



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:41 am GMT

PDB ID : 1L7X
Title : Human liver glycogen phosphorylase b complexed with caffeine, 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 : 2002-03-18
Resolution : 2.30 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

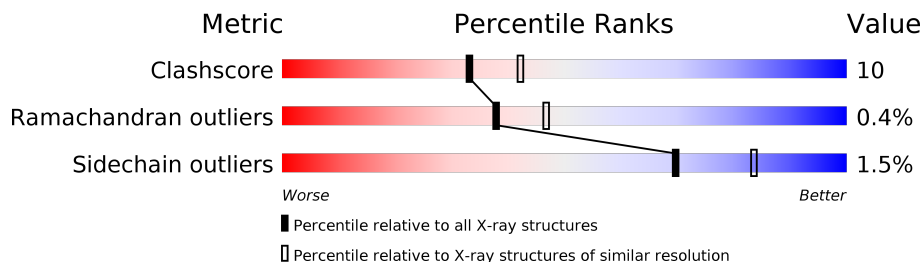
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)

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	

2 Entry composition [i](#)

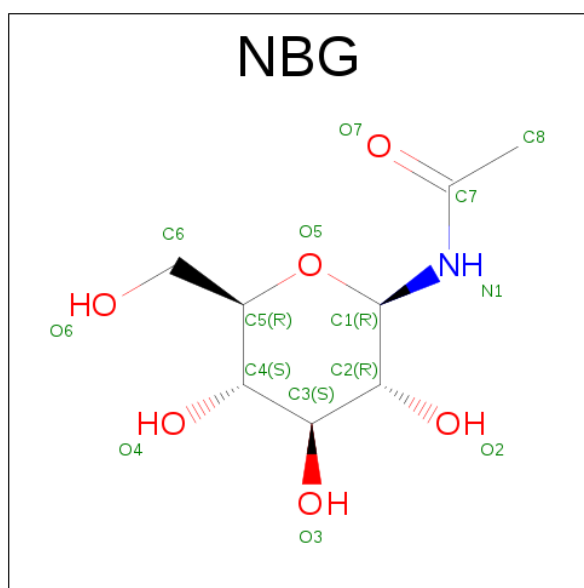
There are 7 unique types of molecules in this entry. The entry contains 13542 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

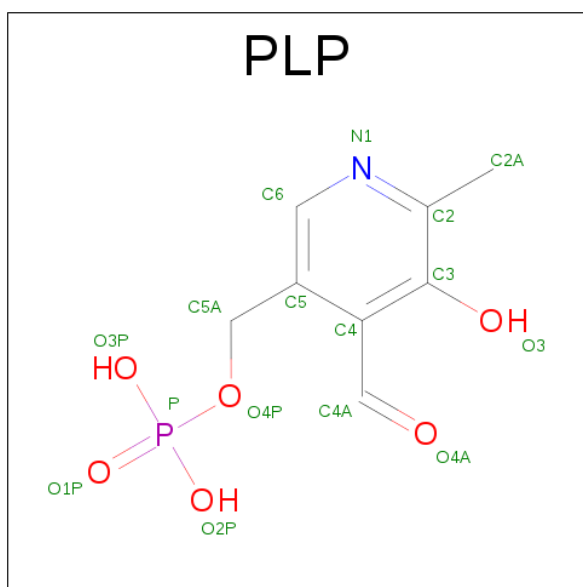
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	793	Total	C	N	O	S	0	0	0
			6436	4135	1092	1180	29			
1	B	795	Total	C	N	O	S	0	0	0
			6446	4141	1094	1182	29			

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



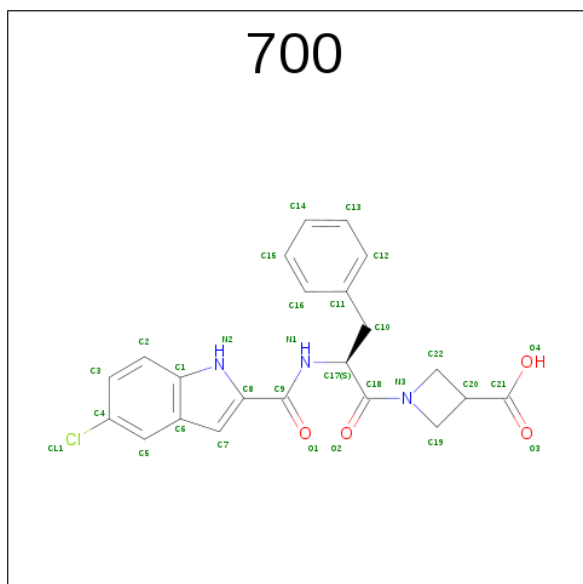
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- 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).



