



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:37 PM GMT

PDB ID : 1L5S
Title : Human liver glycogen phosphorylase complexed with uric acid, N-Acetyl-beta-D-glucopyranosylamine, and CP-403,700
Authors : Ekstrom, J.L.; Pauly, T.A.; Carty, M.D.; Soeller, W.C.; Culp, J.; Danley, D.E.; Hoover, D.J.; Treadway, J.L.; Gibbs, E.M.; Fletterick, R.J.; Day, Y.S.N.; Myszka, D.G.; Rath, V.L.
Deposited on : 2002-03-07
Resolution : 2.10 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

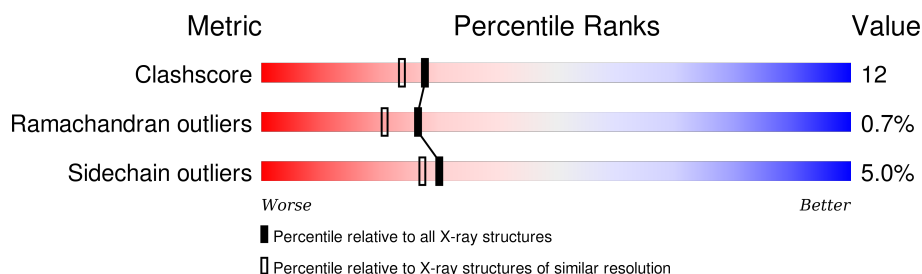
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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	847	
1	B	847	

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	MRD	B	903	-	-	X	-

2 Entry composition [i](#)

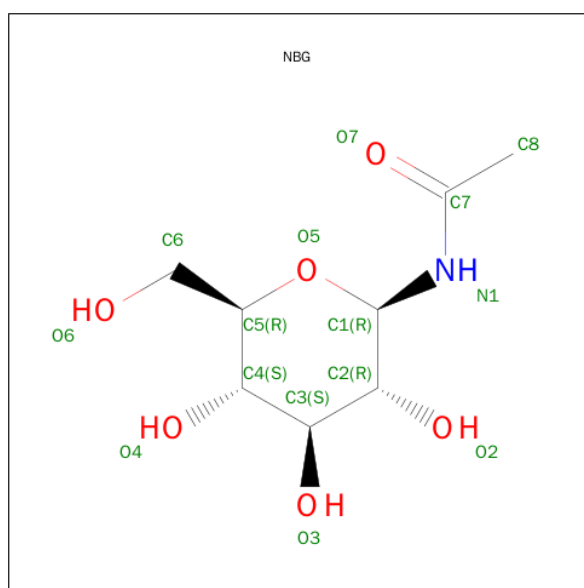
There are 7 unique types of molecules in this entry. The entry contains 13826 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	793	Total	C	N	O	S	0	0	0
			6437	4134	1092	1182	29			
1	B	791	Total	C	N	O	S	0	0	0
			6420	4125	1090	1176	29			

- Molecule 2 is SUGAR (1-N-ACETYL-BETA-D-GLUCOSAMINE) (three-letter code: NBG) (formula: $C_8H_{15}NO_6$).



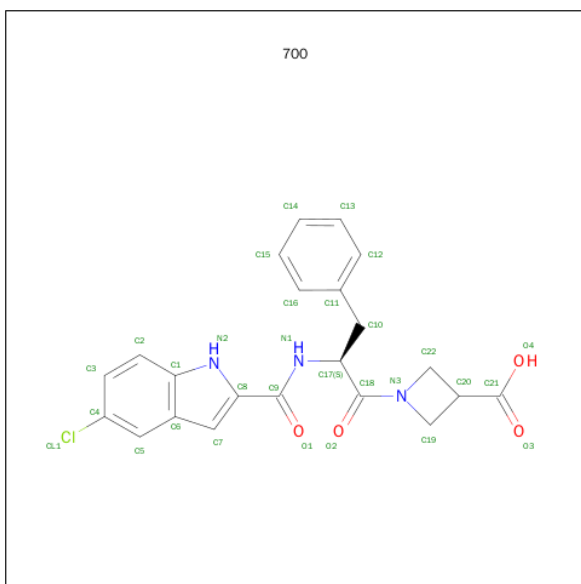
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 4 is [5-CHLORO-1H-INDOL-2-CARBONYL-PHENYLALANINYL]-AZETIDINE-3-CARBOXYLIC ACID (three-letter code: 700) (formula: C₂₂H₂₀ClN₃O₄).



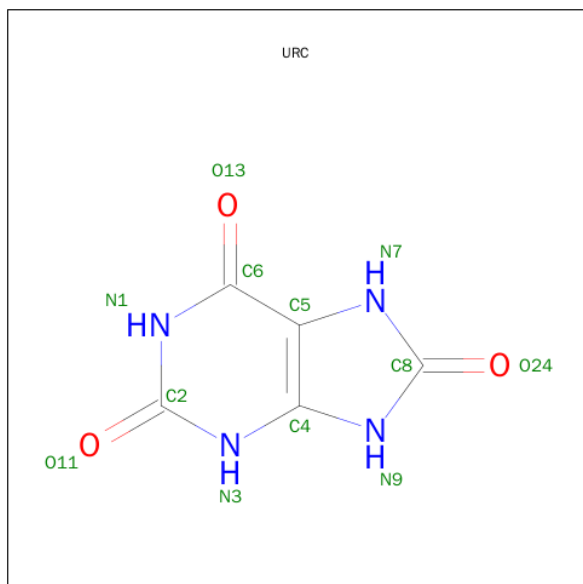
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	B	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

- Molecule 5 is URIC ACID (three-letter code: URC) (formula: $C_5H_4N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			12	5	4	3		
5	B	1	Total	C	N	O	0	0
			12	5	4	3		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



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

- Molecule 7 is water.

