Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 10:36 AM EDT

PDB ID	:	3CDU
Title	:	Crystal structure of coxsackievirus B3 RNA-dependent RNA polymerase (3Dpol) in complex with a pyrophosphate
Authors	:	Gruez, A.; Selisko, B.; Roberts, M.; Bricogne, G.; Bussetta, C.; Canard, B.
Deposited on	:	2008-02-27
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
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 (i)) were used in the production of this report:

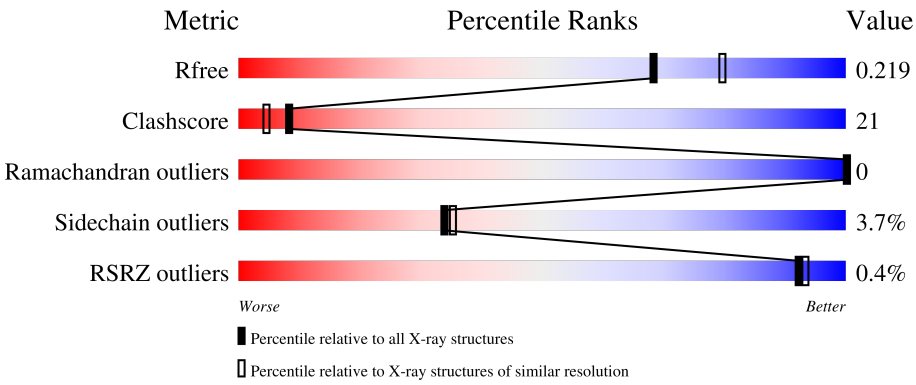
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 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% 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.

Mol	Chain	Length	Quality of chain
1	A	468	80% 19% •

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
4	ACT	A	477	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	A	478	-	X	X	-
5	POP	A	482	-	X	X	-
6	GOL	A	487	-	-	X	-
6	GOL	A	489	-	-	X	-
6	GOL	A	491	-	X	-	-
6	GOL	A	492	-	-	X	-
6	GOL	A	498	-	-	X	-
6	GOL	A	500	-	-	X	-
6	GOL	A	501	-	-	X	-
6	GOL	A	502	-	-	X	-
6	GOL	A	505	-	-	X	-
6	GOL	A	506	-	X	X	-
6	GOL	A	510	-	X	-	-
6	GOL	A	511	-	-	X	X
6	GOL	A	512	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4323 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 RNA-directed RNA polymerase 3D-POL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	468	3778	2420	641	695	22	0	6	0

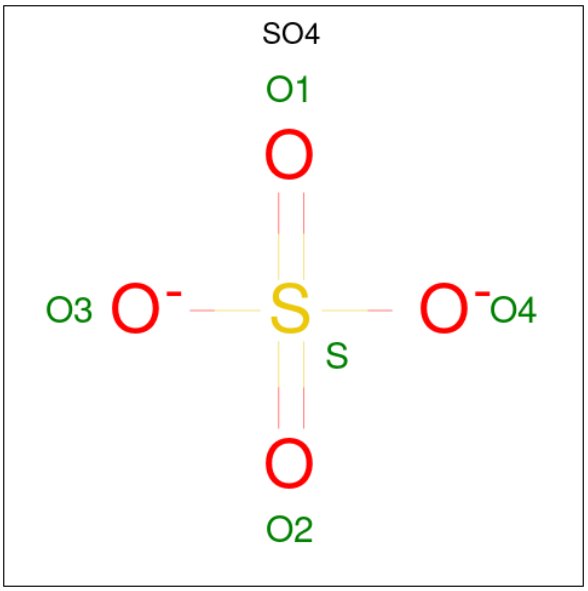
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	463	HIS	-	expression tag	UNP P03313
A	464	HIS	-	expression tag	UNP P03313
A	465	HIS	-	expression tag	UNP P03313
A	466	HIS	-	expression tag	UNP P03313
A	467	HIS	-	expression tag	UNP P03313
A	468	HIS	-	expression tag	UNP P03313

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

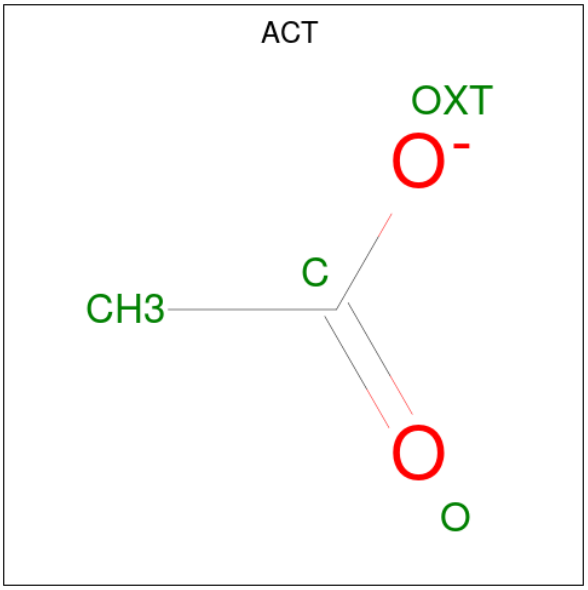
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	6	6	6	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

