



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:28 pm BST

PDB ID : 5CX6
Title : Crystal structure of Thosea asigna virus RNA-dependent RNA polymerase (RdRP) complexed with CDP
Authors : Ferrero, D.S.; Buxaderas, M.; Rodriguez, J.F.; Verdaguer, N.
Deposited on : 2015-07-28
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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
buster-report : 1.1.7 (2018)
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) : 2.11

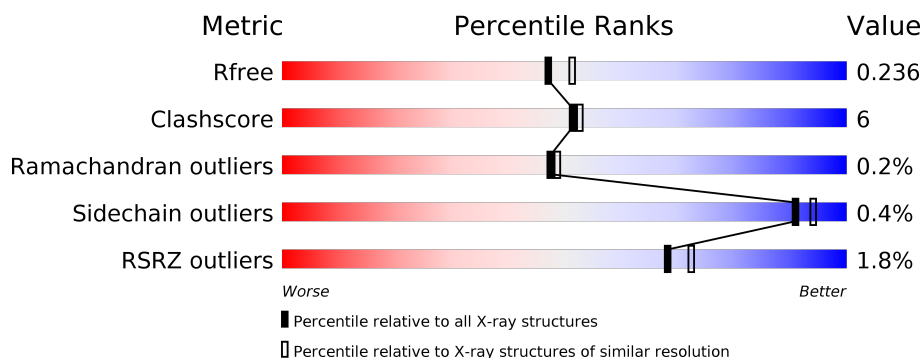
1 Overall quality at a glance

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))
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 on 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	705	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, orange 1%, yellow 85%, green 94%, grey 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">85% 8% 6%</div> </div> </div>
1	B	705	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">3%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, orange 3%, yellow 84%, green 94%, grey 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">84% 10% 6%</div> </div> </div>

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
2	SO4	A	707	-	-	X	-
5	CDP	A	721	-	-	-	X
5	CDP	B	713	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11360 atoms, of which 24 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-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	0	0	0
			5247	3331	909	981	26			
1	B	665	Total	C	N	O	S	0	0	0
			5265	3341	911	987	26			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	initiating methionine	UNP Q6A562
A	-29	SER	-	expression tag	UNP Q6A562
A	-28	TYR	-	expression tag	UNP Q6A562
A	-27	TYR	-	expression tag	UNP Q6A562
A	-26	HIS	-	expression tag	UNP Q6A562
A	-25	HIS	-	expression tag	UNP Q6A562
A	-24	HIS	-	expression tag	UNP Q6A562
A	-23	HIS	-	expression tag	UNP Q6A562
A	-22	HIS	-	expression tag	UNP Q6A562
A	-21	HIS	-	expression tag	UNP Q6A562
A	-20	ASP	-	expression tag	UNP Q6A562
A	-19	TYR	-	expression tag	UNP Q6A562
A	-18	ASP	-	expression tag	UNP Q6A562
A	-17	ILE	-	expression tag	UNP Q6A562
A	-16	PRO	-	expression tag	UNP Q6A562
A	-15	THR	-	expression tag	UNP Q6A562
A	-14	THR	-	expression tag	UNP Q6A562
A	-13	GLU	-	expression tag	UNP Q6A562
A	-12	ASN	-	expression tag	UNP Q6A562
A	-11	LEU	-	expression tag	UNP Q6A562
A	-10	TYR	-	expression tag	UNP Q6A562
A	-9	PHE	-	expression tag	UNP Q6A562
A	-8	GLN	-	expression tag	UNP Q6A562
A	-7	GLY	-	expression tag	UNP Q6A562
A	-6	ALA	-	expression tag	UNP Q6A562

