



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:03 AM GMT

PDB ID : 2ZB2
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

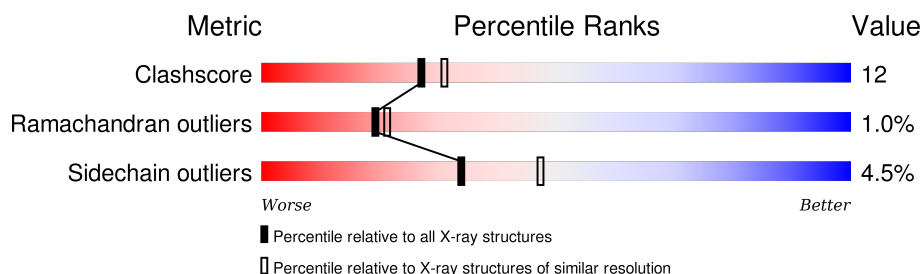
1 Overall quality at a glance

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	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

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.

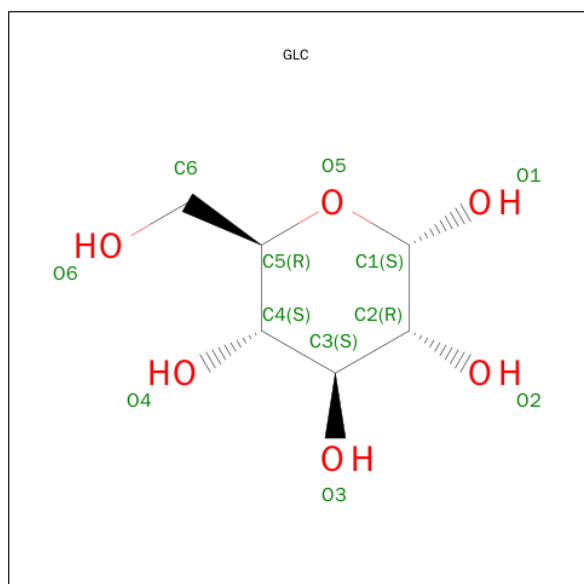
- Molecule 1 is a protein called Glycogen phosphorylase, liver form.

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:

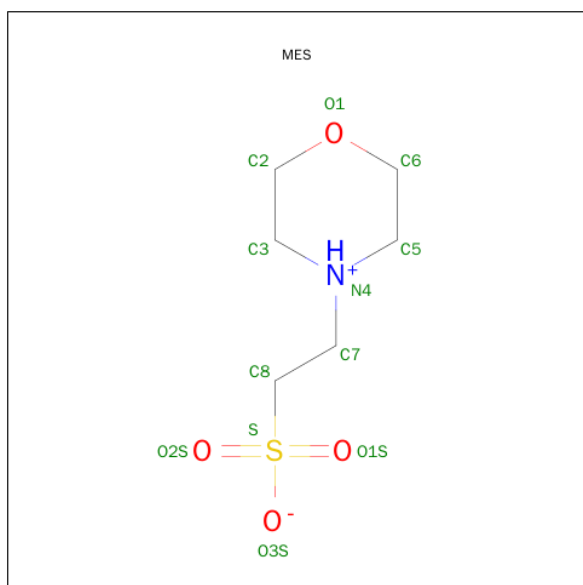
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P06737
A	-1	SER	-	EXPRESSION TAG	UNP P06737
B	-2	GLY	-	EXPRESSION TAG	UNP P06737
B	-1	SER	-	EXPRESSION TAG	UNP P06737

- Molecule 2 is SUGAR (ALPHA-D-GLUCOSE) (three-letter code: 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 (three-letter code: MES) (formula: C₆H₁₃NO₄S).



