Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2023 – 07:40 AM EDT

PDB ID	:	1FU8
Title	:	STRUCTURES OF GLYCOGEN PHOSPHORYLASE-INHIBITOR COMPLEXES AND THE IMPLICATIONS FOR STRUCTURE-BASED DRUG DESIGN
Authors	:	Watson, K.A.; Tsitsanou, K.E.; Gregoriou, M.; Zographos, S.E.; Skamnaki, V.T.; Oikonomakos, N.G.; Fleet, G.W.; Johnson, L.N.
Deposited on	:	2000-09-14
Resolution	:	2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

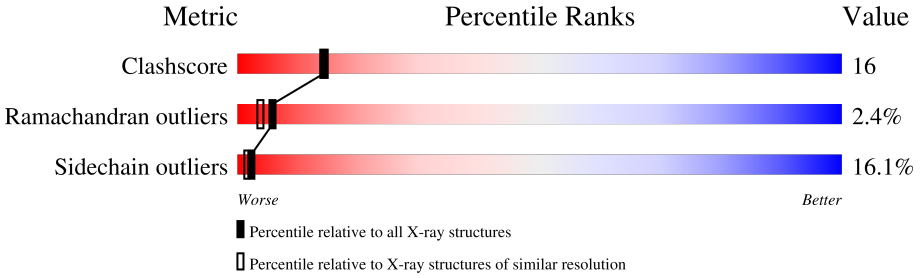
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6974 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.

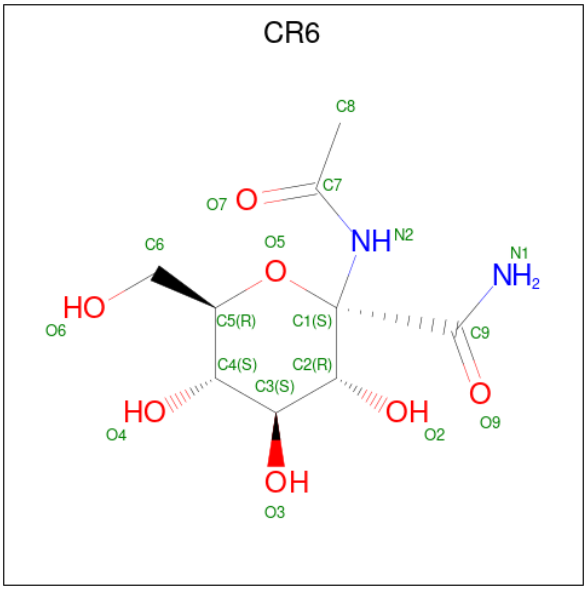
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	830	6749	4303	1189	1227	30	0	0	0

There is a discrepancy between the modelled and reference sequences:

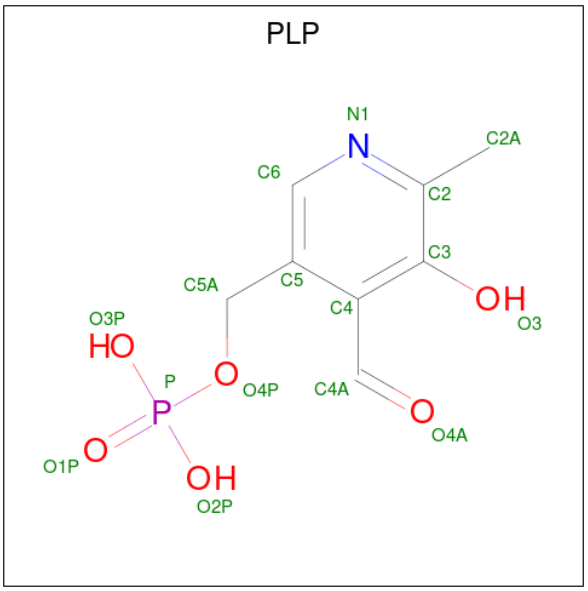
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	SEE REMARK 999	UNP P00489

- Molecule 2 is 1-DEOXY-1-ACETYLAMINO-BETA-D-GLUCO-2-HEPTULOPYRANOSO NAMIDE (three-letter code: CR6) (formula: $C_9H_{16}N_2O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	18	9	2	7	0	0