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP Q6A562
A	-4	GLY	-	expression tag	UNP Q6A562
A	-3	ALA	-	expression tag	UNP Q6A562
A	-2	MET	-	expression tag	UNP Q6A562
A	-1	GLY	-	expression tag	UNP Q6A562
A	0	ILE	-	expression tag	UNP Q6A562
B	-30	MET	-	initiating methionine	UNP Q6A562
B	-29	SER	-	expression tag	UNP Q6A562
B	-28	TYR	-	expression tag	UNP Q6A562
B	-27	TYR	-	expression tag	UNP Q6A562
B	-26	HIS	-	expression tag	UNP Q6A562
B	-25	HIS	-	expression tag	UNP Q6A562
B	-24	HIS	-	expression tag	UNP Q6A562
B	-23	HIS	-	expression tag	UNP Q6A562
B	-22	HIS	-	expression tag	UNP Q6A562
B	-21	HIS	-	expression tag	UNP Q6A562
B	-20	ASP	-	expression tag	UNP Q6A562
B	-19	TYR	-	expression tag	UNP Q6A562
B	-18	ASP	-	expression tag	UNP Q6A562
B	-17	ILE	-	expression tag	UNP Q6A562
B	-16	PRO	-	expression tag	UNP Q6A562
B	-15	THR	-	expression tag	UNP Q6A562
B	-14	THR	-	expression tag	UNP Q6A562
B	-13	GLU	-	expression tag	UNP Q6A562
B	-12	ASN	-	expression tag	UNP Q6A562
B	-11	LEU	-	expression tag	UNP Q6A562
B	-10	TYR	-	expression tag	UNP Q6A562
B	-9	PHE	-	expression tag	UNP Q6A562
B	-8	GLN	-	expression tag	UNP Q6A562
B	-7	GLY	-	expression tag	UNP Q6A562
B	-6	ALA	-	expression tag	UNP Q6A562
B	-5	MET	-	expression tag	UNP Q6A562
B	-4	GLY	-	expression tag	UNP Q6A562
B	-3	ALA	-	expression tag	UNP Q6A562
B	-2	MET	-	expression tag	UNP Q6A562
B	-1	GLY	-	expression tag	UNP Q6A562
B	0	ILE	-	expression tag	UNP Q6A562

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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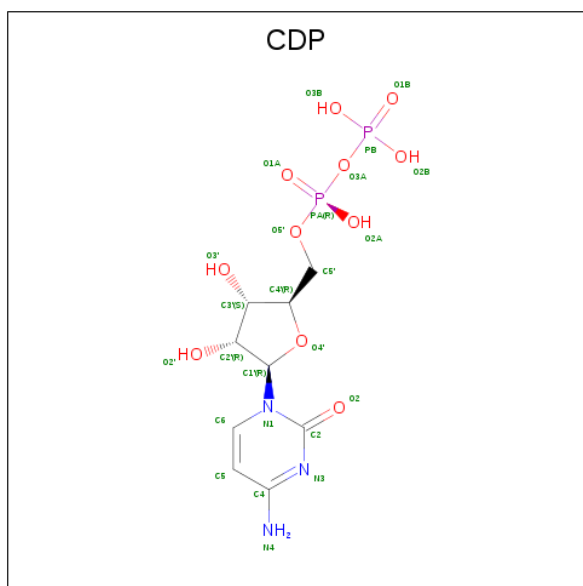
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is CYTIDINE-5'-DIPHOSPHATE (three-letter code: CDP) (formula: C₉H₁₅N₃O₁₁P₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			37	9	12	3	11	2		
5	B	1	Total	C	H	N	O	P	0	0
			33	9	12	3	8	1		

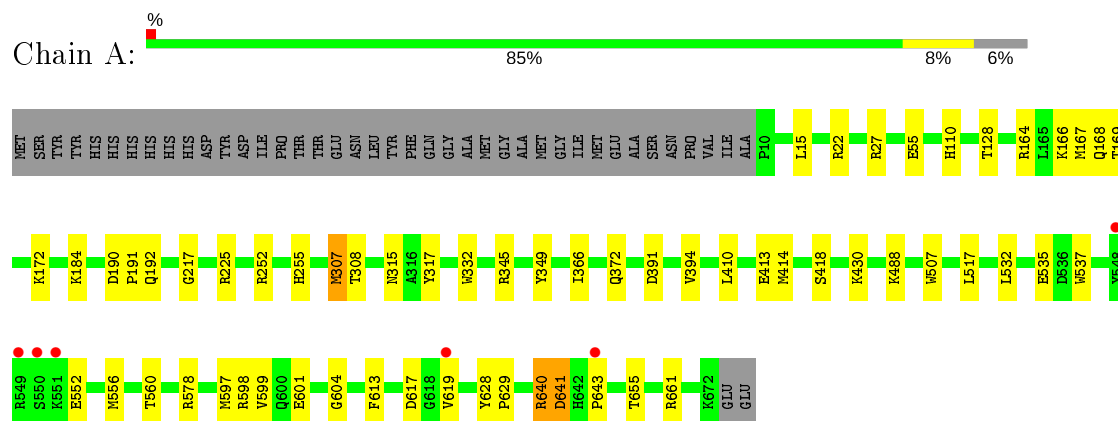
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	306	Total 306	O 306	0	0
6	B	297	Total 297	O 297	0	0