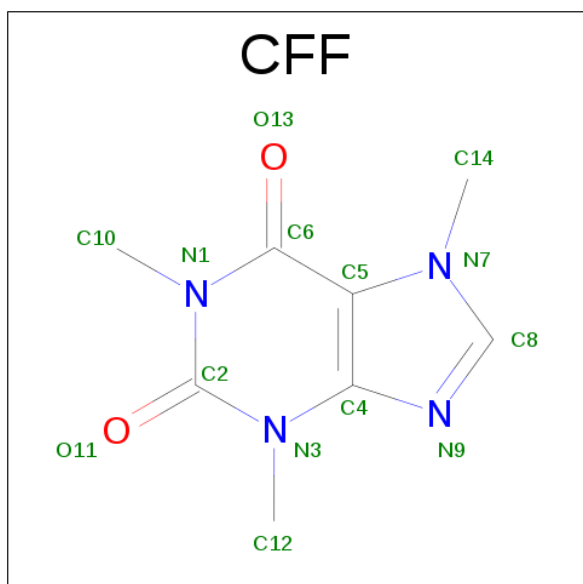
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

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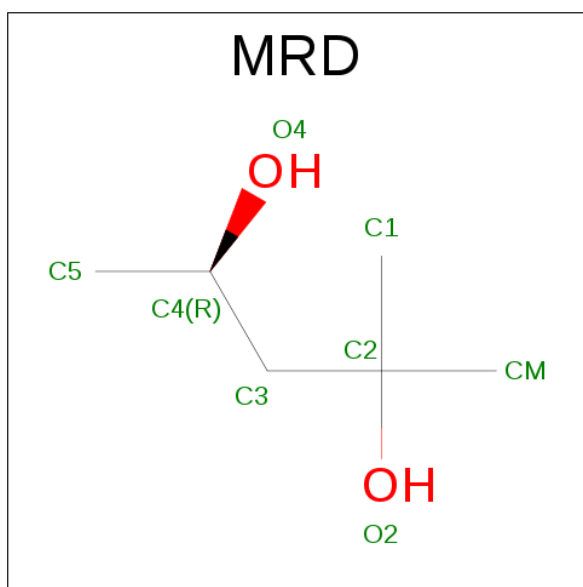
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

- Molecule 5 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	4	2		
5	B	1	Total	C	N	O	0	0
			14	8	4	2		
5	A	1	Total	C	N	O	0	0
			14	8	4	2		

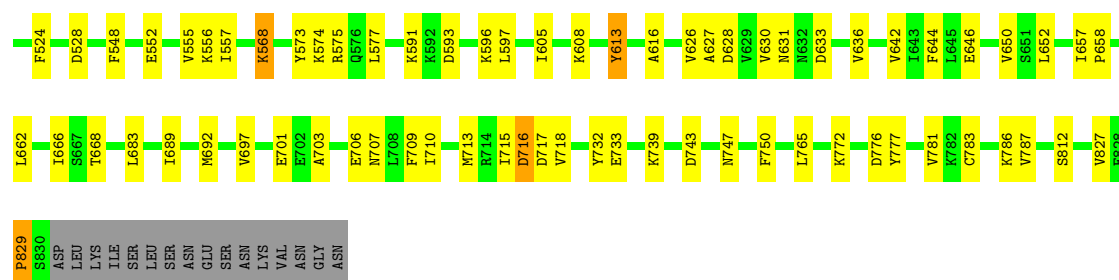
- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	252	Total O 252 252	0	0
7	B	222	Total O 222 222	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	124.07Å 124.07Å 122.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.39 – 2.30	Depositor
% Data completeness (in resolution range)	96.6 (34.39-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13542	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CFF, MRD, 700, NBG, 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	0.36	0/6580	0.59	0/8899
1	B	0.35	0/6590	0.59	0/8912
All	All	0.35	0/13170	0.59	0/17811

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6436	0	6426	126	0
1	B	6446	0	6436	133	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0
3	A	15	0	7	0	0
3	B	15	0	7	0	0
4	A	30	0	19	0	0
4	B	30	0	19	0	0
5	A	28	0	20	0	0
5	B	14	0	10	0	0
6	B	24	0	42	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	252	0	0	7	0
7	B	222	0	0	4	0
All	All	13542	0	13016	256	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 10.