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	192	192	192	0	0

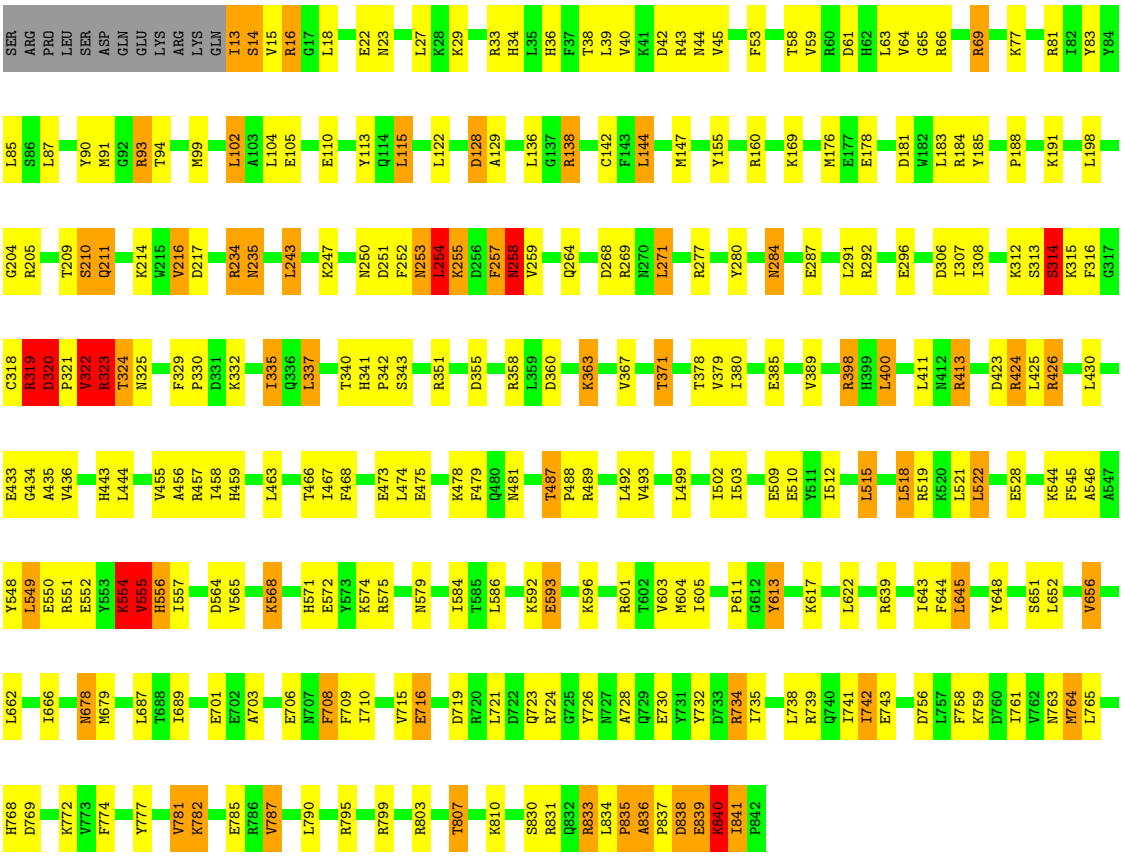
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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

Chain A: 65% 26% 7% ••



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	128.50Å 128.50Å 116.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.40 – 2.35	Depositor
% Data completeness (in resolution range)	88.0 (15.40-2.35)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.198 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6974	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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: PLP, CR6

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	0.47	0/6903	0.67	2/9344 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	554	LYS	N-CA-C	7.23	130.51	111.00
1	A	556	HIS	N-CA-C	5.41	125.62	111.00

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	6749	0	6695	209	0
2	A	18	0	16	3	0
3	A	15	0	7	0	0
4	A	192	0	0	13	1
All	All	6974	0	6718	210	1

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 16.

