	N-CA-C	5.46	116.91	111.07
1	B	646	GLU	N-CA-C	5.45	118.19	110.50
1	A	261	ASP	N-CA-C	-5.40	106.19	112.89
1	A	250	ASN	N-CA-C	5.38	119.85	113.12
1	B	465	THR	N-CA-C	5.29	119.44	112.89
1	B	105	GLN	N-CA-C	5.23	116.67	111.07
1	A	702	GLU	N-CA-C	5.23	116.79	111.14
1	A	465	THR	N-CA-C	5.22	119.36	112.89
1	A	676	THR	N-CA-C	-5.21	107.94	114.56
1	B	166	PHE	N-CA-C	5.20	117.77	110.23
1	A	64	VAL	N-CA-C	5.19	115.81	110.36
1	B	702	GLU	N-CA-C	5.18	116.73	111.14
1	A	689	ILE	N-CA-C	-5.15	100.90	108.11
1	B	64	VAL	N-CA-C	5.11	115.72	110.36

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	6466	0	6451	171	0
1	B	6410	0	6394	166	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	12	0	12	3	0
3	B	12	0	13	3	0
4	A	15	0	7	0	0
4	B	15	0	7	0	0
5	A	23	0	15	0	0
5	B	23	0	15	1	0
6	B	16	0	28	6	0
7	A	199	0	0	8	0
7	B	198	0	0	13	0
All	All	13413	0	12966	334	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 13.