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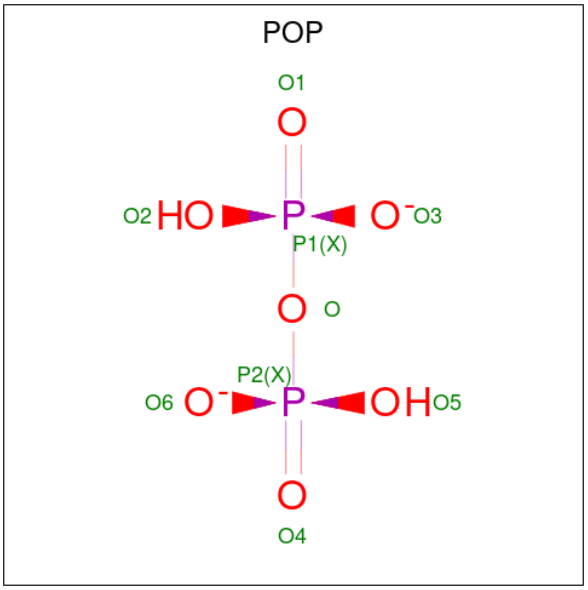
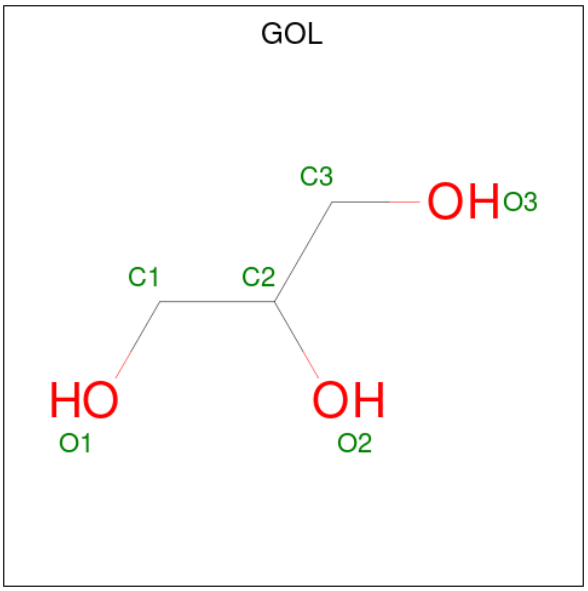
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0
			Total	C	O		
4	A	1	4	2	2	0	0
			Total	C	O		
4	A	1	4	2	2	0	0

- Molecule 5 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
5	A	1	9	7	2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0

- Molecule 7 is water.

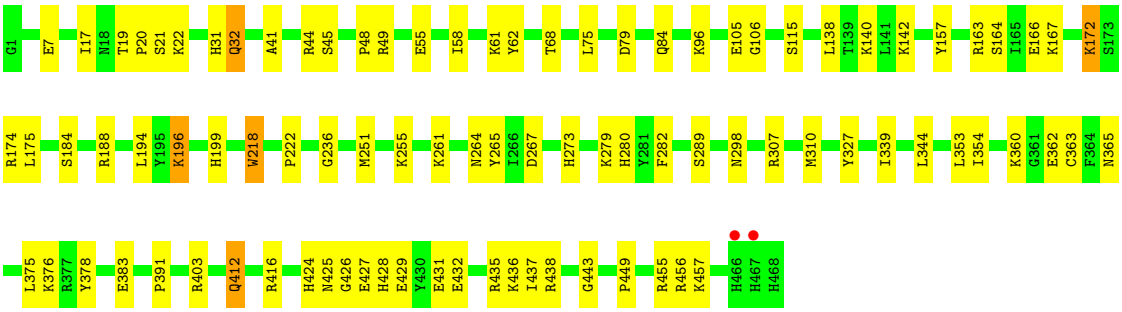
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	321	321	321	0	0

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 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.

• Molecule 1: RNA-directed RNA polymerase 3D-POL

Chain A: 80% 19%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	74.41Å 74.41Å 285.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.98 – 2.10 72.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	84.7 (71.98-2.10) 84.8 (72.01-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	4.95 (at 2.10Å)	Xtriage
Refinement program	BUSTER-TNT 2.3.0	Depositor
R, R_{free}	0.178 , 0.220 0.175 , 0.219	Depositor DCC
R_{free} test set	2045 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4323	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: ACT, POP, SO4, GOL, CL

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	0.64	0/3905	0.71	0/5284

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	3778	0	3723	151	0
2	A	6	0	0	0	0
3	A	5	0	0	0	0
4	A	24	0	18	21	0
5	A	9	0	0	6	0
6	A	180	0	239	91	0
7	A	321	0	0	12	0
All	All	4323	0	3980	168	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 21.