All (210) 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:320:ASP:HB3	1:A:321:PRO:HD2	1.30	1.07
1:A:413:ARG:HG2	1:A:413:ARG:HH21	1.24	1.00
1:A:15:VAL:HB	4:A:1191:HOH:O	1.63	0.96
1:A:251:ASP:CG	1:A:252:PHE:H	1.70	0.95
1:A:320:ASP:HB3	1:A:321:PRO:CD	1.99	0.91
1:A:554:LYS:O	1:A:555:VAL:HG22	1.73	0.88
1:A:764:MET:HE3	4:A:1063:HOH:O	1.73	0.88
1:A:379:VAL:HG22	4:A:1101:HOH:O	1.75	0.86
1:A:319:ARG:HG2	1:A:320:ASP:H	1.42	0.85
1:A:319:ARG:CG	1:A:320:ASP:H	1.92	0.82
1:A:515:LEU:HD22	1:A:518:LEU:HD22	1.60	0.82
1:A:455:VAL:H	1:A:459:HIS:HD2	1.29	0.80
1:A:839:GLU:O	1:A:840:LYS:HG3	1.83	0.78
1:A:322:VAL:O	1:A:323:ARG:HB2	1.84	0.76
1:A:413:ARG:HG2	1:A:413:ARG:NH2	1.98	0.75
1:A:764:MET:HE2	1:A:769:ASP:HA	1.68	0.74
1:A:235:ASN:H	1:A:235:ASN:HD22	1.33	0.74
1:A:66:ARG:HG3	1:A:837:PRO:HB3	1.70	0.74
1:A:546:ALA:HA	1:A:557:ILE:HD11	1.69	0.73
1:A:545:PHE:CZ	1:A:656:VAL:HG13	2.23	0.73
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.71	0.73
1:A:251:ASP:CG	1:A:252:PHE:N	2.42	0.73
1:A:678:ASN:HD22	1:A:679:MET:H	1.36	0.73
1:A:571:HIS:HB2	1:A:574:LYS:HG3	1.71	0.72
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.72	0.72
1:A:703:ALA:HB2	1:A:807:THR:HG21	1.73	0.71
1:A:678:ASN:ND2	1:A:679:MET:H	1.90	0.69
1:A:708:PHE:HB3	1:A:710:ILE:CD1	2.22	0.69
1:A:601:ARG:HD2	4:A:1032:HOH:O	1.91	0.69
1:A:144:LEU:HD12	1:A:147:MET:HE3	1.74	0.68
1:A:13:ILE:O	1:A:14:SER:HB2	1.93	0.67
1:A:69:ARG:NH2	1:A:840:LYS:HG2	2.09	0.67
1:A:323:ARG:O	1:A:325:ASN:N	2.28	0.67
1:A:678:ASN:HD22	1:A:678:ASN:N	1.92	0.67
1:A:703:ALA:CB	1:A:807:THR:HG21	2.25	0.67
1:A:716:GLU:H	1:A:716:GLU:CD	1.97	0.67
1:A:841:ILE:HG23	1:A:841:ILE:O	1.95	0.66
1:A:764:MET:CE	1:A:769:ASP:HA	2.25	0.66
1:A:142:CYS:SG	1:A:487:THR:HG22	2.36	0.66
1:A:488:PRO:O	1:A:492:LEU:HB3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:GLU:O	1:A:734:ARG:HG2	1.96	0.65
1:A:284:ASN:ND2	2:A:998:CR6:H82	2.12	0.65
1:A:367:VAL:O	1:A:371:THR:HG23	1.97	0.64
1:A:65:GLY:O	1:A:69:ARG:HG2	1.96	0.64
1:A:184:ARG:HE	1:A:185:TYR:HE2	1.46	0.63
1:A:257:PHE:O	1:A:258:ASN:HB2	1.98	0.63
1:A:16:ARG:HB3	1:A:105:GLU:HB3	1.79	0.63
1:A:15:VAL:HG21	1:A:509:GLU:CD	2.19	0.63
1:A:795:ARG:O	1:A:799:ARG:HG3	1.99	0.63
1:A:138:ARG:O	1:A:138:ARG:HD3	1.99	0.62
1:A:335:ILE:HD11	1:A:337:LEU:CD1	2.29	0.62
1:A:708:PHE:HB3	1:A:710:ILE:HD12	1.80	0.62