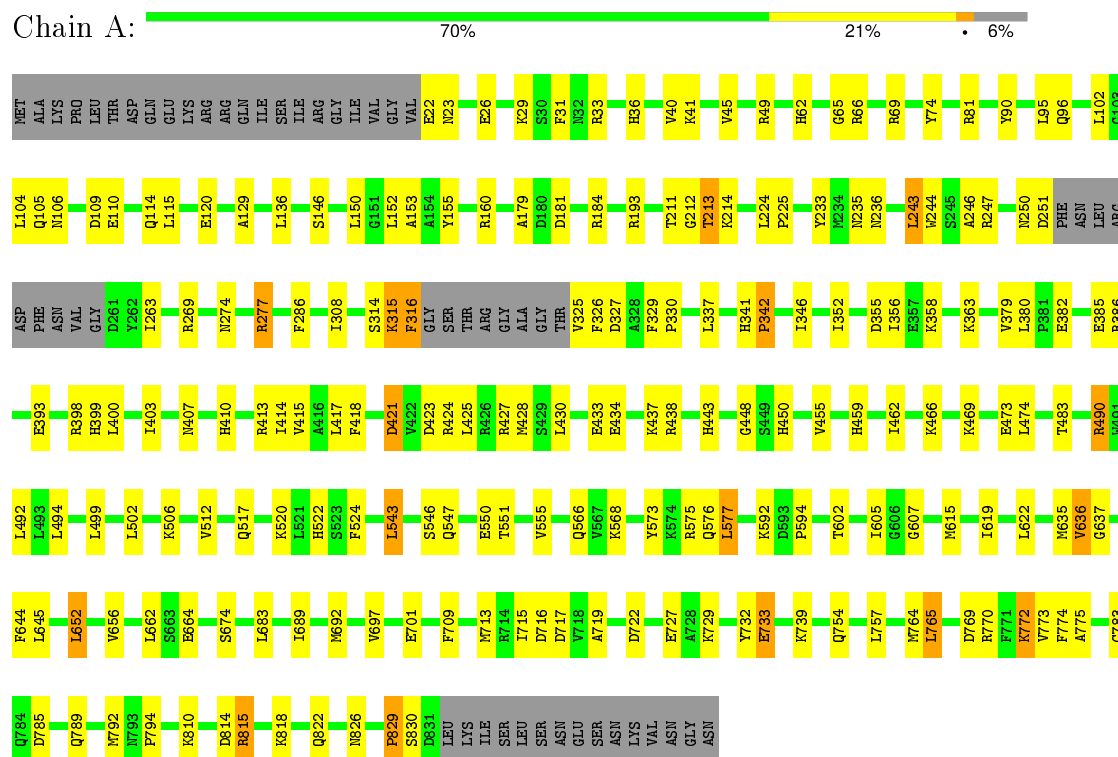
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	433	Total	O	0	0
			433	433		
7	B	352	Total	O	0	0
			352	352		

3 Residue-property plots

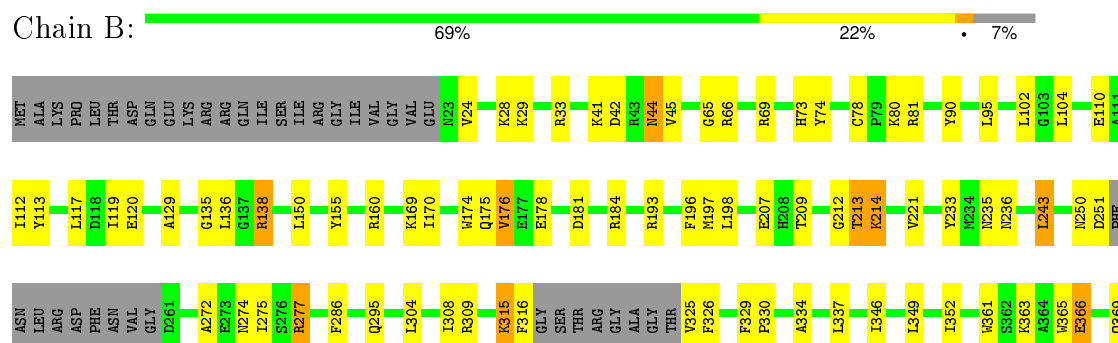
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



- Molecule 1: Glycogen phosphorylase, liver form



V379	L380	P381	E382	E385	R386	V392	E393	L400	E405	K409	R413	I414	V415	K420	D421	V422	D423	R424	L425	E432	E433	E434	G435	S436	K437	R438	I439	G448	S449	H450	V455	H459	V463	K466	V467	F468	L474	R490	V491	L492	L493	L494	
L499	L502	L503	L507	V512	D527	D528	V529	F530	K536	E540	F545	S546	Q547	F548	T551	E552	Y553	R554	V555	N558	P559	S560	Y573	K574	R575	Q576	L577	Y587	K591	K592	D593	P594	K595	K596	L597	F598	I605	Y613	H614	M615	L622	D628	V629
V630	H631	H632	D633	V636	Q637	S638	K639	F644	L645	E646	L652	L662	I666	S674	H678	H679	K680	F681	H682	L683	I689	H692	H699	I715	D716	A719	A728	K729	Y732	E733	K739	D743	P755	K759	D760	I761	H764	L765	F766				
R770	F771	K772	A775	D785	K786	V787	S788	Q789	M792	H793	P794	L802	S808	G809	K810	R815	K818	V827	E828	P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN					

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	124.03Å 124.03Å 123.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.60 – 2.10	Depositor
% Data completeness (in resolution range)	87.8 (40.60-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13826	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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: MRD, NBG, URC, 700, 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	0.48	0/6581	0.70	3/8900 (0.0%)
1	B	0.47	0/6564	0.69	2/8877 (0.0%)
All	All	0.47	0/13145	0.69	5/17777 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	490	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	490	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	129	ALA	N-CA-C	-5.32	96.62	111.00
1	A	129	ALA	N-CA-C	-5.21	96.94	111.00
1	A	602	THR	N-CA-C	-5.08	97.28	111.00