All (168) 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:273[A]:HIS:NE2	1:A:280:HIS:NE2	2.03	1.05
1:A:61:LYS:HD2	6:A:500:GOL:H11	1.39	1.04
1:A:360:LYS:NZ	6:A:492:GOL:H32	1.84	0.93
1:A:61:LYS:HD2	6:A:500:GOL:C1	2.00	0.91
1:A:310:MET:HE1	1:A:339:ILE:HG21	1.51	0.90
1:A:61:LYS:NZ	6:A:500:GOL:H12	1.88	0.88
1:A:455:ARG:HH21	6:A:486:GOL:H12	1.37	0.88
1:A:403:ARG:HH22	6:A:505:GOL:H12	1.40	0.85
1:A:31:HIS:CE1	6:A:505:GOL:H31	2.11	0.85
1:A:403:ARG:NH2	6:A:505:GOL:H12	1.97	0.79
1:A:424:HIS:O	6:A:499:GOL:H12	1.80	0.79
1:A:427:GLU:O	1:A:431[A]:GLU:HG3	1.82	0.78
1:A:429:GLU:HG2	4:A:478:ACT:H2	1.65	0.78
1:A:383:GLU:HB2	6:A:506:GOL:H12	1.66	0.76
1:A:49:ARG:HG3	6:A:511:GOL:H11	1.66	0.76
1:A:45:SER:H	6:A:498:GOL:C3	1.99	0.76
1:A:31:HIS:NE2	6:A:505:GOL:H31	1.99	0.75
1:A:279:LYS:HG3	6:A:497:GOL:H12	1.68	0.75
1:A:167[B]:LYS:NZ	5:A:482:POP:O6	2.21	0.74
1:A:264:ASN:HB3	6:A:495:GOL:H31	1.69	0.74
1:A:429:GLU:HG2	4:A:478:ACT:C	2.19	0.73
1:A:17:ILE:HG22	1:A:19:THR:HG23	1.68	0.73
1:A:172:LYS:HA	1:A:172:LYS:HE2	1.72	0.72
1:A:49:ARG:HD3	6:A:511:GOL:O1	1.91	0.71
1:A:438:ARG:NH1	7:A:813:HOH:O	2.24	0.71
6:A:499:GOL:H31	6:A:506:GOL:O2	1.90	0.71
1:A:49:ARG:CG	6:A:511:GOL:H11	2.21	0.70
1:A:163[B]:ARG:NH2	5:A:482:POP:O1	2.24	0.70
1:A:383:GLU:CB	6:A:506:GOL:H12	2.20	0.70
1:A:61:LYS:HZ2	6:A:500:GOL:H12	1.54	0.70
1:A:429:GLU:HG2	4:A:478:ACT:CH3	2.22	0.69
6:A:489:GOL:H11	7:A:751:HOH:O	1.93	0.68
1:A:45:SER:OG	6:A:498:GOL:H32	1.92	0.68
1:A:22:LYS:CE	4:A:477:ACT:H3	2.26	0.66
6:A:489:GOL:H32	7:A:751:HOH:O	1.95	0.65
1:A:360:LYS:HZ1	6:A:492:GOL:H32	1.60	0.65
1:A:172:LYS:HE2	1:A:172:LYS:CA	2.23	0.65
6:A:484:GOL:H2	6:A:504:GOL:O2	1.98	0.64
1:A:184:SER:O	1:A:188:ARG:HG3	1.98	0.64
6:A:493:GOL:H12	7:A:673:HOH:O	1.97	0.64
1:A:49:ARG:HE	6:A:511:GOL:H32	1.64	0.63
1:A:273[B]:HIS:HB3	1:A:282:PHE:CE1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ALA:HB2	1:A:163[B]:ARG:HG3	1.79	0.63
1:A:84:GLN:NE2	1:A:307:ARG:HH21	1.96	0.62
1:A:412:GLN:NE2	7:A:658:HOH:O	2.31	0.62
1:A:49:ARG:NE	6:A:511:GOL:H32	2.15	0.61
1:A:416:ARG:HD3	7:A:758:HOH:O	1.99	0.61
1:A:19:THR:HB	1:A:20:PRO:HD2	1.83	0.61
1:A:172:LYS:HA	1:A:172:LYS:CE	2.31	0.60
1:A:44:ARG:HH21	4:A:477:ACT:C	2.15	0.60
1:A:61:LYS:HZ3	6:A:500:GOL:H12	1.66	0.60
1:A:45:SER:H	6:A:498:GOL:H32	1.67	0.60
1:A:383:GLU:HB2	6:A:506:GOL:C1	2.31	0.60
6:A:484:GOL:H12	7:A:629:HOH:O	2.02	0.60
1:A:115:SER:N	6:A:510:GOL:O1	2.29	0.60
1:A:360:LYS:HZ3	6:A:492:GOL:H32	1.67	0.60