1:A:316:PHE:HE2	1:A:332:LYS:HZ1	1.46	0.62
1:A:841:ILE:O	1:A:841:ILE:CG2	2.48	0.62
1:A:144:LEU:HA	1:A:147:MET:HE2	1.82	0.61
1:A:15:VAL:HG21	1:A:509:GLU:OE1	2.01	0.61
1:A:493:VAL:CG2	1:A:512:ILE:HD12	2.30	0.61
1:A:554:LYS:C	1:A:555:VAL:HG22	2.21	0.60
1:A:15:VAL:HG13	1:A:15:VAL:O	2.02	0.59
1:A:319:ARG:CG	1:A:320:ASP:N	2.64	0.59
1:A:592:LYS:HG3	1:A:593:GLU:HG2	1.85	0.59
1:A:253:ASN:O	1:A:254:LEU:HB2	2.01	0.58
1:A:564:ASP:O	1:A:603:VAL:HA	2.03	0.58
1:A:61:ASP:O	1:A:64:VAL:HG22	2.03	0.58
1:A:319:ARG:N	1:A:319:ARG:HD3	2.17	0.58
1:A:571:HIS:HB2	1:A:574:LYS:CG	2.33	0.58
1:A:703:ALA:HB2	1:A:807:THR:CG2	2.34	0.57
1:A:424:ARG:NH1	1:A:473:GLU:OE1	2.35	0.57
1:A:703:ALA:CA	1:A:807:THR:HG21	2.35	0.57
1:A:678:ASN:ND2	1:A:678:ASN:N	2.52	0.57
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.88	0.56
1:A:34:HIS:HE1	1:A:61:ASP:OD1	1.89	0.56
1:A:144:LEU:HD12	1:A:147:MET:CE	2.35	0.56
1:A:235:ASN:HD22	1:A:235:ASN:N	1.98	0.56
1:A:66:ARG:CG	1:A:837:PRO:HB3	2.35	0.56
1:A:316:PHE:HE2	1:A:332:LYS:NZ	2.03	0.55
1:A:367:VAL:O	1:A:371:THR:CG2	2.55	0.55
1:A:554:LYS:O	1:A:555:VAL:HG13	2.07	0.55
1:A:709:PHE:CD1	1:A:787:VAL:HG12	2.42	0.55
1:A:604:MET:HB3	1:A:645:LEU:HD22	1.88	0.54
1:A:335:ILE:HD11	1:A:337:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:TYR:HA	1:A:652:LEU:HD23	1.90	0.54
1:A:703:ALA:HA	1:A:807:THR:HG21	1.89	0.54
1:A:689:ILE:HG23	1:A:689:ILE:O	2.07	0.54
1:A:423:ASP:O	1:A:426:ARG:HG3	2.08	0.53
1:A:571:HIS:ND1	4:A:1118:HOH:O	2.34	0.53
1:A:181:ASP:HB3	1:A:184:ARG:NH2	2.24	0.53
1:A:719:ASP:O	1:A:723:GLN:HG2	2.08	0.53
1:A:463:LEU:HA	1:A:467:ILE:HG22	1.90	0.53
1:A:458:ILE:HG22	4:A:1087:HOH:O	2.09	0.52
1:A:413:ARG:NH2	1:A:413:ARG:CG	2.72	0.52
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.09	0.52
1:A:320:ASP:CB	1:A:321:PRO:CD	2.84	0.51
1:A:479:PHE:HB3	4:A:1171:HOH:O	2.10	0.51
1:A:322:VAL:O	1:A:322:VAL:HG12	2.11	0.51
1:A:335:ILE:O	1:A:335:ILE:HG13	2.07	0.51
1:A:554:LYS:O	1:A:555:VAL:CG2	2.53	0.51
1:A:689:ILE:HA	1:A:709:PHE:HB2	1.93	0.51
1:A:732:TYR:CZ	1:A:739:ARG:HG3	2.46	0.51
1:A:360:ASP:OD1	1:A:363:LYS:HB2	2.11	0.51
1:A:280:TYR:OH	1:A:291:LEU:HB3	2.11	0.51
1:A:58:THR:O	1:A:61:ASP:HB2	2.11	0.51
1:A:91:MET:HB2	1:A:129:ALA:HB3	1.91	0.51
1:A:458:ILE:HD11	1:A:715:VAL:HG21	1.92	0.51