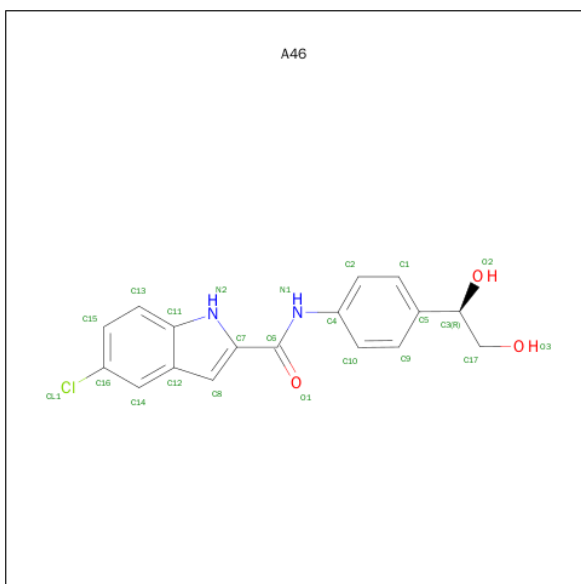
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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 (three-letter code: A46) (formula: C₁₇H₁₅ClN₂O₃).



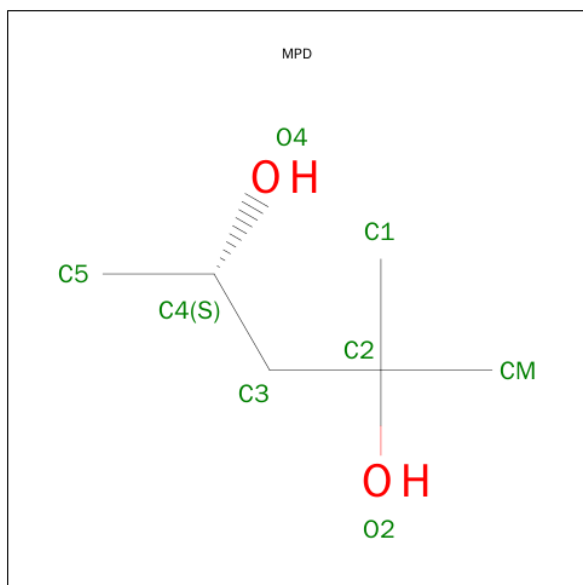
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	0
			23	17	1	2	3		

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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 (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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.

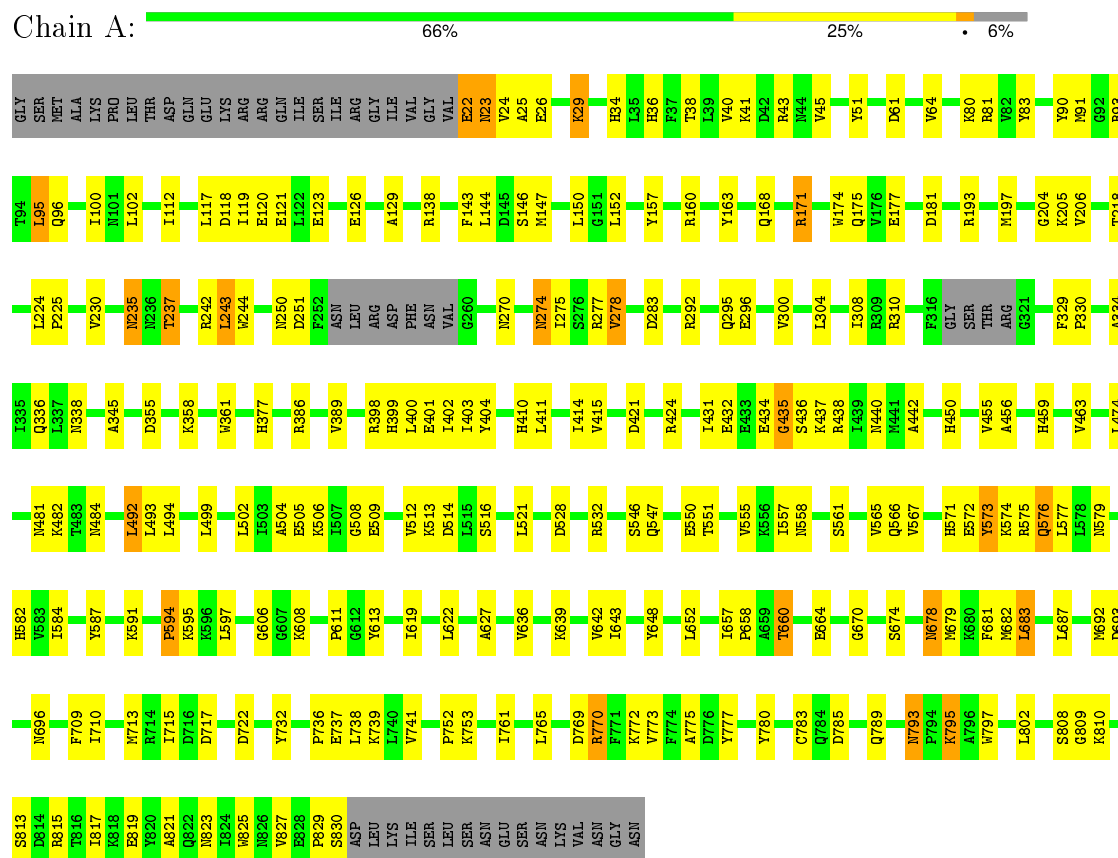
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	199	Total	O		
			199	199		
					0	0
7	B	198	Total	O		
			198	198		
					0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: Glycogen phosphorylase, liver form