1:A:45:SER:H	6:A:498:GOL:H31	1.67	0.60
1:A:310:MET:HE3	1:A:344:LEU:HD21	1.84	0.59
1:A:61:LYS:HB2	6:A:501:GOL:O1	2.02	0.59
1:A:426:GLY:HA3	4:A:478:ACT:O	2.03	0.58
1:A:22:LYS:HE2	4:A:477:ACT:H3	1.86	0.58
1:A:273[A]:HIS:CD2	1:A:280:HIS:NE2	2.70	0.58
1:A:456:ARG:NE	6:A:487:GOL:O1	2.33	0.58
1:A:360:LYS:CE	6:A:492:GOL:H32	2.34	0.58
1:A:425:ASN:O	4:A:478:ACT:O	2.22	0.58
1:A:19:THR:HG22	1:A:157:TYR:CE1	2.40	0.57
6:A:505:GOL:H32	7:A:560:HOH:O	2.05	0.57
1:A:427:GLU:H	6:A:507:GOL:H2	1.69	0.57
1:A:61:LYS:HD2	6:A:500:GOL:H12	1.87	0.56
1:A:44:ARG:NH2	4:A:477:ACT:O	2.38	0.56
1:A:264:ASN:CB	6:A:495:GOL:H31	2.35	0.56
6:A:499:GOL:H31	6:A:506:GOL:O1	2.06	0.56
1:A:44:ARG:HA	6:A:498:GOL:H31	1.89	0.55
1:A:138:LEU:O	1:A:142:LYS:HG3	2.06	0.55
1:A:267:ASP:OD1	6:A:496:GOL:H12	2.06	0.55
4:A:480:ACT:H2	6:A:496:GOL:O3	2.06	0.55
1:A:429:GLU:N	4:A:478:ACT:OXT	2.38	0.55
1:A:378:TYR:CD2	6:A:490:GOL:H12	2.42	0.54
5:A:482:POP:O6	5:A:482:POP:O1	2.26	0.53
1:A:105:GLU:O	1:A:196:LYS:HD2	2.09	0.53
1:A:84:GLN:HE22	1:A:307:ARG:NH2	2.06	0.53
6:A:502:GOL:H32	7:A:650:HOH:O	2.09	0.52
1:A:360:LYS:HE2	6:A:492:GOL:C3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLN:HE22	1:A:307:ARG:HH21	1.58	0.52
1:A:456:ARG:HE	6:A:487:GOL:HO1	1.56	0.52
1:A:7:GLU:OE2	1:A:280:HIS:ND1	2.32	0.51
6:A:487:GOL:O1	6:A:487:GOL:O3	2.28	0.51
1:A:164:SER:N	5:A:482:POP:O5	2.34	0.51
1:A:279:LYS:HG3	6:A:497:GOL:C1	2.38	0.51
1:A:403:ARG:HH22	6:A:505:GOL:C1	2.19	0.51
1:A:22:LYS:HD2	4:A:477:ACT:H2	1.93	0.51
1:A:106:GLY:O	1:A:199:HIS:HD2	1.92	0.51
1:A:435:ARG:HG2	1:A:435:ARG:HH11	1.76	0.51
1:A:429:GLU:CG	4:A:478:ACT:H2	2.38	0.51
1:A:44:ARG:NE	4:A:477:ACT:O	2.42	0.51
1:A:115:SER:H	6:A:510:GOL:H32	1.76	0.51
1:A:416:ARG:HH22	6:A:489:GOL:C1	2.24	0.51
1:A:236:GLY:H	6:A:502:GOL:C1	2.24	0.50
1:A:457:LYS:HE3	6:A:488:GOL:H11	1.92	0.50
1:A:21:SER:N	4:A:476:ACT:OXT	2.29	0.50
1:A:429:GLU:H	4:A:478:ACT:C	2.22	0.50
1:A:383:GLU:CG	6:A:506:GOL:H12	2.42	0.49
1:A:84:GLN:NE2	1:A:307:ARG:NH2	2.61	0.49
1:A:363:CYS:O	1:A:365:ASN:N	2.46	0.49
1:A:218:TRP:CD1	1:A:391:PRO:HA	2.47	0.49
1:A:353:LEU:C	1:A:354:ILE:HD13	2.33	0.49
1:A:174[A]:ARG:NH1	6:A:502:GOL:C3	2.75	0.48
1:A:236:GLY:H	6:A:502:GOL:H12	1.79	0.48
1:A:62:TYR:CZ	6:A:501:GOL:H32	2.49	0.48
1:A:194:LEU:C	1:A:194:LEU:HD23	2.34	0.48
1:A:19:THR:CG2	1:A:157:TYR:CE1	2.96	0.48
1:A:429:GLU:CG	4:A:478:ACT:C	2.89	0.48
1:A:435:ARG:HG2	1:A:435:ARG:NH1	2.29	0.48
1:A:62:TYR:CD2	6:A:501:GOL:H12	2.49	0.47