1:A:87:LEU:HD13	1:A:341:HIS:HB3	1.93	0.51
1:A:758:PHE:HD2	1:A:761:ILE:HD12	1.76	0.51
1:A:110:GLU:O	1:A:113:TYR:HB3	2.11	0.51
1:A:129:ALA:HB2	4:A:1083:HOH:O	2.11	0.51
1:A:456:ALA:C	1:A:481:ASN:HD21	2.15	0.51
1:A:268:ASP:O	1:A:271:LEU:HB2	2.10	0.50
1:A:398:ARG:O	1:A:398:ARG:HG3	2.10	0.50
1:A:235:ASN:HA	1:A:833:ARG:HG3	1.94	0.50
1:A:708:PHE:HB3	1:A:710:ILE:HD11	1.94	0.50
1:A:59:VAL:HG21	1:A:99:MET:HE2	1.94	0.50
1:A:351:ARG:O	1:A:355:ASP:HB2	2.12	0.50
1:A:434:GLY:O	1:A:435:ALA:C	2.50	0.50
1:A:592:LYS:HD2	1:A:592:LYS:O	2.12	0.50
1:A:575:ARG:HD3	1:A:666:ILE:O	2.12	0.49
1:A:284:ASN:HD21	2:A:998:CR6:H82	1.78	0.49
1:A:810:LYS:O	1:A:810:LYS:HG2	2.13	0.49
1:A:466:THR:HG22	1:A:467:ILE:N	2.28	0.49
1:A:836:ALA:HB1	1:A:837:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HD13	1:A:335:ILE:HD12	1.94	0.48
1:A:503:ILE:HG12	1:A:521:LEU:HD11	1.94	0.48
1:A:250:ASN:HA	1:A:269:ARG:HH22	1.78	0.48
1:A:430:LEU:HD22	1:A:443:HIS:HB3	1.96	0.48
1:A:678:ASN:ND2	1:A:679:MET:N	2.60	0.48
1:A:204:GLY:HA2	1:A:217:ASP:O	2.14	0.47
1:A:572:GLU:HG3	1:A:613:TYR:OH	2.14	0.47
1:A:313:SER:O	1:A:314:SER:C	2.51	0.47
1:A:325:ASN:HA	4:A:1169:HOH:O	2.15	0.47
1:A:493:VAL:HG21	1:A:512:ILE:HD12	1.95	0.47
1:A:467:ILE:HG23	1:A:468:PHE:CG	2.49	0.47
1:A:251:ASP:C	1:A:255:LYS:HB3	2.35	0.47
1:A:519:ARG:O	1:A:522:LEU:HB2	2.14	0.47
1:A:836:ALA:HB1	1:A:837:PRO:HD2	1.96	0.47
1:A:604:MET:HB3	1:A:645:LEU:CD2	2.44	0.46
1:A:36:HIS:O	1:A:40:VAL:HA	2.15	0.46
1:A:475:GLU:CD	1:A:478:LYS:HE3	2.36	0.46
1:A:548:TYR:HA	1:A:551:ARG:HH21	1.80	0.46
1:A:209:THR:O	1:A:211:GLN:N	2.47	0.46
1:A:144:LEU:HA	1:A:147:MET:CE	2.44	0.46
1:A:742:ILE:HD11	1:A:774:PHE:CZ	2.50	0.46
1:A:678:ASN:HD22	1:A:679:MET:N	2.06	0.46
1:A:42:ASP:O	1:A:44:ASN:N	2.49	0.46
2:A:998:CR6:O9	2:A:998:CR6:H51	2.15	0.46
1:A:564:ASP:HB3	1:A:603:VAL:HA	1.98	0.46
1:A:716:GLU:CD	1:A:716:GLU:N	2.67	0.45
1:A:728:ALA:HB1	1:A:774:PHE:CD1	2.51	0.45
1:A:467:ILE:HG23	1:A:468:PHE:N	2.31	0.45
1:A:319:ARG:NE	1:A:320:ASP:N	2.63	0.45
1:A:340:THR:O	1:A:343:SER:HB3	2.17	0.45
1:A:251:ASP:O	1:A:255:LYS:N	2.38	0.45
1:A:53:PHE:HE2	1:A:188:PRO:HD3	1.82	0.45
1:A:128:ASP:OD2	1:A:651:SER:HB3	2.17	0.44
1:A:169:LYS:HB2	1:A:176:MET:HB2	1.99	0.44
1:A:296:GLU:OE1	1:A:385:GLU:OE2	2.35	0.44
1:A:739:ARG:O	1:A:743:GLU:HG3	2.18	0.44
1:A:835:PRO:O	1:A:836:ALA:O	2.36	0.44