D785	A673	V567	N440	A1A	V221
Q789	S674	K568	N441	GLY	L224
N793	N678	H571	A442	V325	P225
P794	N679	E572	H450	F326	Y226
K795	N680	Y573	V455	P329	V230
A796	N681	K574	A456	P330	N235
W797	N682	N575	K457	A334	N236
L802	L683	Q576	I458	N236	T237
		N579	H459	T340	R242
	L687	C580	V463	H341	L243
S808	N692	V583	L474	P342	W244
G809	D693	Y587	N481	A346	N250
K810	N696	K591	L492	D355	ASP
S813	N697	P594	L493	K358	PHE
R814	E701	L597	L494	W361	ASN
R815	F709	V603	L499	K370	LEU
T816	I710	I604	L502	PHE	ASP
I817	N713	I604	L503	V379	ASN
K818	R714	I605	A504	R386	VAL
E819	I715	G606	E505	V389	G260
	D717	G607	K506		V266
		Y613	N507		N270
V827	D722	Y617	G508	R398	
E828	Y732	N618	E509	R399	N274
P829	P736	I619	V512	L400	L275
S830	E737	L622	K513	E401	S276
ASP	L738	A627	D514	I402	R277
LEU	K739		L515	I403	V278
LYS	L740	V636	S516	Y404	
ILE	V741		L521	E405	L291
SER	P752	K639	D528	I406	R292
LEU	K753	L640	R532	H410	Q295
SER	I761	K641	S546	L411	E296
ASN	L765	V642	S547	I414	V300
LYS	D769	E646	N647	V415	L304
VAL	R770	N648	Y648	D421	
GLY	F771	L852	E550	R424	R310
ASN	K772	P657	T551	I431	F311
	V773	N558	Y559	E432	K312
	F774	A659	N558	E433	S314
	A775	T660	S561	E434	LYS
	D776	S663	D564	G435	PHE
	Y777	E664	Y565	S436	GLY
	C783	Q665		R437	SER
	Q784			R438	THR
				I439	ARG
					GLY

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	CNX2000	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: A46, MPD, GLC, MES, 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	0.54	0/6611	0.61	0/8940
1	B	0.52	0/6553	0.61	0/8865
All	All	0.53	0/13164	0.61	0/17805

There are no bond length outliers.

There are no bond angle outliers.