All (334) 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:204:GLY:O	1:A:205:LYS:HD2	1.79	0.83
1:B:204:GLY:O	1:B:205:LYS:HD2	1.80	0.80
1:B:678:ASN:HD22	1:B:679:MET:H	1.29	0.77
1:A:678:ASN:HD22	1:A:679:MET:H	1.32	0.76
1:A:310:ARG:HE	3:A:848:MES:H72	1.50	0.76
1:A:96:GLN:HB3	1:A:494:LEU:HD21	1.69	0.75
1:A:547:GLN:O	1:A:551:THR:HG23	1.87	0.74
1:A:95:LEU:HD22	1:A:99:MET:HE2	1.70	0.74
1:B:692:MET:HE2	1:B:710:ILE:HG21	1.69	0.72
1:A:692:MET:HE2	1:A:710:ILE:HG21	1.70	0.72
1:B:168:GLN:NE2	1:B:647:ASN:H	1.87	0.72
1:B:163:TYR:HE1	1:B:181:ASP:HB3	1.54	0.71
1:B:547:GLN:O	1:B:551:THR:HG23	1.89	0.71
1:B:29:LYS:O	1:B:29:LYS:HE3	1.91	0.71
1:A:80:LYS:HB3	1:A:827:VAL:HG12	1.71	0.70
1:A:29:LYS:HE3	1:A:29:LYS:O	1.90	0.70
1:A:174:TRP:HB3	7:A:853:HOH:O	1.91	0.69
1:B:96:GLN:HB3	1:B:494:LEU:HD21	1.75	0.69
1:B:770:ARG:HA	7:B:1079:HOH:O	1.92	0.69
1:A:184:ARG:HD3	1:B:197:MET:HE1	1.75	0.69
1:B:95:LEU:HD22	1:B:99:MET:HE2	1.75	0.68
1:B:492:LEU:HG	1:B:683:LEU:HD22	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:LYS:HA	1:A:595:LYS:HE2	1.74	0.68
1:A:163:TYR:HE1	1:A:181:ASP:HB3	1.58	0.68
1:B:715:ILE:HG13	7:B:979:HOH:O	1.93	0.68
1:A:274:ASN:HD21	1:B:270:ASN:HD21	1.43	0.67
1:B:157:TYR:HD2	1:B:244:TRP:HE1	1.42	0.67
1:B:678:ASN:HD22	1:B:679:MET:N	1.91	0.67
1:A:193:ARG:HH12	6:B:852:MPD:H12	1.59	0.67
1:A:157:TYR:HD2	1:A:244:TRP:HE1	1.43	0.66
1:B:80:LYS:HB3	1:B:827:VAL:HG12	1.77	0.66
1:B:168:GLN:HE21	1:B:647:ASN:H	1.42	0.66
1:A:80:LYS:HE2	1:A:334:ALA:HB2	1.79	0.65
1:A:270:ASN:HD21	1:B:274:ASN:HD21	1.43	0.65
1:A:509:GLU:O	1:A:512:VAL:HG22	1.97	0.64
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.78	0.64
1:B:752:PRO:HG2	1:B:753:LYS:HD2	1.79	0.64
1:A:752:PRO:HG2	1:A:753:LYS:HD2	1.80	0.63
1:A:678:ASN:HD22	1:A:679:MET:N	1.95	0.63
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.79	0.63
1:B:93:ARG:HG2	1:B:126:GLU:HG2	1.80	0.63
1:B:242:ARG:NH2	7:B:941:HOH:O	2.32	0.63
1:A:492:LEU:HG	1:A:683:LEU:HD22	1.80	0.62
1:B:678:ASN:HD22	1:B:678:ASN:N	1.98	0.62
1:B:163:TYR:CE1	1:B:181:ASP:HB3	2.34	0.62
1:B:206:VAL:HG21	1:B:401:GLU:OE1	1.99	0.62
1:A:660:THR:HG21	1:A:681:PHE:HE2	1.64	0.61
1:A:678:ASN:HD22	1:A:678:ASN:N	1.96	0.61
1:A:713:MET:HE1	1:A:772:LYS:HG3	1.80	0.61
1:B:713:MET:HE1	1:B:772:LYS:HG3	1.80	0.61
1:B:678:ASN:ND2	1:B:679:MET:H	1.98	0.61
1:A:678:ASN:ND2	1:A:679:MET:H	1.99	0.61
1:A:93:ARG:HG2	1:A:126:GLU:HG2	1.82	0.61
1:B:509:GLU:O	1:B:512:VAL:HG22	2.01	0.60
1:A:119:ILE:O	1:A:123:GLU:HG3	2.01	0.60
1:B:660:THR:HG21	1:B:681:PHE:HE2	1.66	0.60
1:A:163:TYR:CE1	1:A:181:ASP:HB3	2.35	0.60
1:A:206:VAL:HG21	1:A:401:GLU:OE1	2.01	0.60
1:B:204:GLY:HA3	1:B:218:THR:HG22	1.84	0.60
1:B:119:ILE:O	1:B:123:GLU:HG3	2.02	0.60
1:A:713:MET:HE3	1:A:718:VAL:HG22	1.84	0.59
1:A:204:GLY:HA3	1:A:218:THR:HG22	1.83	0.59
1:A:242:ARG:HH22	3:A:848:MES:H22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:PRO:O	1:A:830:SER:HB2	2.01	0.59
1:A:310:ARG:HH21	3:A:848:MES:H21	1.66	0.59
1:B:170:ILE:HG12	1:B:646:GLU:HG2	1.84	0.59
1:B:340:THR:HG23	7:B:1022:HOH:O	2.02	0.59
1:B:136:LEU:HD23	7:B:1034:HOH:O	2.02	0.58
1:B:168:GLN:HB3	1:B:647:ASN:HA	1.86	0.58
1:B:678:ASN:ND2	1:B:679:MET:N	2.52	0.58
1:A:40:VAL:HG11	6:B:851:MPD:HM2	1.85	0.57
1:A:772:LYS:HB3	1:A:775:ALA:HB3	1.86	0.57
1:B:521:LEU:HB3	1:B:802:LEU:HD11	1.86	0.57
1:A:22:GLU:HG3	1:A:23:ASN:N	2.19	0.57
1:B:657:ILE:HB	1:B:658:PRO:HD3	1.86	0.57
1:A:274:ASN:ND2	1:A:277:ARG:HE	2.03	0.57
1:B:61:ASP:O	1:B:64:VAL:HG22	2.04	0.57
1:B:810:LYS:O	1:B:815:ARG:HD3	2.05	0.57
1:A:197:MET:HE1	1:B:184:ARG:HD3	1.86	0.56
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.88	0.56
1:A:81:ARG:NH1	1:A:310:ARG:HD3	2.21	0.56
1:A:431:ILE:N	1:A:431:ILE:HD12	2.20	0.56
1:A:810:LYS:O	1:A:815:ARG:HD3	2.04	0.56