1:A:79:ASP:OD1	1:A:255:LYS:HE2	2.15	0.47
6:A:511:GOL:O1	6:A:512:GOL:H32	2.14	0.47
1:A:49:ARG:HD3	6:A:511:GOL:C1	2.44	0.47
1:A:75:LEU:HD23	1:A:251:MET:HE1	1.97	0.47
1:A:174[A]:ARG:NH2	5:A:482:POP:O1	2.45	0.47
1:A:45:SER:CB	6:A:498:GOL:H32	2.45	0.47
1:A:375:LEU:O	1:A:376:LYS:HB2	2.15	0.47
1:A:428:HIS:N	4:A:478:ACT:OXT	2.48	0.47
1:A:48:PRO:HG2	6:A:511:GOL:H2	1.97	0.46
1:A:174[A]:ARG:NH1	6:A:502:GOL:H31	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:THR:HG21	1:A:157:TYR:CD1	2.51	0.46
1:A:310:MET:HE1	1:A:339:ILE:CG2	2.36	0.46
1:A:432:GLU:HG3	1:A:436:LYS:HE2	1.97	0.46
1:A:222:PRO:HG2	6:A:491:GOL:H11	1.98	0.46
1:A:251:MET:HE3	1:A:251:MET:HB3	1.80	0.46
1:A:22:LYS:HD2	4:A:477:ACT:CH3	2.46	0.46
1:A:437:ILE:O	1:A:443:GLY:HA3	2.17	0.45
1:A:163[A]:ARG:NH1	1:A:174[A]:ARG:HG3	2.32	0.45
1:A:164:SER:HG	6:A:492:GOL:HO2	1.64	0.45
1:A:62:TYR:CZ	6:A:501:GOL:C3	3.01	0.44
1:A:75:LEU:CD2	1:A:251:MET:HE1	2.47	0.44
1:A:383:GLU:H	6:A:506:GOL:C1	2.31	0.44
1:A:172:LYS:CA	1:A:172:LYS:CE	2.94	0.44
1:A:167[B]:LYS:HE3	6:A:492:GOL:O3	2.18	0.44
1:A:164:SER:OG	6:A:492:GOL:O2	2.31	0.44
6:A:483:GOL:H31	6:A:484:GOL:H31	2.00	0.44
1:A:455:ARG:NH2	6:A:486:GOL:H12	2.18	0.44
1:A:17:ILE:CG2	1:A:19:THR:HG23	2.42	0.43
1:A:174[A]:ARG:HH12	6:A:502:GOL:H31	1.81	0.43
1:A:383:GLU:H	6:A:506:GOL:H12	1.83	0.43
1:A:456:ARG:NH2	6:A:487:GOL:O1	2.47	0.43
1:A:164:SER:OG	1:A:167[A]:LYS:HG2	2.18	0.43
1:A:438:ARG:NH2	7:A:759:HOH:O	2.47	0.43
5:A:482:POP:O4	6:A:492:GOL:O3	2.29	0.43
1:A:174[A]:ARG:NH1	6:A:502:GOL:O3	2.46	0.43
1:A:428:HIS:HB3	4:A:478:ACT:OXT	2.18	0.43
1:A:22:LYS:CD	4:A:477:ACT:CH3	2.97	0.43
1:A:45:SER:N	6:A:498:GOL:H31	2.31	0.43
1:A:61:LYS:HB2	6:A:501:GOL:C1	2.49	0.42
1:A:32:GLN:HB2	7:A:523:HOH:O	2.19	0.42
1:A:58:ILE:HD12	1:A:175:LEU:HD21	2.01	0.42
1:A:456:ARG:HH22	6:A:488:GOL:C1	2.33	0.42
1:A:360:LYS:HE2	6:A:492:GOL:C2	2.49	0.42
1:A:383:GLU:HB2	6:A:506:GOL:C2	2.50	0.41
1:A:438:ARG:NE	7:A:759:HOH:O	2.27	0.41
1:A:61:LYS:CD	6:A:500:GOL:C1	2.87	0.41
1:A:106:GLY:O	1:A:199:HIS:CD2	2.73	0.41
1:A:164:SER:OG	1:A:167[B]:LYS:HG3	2.20	0.41
1:A:449:PRO:HA	6:A:489:GOL:H12	2.01	0.41
1:A:218:TRP:O	1:A:222:PRO:HD3	2.21	0.41
1:A:427:GLU:N	6:A:507:GOL:H2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:OE1	6:A:498:GOL:O3	2.36	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	472/468 (101%)	465 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	415/409 (102%)	400 (96%)	15 (4%)	35	36