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	160	0
1	B	6410	0	6394	153	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	199	0	0	8	0
7	B	198	0	0	13	0
All	All	13413	0	12966	312	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 12.

All (312) 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: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:HE3	1:B:29:LYS:O	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:B:492:LEU:HG	1:B:683:LEU:HD22	1.75	0.68
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:B:157:TYR:HD2	1:B:244:TRP:HE1	1.42	0.67
1:A:274:ASN:HD21	1:B:270:ASN:HD21	1.43	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:168:GLN:HE21	1:B:647:ASN:H	1.42	0.66
1:B:80:LYS:HB3	1:B:827:VAL:HG12	1.77	0.66
1:A:80:LYS:HE2	1:A:334:ALA:HB2	1.79	0.65
1:B:692:MET:HE2	1:B:710:ILE:HG21	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:692:MET:HE2	1:A:710:ILE:HG21	1.80	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:B:93:ARG:HG2	1:B:126:GLU:HG2	1.80	0.63
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.79	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: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:A:829:PRO:O	1:A:830:SER:HB2	2.01	0.60
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: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
1:A:310:ARG:HH21	3:A:848:MES:H21	1.66	0.59
1:B:340:THR:HG23	7:B:1022:HOH:O	2.02	0.59
1:B:170:ILE:HG12	1:B:646:GLU:HG2	1.84	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:22:GLU:HG3	1:A:23:ASN:N	2.19	0.57
1:B:521:LEU:HB3	1:B:802:LEU:HD11	1.86	0.57
1:A:772:LYS:HB3	1:A:775:ALA:HB3	1.86	0.57
1:A:40:VAL:HG11	6:B:851:MPD:HM2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:810:LYS:O	1:A:815:ARG:HD3	2.04	0.56
1:A:431:ILE:N	1:A:431:ILE:HD12	2.20	0.56
1:B:692:MET:HE1	1:B:710:ILE:HG13	1.88	0.56
1:A:678:ASN:ND2	1:A:679:MET:N	2.54	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:692:MET:HE1	1:A:710:ILE:HG13	1.88	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: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:H	1:B:753:LYS:HD2	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: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:A:171:ARG:HA	1:A:171:ARG:HH11	1.73	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:770:ARG:HA	7:A:938:HOH:O	2.08	0.53
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.91	0.53
1:A:512:VAL:HG23	1:A:513:LYS:N	2.25	0.52
1:B:713:MET:HB3	1:B:717:ASP:HB2	1.91	0.52
1:B:80:LYS:HE2	1:B:334:ALA:HB2	1.91	0.52
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.93	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:336:GLN:OE1	1:A:825:TRP:NE1	2.39	0.51
1:A:678:ASN:ND2	1:A:678:ASN:N	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:583:VAL:HG13	1:B:640:LEU:HD21	1.92	0.50
1:A:557:ILE:HD11	1:A:643:ILE:HD11	1.93	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:B:168:GLN:HG3	1:B:175:GLN:HG3	1.94	0.49
6:B:852:MPD:C5	6:B:852:MPD:H11	2.42	0.49
1:A:275:ILE:O	1:A:295:GLN:HG2	2.12	0.49