1:A:115:LEU:HD12	1:A:115:LEU:HA	1.85	0.44
1:A:308:ILE:O	1:A:312:LYS:HG3	2.18	0.44
1:A:322:VAL:O	1:A:322:VAL:CG1	2.66	0.44
1:A:93:ARG:CG	1:A:93:ARG:HH21	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ARG:HH12	1:A:701:GLU:CD	2.20	0.43
1:A:319:ARG:CD	1:A:320:ASP:H	2.30	0.43
1:A:831:ARG:O	1:A:833:ARG:NH1	2.51	0.43
1:A:252:PHE:C	1:A:254:LEU:H	2.20	0.43
1:A:467:ILE:CG2	1:A:468:PHE:N	2.82	0.43
1:A:568:LYS:HE2	4:A:1113:HOH:O	2.17	0.43
1:A:499:LEU:HD12	1:A:502:ILE:HD11	2.00	0.43
1:A:639:ARG:HG2	4:A:1165:HOH:O	2.18	0.43
1:A:234:ARG:NH1	4:A:1024:HOH:O	2.52	0.43
1:A:319:ARG:NE	1:A:320:ASP:H	2.17	0.43
1:A:81:ARG:CG	1:A:155:TYR:HE2	2.31	0.43
1:A:136:LEU:C	1:A:136:LEU:HD23	2.39	0.42
1:A:489:ARG:N	1:A:489:ARG:HD3	2.33	0.42
1:A:169:LYS:O	1:A:176:MET:N	2.48	0.42
1:A:205:ARG:HG2	1:A:216:VAL:HG12	2.00	0.42
1:A:83:TYR:CZ	1:A:307:ILE:HG12	2.55	0.42
1:A:181:ASP:HB3	1:A:184:ARG:HH21	1.84	0.42
1:A:549:LEU:HA	1:A:549:LEU:HD12	1.73	0.42
1:A:777:TYR:O	1:A:781:VAL:HG13	2.20	0.42
1:A:735:ILE:HG22	1:A:738:LEU:H	1.84	0.42
1:A:455:VAL:H	1:A:459:HIS:CD2	2.19	0.42
1:A:341:HIS:N	1:A:342:PRO:CD	2.83	0.42
1:A:235:ASN:N	1:A:235:ASN:ND2	2.66	0.42
1:A:782:LYS:O	1:A:785:GLU:HB2	2.19	0.42
1:A:834:LEU:O	1:A:836:ALA:N	2.53	0.42
1:A:63:LEU:HB3	1:A:102:LEU:HD21	2.01	0.41
1:A:296:GLU:HG2	1:A:341:HIS:O	2.20	0.41
1:A:378:THR:OG1	1:A:380:ILE:HG12	2.20	0.41
1:A:521:LEU:HD23	1:A:521:LEU:HA	1.93	0.41
1:A:730:GLU:O	1:A:734:ARG:CG	2.67	0.41
1:A:678:ASN:ND2	1:A:679:MET:HG3	2.35	0.41
1:A:734:ARG:HG2	1:A:734:ARG:H	1.70	0.41
1:A:93:ARG:HH21	1:A:93:ARG:HG3	1.86	0.41
1:A:605:ILE:O	1:A:644:PHE:HA	2.20	0.41
1:A:522:LEU:HD12	1:A:522:LEU:HA	1.90	0.41
1:A:834:LEU:HA	1:A:834:LEU:HD12	1.82	0.41
1:A:611:PRO:HA	1:A:617:LYS:HE3	2.02	0.40
1:A:355:ASP:OD1	1:A:398:ARG:HD3	2.21	0.40
1:A:550:GLU:O	1:A:554:LYS:HG2	2.21	0.40
1:A:77:LYS:HA	1:A:77:LYS:HD2	1.93	0.40
1:A:216:VAL:HG13	1:A:217:ASP:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:VAL:HG13	1:A:400:LEU:HD11	2.04	0.40
1:A:411:LEU:HD23	1:A:411:LEU:HA	1.90	0.40
1:A:183:LEU:HB2	4:A:1142:HOH:O	2.21	0.40
1:A:216:VAL:HG13	1:A:217:ASP:CG	2.42	0.40
1:A:493:VAL:HG22	1:A:512:ILE:HD12	2.03	0.40
1:A:584:ILE:HG21	1:A:741:ILE:HG23	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1178:HOH:O	4:A:1179:HOH:O[4_555]	2.11	0.09