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	68	THR
1	A	96	LYS
1	A	140	LYS
1	A	166	GLU

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Mol	Chain	Res	Type
1	A	172	LYS
1	A	196	LYS
1	A	218	TRP
1	A	261	LYS
1	A	265	TYR
1	A	289	SER
1	A	298	ASN
1	A	327	TYR
1	A	362	GLU
1	A	412	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	199	HIS
1	A	228	HIS
1	A	271	ASN
1	A	298	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 44 ligands modelled in this entry, 6 are monoatomic - leaving 38 for Mogul analysis.

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	GOL	A	501	-	5,5,5	1.73	2 (40%)	5,5,5	1.31	1 (20%)
4	ACT	A	480	-	3,3,3	0.85	0	3,3,3	0.94	0
6	GOL	A	490	-	5,5,5	0.28	0	5,5,5	1.14	0
6	GOL	A	494	-	5,5,5	0.53	0	5,5,5	1.33	0
6	GOL	A	505	-	5,5,5	0.77	0	5,5,5	0.73	0
6	GOL	A	484	-	5,5,5	1.18	1 (20%)	5,5,5	1.19	0
4	ACT	A	476	-	3,3,3	1.12	0	3,3,3	0.63	0
6	GOL	A	497	-	5,5,5	0.55	0	5,5,5	0.81	0
5	POP	A	482	-	6,8,8	1.58	2 (33%)	13,13,13	3.02	6 (46%)
6	GOL	A	512	-	5,5,5	0.62	0	5,5,5	0.47	0
6	GOL	A	489	-	5,5,5	0.91	0	5,5,5	1.50	1 (20%)
6	GOL	A	507	-	5,5,5	0.81	0	5,5,5	1.02	0
6	GOL	A	510	-	5,5,5	0.80	0	5,5,5	2.63	3 (60%)
6	GOL	A	483	-	5,5,5	0.75	0	5,5,5	1.44	1 (20%)
4	ACT	A	481	-	3,3,3	0.95	0	3,3,3	1.26	0
6	GOL	A	498	-	5,5,5	0.95	0	5,5,5	1.45	1 (20%)
6	GOL	A	503	-	5,5,5	0.52	0	5,5,5	0.53	0
6	GOL	A	496	-	5,5,5	0.31	0	5,5,5	0.83	0
6	GOL	A	485	-	5,5,5	0.39	0	5,5,5	1.24	1 (20%)
6	GOL	A	500	-	5,5,5	1.39	0	5,5,5	1.36	1 (20%)
6	GOL	A	486	-	5,5,5	0.64	0	5,5,5	0.99	0
6	GOL	A	509	-	5,5,5	0.68	0	5,5,5	0.35	0
4	ACT	A	479	-	3,3,3	1.19	0	3,3,3	1.17	0
4	ACT	A	478	-	3,3,3	1.53	1 (33%)	3,3,3	2.23	2 (66%)
6	GOL	A	487	-	5,5,5	0.11	0	5,5,5	0.52	0
6	GOL	A	508	-	5,5,5	1.11	0	5,5,5	1.24	0
6	GOL	A	504	-	5,5,5	0.49	0	5,5,5	1.49	1 (20%)
4	ACT	A	477	-	3,3,3	1.10	0	3,3,3	1.12	0
6	GOL	A	499	-	5,5,5	0.80	0	5,5,5	0.92	0
6	GOL	A	511	-	5,5,5	0.83	0	5,5,5	0.99	0
3	SO4	A	475	-	4,4,4	0.59	0	6,6,6	0.20	0
6	GOL	A	502	-	5,5,5	0.81	0	5,5,5	0.55	0
6	GOL	A	506	-	5,5,5	0.63	0	5,5,5	1.61	2 (40%)
6	GOL	A	491	-	5,5,5	0.74	0	5,5,5	1.93	2 (40%)
6	GOL	A	488	-	5,5,5	0.56	0	5,5,5	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GOL	A	495	-	5,5,5	0.51	0	5,5,5	1.11	0
6	GOL	A	492	-	5,5,5	0.83	0	5,5,5	0.60	0
6	GOL	A	493	-	5,5,5	0.78	0	5,5,5	0.90	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	GOL	A	501	-	-	2/4/4/4	-
6	GOL	A	490	-	-	0/4/4/4	-
6	GOL	A	494	-	-	4/4/4/4	-
6	GOL	A	505	-	-	2/4/4/4	-
6	GOL	A	484	-	-	3/4/4/4	-
6	GOL	A	497	-	-	2/4/4/4	-
5	POP	A	482	-	-	4/6/6/6	-
6	GOL	A	512	-	-	2/4/4/4	-
6	GOL	A	489	-	-	4/4/4/4	-
6	GOL	A	507	-	-	2/4/4/4	-
6	GOL	A	510	-	-	4/4/4/4	-
6	GOL	A	483	-	-	4/4/4/4	-
6	GOL	A	498	-	-	3/4/4/4	-
6	GOL	A	503	-	-	0/4/4/4	-
6	GOL	A	496	-	-	3/4/4/4	-
6	GOL	A	485	-	-	2/4/4/4	-
6	GOL	A	500	-	-	2/4/4/4	-
6	GOL	A	486	-	-	1/4/4/4	-
6	GOL	A	509	-	-	0/4/4/4	-
6	GOL	A	487	-	-	4/4/4/4	-
6	GOL	A	508	-	-	3/4/4/4	-
6	GOL	A	504	-	-	2/4/4/4	-
6	GOL	A	499	-	-	2/4/4/4	-
6	GOL	A	511	-	-	0/4/4/4	-
6	GOL	A	502	-	-	0/4/4/4	-
6	GOL	A	506	-	-	4/4/4/4	-
6	GOL	A	491	-	-	4/4/4/4	-
6	GOL	A	488	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	495	-	-	4/4/4/4	-
6	GOL	A	492	-	-	2/4/4/4	-
6	GOL	A	493	-	-	4/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	482	POP	P2-O4	3.04	1.60	1.50
6	A	501	GOL	O2-C2	-2.59	1.35	1.43
5	A	482	POP	P1-O2	2.04	1.62	1.54
6	A	501	GOL	C1-C2	2.04	1.60	1.51
4	A	478	ACT	OXT-C	-2.02	1.21	1.30
6	A	484	GOL	O2-C2	2.01	1.49	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	482	POP	P2-O-P1	-6.92	109.09	132.83
5	A	482	POP	O3-P1-O1	-4.24	94.10	110.68
5	A	482	POP	O6-P2-O4	-4.17	94.35	110.68
5	A	482	POP	O5-P2-O	4.00	118.07	104.64
6	A	510	GOL	C3-C2-C1	-3.94	96.40	111.70
6	A	510	GOL	O1-C1-C2	-3.55	93.17	110.20
6	A	491	GOL	C3-C2-C1	-2.98	100.11	111.70
4	A	478	ACT	OXT-C-CH3	2.84	126.90	115.18
5	A	482	POP	O2-P1-O	2.75	113.87	104.64
6	A	504	GOL	O3-C3-C2	-2.67	97.40	110.20
6	A	489	GOL	O2-C2-C1	-2.56	97.85	109.12
4	A	478	ACT	OXT-C-O	-2.56	112.62	122.05
6	A	491	GOL	O3-C3-C2	-2.52	98.12	110.20
6	A	506	GOL	O1-C1-C2	-2.47	98.38	110.20
5	A	482	POP	O3-P1-O	2.45	112.84	104.64
6	A	483	GOL	C3-C2-C1	2.28	120.58	111.70
6	A	501	GOL	O2-C2-C3	-2.20	99.42	109.12
6	A	498	GOL	O1-C1-C2	2.12	120.38	110.20
6	A	506	GOL	O2-C2-C1	-2.05	100.07	109.12
6	A	500	GOL	O2-C2-C3	2.03	118.08	109.12
6	A	485	GOL	O2-C2-C1	-2.02	100.20	109.12
6	A	510	GOL	O2-C2-C1	-2.02	100.23	109.12