1:A:648:TYR:HA	1:A:652:LEU:HD23	1.94	0.49
1:B:648:TYR:HA	1:B:652:LEU:HD23	1.95	0.49
1:B:41:LYS:HD2	1:B:45:VAL:HG23	1.93	0.49
1:A:753:LYS:N	1:A:753:LYS:HD2	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:ND2	1:B:678:ASN:N	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
1:B:693:ASP:O	1:B:696:ASN:HB2	2.13	0.48
1:A:576:GLN:H	1:A:576:GLN:HE21	1.62	0.48
1:A:146:SER:O	1:A:150:LEU:HD13	2.14	0.48
1:A:143:PHE:O	1:A:147:MET:HG3	2.12	0.48
1:A:456:ALA:C	1:A:481:ASN:HD21	2.17	0.48
1:A:829:PRO:O	1:A:830:SER:CB	2.62	0.48
1:B:171:ARG:HH11	1:B:171:ARG:HA	1.77	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:B:753:LYS:N	1:B:753:LYS:HD2	2.28	0.48
1:B:275:ILE:O	1:B:295:GLN:HG2	2.13	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:514:ASP:OD2	1:B:516:SER:HB3	2.14	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:100:ILE:HD12	1:A:494:LEU:CD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.96	0.47
1:B:436:SER:O	1:B:438:ARG:HG3	2.14	0.47
1:A:482:LYS:NZ	1:A:823:ASN:HB2	2.29	0.47
1:A:627:ALA:HA	1:A:642:VAL:HB	1.95	0.47
1:A:584:ILE:HG21	1:A:741:VAL:HG13	1.97	0.47
1:B:558:ASN:HB3	1:B:561:SER:HB3	1.96	0.47
1:B:386:ARG:HD2	1:B:432:GLU:OE2	2.15	0.47
1:A:567:VAL:HB	1:A:648:TYR:CZ	2.50	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:A:91:MET:HB2	1:A:129:ALA:HB3	1.95	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: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
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:A:434:GLU:O	1:A:435:GLY:C	2.54	0.46
1:B:566:GLN:HA	7:B:1011:HOH:O	2.14	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:118:ASP:HB3	1:A:121:GLU:HB3	1.97	0.46
1:A:100:ILE:CD1	1:A:494:LEU:HA	2.45	0.46
1:B:619:ILE:HD13	7:B:989:HOH:O	2.16	0.46
1:A:795:LYS:H	1:A:795:LYS:HD2	1.80	0.46
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.51	0.46
1:A:152:LEU:CD2	1:A:829:PRO:HA	2.46	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: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:119:ILE:HG23	1:A:120:GLU:N	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:91:MET:HB2	1:B:129:ALA:HB3	1.98	0.45
1:A:514:ASP:OD2	1:A:516:SER:HB3	2.17	0.45
1:A:636:VAL:O	1:A:639:LYS:HB2	2.16	0.45
1:A:504:ALA:HA	1:A:508:GLY:O	2.17	0.45
1:B:193:ARG:HH22	3:B:848:MES:H61	1.82	0.45
1:A:197:MET:HE3	1:A:224:LEU:HD13	1.99	0.45
1:B:456:ALA:C	1:B:481:ASN:HD21	2.21	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: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: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: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:A:809:GLY:HA3	7:A:1021:HOH:O	2.16	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:573:TYR:O	1:A:575:ARG:HG3	2.18	0.43
1:B:434:GLU:O	1:B:435:GLY:C	2.55	0.43
1:A:571:HIS:HD2	1:A:574:LYS:HD2	1.83	0.43
1:B:580:CYS:SG	1:B:622:LEU:HD22	2.57	0.43
1:A:687:LEU:HD13	1:A:709:PHE:HE1	1.83	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: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:714:ARG:HB3	7:B:979:HOH:O	2.18	0.43
1:B:81:ARG:HG3	7:B:1041:HOH:O	2.18	0.43