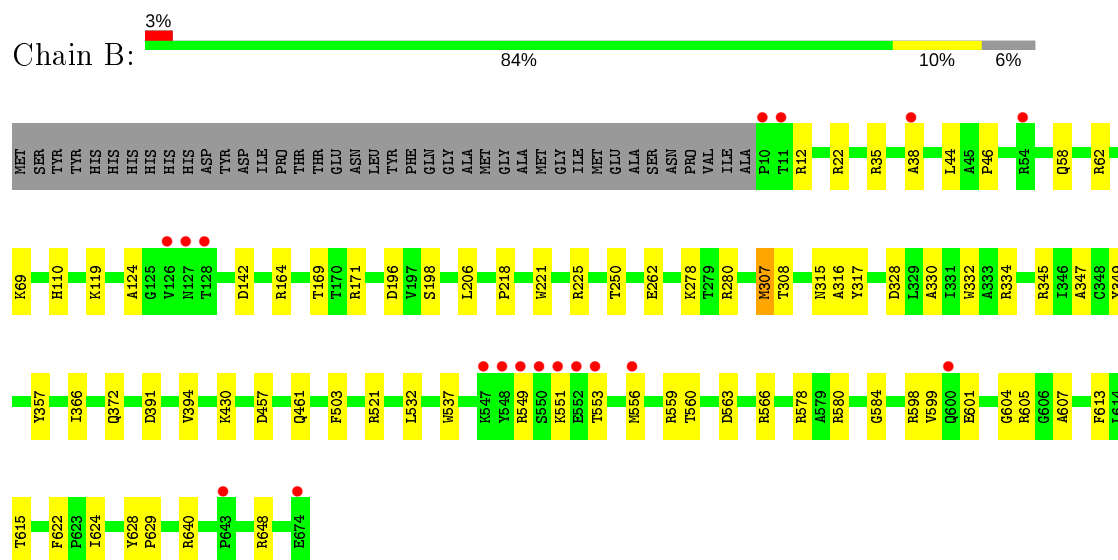
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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-dependent RNA polymerase



• Molecule 1: RNA-dependent RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	133.70 Å 149.60 Å 100.11 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.85 – 2.10 66.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.3 (66.85-2.10) 98.3 (66.85-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.10 Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.184 , 0.232 0.193 , 0.236	Depositor DCC
R_{free} test set	5790 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11360	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 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CDP, SO4

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	0.40	1/5366 (0.0%)	0.54	1/7267 (0.0%)
1	B	0.37	0/5384	0.53	1/7291 (0.0%)
All	All	0.39	1/10750 (0.0%)	0.53	2/14558 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	MET	CG-SD	-5.01	1.68	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	MET	CA-CB-CG	-8.01	99.68	113.30
1	B	142	ASP	CB-CG-OD2	5.22	123.00	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	640	ARG	Peptide

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	5247	0	5210	53	0
1	B	5265	0	5222	60	1
2	A	35	0	0	4	0
2	B	25	0	0	0	0
3	A	72	0	96	8	1
3	B	42	0	56	10	0
4	A	1	0	0	0	0
5	A	25	12	12	7	0
5	B	21	12	12	10	0
6	A	306	0	0	12	1
6	B	297	0	0	9	1
All	All	11336	24	10608	119	2

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 6.