1:A:678:ASN:ND2	1:A:679:MET:N	2.54	0.55
1:B:692:MET:HE2	1:B:710:ILE:HG13	1.89	0.55
1:A:521:LEU:HB3	1:A:802:LEU:HD11	1.88	0.55
1:A:591:LYS:O	1:A:594:PRO:HD3	2.06	0.55
1:B:170:ILE:CG1	1:B:646:GLU:HG2	2.38	0.54
1:B:772:LYS:HB3	1:B:775:ALA:HB3	1.87	0.54
1:A:61:ASP:O	1:A:64:VAL:HG22	2.08	0.54
1:A:410:HIS:O	1:A:414:ILE:HG12	2.08	0.54
1:B:713:MET:HE3	1:B:718:VAL:HG22	1.88	0.54
1:A:177:GLU:HG2	1:A:611:PRO:HG3	1.88	0.54
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.90	0.54
1:A:168:GLN:OE1	1:A:608:LYS:HA	2.08	0.54
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.90	0.54
1:B:568:LYS:O	1:B:607:GLY:HA3	2.07	0.54
1:B:112:ILE:HG23	1:B:117:LEU:HB2	1.90	0.54
1:B:379:VAL:HG22	7:B:982:HOH:O	2.09	0.53
1:B:591:LYS:O	1:B:594:PRO:HD3	2.09	0.53
1:B:753:LYS:HD2	1:B:753:LYS:H	1.73	0.53
1:A:753:LYS:HD2	1:A:753:LYS:H	1.73	0.53
1:B:410:HIS:O	1:B:414:ILE:HG12	2.09	0.53
1:A:171:ARG:HA	1:A:171:ARG:HH11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ASN:ND2	1:B:277:ARG:HE	2.07	0.53
1:B:813:SER:O	1:B:817:ILE:HG12	2.08	0.53
1:B:431:ILE:N	1:B:431:ILE:HD12	2.24	0.53
1:B:583:VAL:HG11	1:B:642:VAL:HG21	1.89	0.53
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.91	0.53
1:A:770:ARG:HA	7:A:938:HOH:O	2.08	0.53
1:A:512:VAL:HG23	1:A:513:LYS:N	2.25	0.52
1:A:692:MET:HE2	1:A:710:ILE:HG13	1.92	0.52
1:B:713:MET:HB3	1:B:717:ASP:HB2	1.91	0.52
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.93	0.52
1:B:80:LYS:HE2	1:B:334:ALA:HB2	1.91	0.52
1:B:118:ASP:HB3	1:B:121:GLU:HB3	1.92	0.52
1:B:512:VAL:HG23	1:B:513:LYS:N	2.24	0.51
1:A:456:ALA:C	1:A:481:ASN:HD21	2.17	0.51
1:A:336:GLN:OE1	1:A:825:TRP:NE1	2.39	0.51
1:A:41:LYS:HD2	1:A:45:VAL:HG23	1.92	0.51
1:A:112:ILE:HG23	1:A:117:LEU:HB2	1.91	0.51
1:A:434:GLU:O	1:A:435:GLY:C	2.54	0.51
1:A:100:ILE:HD12	1:A:494:LEU:HD23	1.92	0.50
1:A:785:ASP:O	1:A:789:GLN:HG3	2.11	0.50
1:B:311:PHE:CE2	1:B:325:VAL:HG12	2.46	0.50
1:A:813:SER:O	1:A:817:ILE:HG12	2.10	0.50
1:A:557:ILE:HD11	1:A:643:ILE:HD11	1.93	0.50
1:B:583:VAL:HG13	1:B:640:LEU:HD21	1.92	0.50
1:A:411:LEU:O	1:A:415:VAL:HG23	2.12	0.50
1:B:81:ARG:NH1	1:B:310:ARG:HD3	2.25	0.50
6:B:852:MPD:H53	6:B:852:MPD:H11	1.94	0.50
1:B:411:LEU:O	1:B:415:VAL:HG23	2.12	0.50
1:A:275:ILE:O	1:A:295:GLN:HG2	2.12	0.49
1:B:168:GLN:HG3	1:B:175:GLN:HG3	1.94	0.49
6:B:852:MPD:H11	6:B:852:MPD:C5	2.42	0.49
1:A:648:TYR:HA	1:A:652:LEU:HD23	1.94	0.49
1:B:41:LYS:HD2	1:B:45:VAL:HG23	1.93	0.49
1:B:648:TYR:HA	1:B:652:LEU:HD23	1.95	0.49
1:A:753:LYS:HD2	1:A:753:LYS:N	2.27	0.49
1:B:193:ARG:HH22	3:B:848:MES:C6	2.26	0.49
1:A:152:LEU:HD21	1:A:829:PRO:HA	1.93	0.49
1:B:678:ASN:N	1:B:678:ASN:ND2	2.60	0.49
1:B:450:HIS:HE1	7:B:1035:HOH:O	1.96	0.49
1:A:587:TYR:CZ	1:A:591:LYS:HD2	2.48	0.49
1:B:785:ASP:O	1:B:789:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:MET:HE2	1:B:224:LEU:HD13	1.95	0.48
1:B:693:ASP:O	1:B:696:ASN:HB2	2.13	0.48
1:A:146:SER:O	1:A:150:LEU:HD13	2.14	0.48
1:A:576:GLN:H	1:A:576:GLN:HE21	1.62	0.48
1:A:143:PHE:O	1:A:147:MET:HG3	2.12	0.48
1:B:434:GLU:O	1:B:435:GLY:C	2.55	0.48
1:A:829:PRO:O	1:A:830:SER:CB	2.62	0.48
1:B:171:ARG:HA	1:B:171:ARG:HH11	1.77	0.48
1:B:456:ALA:C	1:B:481:ASN:HD21	2.21	0.48
1:B:221:VAL:HG11	1:B:275:ILE:HD12	1.96	0.48
1:A:436:SER:O	1:A:438:ARG:HG3	2.14	0.48
1:A:678:ASN:N	1:A:678:ASN:ND2	2.58	0.48
1:A:24:VAL:HG23	1:A:25:ALA:N	2.29	0.48
1:B:144:LEU:HB3	1:B:230:VAL:HG11	1.96	0.48
1:B:275:ILE:O	1:B:295:GLN:HG2	2.13	0.48
1:B:514:ASP:OD2	1:B:516:SER:HB3	2.14	0.48
1:B:753:LYS:HD2	1:B:753:LYS:N	2.28	0.48
1:A:693:ASP:O	1:A:696:ASN:HB2	2.14	0.48
1:B:627:ALA:HA	1:B:642:VAL:HB	1.96	0.47
1:A:138:ARG:HB3	7:A:959:HOH:O	2.15	0.47
1:A:197:MET:HE2	1:A:224:LEU:HD13	1.96	0.47
1:A:100:ILE:HD12	1:A:494:LEU:CD2	2.44	0.47