1:B:146:SER:O	1:B:150:LEU:HD13	2.18	0.43
1:A:566:GLN:HA	7:A:912:HOH:O	2.18	0.43
1:A:484:ASN:HA	1:A:484:ASN:HD22	1.64	0.43
1:A:687:LEU:HD12	1:A:797:TRP:CZ3	2.54	0.43
1:A:235:ASN:ND2	1:A:237:THR:HG23	2.33	0.43
1:B:732:TYR:CZ	1:B:739:LYS:HG3	2.54	0.43
1:B:761:ILE:O	1:B:765:LEU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:VAL:HG23	1:B:65:GLY:N	2.33	0.43
1:A:682:MET:HG2	1:A:808:SER:OG	2.18	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: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:821:ALA:HB1	1:A:827:VAL:HG23	2.00	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:B:312:LYS:HE3	1:B:326:PHE:HZ	1.84	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:A:738:LEU:HD13	1:A:777:TYR:CG	2.55	0.42
1:B:274:ASN:ND2	1:B:277:ARG:HH21	2.18	0.42
1:B:60:ARG:HD2	5:B:850:A46:C13	2.50	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:577:LEU:HG	1:A:619:ILE:CD1	2.50	0.42
1:B:421:ASP:CG	1:B:424:ARG:HB2	2.40	0.42
1:B:815:ARG:O	1:B:819: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:197:MET:HE3	1:B:224:LEU:HD13	2.01	0.42
1:A:283:ASP:OD1	1:A:571:HIS:NE2	2.51	0.42
1:A:738:LEU:HD13	1:A:777:TYR:CD2	2.55	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:A:237:THR:HG22	7:A:963:HOH:O	2.20	0.41
1:B:567:VAL:HA	1:B:606:GLY:O	2.19	0.41
1:B:715:ILE:HG13	1:B:715:ILE:H	1.64	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:A:761:ILE:O	1:A:765:LEU:HB2	2.19	0.41
1:A:338:ASN:OD1	1:A:377:HIS:NE2	2.53	0.41
1:B:402:ILE:O	1:B:406:ILE:HG13	2.20	0.41
1:A:399:HIS:O	1:A:403:ILE:HG13	2.20	0.41
1:A:456:ALA:C	1:A:481:ASN:ND2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:168:GLN:O	1:B:647:ASN:HB2	2.21	0.41
1:B:398:ARG:O	1:B:402:ILE:HG13	2.21	0.41
1:B:341:HIS:HB2	1:B:342:PRO:HD3	2.02	0.41
1:A:769:ASP:OD2	1:A:773:VAL:HG23	2.20	0.41
1:B:737:GLU:O	1:B:741:VAL:HG23	2.21	0.41
1:B:389:VAL:HG23	1:B:437:LYS:O	2.20	0.41
1:B:274:ASN:HA	1:B:274:ASN:HD22	1.64	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
1:A:493:LEU:HD21	1:A:512:VAL:HG12	2.02	0.41
1:B:300:VAL:CG1	1:B:345:ALA:HA	2.51	0.41
1:A:440:ASN:OD1	1:A:442:ALA:HB3	2.21	0.41
1:A:793:ASN:C	1:A:793:ASN:HD22	2.24	0.41
1:A:528:ASP:O	1:A:532:ARG:HG3	2.21	0.41
1:B:330:PRO:HB3	1:B:370:LYS:HB3	2.02	0.40
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.61	0.40
1:A:400:LEU:HG	1:A:404:TYR:CE2	2.56	0.40
1:B:738:LEU:HB2	1:B:777:TYR:CE2	2.56	0.40
1:B:564:ASP:O	1:B:603:VAL:HA	2.20	0.40
1:A:670:GLY:H	1:A:693:ASP:CG	2.23	0.40
1:A:582:HIS:HB2	1:A:780:TYR:HE2	1.84	0.40
1:A:566:GLN:HB2	1:A:664:GLU:HB2	2.03	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: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:B:663:SER:HG	1:B:665:GLN:HE21	1.68	0.40
1:A:421:ASP:CG	1:A:424:ARG:HB2	2.41	0.40
1:A:567:VAL:HA	1:A:606:GLY:O	2.22	0.40
1:B:440:ASN:OD1	1:B:442:ALA:HB3	2.22	0.40
1:B:192:SER:HB3	1:B:226:TYR:CE1	2.56	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	792/849 (93%)	739 (93%)	45 (6%)	8 (1%)	19	21
1	B	785/849 (92%)	734 (94%)	43 (6%)	8 (1%)	19	21
All	All	1577/1698 (93%)	1473 (93%)	88 (6%)	16 (1%)	19	21