All (119) 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)
5:B:713:CDP:H2'	5:B:713:CDP:O2	1.52	1.04
1:A:560:THR:HA	5:A:721:CDP:O1A	1.59	1.03
5:B:713:CDP:C2'	5:B:713:CDP:O2	2.20	0.89
3:A:710:GOL:H32	3:A:711:GOL:H12	1.57	0.86
1:B:563:ASP:OD2	5:B:713:CDP:O1A	1.93	0.86
5:A:721:CDP:O2	5:A:721:CDP:C2'	2.25	0.84
1:A:168:GLN:HE21	1:A:372:GLN:HE21	1.28	0.81
1:A:110:HIS:H	3:A:716:GOL:H32	1.48	0.78
1:B:598:ARG:NH1	1:B:599:VAL:O	2.18	0.76
5:A:721:CDP:H2'	5:A:721:CDP:O2	1.84	0.76
1:B:328:ASP:OD1	1:B:640:ARG:NH2	2.25	0.70
1:B:372:GLN:OE1	6:B:801:HOH:O	2.10	0.69
1:B:12:ARG:NH2	6:B:805:HOH:O	2.26	0.68
1:A:307:MET:HG2	1:A:308:THR:N	2.07	0.67
1:B:110:HIS:HA	3:B:708:GOL:H2	1.77	0.67
1:B:549:ARG:HH22	1:B:551:LYS:HD3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:MET:HE3	5:A:721:CDP:H1'	1.78	0.66
1:B:615:THR:HB	3:B:706:GOL:H12	1.79	0.65
1:B:553:THR:H	1:B:556:MET:HE3	1.63	0.63
1:A:225:ARG:O	1:B:22:ARG:HD2	1.99	0.63
1:B:35:ARG:NH1	6:B:807:HOH:O	2.31	0.63
1:B:601:GLU:OE2	5:B:713:CDP:H3'	2.01	0.61
1:A:488:LYS:NZ	6:A:811:HOH:O	2.35	0.60
1:A:601:GLU:OE1	5:A:721:CDP:H3'	2.02	0.59
1:A:252:ARG:NH2	1:A:413:GLU:OE1	2.34	0.58
1:A:164:ARG:NH2	2:A:707:SO4:S	2.77	0.58
1:B:556:MET:HG3	5:B:713:CDP:C6	2.39	0.57
1:A:655:THR:OG1	1:A:661:ARG:NH2	2.37	0.57
1:A:55:GLU:OE1	6:A:802:HOH:O	2.17	0.56
1:B:559:ARG:HG2	5:B:713:CDP:H4'	1.87	0.56
1:A:640:ARG:O	1:A:641:ASP:HB2	2.06	0.56
1:A:307:MET:CG	1:A:308:THR:N	2.69	0.55
1:A:391:ASP:HA	1:A:394:VAL:HG22	1.88	0.55
1:A:619:VAL:HA	6:A:988:HOH:O	2.07	0.55
1:A:532:LEU:HB2	1:A:537:TRP:CE2	2.43	0.54
1:B:391:ASP:HA	1:B:394:VAL:HG22	1.88	0.54
1:A:410:LEU:O	1:A:414:MET:HG3	2.07	0.54
1:A:22:ARG:HD2	1:B:225:ARG:O	2.08	0.54
1:B:110:HIS:H	3:B:708:GOL:H12	1.73	0.53
1:A:332:TRP:CE2	1:A:345:ARG:HD2	2.43	0.53
1:B:532:LEU:HB2	1:B:537:TRP:CE2	2.44	0.53
1:B:44:LEU:HD11	3:B:712:GOL:H32	1.91	0.53
1:B:119:LYS:HE2	3:B:708:GOL:H32	1.90	0.53
1:A:164:ARG:NH2	2:A:707:SO4:O2	2.38	0.53
1:A:22:ARG:HH22	3:A:714:GOL:H2	1.73	0.53
1:A:307:MET:HG2	1:A:308:THR:H	1.73	0.53
1:B:171:ARG:NH1	6:B:819:HOH:O	2.42	0.52
2:A:707:SO4:O3	6:A:803:HOH:O	2.19	0.52
1:A:641:ASP:CG	1:A:643:PRO:HG3	2.30	0.52
1:B:58:GLN:O	1:B:62:ARG:HG3	2.11	0.51
1:B:580:ARG:HD3	6:B:871:HOH:O	2.10	0.51
1:B:332:TRP:CE2	1:B:345:ARG:HD2	2.46	0.51
1:B:457:ASP:O	1:B:461:GLN:HG2	2.11	0.50
1:B:69:LYS:NZ	1:B:124:ALA:HB1	2.26	0.50
1:B:648:ARG:NH1	6:B:803:HOH:O	2.43	0.50
1:A:597:MET:CE	5:A:721:CDP:H1'	2.41	0.49
1:A:184:LYS:NZ	6:A:820:HOH:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:721:CDP:O2'	5:A:721:CDP:O2	2.28	0.49