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	6437	0	6418	149	0
1	B	6420	0	6408	153	0
2	A	15	0	15	0	0
2	B	15	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	15	0	7	0	0
3	B	15	0	7	1	0
4	A	30	0	18	0	0
4	B	30	0	18	0	0
5	A	12	0	4	0	0
5	B	12	0	4	0	0
6	A	24	0	42	3	0
6	B	16	0	28	9	0
7	A	433	0	0	16	0
7	B	352	0	0	21	0
All	All	13826	0	12984	307	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 (307) 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:109:ASP:HB3	7:A:2741:HOH:O	1.53	1.05
1:A:49:ARG:HH22	6:A:905:MRD:H1C2	1.26	1.01
1:A:754:GLN:HG2	1:A:757:LEU:HB2	1.43	1.00
1:B:818:LYS:HB3	1:B:818:LYS:NZ	1.81	0.95
1:A:547:GLN:O	1:A:551:THR:HG23	1.72	0.90
1:B:110:GLU:HA	7:B:2762:HOH:O	1.79	0.82
1:A:308:ILE:HD13	1:A:352:ILE:HG21	1.61	0.81
1:B:770:ARG:HA	7:B:2481:HOH:O	1.81	0.79
1:B:789:GLN:HA	1:B:792:MET:HE2	1.63	0.79
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.65	0.78
1:B:818:LYS:HB3	1:B:818:LYS:HZ3	1.47	0.76
1:B:169:LYS:HB2	1:B:176:VAL:HG12	1.69	0.75
1:A:29:LYS:HE2	1:A:33:ARG:HH21	1.51	0.74
1:A:29:LYS:HG2	1:A:33:ARG:NH2	2.04	0.73
1:B:729:LYS:O	1:B:733:GLU:HG2	1.90	0.72
1:B:592:LYS:HD3	1:B:592:LYS:C	2.09	0.72
1:A:466:LYS:HE3	7:A:2665:HOH:O	1.88	0.72
1:A:433:GLU:HG2	1:A:437:LYS:HE3	1.73	0.71
1:B:450:HIS:HD2	7:B:2730:HOH:O	1.72	0.71
1:B:196:PHE:CZ	6:B:903:MRD:H1C3	2.25	0.70
6:B:903:MRD:H5C1	7:B:2596:HOH:O	1.90	0.70
1:B:434:GLU:CD	1:B:434:GLU:H	1.94	0.70
1:B:33:ARG:HD2	7:B:2480:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:VAL:HG22	1:A:425:LEU:HD11	1.72	0.70
1:A:106:ASN:ND2	7:A:2586:HOH:O	2.24	0.70
1:A:29:LYS:HE2	1:A:33:ARG:NH2	2.07	0.69
1:B:547:GLN:O	1:B:551:THR:HG23	1.92	0.69
1:A:506:LYS:HD2	1:A:524:PHE:CE2	2.28	0.69
1:A:146:SER:O	1:A:150:LEU:HD13	1.93	0.69
1:A:66:ARG:HD2	1:A:236:ASN:HA	1.73	0.69
1:B:170:ILE:HG12	1:B:646:GLU:HG2	1.75	0.69
1:A:96:GLN:HG2	1:A:105:GLN:HE22	1.58	0.69
1:B:29:LYS:HG2	1:B:33:ARG:NH2	2.08	0.68
1:A:522:HIS:NE2	7:A:2517:HOH:O	2.26	0.68
1:B:315:LYS:HA	1:B:315:LYS:HE3	1.76	0.68
1:B:42:ASP:OD2	1:B:44:ASN:ND2	2.27	0.67
1:A:789:GLN:HA	1:A:792:MET:HE2	1.75	0.67
1:B:792:MET:O	1:B:794:PRO:HD3	1.94	0.67
1:A:379:VAL:HG12	1:A:379:VAL:O	1.94	0.67
1:B:450:HIS:HE1	7:B:2135:HOH:O	1.77	0.67
1:A:592:LYS:C	1:A:592:LYS:HD3	2.14	0.66
1:A:455:VAL:H	1:A:459:HIS:HD2	1.44	0.66
1:B:433:GLU:HG3	1:B:437:LYS:HE3	1.77	0.65
1:B:66:ARG:CD	1:B:236:ASN:HA	2.26	0.65
1:B:455:VAL:H	1:B:459:HIS:HD2	1.45	0.64
1:A:772:LYS:HB3	1:A:775:ALA:HB3	1.79	0.64
1:B:361:TRP:CH2	1:B:405:GLU:HG2	2.32	0.64
1:B:325:VAL:O	1:B:326:PHE:HB2	1.96	0.64
1:B:764:MET:HE3	1:B:765:LEU:HD13	1.79	0.64
1:A:96:GLN:HG2	1:A:105:GLN:NE2	2.13	0.64
1:A:421:ASP:CG	1:A:424:ARG:HB2	2.19	0.63
1:B:633:ASP:O	1:B:636:VAL:HG22	1.99	0.63
1:B:818:LYS:HB3	1:B:818:LYS:HZ2	1.61	0.63
1:B:493:LEU:HD11	1:B:512:VAL:HG11	1.81	0.63
1:A:65:GLY:O	1:A:69:ARG:HG3	1.98	0.62
1:B:493:LEU:HD21	1:B:512:VAL:HG22	1.81	0.62
1:B:633:ASP:HB3	1:B:636:VAL:HG22	1.81	0.62
1:A:729:LYS:O	1:A:733:GLU:HG2	1.98	0.62
1:A:96:GLN:HE21	1:A:105:GLN:HE22	1.47	0.62
1:A:41:LYS:HE3	1:A:45:VAL:HG12	1.82	0.62
1:B:592:LYS:HD3	1:B:592:LYS:O	1.98	0.62
1:B:382:GLU:CD	1:B:770:ARG:HH22	2.03	0.62
1:A:415:VAL:CG2	1:A:425:LEU:HD11	2.29	0.62
1:A:414:ILE:HD13	1:A:428:MET:SD	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:GLU:HA	1:B:437:LYS:HG2	1.82	0.61
1:A:469:LYS:O	1:A:473:GLU:HG3	2.00	0.60
1:A:382:GLU:CD	1:A:770:ARG:HH22	2.04	0.60
1:A:308:ILE:CD1	1:A:352:ILE:HG21	2.29	0.60
1:B:645:LEU:HD13	1:B:652:LEU:HD13	1.83	0.60
1:A:433:GLU:HA	1:A:437:LYS:HG2	1.83	0.60
1:A:23:ASN:HD21	1:A:26:GLU:CG	2.14	0.59
1:A:810:LYS:O	1:A:815:ARG:HD3	2.02	0.59
1:A:23:ASN:HD21	1:A:26:GLU:HG2	1.66	0.59
1:A:233:TYR:CE2	1:A:512:VAL:HG11	2.38	0.58
1:B:346:ILE:HD13	1:B:448:GLY:HA3	1.85	0.58
6:A:904:MRD:H1C3	7:A:2758:HOH:O	2.03	0.58
1:A:754:GLN:HG2	1:A:757:LEU:CB	2.28	0.58
6:B:903:MRD:H1C1	7:B:2597:HOH:O	2.03	0.58
1:A:615:MET:HE3	1:A:619:ILE:HG13	1.85	0.58
1:B:65:GLY:O	1:B:69:ARG:HG3	2.02	0.58
1:B:363:LYS:HD2	1:B:366:GLU:OE1	2.04	0.58
1:B:432:GLU:O	1:B:437:LYS:HA	2.05	0.57
1:A:415:VAL:HG23	1:A:425:LEU:HD21	1.87	0.57
1:B:761:ILE:O	1:B:765:LEU:HD22	2.04	0.57
1:B:810:LYS:O	1:B:815:ARG:HD3	2.05	0.57
1:B:81:ARG:NH1	1:B:155:TYR:OH	2.38	0.57
1:A:792:MET:O	1:A:794:PRO:HD3	2.04	0.56
1:A:494:LEU:HD23	1:A:494:LEU:C	2.25	0.56
1:B:545:PHE:O	1:B:548:PHE:HB3	2.05	0.56
1:A:325:VAL:O	1:A:326:PHE:HB2	2.04	0.56
1:B:392:VAL:HG21	1:B:439:ILE:HD12	1.87	0.56
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.87	0.56
1:B:66:ARG:HD2	1:B:236:ASN:HA	1.87	0.56
1:B:325:VAL:N	7:B:2742:HOH:O	2.38	0.56
1:A:179:ALA:O	1:B:250:ASN:ND2	2.38	0.56
1:A:785:ASP:O	1:A:789:GLN:HG2	2.05	0.56
1:A:213:THR:HG23	1:A:355:ASP:OD1	2.06	0.56