All (256) 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:350:MET:HE1	1:A:364:ALA:HB1	1.56	0.86
1:B:77:LYS:HA	1:B:77:LYS:HE3	1.59	0.84
1:A:80:LYS:HB3	1:A:827:VAL:HG12	1.60	0.83
1:A:721:LEU:HD23	1:A:772:LYS:HD3	1.60	0.83
1:B:80:LYS:HB3	1:B:827:VAL:HG12	1.62	0.82
1:B:170:ILE:HG12	1:B:646:GLU:HG2	1.61	0.81
1:A:597:LEU:H	1:A:597:LEU:HD22	1.45	0.80
1:B:597:LEU:HD22	1:B:597:LEU:H	1.47	0.79
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.63	0.79
1:A:308:ILE:HD13	1:A:352:ILE:HG21	1.64	0.78
1:B:350:MET:HE1	1:B:364:ALA:HB1	1.64	0.78
1:A:308:ILE:CD1	1:A:352:ILE:HG21	2.14	0.77
1:B:633:ASP:O	1:B:636:VAL:HG12	1.84	0.76
1:B:181:ASP:OD2	1:B:184:ARG:HB2	1.85	0.76
1:B:30:SER:HA	1:B:33:ARG:NH1	2.02	0.75
1:B:575:ARG:HD3	1:B:666:ILE:O	1.88	0.74
1:A:209:THR:HG21	1:A:214:LYS:HE2	1.70	0.72
1:B:170:ILE:HG22	7:B:2366:HOH:O	1.89	0.71
1:A:77:LYS:HA	1:A:77:LYS:HE3	1.73	0.70
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.73	0.69
1:A:350:MET:HE3	1:A:364:ALA:O	1.92	0.69
1:B:568:LYS:HD3	1:B:574:LYS:HD3	1.74	0.69
1:A:633:ASP:O	1:A:636:VAL:HG12	1.94	0.68
1:A:350:MET:HA	1:A:350:MET:CE	2.24	0.67
1:B:575:ARG:NH2	1:B:776:ASP:HB2	2.09	0.67
1:A:568:LYS:HD3	1:A:574:LYS:HD3	1.78	0.66
1:B:575:ARG:HH22	1:B:776:ASP:HB2	1.61	0.65
1:B:247:ARG:HD2	7:B:2449:HOH:O	1.96	0.65
1:A:613:TYR:CD2	1:A:616:ALA:HB2	2.32	0.65
1:A:786:LYS:NZ	1:A:786:LYS:HB3	2.10	0.65
1:A:150:LEU:O	1:A:829:PRO:HB3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:MET:HE3	1:B:364:ALA:O	1.97	0.64
1:B:142:CYS:SG	1:B:487:THR:HG22	2.37	0.64
1:A:415:VAL:HG22	1:A:425:LEU:HD11	1.80	0.63
1:B:93:ARG:HG3	1:B:128:ASP:OD2	1.97	0.63
1:A:732:TYR:CE1	1:A:739:LYS:HG3	2.33	0.62
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.81	0.62
1:B:548:PHE:O	1:B:552:GLU:HG2	2.01	0.61
1:A:365:TRP:CD1	1:A:369:GLN:NE2	2.69	0.60
1:A:515:LEU:HG	1:A:809:GLY:HA2	1.82	0.60
1:A:462:ILE:HG12	1:A:466:LYS:NZ	2.16	0.60
1:A:181:ASP:OD2	1:A:184:ARG:NE	2.34	0.60
1:B:469:LYS:O	1:B:473:GLU:HG3	2.02	0.60
1:A:209:THR:CG2	1:A:214:LYS:HE2	2.32	0.59
1:B:109:ASP:OD1	1:B:119:ILE:HD13	2.03	0.58
1:B:207:GLU:HG2	1:B:209:THR:HG23	1.85	0.58
1:A:462:ILE:HA	1:A:466:LYS:HD2	1.84	0.58
1:A:548:PHE:O	1:A:552:GLU:HG2	2.03	0.58
1:B:386:ARG:HD2	1:B:432:GLU:OE2	2.04	0.58
1:B:697:VAL:O	1:B:701:GLU:HG3	2.03	0.58
1:A:292:ARG:O	1:A:296:GLU:HG3	2.02	0.58
1:B:66:ARG:HD2	1:B:236:ASN:HA	1.85	0.57
1:B:555:VAL:CG2	1:B:631:ASN:HD22	2.17	0.57
1:B:662:LEU:HD22	1:B:787:VAL:HG11	1.85	0.57
1:A:365:TRP:NE1	1:A:369:GLN:NE2	2.53	0.57
1:A:597:LEU:H	1:A:597:LEU:CD2	2.17	0.57
1:B:458:ILE:O	1:B:462:ILE:HG13	2.04	0.57
1:A:45:VAL:O	1:A:45:VAL:HG12	2.05	0.57
1:A:556:LYS:HD3	1:A:557:ILE:N	2.20	0.57
1:A:170:ILE:HG12	1:A:646:GLU:HG2	1.86	0.57
1:A:357:GLU:HA	1:A:357:GLU:OE2	2.04	0.56
1:A:250:ASN:HD21	1:B:184:ARG:NH1	2.02	0.56
1:A:458:ILE:HG22	7:A:2145:HOH:O	2.04	0.56