1:A:164:ARG:NH2	2:A:707:SO4:O3	2.46	0.48
1:B:307:MET:HG3	1:B:308:THR:H	1.78	0.48
1:B:566:ARG:NH2	1:B:624:ILE:O	2.38	0.48
1:A:507:TRP:CG	1:A:517:LEU:HD23	2.49	0.48
1:A:641:ASP:OD2	1:A:643:PRO:HG3	2.13	0.48
1:B:613:PHE:CE2	3:B:711:GOL:H31	2.47	0.48
1:B:69:LYS:HZ3	1:B:124:ALA:HB1	1.79	0.48
3:A:710:GOL:H32	3:A:711:GOL:H32	1.95	0.48
1:B:278:LYS:O	6:B:802:HOH:O	2.20	0.47
1:A:617:ASP:OD1	1:A:617:ASP:N	2.47	0.47
1:A:172:LYS:HG2	6:A:969:HOH:O	2.15	0.47
1:B:262:GLU:OE2	3:B:707:GOL:H2	2.14	0.47
1:A:578:ARG:NH1	6:A:806:HOH:O	2.25	0.47
1:B:599:VAL:O	1:B:604:GLY:HA2	2.15	0.47
1:A:599:VAL:O	1:A:604:GLY:HA2	2.15	0.46
1:B:315:ASN:OD1	1:B:317:TYR:HB3	2.15	0.46
1:B:316:ALA:HB2	1:B:347:ALA:HB1	1.96	0.46
1:A:166:LYS:HD3	6:A:865:HOH:O	2.15	0.46
1:B:549:ARG:NH2	1:B:551:LYS:HD3	2.30	0.45
1:A:613:PHE:HE2	3:A:712:GOL:H11	1.80	0.45
1:A:255:HIS:ND1	3:A:719:GOL:H31	2.32	0.45
1:A:578:ARG:NH2	6:A:816:HOH:O	2.40	0.45
1:A:128:THR:HG23	6:A:883:HOH:O	2.15	0.45
1:B:560:THR:HA	5:B:713:CDP:O2A	2.16	0.45
1:A:414:MET:HA	1:A:418:SER:OG	2.17	0.44
1:B:280:ARG:HD2	6:B:824:HOH:O	2.17	0.44
1:A:217:GLY:HA2	6:A:885:HOH:O	2.18	0.44
1:A:15:LEU:HB2	1:B:206:LEU:HA	2.00	0.44
1:A:535:GLU:OE2	6:A:804:HOH:O	2.21	0.44
1:B:280:ARG:HG2	6:B:801:HOH:O	2.18	0.43
1:B:503:PHE:CD1	1:B:521:ARG:HB2	2.54	0.43
1:B:605:ARG:HD2	1:B:622:PHE:O	2.19	0.43
1:B:560:THR:OG1	5:B:713:CDP:O2A	2.28	0.43
1:B:330:ALA:O	1:B:334:ARG:HG3	2.18	0.43
1:B:196:ASP:OD1	1:B:198:SER:OG	2.26	0.43
1:A:110:HIS:N	3:A:716:GOL:H32	2.26	0.43
1:A:628:TYR:HA	1:A:629:PRO:HD3	1.87	0.43
1:A:167:MET:HE2	1:A:167:MET:HB3	1.72	0.42
1:B:599:VAL:HB	5:B:713:CDP:O3'	2.19	0.42
1:B:615:THR:CB	3:B:706:GOL:H12	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:HA	1:A:164:ARG:HD2	1.67	0.42
1:A:315:ASN:OD1	1:A:317:TYR:HB3	2.19	0.42
1:B:164:ARG:HA	1:B:164:ARG:HD3	1.75	0.42
1:B:44:LEU:HD11	3:B:712:GOL:H11	2.00	0.42
1:B:218:PRO:HG3	1:B:221:TRP:CZ2	2.55	0.42
1:B:598:ARG:HH12	1:B:604:GLY:HA2	1.84	0.42
1:A:190:ASP:HA	1:A:191:PRO:HD3	1.93	0.42
1:B:169:THR:HG22	1:B:430:LYS:HD3	2.02	0.42
1:A:27:ARG:NH1	1:A:598:ARG:HH11	2.16	0.41
1:A:345:ARG:HD3	1:A:345:ARG:HA	1.94	0.41
1:B:44:LEU:HD21	3:B:712:GOL:H11	2.03	0.41
1:A:552:GLU:HG2	1:A:556:MET:SD	2.61	0.41
1:B:307:MET:HG3	1:B:308:THR:N	2.36	0.41
1:B:357:TYR:HE2	1:B:366:ILE:HD11	1.86	0.41
1:B:46:PRO:O	1:B:584:GLY:HA3	2.22	0.40
1:B:607:ALA:CB	5:B:713:CDP:O3A	2.69	0.40
1:A:168:GLN:HE21	1:A:372:GLN:NE2	2.06	0.40
1:A:169:THR:HG22	1:A:430:LYS:HD3	2.03	0.40
1:B:332:TRP:NE1	1:B:345:ARG:HD2	2.36	0.40
3:A:713:GOL:O3	3:A:716:GOL:O1	2.29	0.40
1:B:628:TYR:HA	1:B:629:PRO:HD3	1.94	0.40