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.96	0.47
1:A:482:LYS:NZ	1:A:823:ASN:HB2	2.29	0.47
1:B:436:SER:O	1:B:438:ARG:HG3	2.14	0.47
1:A:584:ILE:HG21	1:A:741:VAL:HG13	1.97	0.47
1:A:627:ALA:HA	1:A:642:VAL:HB	1.95	0.47
1:B:386:ARG:HD2	1:B:432:GLU:OE2	2.15	0.47
1:B:558:ASN:HB3	1:B:561:SER:HB3	1.96	0.47
1:A:567:VAL:HB	1:A:648:TYR:CZ	2.50	0.47
1:A:91:MET:HB2	1:A:129:ALA:HB3	1.95	0.47
1:B:587:TYR:CZ	1:B:591:LYS:HD2	2.50	0.47
1:B:617:LYS:HD3	7:B:1045:HOH:O	2.14	0.47
1:B:43:ARG:NH1	1:B:51:TYR:OH	2.48	0.47
1:A:582:HIS:HB2	1:A:780:TYR:CE2	2.50	0.47
1:A:670:GLY:H	1:A:693:ASP:CG	2.23	0.47
1:B:421:ASP:CG	1:B:424:ARG:HB2	2.40	0.47
1:A:193:ARG:NH1	6:B:852:MPD:H12	2.28	0.46
1:B:24:VAL:HG23	1:B:25:ALA:N	2.30	0.46
1:B:504:ALA:HA	1:B:508:GLY:O	2.14	0.46
1:B:300:VAL:HG13	1:B:345:ALA:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ARG:O	1:B:296:GLU:HG3	2.14	0.46
1:A:558:ASN:HB3	1:A:561:SER:HB3	1.97	0.46
1:A:355:ASP:O	1:A:358:LYS:HE3	2.16	0.46
1:B:566:GLN:HA	7:B:1011:HOH:O	2.14	0.46
1:A:118:ASP:HB3	1:A:121:GLU:HB3	1.97	0.46
1:B:34:HIS:HD2	1:B:38:THR:OG1	1.99	0.46
1:B:682:MET:HG2	1:B:808:SER:OG	2.15	0.46
1:A:100:ILE:CD1	1:A:494:LEU:HA	2.45	0.46
1:A:795:LYS:H	1:A:795:LYS:HD2	1.80	0.46
1:B:619:ILE:HD13	7:B:989:HOH:O	2.16	0.46
1:A:40:VAL:CG1	6:B:851:MPD:HM2	2.46	0.46
1:A:144:LEU:HD22	7:A:949:HOH:O	2.15	0.46
1:A:144:LEU:HB3	1:A:230:VAL:HG11	1.97	0.46
1:A:152:LEU:CD2	1:A:829:PRO:HA	2.46	0.46
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.51	0.46
1:A:450:HIS:HD2	7:A:1039:HOH:O	1.98	0.46
1:B:235:ASN:ND2	1:B:237:THR:HG23	2.30	0.46
1:A:572:GLU:O	1:A:575:ARG:HG2	2.15	0.45
1:A:292:ARG:O	1:A:296:GLU:HG3	2.16	0.45
1:A:456:ALA:C	1:A:481:ASN:ND2	2.74	0.45
1:A:421:ASP:CG	1:A:424:ARG:HB2	2.41	0.45
1:A:459:HIS:O	1:A:463:VAL:HG23	2.16	0.45
1:B:355:ASP:OD2	1:B:398:ARG:HD3	2.17	0.45
1:B:795:LYS:H	1:B:795:LYS:HD2	1.81	0.45
1:A:43:ARG:NH1	1:A:51:TYR:OH	2.50	0.45
1:A:386:ARG:HD2	1:A:432:GLU:OE2	2.17	0.45
1:A:514:ASP:OD2	1:A:516:SER:HB3	2.17	0.45
1:B:91:MET:HB2	1:B:129:ALA:HB3	1.98	0.45
1:A:504:ALA:HA	1:A:508:GLY:O	2.17	0.45
1:A:636:VAL:O	1:A:639:LYS:HB2	2.16	0.45
1:B:193:ARG:HH22	3:B:848:MES:H61	1.82	0.45
1:A:300:VAL:HG13	1:A:345:ALA:HA	1.99	0.44
1:B:143:PHE:O	1:B:147:MET:HG3	2.17	0.44
1:A:793:ASN:C	1:A:793:ASN:HD22	2.24	0.44
1:B:455:VAL:HG23	1:B:674:SER:HB2	1.99	0.44
1:B:572:GLU:O	1:B:575:ARG:HG2	2.17	0.44
1:B:579:ASN:C	1:B:579:ASN:HD22	2.24	0.44
1:A:579:ASN:C	1:A:579:ASN:HD22	2.24	0.44
1:B:455:VAL:H	1:B:459:HIS:HD2	1.64	0.44
1:B:571:HIS:HD2	1:B:574:LYS:HD2	1.82	0.44
1:A:119:ILE:HG23	1:A:120:GLU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:GLY:HA3	7:A:1021:HOH:O	2.16	0.44
1:B:300:VAL:O	1:B:304:LEU:HD23	2.18	0.44
1:B:355:ASP:O	1:B:358:LYS:HE3	2.18	0.44
1:B:427:ARG:HH21	1:B:470:ASP:CG	2.25	0.44
1:B:456:ALA:HB3	1:B:673:ALA:O	2.18	0.44
1:A:815:ARG:O	1:A:819:GLU:HG3	2.18	0.44
1:A:274:ASN:HD22	1:A:277:ARG:HE	1.64	0.44
1:B:458:ILE:HG22	7:B:1004:HOH:O	2.18	0.44
1:A:571:HIS:HD2	1:A:574:LYS:HD2	1.83	0.43
1:A:573:TYR:O	1:A:575:ARG:HG3	2.18	0.43
1:A:687:LEU:HD13	1:A:709:PHE:HE1	1.83	0.43
1:B:580:CYS:SG	1:B:622:LEU:HD22	2.57	0.43
1:A:300:VAL:O	1:A:304:LEU:HD23	2.17	0.43
1:A:546:SER:O	1:A:550:GLU:HG3	2.18	0.43
1:B:636:VAL:O	1:B:639:LYS:HB2	2.18	0.43
1:B:714:ARG:O	1:B:715:ILE:C	2.61	0.43
1:A:737:GLU:O	1:A:741:VAL:HG23	2.19	0.43
1:B:546:SER:O	1:B:550:GLU:HG3	2.18	0.43
1:B:81:ARG:HG3	7:B:1041:HOH:O	2.18	0.43
1:B:714:ARG:HB3	7:B:979:HOH:O	2.18	0.43
1:A:484:ASN:HD22	1:A:484:ASN:HA	1.64	0.43
1:A:566:GLN:HA	7:A:912:HOH:O	2.18	0.43
1:B:146:SER:O	1:B:150:LEU:HD13	2.18	0.43
1:A:235:ASN:ND2	1:A:237:THR:HG23	2.33	0.43
1:A:427:ARG:HH21	1:A:470:ASP:CG	2.26	0.43
1:A:687:LEU:HD12	1:A:797:TRP:CZ3	2.54	0.43