1:B:421:ASP:CG	1:B:424:ARG:HB2	2.27	0.56
1:B:433:GLU:CG	1:B:437:LYS:HE3	2.36	0.55
1:A:382:GLU:OE2	1:A:770:ARG:NH2	2.39	0.55
1:A:732:TYR:CZ	1:A:739:LYS:HG3	2.41	0.55
1:B:379:VAL:HG12	1:B:379:VAL:O	2.06	0.55
1:A:433:GLU:CG	1:A:437:LYS:HE3	2.36	0.55
1:B:592:LYS:C	1:B:594:PRO:HD3	2.27	0.55
1:A:49:ARG:NH2	6:A:905:MRD:H1C2	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:HIS:HE1	7:A:2334:HOH:O	1.89	0.54
1:A:45:VAL:O	1:A:45:VAL:HG12	2.07	0.54
1:A:814:ASP:O	1:A:818:LYS:HG3	2.07	0.54
1:A:327:ASP:OD1	1:A:363:LYS:HE2	2.07	0.54
1:B:772:LYS:HB3	1:B:775:ALA:HB3	1.90	0.54
1:B:785:ASP:O	1:B:789:GLN:HG2	2.08	0.53
1:A:822:GLN:HB2	7:A:2748:HOH:O	2.08	0.53
1:B:66:ARG:HD3	1:B:236:ASN:HA	1.89	0.53
1:B:466:LYS:NZ	1:B:715:ILE:HD11	2.23	0.53
1:A:455:VAL:HG23	1:A:674:SER:HB2	1.91	0.53
1:A:826:ASN:ND2	7:A:2682:HOH:O	2.39	0.53
1:B:463:VAL:HG13	1:B:468:PHE:CD1	2.44	0.53
1:A:407:ASN:O	1:A:410:HIS:HB3	2.08	0.53
1:A:136:LEU:C	1:A:136:LEU:HD23	2.29	0.52
1:B:455:VAL:HG23	1:B:674:SER:HB2	1.92	0.52
1:B:493:LEU:HD11	1:B:512:VAL:CG1	2.39	0.52
1:A:399:HIS:O	1:A:403:ILE:HG13	2.09	0.52
1:B:503:ILE:O	1:B:507:ILE:HG12	2.10	0.52
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.92	0.52
6:B:902:MRD:H5C1	7:B:2274:HOH:O	2.10	0.52
1:A:269:ARG:NH2	7:A:2224:HOH:O	2.25	0.52
1:B:662:LEU:HG	1:B:787:VAL:HG11	1.92	0.51
1:A:789:GLN:OE1	1:A:792:MET:HE2	2.10	0.51
1:B:135:GLY:HA3	7:B:2013:HOH:O	2.10	0.51
1:B:636:VAL:HG23	1:B:637:GLY:N	2.24	0.51
1:A:697:VAL:O	1:A:701:GLU:HG3	2.10	0.51
1:A:417:LEU:HB2	1:A:418:PHE:CD1	2.46	0.51
6:B:903:MRD:HMC2	7:B:2100:HOH:O	2.11	0.51
1:A:727:GLU:OE1	1:A:729:LYS:HE3	2.11	0.51
1:A:462:ILE:HG23	1:A:466:LYS:HD2	1.93	0.51
1:B:818:LYS:CB	1:B:818:LYS:NZ	2.62	0.50
1:B:386:ARG:HA	1:B:439:ILE:O	2.10	0.50
1:B:536:LYS:O	1:B:540:GLU:HG3	2.11	0.50
1:A:352:ILE:O	1:A:356:ILE:HB	2.11	0.50
1:B:587:TYR:O	1:B:591:LYS:HG2	2.12	0.50
1:A:466:LYS:NZ	1:A:715:ILE:HD11	2.26	0.50
1:A:455:VAL:H	1:A:459:HIS:CD2	2.28	0.50
1:B:136:LEU:HD23	1:B:136:LEU:C	2.32	0.50
1:B:169:LYS:NZ	7:B:2525:HOH:O	2.44	0.50
1:A:213:THR:HG21	1:A:398:ARG:NH2	2.26	0.49
1:B:772:LYS:HD3	7:B:2158:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:ILE:HG22	1:B:765:LEU:CD2	2.42	0.49
6:B:902:MRD:H5C1	6:B:903:MRD:H5C3	1.95	0.49
1:A:23:ASN:ND2	1:A:26:GLU:HB2	2.27	0.49
1:B:81:ARG:NH2	7:B:2469:HOH:O	2.44	0.49
1:B:463:VAL:HG13	1:B:468:PHE:HD1	1.76	0.49
1:A:346:ILE:HD13	1:A:448:GLY:HA3	1.95	0.49
1:B:41:LYS:HE2	1:B:45:VAL:HG12	1.94	0.49
1:A:594:PRO:HG3	1:A:635:MET:SD	2.52	0.49
1:B:365:TRP:CD1	1:B:369:GLN:NE2	2.81	0.49
1:A:423:ASP:O	1:A:427:ARG:HG3	2.12	0.49
1:A:719:ALA:O	1:A:722:ASP:HB2	2.13	0.49
1:A:41:LYS:CE	1:A:45:VAL:HG12	2.42	0.49
1:B:415:VAL:HG23	1:B:425:LEU:HD21	1.95	0.48
1:A:246:ALA:O	1:A:247:ARG:HD3	2.13	0.48
1:A:689:ILE:O	1:A:689:ILE:HG23	2.13	0.48
1:A:592:LYS:C	1:A:594:PRO:HD3	2.34	0.48
1:A:765:LEU:HG	1:A:774:PHE:CE2	2.49	0.48
1:B:221:VAL:HG22	1:B:272:ALA:HB1	1.95	0.48
1:B:422:VAL:HG23	1:B:423:ASP:N	2.28	0.48
1:A:66:ARG:CD	1:A:236:ASN:HA	2.42	0.48
1:A:729:LYS:HG3	7:A:2676:HOH:O	2.14	0.48
1:A:605:ILE:O	1:A:644:PHE:HA	2.14	0.48
1:A:421:ASP:OD1	1:A:424:ARG:HD2	2.14	0.47
1:B:689:ILE:HG23	1:B:689:ILE:O	2.14	0.47
1:A:224:LEU:HD12	1:A:225:PRO:HD2	1.96	0.47
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.96	0.47
1:A:314:SER:C	1:A:316:PHE:H	2.18	0.47
1:B:596:LYS:HG2	1:B:597:LEU:N	2.29	0.47
1:A:308:ILE:HD13	1:A:352:ILE:CG2	2.39	0.47
1:B:80:LYS:HE2	1:B:334:ALA:HB2	1.96	0.47
1:B:361:TRP:CZ3	1:B:405:GLU:HG2	2.49	0.47
1:B:729:LYS:O	1:B:732:TYR:HB3	2.15	0.47
1:B:235:ASN:O	1:B:236:ASN:HB2	2.14	0.47
1:B:308:ILE:CD1	1:B:352:ILE:HG21	2.45	0.47
1:B:275:ILE:O	1:B:295:GLN:HG2	2.14	0.47
1:B:420:LYS:O	1:B:422:VAL:N	2.48	0.47
1:B:81:ARG:NE	7:B:2469:HOH:O	2.48	0.47
1:A:413:ARG:O	1:A:417:LEU:HG	2.15	0.46
1:A:546:SER:O	1:A:550:GLU:HG3	2.15	0.46
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.95	0.46
1:B:605:ILE:O	1:B:644:PHE:HA	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:902:MRD:H5C2	6:B:903:MRD:H3C2	1.96	0.46
1:B:170:ILE:HD13	1:B:175:GLN:HA	1.97	0.46
1:B:42:ASP:CG	1:B:44:ASN:HD21	2.18	0.46
1:B:405:GLU:O	1:B:409:LYS:HG2	2.14	0.46
1:A:393:GLU:HB2	1:A:400:LEU:HD22	1.97	0.46
1:A:592:LYS:HD3	1:A:592:LYS:O	2.14	0.46
1:B:80:LYS:HB3	1:B:827:VAL:HG12	1.96	0.46
1:B:639:LYS:NZ	7:B:2615:HOH:O	2.48	0.46
1:B:558:ASN:OD1	1:B:560:SER:HB3	2.14	0.46
1:A:732:TYR:CE1	1:A:739:LYS:HG3	2.50	0.46
1:A:566:GLN:HB2	1:A:664:GLU:HB2	1.98	0.46
1:A:41:LYS:HE2	1:A:45:VAL:O	2.16	0.46
1:A:247:ARG:HB3	1:B:184:ARG:NH2	2.30	0.46
1:B:24:VAL:O	1:B:28:LYS:HG3	2.16	0.46
1:A:235:ASN:O	1:A:236:ASN:HB2	2.16	0.45
1:B:45:VAL:HG12	1:B:45:VAL:O	2.16	0.45