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	828/842 (98%)	760 (92%)	48 (6%)	20 (2%)	6 4

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	210	SER
1	A	254	LEU
1	A	258	ASN
1	A	320	ASP
1	A	323	ARG
1	A	324	THR
1	A	555	VAL
1	A	556	HIS
1	A	839	GLU

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Mol	Chain	Res	Type
1	A	840	LYS
1	A	43	ARG
1	A	259	VAL
1	A	835	PRO
1	A	836	ALA
1	A	838	ASP
1	A	314	SER
1	A	554	LYS
1	A	319	ARG
1	A	322	VAL

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	719/731 (98%)	603 (84%)	116 (16%)	2 1

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	16	ARG
1	A	18	LEU
1	A	22	GLU
1	A	23	ASN
1	A	27	LEU
1	A	29	LYS
1	A	33	ARG
1	A	39	LEU
1	A	45	VAL
1	A	69	ARG
1	A	90	TYR
1	A	93	ARG
1	A	94	THR
1	A	102	LEU
1	A	104	LEU

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Mol	Chain	Res	Type
1	A	115	LEU
1	A	122	LEU
1	A	128	ASP
1	A	138	ARG
1	A	144	LEU
1	A	178	GLU
1	A	191	LYS
1	A	198	LEU
1	A	210	SER
1	A	211	GLN
1	A	214	LYS
1	A	216	VAL
1	A	234	ARG
1	A	235	ASN
1	A	243	LEU
1	A	247	LYS
1	A	253	ASN
1	A	254	LEU
1	A	255	LYS
1	A	257	PHE
1	A	258	ASN
1	A	264	GLN
1	A	271	LEU
1	A	277	ARG
1	A	284	ASN
1	A	287	GLU
1	A	292	ARG
1	A	306	ASP
1	A	314	SER
1	A	315	LYS
1	A	318	CYS
1	A	319	ARG
1	A	320	ASP
1	A	322	VAL
1	A	323	ARG
1	A	324	THR
1	A	335	ILE
1	A	337	LEU
1	A	358	ARG
1	A	363	LYS
1	A	371	THR
1	A	398	ARG

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Mol	Chain	Res	Type
1	A	400	LEU
1	A	413	ARG
1	A	424	ARG
1	A	425	LEU
1	A	426	ARG
1	A	433	GLU
1	A	436	VAL
1	A	444	LEU
1	A	474	LEU
1	A	487	THR
1	A	510	GLU
1	A	515	LEU
1	A	518	LEU
1	A	522	LEU
1	A	528	GLU
1	A	544	LYS
1	A	549	LEU
1	A	552	GLU
1	A	555	VAL
1	A	565	VAL
1	A	568	LYS
1	A	579	ASN
1	A	586	LEU
1	A	593	GLU
1	A	596	LYS
1	A	613	TYR
1	A	622	LEU
1	A	643	ILE
1	A	645	LEU
1	A	656	VAL
1	A	662	LEU
1	A	678	ASN
1	A	687	LEU
1	A	706	GLU
1	A	708	PHE
1	A	716	GLU
1	A	721	LEU
1	A	724	ARG
1	A	734	ARG
1	A	742	ILE
1	A	756	ASP
1	A	759	LYS

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Mol	Chain	Res	Type
1	A	763	ASN
1	A	764	MET
1	A	765	LEU
1	A	768	HIS
1	A	772	LYS
1	A	781	VAL
1	A	782	LYS
1	A	787	VAL
1	A	790	LEU
1	A	803	ARG
1	A	807	THR
1	A	830	SER
1	A	833	ARG
1	A	838	ASP
1	A	840	LYS
1	A	841	ILE

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

Mol	Chain	Res	Type
1	A	34	HIS
1	A	211	GLN
1	A	235	ASN
1	A	253	ASN
1	A	284	ASN
1	A	412	ASN
1	A	450	HIS
1	A	459	HIS
1	A	477	HIS
1	A	481	ASN
1	A	484	ASN
1	A	560	ASN
1	A	566	GLN
1	A	579	ASN
1	A	678	ASN
1	A	763	ASN
1	A	832	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	CR6	A	998	-	16,18,18	1.45	4 (25%)	17,27,27	1.86	4 (23%)
3	PLP	A	999	1	15,15,16	2.02	5 (33%)	20,22,23	1.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CR6	A	998	-	-	0/8/36/36	0/1/1/1
3	PLP	A	999	1	-	2/6/6/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	P-O2P	4.78	1.73	1.54
2	A	998	CR6	C4-C5	3.29	1.60	1.53
3	A	999	PLP	C4A-C4	3.02	1.57	1.51
2	A	998	CR6	C3-C4	2.87	1.59	1.52
3	A	999	PLP	C2A-C2	2.78	1.55	1.50
2	A	998	CR6	C1-C9	2.55	1.58	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	P-O3P	-2.19	1.46	1.54
2	A	998	CR6	O4-C4	-2.04	1.38	1.43
3	A	999	PLP	P-O4P	-2.01	1.53	1.60