1:B:732:TYR:CZ	1:B:739:LYS:HG3	2.54	0.43
1:A:430:LEU:C	1:A:431:ILE:HD12	2.44	0.43
1:B:761:ILE:O	1:B:765:LEU:HB2	2.19	0.43
1:A:682:MET:HG2	1:A:808:SER:OG	2.18	0.43
1:B:64:VAL:HG23	1:B:65:GLY:N	2.33	0.43
1:B:505:GLU:O	1:B:506:LYS:HD3	2.19	0.42
1:A:455:VAL:H	1:A:459:HIS:HD2	1.67	0.42
1:A:714:ARG:O	1:A:715:ILE:C	2.61	0.42
1:B:459:HIS:O	1:B:463:VAL:HG23	2.18	0.42
1:B:709:PHE:HB3	1:B:783:CYS:SG	2.59	0.42
1:A:83:TYR:OH	1:A:310:ARG:HD2	2.19	0.42
1:A:355:ASP:OD2	1:A:398:ARG:HD3	2.19	0.42
1:A:732:TYR:CZ	1:A:739:LYS:HG3	2.55	0.42
1:A:738:LEU:HB2	1:A:777:TYR:CE2	2.55	0.42
1:A:821:ALA:HB1	1:A:827:VAL:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:LYS:HE3	1:B:326:PHE:HZ	1.84	0.42
1:A:738:LEU:HD13	1:A:777:TYR:CG	2.55	0.42
1:B:119:ILE:HG23	1:B:120:GLU:N	2.34	0.42
1:B:386:ARG:HA	1:B:439:ILE:O	2.20	0.42
1:B:687:LEU:HD12	1:B:797:TRP:CZ3	2.55	0.42
1:B:793:ASN:C	1:B:793:ASN:HD22	2.28	0.42
1:A:577:LEU:HG	1:A:619:ILE:CD1	2.50	0.42
1:B:60:ARG:HD2	5:B:850:A46:C13	2.50	0.42
1:B:274:ASN:ND2	1:B:277:ARG:HH21	2.18	0.42
1:B:576:GLN:H	1:B:576:GLN:HE21	1.66	0.42
1:B:697:VAL:O	1:B:701:GLU:HG3	2.20	0.42
1:A:45:VAL:HB	3:B:848:MES:H51	2.01	0.42
1:B:291:LEU:O	1:B:295:GLN:HG3	2.19	0.42
1:B:687:LEU:HD13	1:B:709:PHE:HE1	1.83	0.42
1:B:815:ARG:O	1:B:819:GLU:HG3	2.20	0.42
1:A:283:ASP:OD1	1:A:571:HIS:NE2	2.51	0.42
1:B:430:LEU:C	1:B:431:ILE:HD12	2.45	0.42
1:A:738:LEU:HD13	1:A:777:TYR:CD2	2.55	0.41
1:B:670:GLY:H	1:B:693:ASP:CG	2.28	0.41
1:A:237:THR:HG22	7:A:963:HOH:O	2.20	0.41
1:A:274:ASN:ND2	1:A:277:ARG:HH21	2.18	0.41
1:A:584:ILE:CG2	1:A:741:VAL:HG13	2.50	0.41
1:B:567:VAL:HA	1:B:606:GLY:O	2.19	0.41
1:A:338:ASN:OD1	1:A:377:HIS:NE2	2.53	0.41
1:A:761:ILE:O	1:A:765:LEU:HB2	2.19	0.41
1:B:74:TYR:CZ	1:B:153:ALA:HA	2.56	0.41
1:B:528:ASP:O	1:B:532:ARG:HG3	2.20	0.41
1:B:715:ILE:HG13	1:B:715:ILE:H	1.64	0.41
1:A:399:HIS:O	1:A:403:ILE:HG13	2.20	0.41
1:B:402:ILE:O	1:B:406:ILE:HG13	2.20	0.41
1:A:398:ARG:O	1:A:402:ILE:HG13	2.21	0.41
1:B:565:VAL:HA	1:B:604:ILE:O	2.20	0.41
1:B:593:ASP:C	1:B:595:LYS:H	2.29	0.41
1:B:168:GLN:O	1:B:647:ASN:HB2	2.21	0.41
1:A:769:ASP:OD2	1:A:773:VAL:HG23	2.20	0.41
1:B:341:HIS:HB2	1:B:342:PRO:HD3	2.02	0.41
1:B:389:VAL:HG23	1:B:437:LYS:O	2.20	0.41
1:B:398:ARG:O	1:B:402:ILE:HG13	2.21	0.41
1:B:737:GLU:O	1:B:741:VAL:HG23	2.21	0.41
1:A:36:HIS:O	1:A:40:VAL:HA	2.20	0.41
1:B:184:ARG:HG2	1:B:185:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ASN:HD22	1:B:274:ASN:HA	1.64	0.41
1:A:440:ASN:OD1	1:A:442:ALA:HB3	2.21	0.41
1:A:493:LEU:HD21	1:A:512:VAL:HG12	2.02	0.41
1:A:528:ASP:O	1:A:532:ARG:HG3	2.21	0.41
1:A:764:MET:HE1	1:A:765:LEU:HD13	2.03	0.41
1:B:300:VAL:CG1	1:B:345:ALA:HA	2.51	0.41
1:A:42:ASP:OD2	1:A:42:ASP:C	2.64	0.40
1:A:400:LEU:HG	1:A:404:TYR:CE2	2.56	0.40
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.61	0.40
1:B:330:PRO:HB3	1:B:370:LYS:HB3	2.02	0.40
1:B:456:ALA:C	1:B:481:ASN:ND2	2.79	0.40
1:B:494:LEU:HD13	1:B:494:LEU:C	2.45	0.40
1:B:564:ASP:O	1:B:603:VAL:HA	2.20	0.40
1:B:738:LEU:HB2	1:B:777:TYR:CE2	2.56	0.40
1:A:278:VAL:HG13	1:B:266:VAL:HG11	2.02	0.40
1:A:505:GLU:O	1:A:506:LYS:HD3	2.21	0.40
1:A:566:GLN:HB2	1:A:664:GLU:HB2	2.03	0.40
1:A:582:HIS:HB2	1:A:780:TYR:HE2	1.84	0.40
1:B:769:ASP:OD2	1:B:773:VAL:HG23	2.22	0.40
1:A:389:VAL:HG23	1:A:437:LYS:O	2.22	0.40
1:A:567:VAL:HA	1:A:606:GLY:O	2.22	0.40
1:B:192:SER:HB3	1:B:226:TYR:CE1	2.56	0.40
1:B:440:ASN:OD1	1:B:442:ALA:HB3	2.22	0.40
1:A:304:LEU:O	1:A:308:ILE:HG12	2.22	0.40
1:B:400:LEU:HG	1:B:404:TYR:CE2	2.56	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	792/849 (93%)	739 (93%)	45 (6%)	8 (1%)	12 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	785/849 (92%)	734 (94%)	43 (6%)	8 (1%)	12	14
All	All	1577/1698 (93%)	1473 (93%)	88 (6%)	16 (1%)	12	14