1:A:494:LEU:HD23	1:A:494:LEU:C	2.25	0.56
1:B:30:SER:HA	1:B:33:ARG:HH12	1.70	0.56
1:A:224:LEU:HD12	1:A:225:PRO:HD2	1.88	0.56
1:B:20:GLY:HA2	1:B:23:ASN:HD22	1.71	0.56
1:A:350:MET:HE3	1:A:364:ALA:C	2.26	0.56
1:B:150:LEU:O	1:B:829:PRO:HB3	2.07	0.55
1:A:109:ASP:OD1	1:A:119:ILE:HD13	2.05	0.55
1:A:505:GLU:HG3	7:A:2296:HOH:O	2.05	0.55
1:B:597:LEU:HD22	1:B:597:LEU:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:777:TYR:O	1:B:781:VAL:HG23	2.06	0.55
1:B:515:LEU:HD22	1:B:812:SER:HB2	1.88	0.55
1:A:469:LYS:O	1:A:473:GLU:HG3	2.07	0.54
1:A:73:HIS:CE1	1:A:77:LYS:HG3	2.43	0.54
1:B:350:MET:CE	1:B:368:THR:OG1	2.56	0.54
1:B:575:ARG:HH22	1:B:776:ASP:CB	2.20	0.54
1:B:597:LEU:CD2	1:B:597:LEU:H	2.17	0.54
1:A:246:ALA:O	1:A:247:ARG:HD3	2.07	0.54
1:A:350:MET:HA	1:A:350:MET:HE2	1.89	0.54
1:B:22:GLU:O	1:B:26:GLU:HG2	2.08	0.54
1:B:293:LEU:HD23	1:B:395:LEU:HD23	1.90	0.54
1:B:556:LYS:HD3	1:B:557:ILE:N	2.22	0.54
1:B:207:GLU:OE1	1:B:214:LYS:HE3	2.08	0.53
1:B:209:THR:OG1	1:B:214:LYS:HE2	2.08	0.53
1:B:463:VAL:HG13	1:B:468:PHE:CD1	2.44	0.53
1:B:786:LYS:HB3	1:B:786:LYS:NZ	2.24	0.53
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.44	0.53
1:A:536:LYS:HD3	7:A:2237:HOH:O	2.08	0.53
1:B:308:ILE:CD1	1:B:352:ILE:HG21	2.39	0.53
1:B:591:LYS:HD3	1:B:633:ASP:OD1	2.09	0.53
1:A:470:ASP:O	1:A:474:LEU:HD13	2.09	0.53
1:A:143:PHE:CG	1:A:817:ILE:HD11	2.44	0.52
1:B:657:ILE:HB	1:B:658:PRO:HD3	1.91	0.52
1:A:575:ARG:HD3	1:A:666:ILE:O	2.09	0.52
1:A:740:LEU:O	1:A:744:GLN:HG3	2.10	0.52
1:B:510:ASP:OD2	1:B:510:ASP:N	2.38	0.52
1:B:555:VAL:HG21	1:B:631:ASN:HD22	1.75	0.52
1:B:315:LYS:O	1:B:316:PHE:O	2.27	0.52
1:A:374:TYR:O	1:A:452:VAL:HA	2.10	0.52
1:B:405:GLU:OE1	1:B:409:LYS:NZ	2.42	0.52
1:B:80:LYS:HB3	1:B:827:VAL:CG1	2.39	0.52
1:B:492:LEU:HD22	1:B:683:LEU:HD11	1.92	0.51
1:B:45:VAL:HG12	1:B:45:VAL:O	2.10	0.51
1:B:575:ARG:HD2	1:B:668:THR:N	2.26	0.51
1:B:555:VAL:HG21	1:B:631:ASN:ND2	2.25	0.51
1:B:732:TYR:CE1	1:B:739:LYS:HG3	2.46	0.51
1:B:350:MET:HE3	1:B:368:THR:OG1	2.11	0.51
1:B:506:LYS:HD2	1:B:524:PHE:CE2	2.46	0.51
1:A:506:LYS:HE2	1:A:530:PHE:CD1	2.46	0.51
1:B:77:LYS:HA	1:B:77:LYS:CE	2.34	0.51
1:B:22:GLU:HG2	1:B:22:GLU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ALA:O	1:B:305:GLN:HG3	2.11	0.50
1:B:350:MET:HE3	1:B:364:ALA:C	2.30	0.50
1:B:470:ASP:O	1:B:474:LEU:HD13	2.12	0.50
1:A:112:ILE:HG23	1:A:117:LEU:HB2	1.93	0.50
1:A:506:LYS:HE2	1:A:530:PHE:HD1	1.77	0.50
1:A:515:LEU:HD11	1:A:518:LEU:HD11	1.94	0.50
1:A:136:LEU:C	1:A:136:LEU:HD23	2.32	0.49
1:A:330:PRO:HB3	1:A:370:LYS:HB3	1.92	0.49
1:A:453:ASN:ND2	1:A:482:LYS:HB2	2.27	0.49
1:A:786:LYS:HB3	1:A:786:LYS:HZ2	1.76	0.49
1:B:488:PRO:O	1:B:492:LEU:HB3	2.12	0.49
1:A:221:VAL:HG22	1:A:272:ALA:HB1	1.94	0.49
1:A:488:PRO:O	1:A:492:LEU:HB3	2.11	0.49
1:B:718:VAL:HG13	1:B:772:LYS:HE2	1.94	0.49
1:B:168:GLN:HG3	1:B:175:GLN:HG3	1.95	0.49
1:B:423:ASP:OD1	1:B:427:ARG:NH1	2.46	0.49