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	998	CR6	C1-N2-C7	4.81	135.15	124.54
2	A	998	CR6	C4-C3-C2	-4.15	105.58	111.30
2	A	998	CR6	O2-C2-C1	2.41	114.72	108.97
2	A	998	CR6	O2-C2-C3	-2.08	105.42	110.03

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	PLP	C4-C5-C5A-O4P
3	A	999	PLP	C6-C5-C5A-O4P

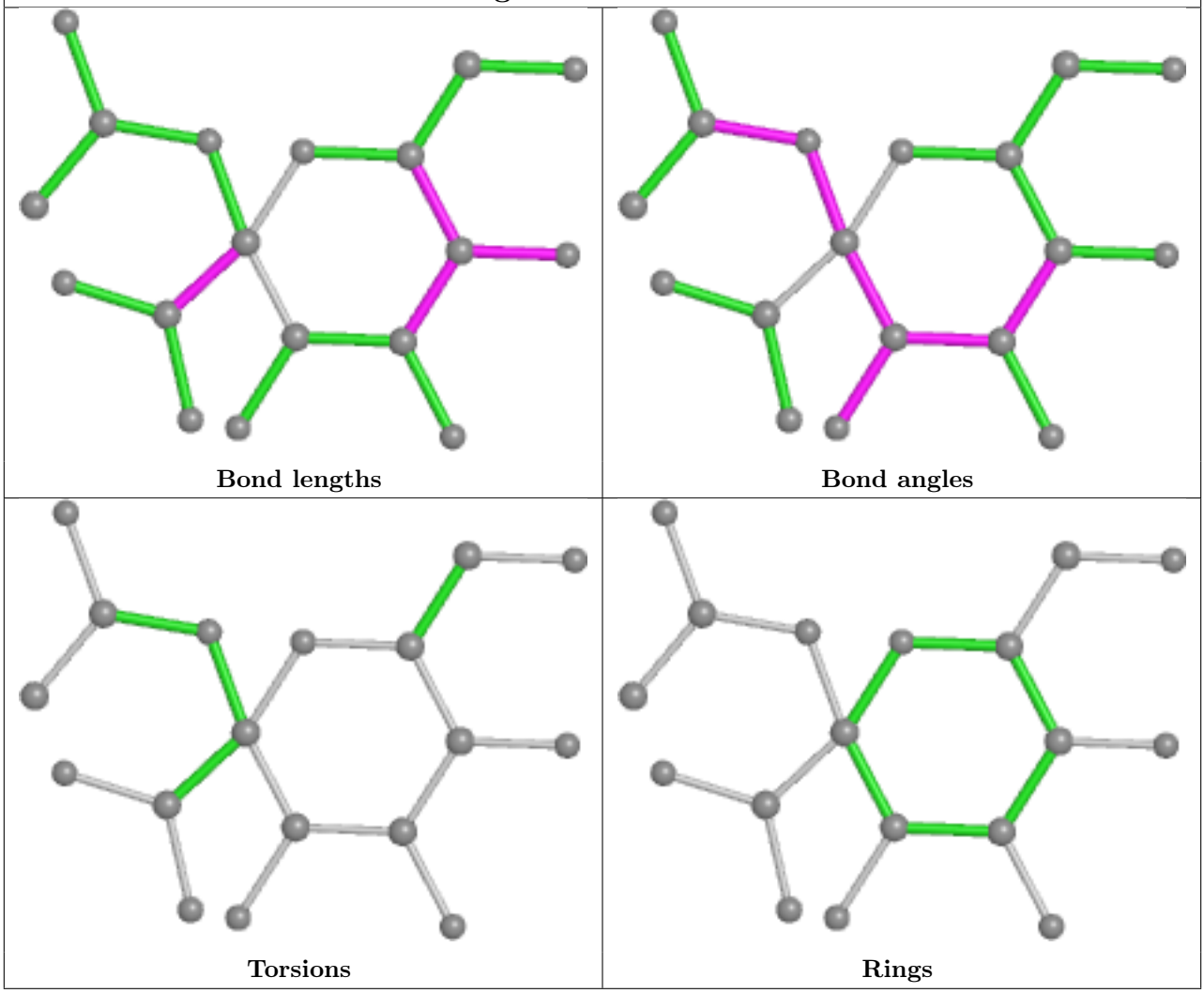
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	998	CR6	3	0

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

Ligand CR6 A 998



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.