All (2) 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)
3:A:711:GOL:O2	6:B:1062:HOH:O[1_554]	2.17	0.03
1:B:250:THR:OG1	6:A:986:HOH:O[1_556]	2.19	0.01

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	661/705 (94%)	645 (98%)	15 (2%)	1 (0%)	47	49
1	B	663/705 (94%)	646 (97%)	15 (2%)	2 (0%)	41	41
All	All	1324/1410 (94%)	1291 (98%)	30 (2%)	3 (0%)	47	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	641	ASP
1	B	307	MET
1	B	38	ALA

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	562/598 (94%)	559 (100%)	3 (0%)	88	92
1	B	564/598 (94%)	562 (100%)	2 (0%)	91	94
All	All	1126/1196 (94%)	1121 (100%)	5 (0%)	91	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	A	349	TYR
1	A	366	ILE
1	B	349	TYR
1	B	578	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 1 is monoatomic - leaving 33 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$
2	SO4	B	702	-	4,4,4	0.15	0	6,6,6	0.16	0
3	GOL	B	708	-	5,5,5	0.36	0	5,5,5	0.68	0
3	GOL	A	712	-	5,5,5	0.36	0	5,5,5	0.17	0
3	GOL	A	716	-	5,5,5	0.32	0	5,5,5	0.39	0
3	GOL	A	718	-	5,5,5	0.37	0	5,5,5	0.30	0
5	CDP	B	713	-	19,22,26	1.17	2 (10%)	24,33,40	1.36	3 (12%)
5	CDP	A	721	-	21,26,26	1.07	2 (9%)	28,40,40	1.23	3 (10%)
2	SO4	A	707	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	B	703	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	B	704	-	4,4,4	0.16	0	6,6,6	0.18	0
3	GOL	B	711	-	5,5,5	0.36	0	5,5,5	0.27	0
2	SO4	A	705	-	4,4,4	0.17	0	6,6,6	0.31	0
2	SO4	B	705	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	701	-	4,4,4	0.17	0	6,6,6	0.14	0
3	GOL	A	711	-	5,5,5	0.42	0	5,5,5	0.25	0
3	GOL	B	712	-	5,5,5	0.39	0	5,5,5	0.26	0
3	GOL	A	708	-	5,5,5	0.32	0	5,5,5	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	706	-	4,4,4	0.15	0	6,6,6	0.08	0
3	GOL	A	713	-	5,5,5	0.32	0	5,5,5	0.44	0
3	GOL	A	717	-	5,5,5	0.38	0	5,5,5	0.72	0
3	GOL	B	710	-	5,5,5	0.36	0	5,5,5	0.34	0
3	GOL	B	707	-	5,5,5	0.38	0	5,5,5	0.18	0
3	GOL	A	709	-	5,5,5	0.35	0	5,5,5	0.59	0
3	GOL	A	715	-	5,5,5	0.37	0	5,5,5	0.21	0
3	GOL	B	709	-	5,5,5	0.42	0	5,5,5	0.34	0
2	SO4	A	703	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	A	704	-	4,4,4	0.17	0	6,6,6	0.21	0
3	GOL	B	706	-	5,5,5	0.39	0	5,5,5	0.44	0
2	SO4	A	702	-	4,4,4	0.17	0	6,6,6	0.12	0
3	GOL	A	710	-	5,5,5	0.37	0	5,5,5	0.30	0
3	GOL	A	719	-	5,5,5	0.42	0	5,5,5	0.53	0
3	GOL	A	714	-	5,5,5	0.38	0	5,5,5	0.27	0
2	SO4	A	701	-	4,4,4	0.12	0	6,6,6	0.20	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
3	GOL	A	709	-	-	4/4/4/4	-
3	GOL	A	711	-	-	4/4/4/4	-
3	GOL	B	710	-	-	2/4/4/4	-
3	GOL	A	715	-	-	2/4/4/4	-
3	GOL	B	708	-	-	1/4/4/4	-
3	GOL	A	712	-	-	2/4/4/4	-
3	GOL	B	712	-	-	3/4/4/4	-
3	GOL	A	708	-	-	4/4/4/4	-
3	GOL	A	716	-	-	2/4/4/4	-
3	GOL	A	718	-	-	2/4/4/4	-
3	GOL	B	711	-	-	3/4/4/4	-
3	GOL	B	709	-	-	3/4/4/4	-
3	GOL	A	713	-	-	0/4/4/4	-
3	GOL	B	706	-	-	4/4/4/4	-
3	GOL	A	710	-	-	2/4/4/4	-
3	GOL	A	717	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CDP	B	713	-	-	4/8/26/32	0/2/2/2
3	GOL	A	719	-	-	3/4/4/4	-
3	GOL	A	714	-	-	2/4/4/4	-
5	CDP	A	721	-	-	5/14/32/32	0/2/2/2
3	GOL	B	707	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	713	CDP	O4'-C1'	2.74	1.44	1.41
5	A	721	CDP	O4'-C1'	2.69	1.44	1.41
5	B	713	CDP	C2-N3	-2.29	1.33	1.38
5	A	721	CDP	C2-N3	-2.25	1.33	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	713	CDP	C2-N3-C4	4.23	120.63	116.34
5	A	721	CDP	C2-N3-C4	4.19	120.59	116.34
5	B	713	CDP	N4-C4-N3	2.32	120.16	116.49
5	B	713	CDP	O4'-C1'-C2'	-2.32	103.53	106.93
5	A	721	CDP	O4'-C1'-C2'	-2.31	103.55	106.93
5	A	721	CDP	N4-C4-N3	2.30	120.13	116.49