1:A:413:ARG:HH11	1:A:413:ARG:HG2	1.81	0.45
1:A:543:LEU:HA	1:A:543:LEU:HD12	1.74	0.45
1:A:74:TYR:CZ	1:A:153:ALA:HA	2.51	0.45
1:A:314:SER:O	1:A:316:PHE:HD2	1.98	0.45
1:A:770:ARG:HA	7:A:2270:HOH:O	2.17	0.45
1:B:739:LYS:HG2	1:B:743:ASP:OD2	2.16	0.45
1:A:212:GLY:O	1:A:214:LYS:HD3	2.16	0.45
1:A:66:ARG:HG3	1:A:69:ARG:HH12	1.80	0.45
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.51	0.45
1:B:575:ARG:HD3	1:B:666:ILE:O	2.16	0.45
1:B:413:ARG:HA	1:B:413:ARG:NE	2.31	0.45
1:A:592:LYS:O	1:A:594:PRO:HD3	2.17	0.45
1:A:251:ASP:HB3	1:B:178:GLU:OE1	2.16	0.45
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.57	0.45
1:A:772:LYS:CE	7:A:2270:HOH:O	2.65	0.44
1:B:113:TYR:HB3	7:B:2762:HOH:O	2.16	0.44
1:B:530:PHE:HE2	1:B:802:LEU:HD22	1.82	0.44
1:A:29:LYS:HG2	1:A:33:ARG:HH21	1.76	0.44
1:B:138:ARG:HD2	1:B:138:ARG:HA	1.82	0.44
1:B:553:TYR:CD1	1:B:553:TYR:N	2.85	0.44
1:A:81:ARG:NH1	1:A:155:TYR:OH	2.51	0.44
1:B:286:PHE:CD1	1:B:385:GLU:HG2	2.52	0.44
1:B:405:GLU:OE1	1:B:409:LYS:HE3	2.17	0.44
1:B:772:LYS:N	1:B:772:LYS:HD2	2.33	0.44
1:B:802:LEU:O	1:B:802:LEU:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1861:NBG:H3	7:B:2452:HOH:O	2.17	0.44
1:A:379:VAL:CG1	1:A:379:VAL:O	2.64	0.44
1:B:197:MET:HE2	1:B:197:MET:HB2	1.91	0.43
1:A:22:GLU:HB3	1:A:62:HIS:CE1	2.52	0.43
1:A:483:THR:O	1:A:815:ARG:NH2	2.47	0.43
1:A:286:PHE:CD1	1:A:385:GLU:HG2	2.53	0.43
1:B:309:ARG:HD2	7:B:2744:HOH:O	2.18	0.43
1:A:517:GLN:OE1	1:A:520:LYS:HE3	2.18	0.43
1:A:772:LYS:HD2	1:A:772:LYS:N	2.33	0.43
1:A:764:MET:CE	1:A:765:LEU:HD13	2.48	0.43
1:A:652:LEU:O	1:A:656:VAL:HG12	2.18	0.43
1:B:434:GLU:CD	1:B:434:GLU:N	2.67	0.43
1:A:109:ASP:CB	7:A:2741:HOH:O	2.33	0.43
1:A:792:MET:C	1:A:794:PRO:HD3	2.39	0.43
1:A:250:ASN:CG	7:A:2224:HOH:O	2.57	0.43
1:B:212:GLY:O	1:B:214:LYS:HD2	2.18	0.43
1:A:74:TYR:HB3	1:A:81:ARG:HH12	1.84	0.42
1:B:196:PHE:CE2	6:B:903:MRD:H1C3	2.54	0.42
1:B:678:ASN:HB2	1:B:699:MET:SD	2.59	0.42
1:B:393:GLU:HB2	1:B:400:LEU:HD22	2.00	0.42
1:A:263:ILE:HG12	7:A:2568:HOH:O	2.18	0.42
1:B:181:ASP:OD2	1:B:184:ARG:NE	2.52	0.42
1:B:80:LYS:HE3	1:B:330:PRO:O	2.20	0.42
1:B:274:ASN:OD1	1:B:277:ARG:HD2	2.20	0.42
1:B:527:ASP:OD2	1:B:529:VAL:HB	2.19	0.42
1:B:420:LYS:O	1:B:422:VAL:HG13	2.20	0.42
1:B:198:LEU:HD21	1:B:309:ARG:CZ	2.49	0.42
1:B:379:VAL:CG1	1:B:379:VAL:O	2.68	0.42
1:B:308:ILE:HD13	1:B:352:ILE:HG21	2.02	0.42
1:B:716:ASP:O	1:B:719:ALA:HB3	2.20	0.42
1:B:555:VAL:HG21	1:B:631:ASN:ND2	2.35	0.42
1:A:152:LEU:HD23	1:A:829:PRO:HA	2.00	0.42
1:B:170:ILE:HA	1:B:174:TRP:O	2.19	0.42
1:B:207:GLU:HG2	1:B:209:THR:HG23	2.02	0.42
1:B:213:THR:O	1:B:213:THR:HG23	2.19	0.42
1:A:235:ASN:O	1:A:236:ASN:CB	2.67	0.42
1:A:769:ASP:OD2	1:A:773:VAL:HG23	2.20	0.41
1:B:592:LYS:C	1:B:592:LYS:CD	2.82	0.41
1:B:250:ASN:O	1:B:251:ASP:C	2.59	0.41
1:A:110:GLU:OE1	1:A:114:GLN:NE2	2.47	0.41
1:B:74:TYR:HB3	1:B:81:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:HB2	1:A:225:PRO:HG2	2.03	0.41
1:B:233:TYR:CZ	1:B:512:VAL:HG11	2.56	0.41
1:A:233:TYR:CZ	1:A:512:VAL:HG11	2.56	0.41
1:B:598:PHE:HE2	1:B:639:LYS:O	2.04	0.41
1:B:119:ILE:HG23	1:B:120:GLU:N	2.35	0.41
1:B:728:ALA:HB3	1:B:766:PHE:HA	2.03	0.41
1:B:193:ARG:HH12	6:B:903:MRD:HMC1	1.86	0.41
1:B:112:ILE:HG23	1:B:117:LEU:HB2	2.01	0.41
1:B:680:LYS:NZ	3:B:1860:PLP:O3	2.53	0.41
1:A:341:HIS:HB2	1:A:342:PRO:HD3	2.02	0.41
1:A:430:LEU:HD23	1:A:443:HIS:HB3	2.03	0.41
1:A:733:GLU:HG2	1:A:733:GLU:H	1.65	0.41
1:B:380:LEU:HA	1:B:381:PRO:HD3	1.85	0.41
1:A:636:VAL:CG2	1:A:637:GLY:N	2.83	0.41
1:B:764:MET:CE	1:B:765:LEU:HD13	2.48	0.41
1:A:421:ASP:OD1	1:A:424:ARG:HB2	2.21	0.41
1:B:630:VAL:O	1:B:636:VAL:HG21	2.21	0.41
1:B:494:LEU:C	1:B:494:LEU:HD23	2.41	0.41
1:A:315:LYS:C	7:A:2780:HOH:O	2.58	0.41
1:A:274:ASN:OD1	1:A:277:ARG:HD2	2.20	0.41
1:A:211:THR:O	1:A:358:LYS:NZ	2.47	0.41
1:B:73:HIS:HA	7:B:2595:HOH:O	2.21	0.41
1:B:304:LEU:HD22	1:B:349:LEU:HD13	2.01	0.41
1:B:682:MET:HG2	1:B:808:SER:HB3	2.03	0.41
1:A:715:ILE:HG23	1:A:716:ASP:N	2.35	0.41
1:B:315:LYS:HD3	1:B:315:LYS:O	2.20	0.41
1:B:386:ARG:NH2	1:B:438:ARG:HD2	2.36	0.40
1:A:36:HIS:O	1:A:40:VAL:HA	2.21	0.40
1:A:568:LYS:O	1:A:607:GLY:HA3	2.21	0.40
1:A:181:ASP:OD2	1:A:184:ARG:NE	2.54	0.40
1:B:678:ASN:OD1	1:B:679:MET:N	2.50	0.40
1:A:31:PHE:CD1	1:A:115:LEU:HD13	2.57	0.40
1:B:44:ASN:HD22	1:B:45:VAL:HG23	1.86	0.40
1:A:417:LEU:HB2	1:A:418:PHE:CE1	2.56	0.40
1:B:759:LYS:HA	1:B:759:LYS:HD2	1.92	0.40
1:A:386:ARG:HB3	1:A:438:ARG:HD3	2.03	0.40
1:B:81:ARG:CZ	7:B:2469:HOH:O	2.68	0.40
1:A:575:ARG:C	1:A:577:LEU:N	2.75	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	787/847 (93%)	743 (94%)	38 (5%)	6 (1%)	24	17
1	B	785/847 (93%)	747 (95%)	33 (4%)	5 (1%)	30	24
All	All	1572/1694 (93%)	1490 (95%)	71 (4%)	11 (1%)	26	21