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	482	POP	P1-O-P2-O6
6	A	486	GOL	C1-C2-C3-O3
6	A	487	GOL	O1-C1-C2-O2
6	A	487	GOL	O1-C1-C2-C3
6	A	488	GOL	C1-C2-C3-O3
6	A	489	GOL	O1-C1-C2-C3
6	A	489	GOL	C1-C2-C3-O3
6	A	491	GOL	O1-C1-C2-O2
6	A	491	GOL	O1-C1-C2-C3
6	A	492	GOL	C1-C2-C3-O3
6	A	493	GOL	O1-C1-C2-C3
6	A	493	GOL	C1-C2-C3-O3
6	A	494	GOL	O1-C1-C2-C3
6	A	494	GOL	C1-C2-C3-O3
6	A	496	GOL	C1-C2-C3-O3
6	A	497	GOL	C1-C2-C3-O3
6	A	498	GOL	O1-C1-C2-C3
6	A	499	GOL	O1-C1-C2-C3
6	A	501	GOL	C1-C2-C3-O3
6	A	504	GOL	C1-C2-C3-O3
6	A	506	GOL	O1-C1-C2-C3
6	A	507	GOL	O1-C1-C2-O2
6	A	507	GOL	O1-C1-C2-C3
6	A	510	GOL	C1-C2-C3-O3
6	A	510	GOL	O2-C2-C3-O3
6	A	512	GOL	C1-C2-C3-O3
6	A	492	GOL	O2-C2-C3-O3
6	A	499	GOL	O1-C1-C2-O2
6	A	483	GOL	O1-C1-C2-C3
6	A	484	GOL	O1-C1-C2-C3
6	A	484	GOL	C1-C2-C3-O3
6	A	485	GOL	O1-C1-C2-C3
6	A	487	GOL	C1-C2-C3-O3
6	A	491	GOL	C1-C2-C3-O3
6	A	495	GOL	O1-C1-C2-C3
6	A	495	GOL	C1-C2-C3-O3
6	A	500	GOL	C1-C2-C3-O3
6	A	505	GOL	O1-C1-C2-C3
6	A	506	GOL	C1-C2-C3-O3
6	A	508	GOL	O1-C1-C2-C3
6	A	510	GOL	O1-C1-C2-C3
6	A	484	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	A	487	GOL	O2-C2-C3-O3
6	A	488	GOL	O2-C2-C3-O3
6	A	489	GOL	O2-C2-C3-O3
6	A	493	GOL	O2-C2-C3-O3
6	A	494	GOL	O1-C1-C2-O2
6	A	494	GOL	O2-C2-C3-O3
6	A	498	GOL	O1-C1-C2-O2
6	A	500	GOL	O2-C2-C3-O3
6	A	506	GOL	O1-C1-C2-O2
6	A	512	GOL	O2-C2-C3-O3
6	A	483	GOL	O2-C2-C3-O3
6	A	489	GOL	O1-C1-C2-O2
6	A	493	GOL	O1-C1-C2-O2
6	A	495	GOL	O1-C1-C2-O2
6	A	496	GOL	O2-C2-C3-O3
6	A	501	GOL	O2-C2-C3-O3
6	A	504	GOL	O2-C2-C3-O3
6	A	508	GOL	O1-C1-C2-O2
6	A	483	GOL	O1-C1-C2-O2
6	A	485	GOL	O1-C1-C2-O2
6	A	491	GOL	O2-C2-C3-O3
6	A	497	GOL	O2-C2-C3-O3
6	A	506	GOL	O2-C2-C3-O3
5	A	482	POP	P2-O-P1-O3
6	A	508	GOL	O2-C2-C3-O3
6	A	505	GOL	O1-C1-C2-O2
6	A	483	GOL	C1-C2-C3-O3
6	A	510	GOL	O1-C1-C2-O2
5	A	482	POP	P1-O-P2-O4
5	A	482	POP	P1-O-P2-O5
6	A	495	GOL	O2-C2-C3-O3
6	A	496	GOL	O1-C1-C2-O2
6	A	498	GOL	C1-C2-C3-O3

There are no ring outliers.