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	716	GOL	O1-C1-C2-C3
3	A	718	GOL	O1-C1-C2-C3
5	B	713	CDP	O4'-C1'-N1-C6
5	B	713	CDP	C2'-C1'-N1-C6
5	A	721	CDP	O4'-C4'-C5'-O5'
5	A	721	CDP	C3'-C4'-C5'-O5'
5	A	721	CDP	C2'-C1'-N1-C6
3	B	711	GOL	C1-C2-C3-O3
3	B	711	GOL	O2-C2-C3-O3
3	A	711	GOL	O1-C1-C2-C3
3	A	711	GOL	C1-C2-C3-O3
3	B	712	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	708	GOL	O1-C1-C2-C3
3	A	708	GOL	C1-C2-C3-O3
3	B	710	GOL	O1-C1-C2-C3
3	B	707	GOL	O1-C1-C2-C3
3	A	709	GOL	O1-C1-C2-C3
3	A	709	GOL	C1-C2-C3-O3
3	A	715	GOL	C1-C2-C3-O3
3	B	706	GOL	O1-C1-C2-C3
3	A	710	GOL	C1-C2-C3-O3
3	A	719	GOL	O1-C1-C2-C3
3	A	714	GOL	O1-C1-C2-C3
3	A	708	GOL	O1-C1-C2-O2
3	A	709	GOL	O1-C1-C2-O2
3	B	706	GOL	O1-C1-C2-O2
3	B	706	GOL	C1-C2-C3-O3
3	A	716	GOL	O1-C1-C2-O2
3	A	718	GOL	O1-C1-C2-O2
3	B	712	GOL	O2-C2-C3-O3
3	A	708	GOL	O2-C2-C3-O3
3	B	710	GOL	O1-C1-C2-O2
3	B	707	GOL	O1-C1-C2-O2
3	A	709	GOL	O2-C2-C3-O3
3	B	706	GOL	O2-C2-C3-O3
3	A	711	GOL	O1-C1-C2-O2
3	A	710	GOL	O2-C2-C3-O3
3	A	719	GOL	O1-C1-C2-O2
3	B	708	GOL	O1-C1-C2-C3
3	A	717	GOL	O1-C1-C2-C3
3	A	711	GOL	O2-C2-C3-O3
3	A	715	GOL	O2-C2-C3-O3
3	A	714	GOL	O1-C1-C2-O2
5	A	721	CDP	PB-O3A-PA-O5'
3	A	712	GOL	O1-C1-C2-O2
3	B	711	GOL	O1-C1-C2-O2
3	B	709	GOL	O1-C1-C2-O2
3	B	709	GOL	O1-C1-C2-C3
5	B	713	CDP	C4'-C5'-O5'-PA
5	A	721	CDP	C4'-C5'-O5'-PA
3	B	712	GOL	O1-C1-C2-C3
3	A	717	GOL	O1-C1-C2-O2
3	A	712	GOL	O1-C1-C2-C3
3	A	717	GOL	O2-C2-C3-O3