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	ASP
1	A	555	VAL
1	B	421	ASP
1	B	435	GLY
1	A	829	PRO
1	A	434	GLU
1	A	830	SER
1	B	213	THR
1	B	829	PRO
1	B	755	PRO
1	A	342	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	694/740 (94%)	662 (95%)	32 (5%)	33	31
1	B	692/740 (94%)	655 (95%)	37 (5%)	28	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1386/1480 (94%)	1317 (95%)	69 (5%)	30	27

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	TYR
1	A	95	LEU
1	A	102	LEU
1	A	104	LEU
1	A	120	GLU
1	A	213	THR
1	A	243	LEU
1	A	277	ARG
1	A	315	LYS
1	A	316	PHE
1	A	337	LEU
1	A	380	LEU
1	A	474	LEU
1	A	490	ARG
1	A	492	LEU
1	A	499	LEU
1	A	502	LEU
1	A	543	LEU
1	A	573	TYR
1	A	576	GLN
1	A	577	LEU
1	A	622	LEU
1	A	636	VAL
1	A	645	LEU
1	A	652	LEU
1	A	662	LEU
1	A	683	LEU
1	A	692	MET
1	A	733	GLU
1	A	765	LEU
1	A	772	LYS
1	A	815	ARG
1	B	44	ASN
1	B	78	CYS
1	B	90	TYR
1	B	95	LEU
1	B	102	LEU