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	ASP
1	A	435	GLY
1	A	555	VAL
1	A	715	ILE
1	B	23	ASN
1	B	435	GLY
1	B	555	VAL
1	B	715	ILE
1	A	95	LEU
1	B	95	LEU
1	A	736	PRO
1	B	736	PRO
1	A	674	SER
1	B	594	PRO
1	A	594	PRO
1	B	829	PRO

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	696/741 (94%)	662 (95%)	34 (5%)	22	33
1	B	691/741 (93%)	659 (95%)	32 (5%)	24	36
All	All	1387/1482 (94%)	1321 (95%)	66 (5%)	23	34

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	26	GLU
1	A	29	LYS
1	A	90	TYR
1	A	95	LEU
1	A	102	LEU
1	A	235	ASN
1	A	237	THR
1	A	243	LEU
1	A	250	ASN
1	A	278	VAL
1	A	279	LEU
1	A	325	VAL
1	A	361	TRP
1	A	366	GLU
1	A	396	LEU
1	A	411	LEU
1	A	466	LYS
1	A	474	LEU
1	A	492	LEU
1	A	499	LEU
1	A	502	LEU
1	A	505	GLU
1	A	565	VAL
1	A	573	TYR
1	A	576	GLN
1	A	597	LEU
1	A	622	LEU
1	A	660	THR
1	A	678	ASN
1	A	683	LEU
1	A	722	ASP
1	A	765	LEU
1	A	795	LYS
1	B	26	GLU
1	B	29	LYS
1	B	90	TYR
1	B	95	LEU
1	B	102	LEU
1	B	235	ASN
1	B	237	THR
1	B	243	LEU
1	B	278	VAL