30 monomers are involved in 116 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	501	GOL	5	0
4	A	480	ACT	1	0
6	A	490	GOL	1	0
6	A	505	GOL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	484	GOL	3	0
4	A	476	ACT	1	0
6	A	497	GOL	2	0
5	A	482	POP	6	0
6	A	512	GOL	1	0
6	A	489	GOL	4	0
6	A	507	GOL	2	0
6	A	510	GOL	2	0
6	A	483	GOL	1	0
6	A	498	GOL	8	0
6	A	496	GOL	2	0
6	A	500	GOL	9	0
6	A	486	GOL	2	0
4	A	478	ACT	11	0
6	A	487	GOL	4	0
6	A	504	GOL	1	0
4	A	477	ACT	8	0
6	A	499	GOL	3	0
6	A	511	GOL	8	0
6	A	502	GOL	7	0
6	A	506	GOL	9	0
6	A	491	GOL	1	0
6	A	488	GOL	2	0
6	A	495	GOL	2	0
6	A	492	GOL	10	0
6	A	493	GOL	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	468/468 (100%)	-0.39	2 (0%)	92	93	16, 26, 50, 75	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	467	HIS	4.8
1	A	466	HIS	3.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	A	479	4/4	0.33	0.35	89,90,91,91	0
6	GOL	A	512	6/6	0.59	0.41	84,85,85,87	0
6	GOL	A	508	6/6	0.62	0.30	63,65,65,66	0
6	GOL	A	484	6/6	0.64	0.33	60,63,63,65	0
4	ACT	A	477	4/4	0.69	0.42	60,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	A	505	6/6	0.72	0.23	58,61,62,63	0
6	GOL	A	502	6/6	0.76	0.27	63,68,69,69	0
6	GOL	A	498	6/6	0.78	0.30	63,63,64,65	0
4	ACT	A	476	4/4	0.79	0.17	63,64,64,65	0
6	GOL	A	507	6/6	0.80	0.29	51,54,54,57	0
6	GOL	A	497	6/6	0.80	0.27	58,60,61,63	0
6	GOL	A	509	6/6	0.80	0.21	65,67,67,68	0
6	GOL	A	511	6/6	0.80	0.68	52,58,60,61	0
6	GOL	A	500	6/6	0.80	0.41	36,40,41,42	0
4	ACT	A	478	4/4	0.83	0.43	65,65,65,66	0
4	ACT	A	480	4/4	0.84	0.28	72,72,73,73	0
6	GOL	A	499	6/6	0.86	0.23	45,47,47,49	0
5	POP	A	482	9/9	0.86	0.24	35,36,39,39	9
6	GOL	A	492	6/6	0.86	0.28	56,57,58,58	0
6	GOL	A	486	6/6	0.87	0.13	51,51,51,53	0
2	CL	A	474	1/1	0.87	0.09	91,91,91,91	0
6	GOL	A	483	6/6	0.87	0.27	40,44,45,49	0
4	ACT	A	481	4/4	0.87	0.17	70,70,70,71	0
6	GOL	A	506	6/6	0.87	0.43	57,61,62,64	0
6	GOL	A	489	6/6	0.88	0.20	45,48,48,50	0
6	GOL	A	488	6/6	0.89	0.23	82,83,84,84	0
6	GOL	A	510	6/6	0.89	0.28	53,55,55,57	0
3	SO4	A	475	5/5	0.90	0.18	82,85,86,87	0
6	GOL	A	493	6/6	0.91	0.20	39,47,48,51	0
6	GOL	A	495	6/6	0.91	0.17	63,64,65,66	0
6	GOL	A	496	6/6	0.91	0.18	54,56,56,58	0
6	GOL	A	487	6/6	0.91	0.29	64,64,65,66	0
6	GOL	A	501	6/6	0.92	0.23	42,43,43,44	0
6	GOL	A	494	6/6	0.93	0.25	54,57,58,59	0
6	GOL	A	491	6/6	0.94	0.18	47,49,50,52	0
6	GOL	A	485	6/6	0.94	0.17	30,37,39,43	0
6	GOL	A	490	6/6	0.94	0.20	58,61,62,63	0
6	GOL	A	504	6/6	0.94	0.19	38,38,39,42	0
2	CL	A	473	1/1	0.97	0.08	48,48,48,48	0
6	GOL	A	503	6/6	0.98	0.09	30,32,34,37	0
2	CL	A	469	1/1	0.99	0.10	30,30,30,30	0
2	CL	A	470	1/1	0.99	0.09	31,31,31,31	0
2	CL	A	471	1/1	1.00	0.07	34,34,34,34	0
2	CL	A	472	1/1	1.00	0.05	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.