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Mol	Chain	Res	Type
1	B	104	LEU
1	B	138	ARG
1	B	150	LEU
1	B	176	VAL
1	B	214	LYS
1	B	243	LEU
1	B	277	ARG
1	B	315	LYS
1	B	316	PHE
1	B	337	LEU
1	B	366	GLU
1	B	474	LEU
1	B	490	ARG
1	B	492	LEU
1	B	499	LEU
1	B	502	LEU
1	B	573	TYR
1	B	576	GLN
1	B	577	LEU
1	B	613	TYR
1	B	615	MET
1	B	622	LEU
1	B	628	ASP
1	B	645	LEU
1	B	652	LEU
1	B	662	LEU
1	B	683	LEU
1	B	692	MET
1	B	755	PRO
1	B	765	LEU
1	B	772	LYS
1	B	815	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	62	HIS
1	A	71	GLN
1	A	72	GLN
1	A	105	GLN
1	A	450	HIS

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Mol	Chain	Res	Type
1	A	459	HIS
1	B	44	ASN
1	B	96	GLN
1	B	105	GLN
1	B	369	GLN
1	B	408	GLN
1	B	450	HIS
1	B	459	HIS
1	B	822	GLN
1	B	823	ASN
1	B	826	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

13 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	MRD	A	1902	-	6,7,7	0.49	0	7,10,10	0.63	0
3	PLP	A	860	1	15,15,16	2.18	9 (60%)	21,22,23	1.20	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NBG	A	861	-	15,15,15	1.43	3 (20%)	21,21,21	1.19	2 (9%)
4	700	A	862	-	26,33,33	1.80	8 (30%)	33,47,47	1.65	7 (21%)
5	URC	A	863	-	12,13,13	5.24	6 (50%)	10,19,19	4.56	4 (40%)
6	MRD	A	904	-	6,7,7	0.71	0	7,10,10	1.00	1 (14%)
6	MRD	A	905	-	6,7,7	0.65	0	7,10,10	0.88	0
3	PLP	B	1860	1	15,15,16	2.03	4 (26%)	21,22,23	1.22	2 (9%)
2	NBG	B	1861	-	15,15,15	1.70	4 (26%)	21,21,21	1.34	3 (14%)
4	700	B	1862	-	26,33,33	1.71	8 (30%)	33,47,47	1.63	6 (18%)
5	URC	B	1863	-	12,13,13	5.18	7 (58%)	10,19,19	4.69	4 (40%)
6	MRD	B	902	-	6,7,7	0.55	0	7,10,10	0.59	0
6	MRD	B	903	-	6,7,7	1.28	0	7,10,10	0.96	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
6	MRD	A	1902	-	-	0/5/5/5	0/0/0/0
3	PLP	A	860	1	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/5/26/26	0/1/1/1
4	700	A	862	-	-	0/15/32/32	0/4/4/4
5	URC	A	863	-	-	0/0/24/24	0/2/2/2
6	MRD	A	904	-	-	0/5/5/5	0/0/0/0
6	MRD	A	905	-	-	0/5/5/5	0/0/0/0
3	PLP	B	1860	1	-	0/6/6/8	0/1/1/1
2	NBG	B	1861	-	-	0/5/26/26	0/1/1/1
4	700	B	1862	-	-	0/15/32/32	0/4/4/4
5	URC	B	1863	-	-	0/0/24/24	0/2/2/2
6	MRD	B	902	-	-	0/5/5/5	0/0/0/0
6	MRD	B	903	-	-	0/5/5/5	0/0/0/0