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Mol	Chain	Res	Type
1	B	279	LEU
1	B	361	TRP
1	B	366	GLU
1	B	396	LEU
1	B	411	LEU
1	B	466	LYS
1	B	474	LEU
1	B	492	LEU
1	B	499	LEU
1	B	502	LEU
1	B	505	GLU
1	B	565	VAL
1	B	573	TYR
1	B	576	GLN
1	B	597	LEU
1	B	622	LEU
1	B	660	THR
1	B	678	ASN
1	B	683	LEU
1	B	722	ASP
1	B	765	LEU
1	B	795	LYS
1	B	815	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	73	HIS
1	A	96	GLN
1	A	106	ASN
1	A	167	ASN
1	A	168	GLN
1	A	235	ASN
1	A	236	ASN
1	A	239	ASN
1	A	274	ASN
1	A	295	GLN
1	A	341	HIS
1	A	459	HIS
1	A	480	GLN
1	A	481	ASN

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Mol	Chain	Res	Type
1	A	541	ASN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	632	ASN
1	A	678	ASN
1	A	789	GLN
1	A	793	ASN
1	A	822	GLN
1	A	826	ASN
1	B	34	HIS
1	B	73	HIS
1	B	96	GLN
1	B	106	ASN
1	B	167	ASN
1	B	168	GLN
1	B	208	HIS
1	B	235	ASN
1	B	239	ASN
1	B	274	ASN
1	B	284	ASN
1	B	295	GLN
1	B	450	HIS
1	B	459	HIS
1	B	480	GLN
1	B	481	ASN
1	B	541	ASN
1	B	566	GLN
1	B	576	GLN
1	B	579	ASN
1	B	678	ASN
1	B	789	GLN
1	B	793	ASN
1	B	822	GLN
1	B	823	ASN
1	B	826	ASN

5.3.3 RNA ⓘ

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](#)

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$
6	MPD	B	851	-	7,7,7	1.30	2 (28%)	9,10,10	1.24	0
5	A46	A	850	-	24,25,25	1.80	7 (29%)	32,35,35	1.85	9 (28%)
6	MPD	B	852	-	7,7,7	0.72	0	9,10,10	1.18	1 (11%)
4	PLP	A	849	1	15,15,16	1.83	4 (26%)	21,22,23	1.18	0
3	MES	A	848	-	12,12,12	1.58	2 (16%)	15,16,16	2.39	5 (33%)
3	MES	B	848	-	12,12,12	1.07	1 (8%)	15,16,16	2.00	6 (40%)
2	GLC	A	847	-	12,12,12	0.46	0	17,17,17	0.64	0
4	PLP	B	849	1	15,15,16	1.48	4 (26%)	21,22,23	1.15	0
2	GLC	B	847	-	12,12,12	0.38	0	17,17,17	0.46	0
5	A46	B	850	-	24,25,25	2.17	6 (25%)	32,35,35	2.27	9 (28%)

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
6	MPD	B	851	-	-	1/5/5/5	-
5	A46	A	850	-	-	2/14/14/14	0/3/3/3
2	GLC	A	847	-	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	A	848	-	-	4/6/14/14	0/1/1/1
3	MES	B	848	-	-	3/6/14/14	0/1/1/1
4	PLP	A	849	1	-	0/6/6/8	0/1/1/1
6	MPD	B	852	-	1/1/2/2	2/5/5/5	-
4	PLP	B	849	1	-	0/6/6/8	0/1/1/1
2	GLC	B	847	-	-	0/2/22/22	0/1/1/1
5	A46	B	850	-	-	0/14/14/14	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	850	A46	C16-CL1	-5.02	1.62	1.74
5	B	850	A46	C8-C7	5.02	1.45	1.37
3	A	848	MES	O3S-S	4.49	1.64	1.47
4	A	849	PLP	C5-C4	4.49	1.45	1.40
5	A	850	A46	C7-N2	-4.46	1.32	1.38
5	B	850	A46	C4-N1	-3.83	1.33	1.41
4	A	849	PLP	C3-C4	3.61	1.47	1.40
5	A	850	A46	C8-C7	3.26	1.42	1.37
4	B	849	PLP	C4A-C4	-3.18	1.45	1.51
5	B	850	A46	C12-C11	2.98	1.45	1.41
5	B	850	A46	C5-C3	-2.97	1.46	1.51
3	B	848	MES	O3S-S	2.90	1.58	1.47
5	A	850	A46	C1-C2	2.67	1.43	1.38
5	A	850	A46	C15-C13	2.63	1.43	1.38
4	B	849	PLP	C6-C5	2.62	1.42	1.37
4	B	849	PLP	C3-C4	2.58	1.45	1.40
4	A	849	PLP	C6-C5	2.56	1.42	1.37
3	A	848	MES	C8-S	2.49	1.81	1.77
5	A	850	A46	C14-C16	2.48	1.42	1.38
5	B	850	A46	C10-C4	2.28	1.43	1.39
6	B	851	MPD	C1-C2	2.19	1.58	1.52
5	A	850	A46	C11-N2	-2.15	1.34	1.38
4	A	849	PLP	C3-C2	2.15	1.43	1.41
4	B	849	PLP	C5-C4	2.08	1.42	1.40
5	A	850	A46	C6-N1	2.07	1.40	1.35
6	B	851	MPD	CM-C2	2.01	1.58	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	850	A46	C12-C8-C7	-6.98	101.17	107.41
3	A	848	MES	C5-N4-C3	5.51	120.71	108.84
5	B	850	A46	C11-C12-C8	5.26	111.11	106.80
5	A	850	A46	C7-C6-N1	4.76	121.94	116.07
5	A	850	A46	C14-C16-CL1	4.68	125.03	119.17
3	A	848	MES	O1S-S-C8	4.10	112.92	106.73
3	B	848	MES	C2-C3-N4	3.48	115.41	110.12
3	A	848	MES	O2S-S-C8	-3.46	101.50	106.73
5	B	850	A46	C14-C12-C11	-3.46	116.99	119.13
5	B	850	A46	C10-C9-C5	-3.40	117.79	121.18
5	B	850	A46	C7-C6-N1	3.27	120.09	116.07
3	B	848	MES	O3S-S-C8	3.10	112.08	106.00
5	B	850	A46	C13-C15-C16	-2.97	116.26	119.24
3	B	848	MES	C6-C5-N4	2.91	114.55	110.12
5	B	850	A46	C8-C7-N2	2.79	111.92	109.15
5	A	850	A46	C12-C8-C7	-2.77	104.93	107.41
3	B	848	MES	C5-N4-C3	2.76	114.78	108.84
5	A	850	A46	O1-C6-C7	-2.64	117.69	121.09
3	B	848	MES	O3S-S-O2S	-2.58	104.96	111.40
5	A	850	A46	C13-C11-C12	-2.53	119.84	122.13
5	B	850	A46	C9-C5-C1	2.51	121.42	118.30
5	A	850	A46	C4-N1-C6	2.36	131.65	127.45
5	A	850	A46	C15-C16-C14	-2.36	118.45	121.53
5	B	850	A46	C13-C11-C12	-2.31	120.04	122.13
3	A	848	MES	C6-C5-N4	2.31	113.63	110.12
3	A	848	MES	O3S-S-O1S	-2.20	105.90	111.40
5	A	850	A46	C9-C10-C4	2.09	122.71	120.30
6	B	852	MPD	CM-C2-C1	2.06	115.24	110.63
5	A	850	A46	C11-N2-C7	2.02	111.18	109.01
3	B	848	MES	O2S-S-O1S	2.01	120.37	113.82