1:B:593:ASP:OD1	1:B:596:LYS:N	2.46	0.49
1:A:415:VAL:CG2	1:A:425:LEU:HD11	2.42	0.49
1:A:369:GLN:O	1:A:450:HIS:HB3	2.13	0.49
1:B:626:VAL:HA	1:B:750:PHE:CD1	2.48	0.49
1:B:196:PHE:CZ	6:B:903:MRD:H1C3	2.47	0.49
1:B:743:ASP:O	1:B:747:ASN:ND2	2.46	0.49
1:B:346:ILE:HD13	1:B:448:GLY:HA3	1.94	0.49
1:A:207:GLU:OE1	1:A:214:LYS:HE3	2.12	0.49
1:A:81:ARG:HD3	1:A:83:TYR:OH	2.13	0.48
1:B:613:TYR:CD2	1:B:616:ALA:HB2	2.48	0.48
1:B:73:HIS:CE1	1:B:77:LYS:HG3	2.48	0.48
1:A:462:ILE:HG12	1:A:466:LYS:HZ3	1.78	0.48
1:B:474:LEU:O	1:B:476:PRO:HD3	2.12	0.48
1:B:455:VAL:CG1	1:B:484:ASN:HD21	2.26	0.48
1:B:713:MET:HB3	1:B:717:ASP:HB2	1.95	0.48
1:B:393:GLU:HB2	1:B:400:LEU:CD2	2.44	0.48
1:A:459:HIS:O	1:A:463:VAL:HG23	2.14	0.48
1:A:348:GLU:O	1:A:352:ILE:HG13	2.13	0.48
1:B:493:LEU:HD21	1:B:512:VAL:HG11	1.96	0.48
1:B:515:LEU:CD2	1:B:812:SER:HB2	2.44	0.48
1:A:605:ILE:O	1:A:644:PHE:HA	2.14	0.48
1:B:350:MET:HA	1:B:350:MET:CE	2.44	0.47
1:B:63:LEU:HD23	1:B:102:LEU:HD11	1.96	0.47
1:A:350:MET:CE	1:A:368:THR:OG1	2.62	0.47
1:A:557:ILE:O	1:A:559:PRO:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ASP:OD1	1:B:340:THR:N	2.43	0.47
1:B:689:ILE:HG23	1:B:689:ILE:O	2.14	0.47
1:B:83:TYR:OH	1:B:310:ARG:HD2	2.15	0.47
1:B:386:ARG:HA	1:B:439:ILE:O	2.14	0.47
1:A:205:LYS:HE2	1:A:217:ASP:OD2	2.14	0.47
1:B:80:LYS:HE2	1:B:334:ALA:HB2	1.95	0.47
1:B:568:LYS:HB3	1:B:568:LYS:NZ	2.30	0.47
1:B:365:TRP:CD1	1:B:369:GLN:NE2	2.83	0.47
1:B:505:GLU:HG2	1:B:505:GLU:O	2.15	0.47
1:A:157:TYR:HD2	1:A:244:TRP:HE1	1.63	0.47
1:A:566:GLN:HB2	1:A:664:GLU:HB2	1.96	0.47
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.15	0.47
1:B:66:ARG:CD	1:B:236:ASN:HA	2.44	0.47
1:B:577:LEU:HD13	1:B:765:LEU:HD21	1.96	0.47
1:A:233:TYR:CE2	1:A:512:VAL:HG11	2.50	0.46
1:A:308:ILE:HD12	1:A:352:ILE:HD13	1.96	0.46
1:A:626:VAL:O	1:A:630:VAL:HG23	2.16	0.46
1:A:492:LEU:HD22	1:A:683:LEU:HD11	1.97	0.46
1:A:78:CYS:HB3	1:A:332:GLN:HE22	1.80	0.46
1:B:630:VAL:O	1:B:636:VAL:HG11	2.14	0.46
1:B:605:ILE:O	1:B:644:PHE:HA	2.15	0.46
1:A:506:LYS:HG3	1:A:530:PHE:CE1	2.49	0.46
1:A:420:LYS:O	1:A:422:VAL:HG13	2.15	0.46
1:B:55:LEU:HD13	1:B:112:ILE:HD11	1.96	0.46
1:A:778:GLU:CG	1:A:782:LYS:HE2	2.46	0.46
1:B:308:ILE:HD13	1:B:352:ILE:HG21	1.98	0.46
1:B:463:VAL:HG13	1:B:468:PHE:HD1	1.79	0.46
1:B:55:LEU:O	1:B:59:VAL:HG23	2.15	0.46
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.97	0.45
1:B:181:ASP:OD2	1:B:184:ARG:NE	2.49	0.45
1:A:693:ASP:O	1:A:696:ASN:HB2	2.16	0.45
1:A:376:ASN:O	1:A:459:HIS:HE1	1.98	0.45
1:B:225:PRO:HB3	1:B:244:TRP:CZ3	2.52	0.45
1:B:293:LEU:HD23	1:B:395:LEU:CD2	2.47	0.45
1:A:732:TYR:CZ	1:A:739:LYS:HG3	2.52	0.45
1:A:405:GLU:HA	1:A:405:GLU:OE2	2.16	0.45
1:A:83:TYR:CD1	1:A:155:TYR:HB2	2.53	0.44
1:B:300:VAL:HG13	1:B:345:ALA:HA	1.99	0.44
1:A:670:GLY:H	1:A:693:ASP:CG	2.21	0.44
1:B:131:LEU:HD22	1:B:161:TYR:HB2	2.00	0.44