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	696/741 (94%)	663 (95%)	33 (5%)	32	45
1	B	691/741 (93%)	661 (96%)	30 (4%)	35	50
All	All	1387/1482 (94%)	1324 (96%)	63 (4%)	34	47

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	23	ASN
1	A	26	GLU
1	A	29	LYS
1	A	90	TYR
1	A	95	LEU
1	A	102	LEU
1	A	171	ARG
1	A	235	ASN
1	A	237	THR
1	A	243	LEU
1	A	250	ASN
1	A	274	ASN
1	A	278	VAL
1	A	361	TRP
1	A	474	LEU
1	A	492	LEU
1	A	499	LEU
1	A	502	LEU
1	A	565	VAL
1	A	573	TYR
1	A	576	GLN
1	A	579	ASN
1	A	597	LEU
1	A	613	TYR
1	A	622	LEU
1	A	660	THR
1	A	678	ASN
1	A	683	LEU
1	A	722	ASP
1	A	770	ARG
1	A	793	ASN
1	A	795	LYS
1	B	23	ASN
1	B	26	GLU

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Mol	Chain	Res	Type
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	274	ASN
1	B	278	VAL
1	B	361	TRP
1	B	474	LEU
1	B	492	LEU
1	B	499	LEU
1	B	502	LEU
1	B	565	VAL
1	B	573	TYR
1	B	576	GLN
1	B	579	ASN
1	B	597	LEU
1	B	613	TYR
1	B	622	LEU
1	B	660	THR
1	B	678	ASN
1	B	683	LEU
1	B	722	ASP
1	B	770	ARG
1	B	793	ASN
1	B	795	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	167	ASN
1	A	168	GLN
1	A	235	ASN
1	A	239	ASN
1	A	274	ASN
1	A	284	ASN
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN

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Mol	Chain	Res	Type
1	A	541	ASN
1	A	547	GLN
1	A	566	GLN
1	A	576	GLN
1	A	579	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	106	ASN
1	B	167	ASN
1	B	168	GLN
1	B	235	ASN
1	B	239	ASN
1	B	250	ASN
1	B	274	ASN
1	B	284	ASN
1	B	459	HIS
1	B	481	ASN
1	B	484	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	826	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 carbohydrates 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$
2	GLC	A	847	-	12,12,12	0.43	0	17,17,17	0.68	0
3	MES	A	848	-	11,12,12	2.14	1 (9%)	14,16,16	3.23	5 (35%)
4	PLP	A	849	1	15,15,16	1.82	4 (26%)	21,22,23	1.16	2 (9%)
5	A46	A	850	-	22,25,25	1.49	4 (18%)	29,35,35	1.87	7 (24%)
2	GLC	B	847	-	12,12,12	0.37	0	17,17,17	0.52	0
3	MES	B	848	-	11,12,12	1.46	1 (9%)	14,16,16	2.04	4 (28%)
4	PLP	B	849	1	15,15,16	1.39	4 (26%)	21,22,23	1.11	1 (4%)
5	A46	B	850	-	22,25,25	2.06	7 (31%)	29,35,35	2.10	9 (31%)
6	MPD	B	851	-	6,7,7	1.15	0	7,10,10	0.93	0
6	MPD	B	852	-	6,7,7	0.64	0	7,10,10	1.12	1 (14%)