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	863	URC	C4-N9	-12.02	1.30	1.44
5	B	1863	URC	C4-N9	-11.64	1.30	1.44
5	B	1863	URC	C4-N3	-10.89	1.33	1.46
5	A	863	URC	C4-N3	-10.65	1.33	1.46
5	A	863	URC	C5-N7	-7.01	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1863	URC	C5-N7	-6.73	1.31	1.45
3	B	1860	PLP	C4A-C4	-5.86	1.39	1.51
3	A	860	PLP	C4A-C4	-4.32	1.42	1.51
3	B	1860	PLP	C3-C2	-2.94	1.38	1.40
4	A	862	700	C7-C8	-2.78	1.34	1.40
5	A	863	URC	C8-N9	-2.58	1.31	1.35
5	A	863	URC	C8-N7	-2.57	1.31	1.35
5	B	1863	URC	C8-N7	-2.50	1.31	1.35
3	A	860	PLP	P-O3P	-2.30	1.46	1.54
4	B	1862	700	C22-N3	-2.25	1.44	1.47
3	A	860	PLP	C3-C2	-2.25	1.39	1.40
5	A	863	URC	C5-C6	-2.16	1.49	1.53
5	B	1863	URC	C2-N1	-2.16	1.34	1.37
5	B	1863	URC	C6-N1	-2.11	1.33	1.37
5	B	1863	URC	C8-N9	-2.11	1.32	1.35
3	B	1860	PLP	P-O3P	-2.11	1.47	1.54
3	B	1860	PLP	C5-C4	-2.11	1.38	1.40
3	A	860	PLP	O3-C3	2.03	1.41	1.37
4	A	862	700	C10-C11	2.06	1.56	1.51
4	A	862	700	C17-N1	2.06	1.50	1.45
4	B	1862	700	C15-C14	2.11	1.43	1.38
2	A	861	NBG	C3-C2	2.15	1.58	1.52
4	B	1862	700	C3-C4	2.16	1.42	1.38
2	B	1861	NBG	C3-C2	2.19	1.58	1.52
2	B	1861	NBG	C4-C5	2.24	1.57	1.53
3	A	860	PLP	P-O4P	2.31	1.68	1.60
4	B	1862	700	C2-C3	2.37	1.41	1.36
3	A	860	PLP	C3-C4	2.37	1.46	1.40
3	A	860	PLP	C5A-C5	2.41	1.57	1.50
4	A	862	700	C7-C6	2.47	1.50	1.41
4	B	1862	700	C16-C11	2.52	1.44	1.38
4	A	862	700	C2-C3	2.53	1.41	1.36
4	A	862	700	C12-C11	2.53	1.44	1.38
3	A	860	PLP	C2A-C2	2.54	1.55	1.50
4	B	1862	700	C7-C6	2.57	1.50	1.41
2	A	861	NBG	C1-N1	2.64	1.46	1.43
2	A	861	NBG	C2-C1	2.65	1.55	1.53
4	B	1862	700	C12-C11	2.65	1.44	1.38
3	A	860	PLP	C2-N1	2.72	1.39	1.34
4	A	862	700	C3-C4	2.72	1.43	1.38
4	A	862	700	C5-C4	3.16	1.43	1.36
2	B	1861	NBG	C2-C1	3.25	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1862	700	C5-C4	3.47	1.43	1.36
2	B	1861	NBG	C1-N1	3.90	1.47	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1863	URC	N7-C8-N9	-5.03	105.41	108.88
5	A	863	URC	N7-C8-N9	-4.69	105.64	108.88
4	B	1862	700	C7-C6-C1	-4.39	102.45	106.27
4	A	862	700	C7-C6-C1	-4.36	102.47	106.27
4	B	1862	700	C4-C5-C6	-3.42	117.04	119.19
4	A	862	700	C3-C2-C1	-3.28	117.32	120.88
4	A	862	700	C4-C5-C6	-3.12	117.22	119.19
3	B	1860	PLP	O4P-P-O1P	-3.00	99.51	107.14
3	A	860	PLP	O4P-C5A-C5	-2.98	104.07	108.99
4	B	1862	700	C3-C2-C1	-2.77	117.87	120.88
2	B	1861	NBG	C2-C1-N1	-2.76	108.34	111.44
4	B	1862	700	O1-C9-C8	-2.68	115.53	121.23
2	A	861	NBG	C2-C1-N1	-2.61	108.52	111.44
4	A	862	700	O1-C9-C8	-2.56	115.79	121.23
4	A	862	700	C10-C17-C18	-2.05	105.41	109.88
6	A	904	MRD	C2-C3-C4	2.05	126.34	116.66
2	B	1861	NBG	C3-C2-C1	2.19	113.61	110.09
3	B	1860	PLP	O3P-P-O1P	2.29	117.95	110.58
3	A	860	PLP	O3P-P-O2P	2.48	116.83	107.38
2	A	861	NBG	C5-O5-C1	3.24	117.20	112.49
4	A	862	700	C8-C9-N1	3.49	122.87	115.10
4	B	1862	700	C8-N2-C1	3.50	111.69	104.47
4	B	1862	700	C8-C9-N1	3.56	123.02	115.10
4	A	862	700	C8-N2-C1	3.76	112.21	104.47
2	B	1861	NBG	C5-O5-C1	4.03	118.35	112.49
5	B	1863	URC	N1-C2-N3	4.43	120.99	116.14
5	A	863	URC	N1-C2-N3	4.55	121.13	116.14
5	A	863	URC	C5-C4-N9	6.65	105.64	102.69
5	B	1863	URC	C5-C4-N9	7.32	105.94	102.69
5	A	863	URC	N9-C4-N3	10.58	132.61	112.36
5	B	1863	URC	N9-C4-N3	10.65	132.74	112.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	904	MRD	1	0
6	A	905	MRD	2	0
3	B	1860	PLP	1	0
2	B	1861	NBG	1	0
6	B	902	MRD	3	0
6	B	903	MRD	8	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 ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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