1:B:152:LEU:HD23	1:B:829:PRO:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.58	0.44
1:B:393:GLU:HB2	1:B:400:LEU:HD22	2.00	0.44
1:B:715:ILE:HG23	1:B:716:ASP:N	2.32	0.44
1:A:93:ARG:HG2	1:A:126:GLU:HG2	1.99	0.44
1:A:568:LYS:O	1:A:607:GLY:HA3	2.17	0.43
1:B:650:VAL:HB	7:B:2328:HOH:O	2.18	0.43
1:A:209:THR:HG21	1:A:214:LYS:CE	2.43	0.43
1:A:307:ILE:HG23	7:A:2398:HOH:O	2.18	0.43
1:A:486:ILE:O	1:A:486:ILE:HG13	2.16	0.43
1:A:778:GLU:HG3	1:A:782:LYS:HE2	2.00	0.43
1:B:399:HIS:O	1:B:403:ILE:HG13	2.19	0.43
1:B:42:ASP:C	1:B:42:ASP:OD2	2.57	0.43
1:A:277:ARG:HG2	1:B:267:LEU:HD23	2.01	0.43
1:A:697:VAL:O	1:A:701:GLU:HG3	2.19	0.43
1:A:669:ALA:HA	1:A:693:ASP:HB2	2.00	0.43
1:B:432:GLU:O	1:B:437:LYS:HA	2.19	0.43
1:A:689:ILE:O	1:A:689:ILE:HG23	2.19	0.43
1:B:692:MET:HG2	1:B:710:ILE:HG21	2.01	0.43
1:A:373:ALA:HB3	7:A:2194:HOH:O	2.18	0.43
1:A:572:GLU:HG3	1:A:613:TYR:OH	2.18	0.42
1:A:738:LEU:HB2	1:A:777:TYR:CE2	2.53	0.42
1:A:80:LYS:HE2	1:A:334:ALA:HB2	2.00	0.42
1:A:326:PHE:CZ	1:A:357:GLU:HG3	2.55	0.42
1:A:346:ILE:CD1	1:A:445:CYS:HA	2.49	0.42
1:A:515:LEU:CG	1:A:809:GLY:HA2	2.48	0.42
1:B:350:MET:HE2	1:B:368:THR:OG1	2.19	0.42
1:A:556:LYS:C	1:A:556:LYS:HD3	2.40	0.42
1:B:405:GLU:OE2	1:B:405:GLU:HA	2.20	0.42
1:B:235:ASN:O	1:B:236:ASN:HB2	2.19	0.42
1:B:170:ILE:CG1	1:B:646:GLU:HG2	2.39	0.42
1:A:715:ILE:HG22	7:A:2297:HOH:O	2.19	0.42
1:B:143:PHE:O	1:B:147:MET:HG3	2.20	0.42
1:B:34:HIS:O	1:B:38:THR:HB	2.20	0.42
1:A:702:GLU:CD	1:A:810:LYS:HD2	2.40	0.42
1:B:315:LYS:O	1:B:316:PHE:C	2.58	0.42
1:B:703:ALA:O	1:B:707:ASN:ND2	2.48	0.42
1:A:311:PHE:CE1	1:A:329:PHE:HA	2.55	0.42
1:B:350:MET:HE1	1:B:364:ALA:CB	2.44	0.42
1:A:235:ASN:O	1:A:236:ASN:HB2	2.19	0.41
1:B:503:ILE:HG23	1:B:521:LEU:HD21	2.02	0.41
1:A:143:PHE:O	1:A:147:MET:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:PHE:CZ	1:A:552:GLU:HG3	2.55	0.41
1:A:735:LEU:HA	1:A:736:PRO:HD2	1.97	0.41
1:A:109:ASP:OD1	1:A:119:ILE:HG21	2.20	0.41
1:A:251:ASP:HA	1:B:178:GLU:OE1	2.20	0.41
1:B:314:SER:HB3	7:B:2199:HOH:O	2.20	0.41
1:A:170:ILE:HA	1:A:174:TRP:O	2.21	0.41
1:B:627:ALA:HA	1:B:642:VAL:HB	2.03	0.41
1:A:413:ARG:HH11	1:A:413:ARG:HG2	1.85	0.41
1:A:181:ASP:OD2	1:A:184:ARG:HB2	2.21	0.41
1:A:566:GLN:HA	7:A:2209:HOH:O	2.20	0.41
1:B:455:VAL:HG12	1:B:484:ASN:HD21	1.83	0.41
1:A:715:ILE:HG23	1:A:716:ASP:OD1	2.20	0.41
1:B:168:GLN:NE2	1:B:608:LYS:HA	2.35	0.41
1:A:474:LEU:N	1:A:474:LEU:HD12	2.36	0.41
1:B:206:VAL:HG11	1:B:401:GLU:OE1	2.20	0.41
1:A:136:LEU:O	1:A:136:LEU:HD23	2.21	0.40
1:B:555:VAL:HG22	1:B:631:ASN:HD22	1.86	0.40
1:B:509:GLU:O	1:B:512:VAL:HG23	2.21	0.40
1:B:709:PHE:HB3	1:B:783:CYS:SG	2.61	0.40
1:A:170:ILE:CG1	1:A:646:GLU:HG2	2.50	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	787/847 (93%)	752 (96%)	32 (4%)	3 (0%)	38	47
1	B	789/847 (93%)	743 (94%)	43 (5%)	3 (0%)	38	47
All	All	1576/1694 (93%)	1495 (95%)	75 (5%)	6 (0%)	38	47