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	GLC	A	847	-	-	0/2/22/22	0/1/1/1
3	MES	A	848	-	-	0/6/14/14	0/1/1/1
4	PLP	A	849	1	-	0/6/6/8	0/1/1/1
5	A46	A	850	-	-	0/11/14/14	0/3/3/3
2	GLC	B	847	-	-	0/2/22/22	0/1/1/1
3	MES	B	848	-	-	0/6/14/14	0/1/1/1
4	PLP	B	849	1	-	0/6/6/8	0/1/1/1
5	A46	B	850	-	-	0/11/14/14	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MPD	B	851	-	-	0/5/5/5	0/0/0/0
6	MPD	B	852	-	1/1/2/2	0/5/5/5	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	850	A46	C16-CL1	-5.19	1.62	1.74
5	B	850	A46	C4-N1	-4.06	1.33	1.41
5	B	850	A46	C5-C3	-3.36	1.46	1.52
4	B	849	PLP	C4A-C4	-3.14	1.45	1.51
5	A	850	A46	C5-C3	-2.14	1.48	1.52
4	B	849	PLP	C3-C4	2.01	1.45	1.40
4	B	849	PLP	C5-C4	2.03	1.42	1.40
5	B	850	A46	C14-C16	2.29	1.41	1.36
5	B	850	A46	C13-C15	2.32	1.41	1.36
4	A	849	PLP	C6-C5	2.33	1.42	1.37
5	B	850	A46	C10-C4	2.36	1.43	1.39
4	B	849	PLP	C6-C5	2.38	1.42	1.37
5	A	850	A46	C1-C2	2.43	1.43	1.38
5	A	850	A46	C14-C16	2.73	1.42	1.36
4	A	849	PLP	C3-C4	2.78	1.47	1.40
5	B	850	A46	C8-C7	3.00	1.45	1.40
5	A	850	A46	C13-C15	3.06	1.43	1.36
4	A	849	PLP	C3-C2	3.52	1.43	1.40
4	A	849	PLP	C5-C4	4.37	1.45	1.40
3	B	848	MES	O3S-S	4.52	1.58	1.46
3	A	848	MES	O3S-S	6.84	1.64	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	848	MES	O2S-S-C8	-6.33	101.50	106.91
5	B	850	A46	C7-C8-C12	-4.32	101.17	106.55
5	B	850	A46	C10-C9-C5	-3.32	117.79	121.20
3	B	848	MES	O3S-S-O2S	-2.86	104.96	111.61
5	A	850	A46	C15-C16-C14	-2.62	118.45	121.87
3	A	848	MES	O3S-S-O1S	-2.45	105.90	111.61
5	B	850	A46	C13-C15-C16	-2.43	116.26	119.28
5	B	850	A46	C14-C12-C11	-2.11	116.99	119.89
4	A	849	PLP	C4A-C4-C5	2.00	122.97	120.88
4	A	849	PLP	O3-C3-C2	2.02	121.17	117.66
5	A	850	A46	C4-N1-C6	2.07	131.65	126.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	850	A46	C9-C10-C4	2.16	122.71	120.28
6	B	852	MPD	CM-C2-C1	2.29	115.24	110.24
4	B	849	PLP	O3-C3-C2	2.30	121.65	117.66
3	A	848	MES	C6-C5-N4	2.32	113.63	110.12
5	B	850	A46	C9-C5-C1	2.44	121.42	118.31
5	B	850	A46	C7-C6-N1	2.58	120.09	113.85
3	B	848	MES	C5-N4-C3	2.72	114.78	108.90
5	B	850	A46	C7-N2-C11	2.75	110.14	104.47
3	B	848	MES	C6-C5-N4	2.92	114.55	110.12
5	A	850	A46	C7-N2-C11	3.26	111.18	104.47
5	A	850	A46	C7-C6-N1	3.34	121.94	113.85
3	B	848	MES	C2-C3-N4	3.49	115.41	110.12
5	A	850	A46	C14-C16-CL1	3.72	125.03	119.74
5	B	850	A46	C16-C14-C12	3.90	121.65	119.19
5	A	850	A46	C16-C14-C12	4.80	122.21	119.19
3	A	848	MES	C5-N4-C3	5.45	120.71	108.90
5	B	850	A46	C8-C12-C11	5.55	111.11	106.27
3	A	848	MES	O1S-S-C8	7.05	112.92	106.91

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	852	MPD	C4

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	848	MES	3	0
3	B	848	MES	3	0
5	B	850	A46	1	0
6	B	851	MPD	2	0
6	B	852	MPD	4	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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.