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	852	MPD	C4

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	848	MES	C7-C8-S-O1S
5	A	850	A46	O3-C17-C3-O2
6	B	851	MPD	C2-C3-C4-C5
3	A	848	MES	C7-C8-S-O3S

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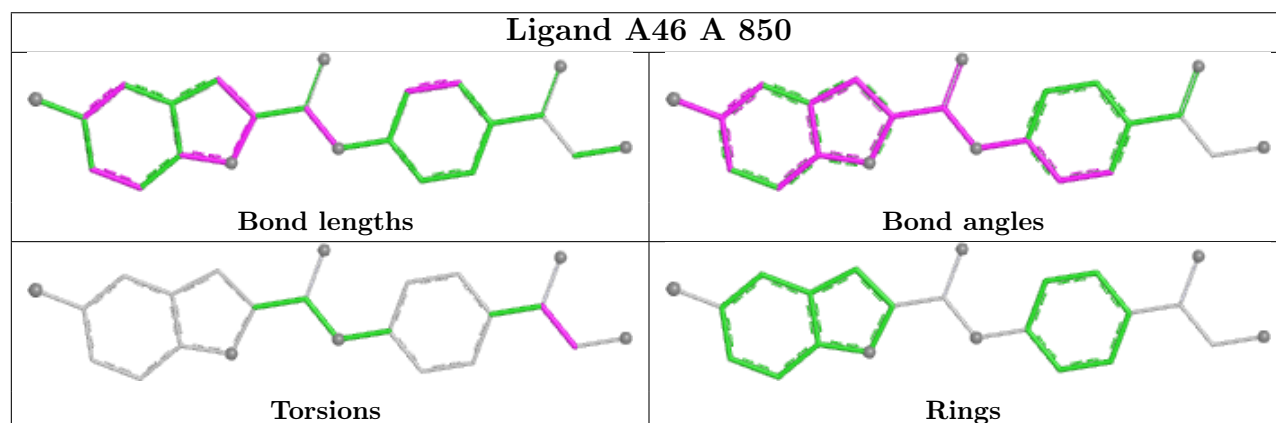
Mol	Chain	Res	Type	Atoms
3	B	848	MES	C8-C7-N4-C5
3	A	848	MES	C7-C8-S-O2S
5	A	850	A46	O3-C17-C3-C5
6	B	852	MPD	O2-C2-C3-C4
6	B	852	MPD	C2-C3-C4-C5
3	A	848	MES	C8-C7-N4-C5
3	B	848	MES	C8-C7-N4-C3
3	B	848	MES	C7-C8-S-O2S

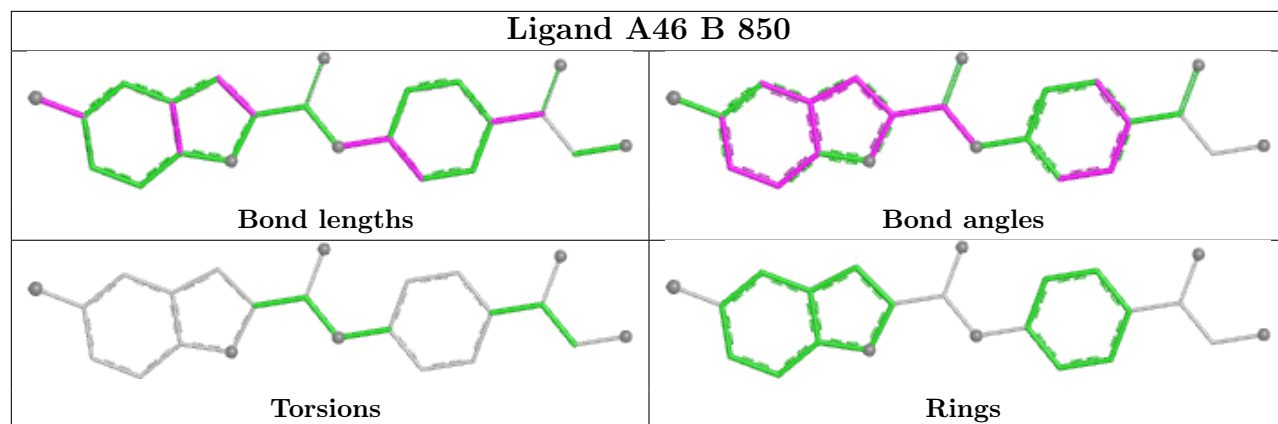
There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	851	MPD	2	0
6	B	852	MPD	4	0
3	A	848	MES	3	0
3	B	848	MES	3	0
5	B	850	A46	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.