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	ASP
1	A	555	VAL
1	B	421	ASP
1	A	434	GLU
1	B	434	GLU
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	694/740 (94%)	688 (99%)	6 (1%)	82	91
1	B	695/740 (94%)	680 (98%)	15 (2%)	57	74
All	All	1389/1480 (94%)	1368 (98%)	21 (2%)	70	83

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LYS
1	A	90	TYR
1	A	120	GLU
1	A	573	TYR
1	A	652	LEU
1	A	733	GLU
1	B	77	LYS
1	B	90	TYR
1	B	120	GLU
1	B	210	ASN
1	B	251	ASP
1	B	510	ASP
1	B	528	ASP
1	B	568	LYS
1	B	573	TYR
1	B	613	TYR
1	B	628	ASP
1	B	652	LEU

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Mol	Chain	Res	Type
1	B	706	GLU
1	B	716	ASP
1	B	733	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	73	HIS
1	A	96	GLN
1	A	105	GLN
1	A	250	ASN
1	A	332	GLN
1	A	369	GLN
1	A	484	ASN
1	A	517	GLN
1	A	822	GLN
1	B	23	ASN
1	B	62	HIS
1	B	73	HIS
1	B	219	GLN
1	B	332	GLN
1	B	369	GLN
1	B	484	ASN
1	B	539	GLN
1	B	747	ASN
1	B	793	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

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	PLP	A	860	1	15,15,16	2.11	3 (20%)	20,22,23	1.08	1 (5%)
2	NBG	A	861	-	15,15,15	1.47	3 (20%)	21,21,21	1.19	1 (4%)
4	700	A	862	-	24,33,33	1.86	9 (37%)	33,47,47	1.64	6 (18%)
5	CFF	A	863	-	7,15,15	1.22	0	8,23,23	1.17	2 (25%)
5	CFF	A	864	-	7,15,15	1.39	1 (14%)	8,23,23	1.20	2 (25%)
3	PLP	B	1860	1	15,15,16	1.75	2 (13%)	20,22,23	1.38	4 (20%)
2	NBG	B	1861	-	15,15,15	1.65	2 (13%)	21,21,21	1.33	2 (9%)
4	700	B	1862	-	24,33,33	1.88	7 (29%)	33,47,47	1.62	6 (18%)
5	CFF	B	1863	-	7,15,15	1.16	0	8,23,23	1.16	2 (25%)
6	MRD	B	1902	-	7,7,7	0.53	0	9,10,10	0.64	0
6	MRD	B	902	-	7,7,7	0.56	0	9,10,10	0.60	0
6	MRD	B	903	-	7,7,7	0.67	0	9,10,10	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	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	CFF	A	863	-	-	0/0/0/0	0/2/2/2
5	CFF	A	864	-	-	0/0/0/0	0/2/2/2
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	CFF	B	1863	-	-	0/0/0/0	0/2/2/2
6	MRD	B	1902	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1860	PLP	C4A-C4	-5.18	1.41	1.51
3	A	860	PLP	C4A-C4	-5.15	1.41	1.51
3	A	860	PLP	C3-C2	-4.11	1.37	1.40
4	B	1862	700	C7-C8	-2.27	1.35	1.39
3	B	1860	PLP	C3-C2	-2.13	1.39	1.40
4	A	862	700	C10-C11	2.01	1.56	1.51
4	B	1862	700	C10-C17	2.01	1.58	1.54
5	A	864	CFF	C6-C5	2.04	1.44	1.41
3	A	860	PLP	C5-C4	2.12	1.43	1.40
4	A	862	700	C16-C11	2.12	1.43	1.38
4	A	862	700	C12-C11	2.17	1.43	1.38
4	A	862	700	C15-C14	2.30	1.43	1.38
4	A	862	700	C13-C12	2.41	1.43	1.38
2	A	861	NBG	C3-C2	2.43	1.58	1.52
4	B	1862	700	C3-C4	2.46	1.42	1.38
4	A	862	700	C3-C4	2.51	1.42	1.38
4	B	1862	700	C7-C6	2.67	1.51	1.41
4	A	862	700	C7-C6	2.72	1.51	1.41
4	B	1862	700	C2-C3	2.75	1.42	1.36
4	A	862	700	C2-C3	2.80	1.42	1.36
2	A	861	NBG	C1-N1	2.80	1.46	1.43
2	A	861	NBG	C2-C1	2.87	1.56	1.52
2	B	1861	NBG	C1-N1	3.01	1.46	1.43
4	B	1862	700	C12-C11	3.22	1.45	1.38
4	A	862	700	C5-C4	3.49	1.43	1.36
4	B	1862	700	C5-C4	3.57	1.43	1.36
2	B	1861	NBG	C2-C1	4.35	1.57	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	862	700	C7-C6-C1	-4.49	102.36	106.27
4	B	1862	700	C7-C6-C1	-4.41	102.43	106.27
4	B	1862	700	C4-C5-C6	-2.89	117.21	119.18
4	B	1862	700	C3-C2-C1	-2.86	117.33	120.84
3	B	1860	PLP	O4P-P-O1P	-2.85	98.48	106.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	862	700	C3-C2-C1	-2.71	117.51	120.84
4	A	862	700	O1-C9-C8	-2.67	115.42	121.13
4	A	862	700	C4-C5-C6	-2.65	117.37	119.18
4	B	1862	700	O1-C9-C8	-2.62	115.52	121.13
5	A	864	CFF	C10-N1-C2	-2.31	114.15	119.75
2	B	1861	NBG	C2-C1-N1	-2.19	108.74	111.30
5	A	863	CFF	C10-N1-C2	-2.18	114.46	119.75
5	A	863	CFF	C5-C6-N1	-2.11	115.87	118.28
5	B	1863	CFF	C10-N1-C2	-2.11	114.64	119.75
5	A	864	CFF	C5-C6-N1	-2.04	115.94	118.28
5	B	1863	CFF	C5-C6-N1	-2.04	115.95	118.28
3	A	860	PLP	O2P-P-O4P	-2.01	101.39	106.73
3	B	1860	PLP	C6-C5-C4	2.06	119.90	118.18
3	B	1860	PLP	O2P-P-O1P	2.11	118.75	110.50
3	B	1860	PLP	O4P-C5A-C5	2.82	114.99	109.32
4	B	1862	700	C8-C9-N1	3.65	122.64	115.20
4	A	862	700	C8-N2-C1	3.78	112.27	104.47
4	B	1862	700	C8-N2-C1	3.85	112.42	104.47
2	A	861	NBG	C5-O5-C1	3.86	117.85	112.53
4	A	862	700	C8-C9-N1	4.04	123.43	115.20
2	B	1861	NBG	C5-O5-C1	4.38	118.57	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	903	MRD	1	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.