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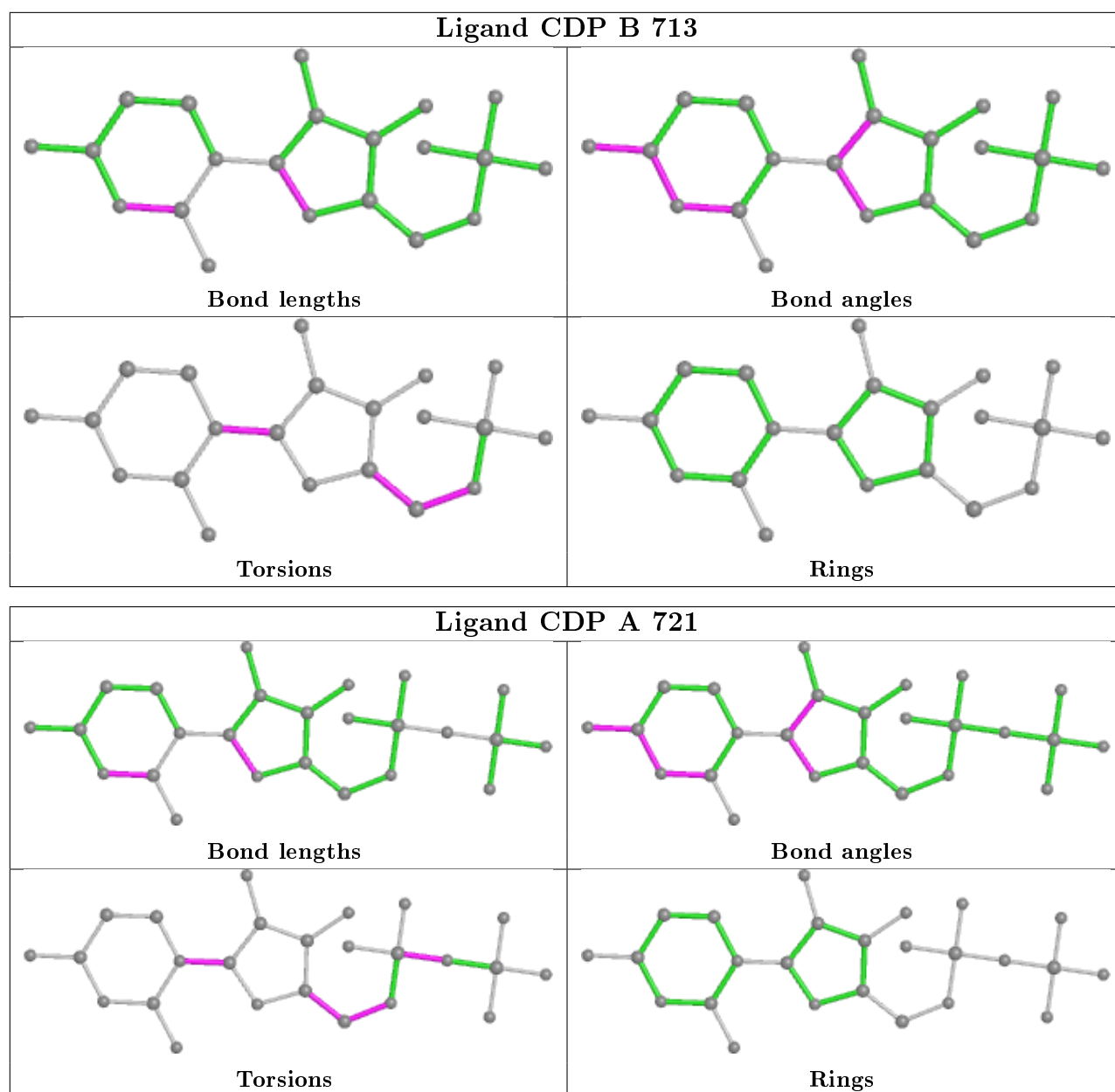
Mol	Chain	Res	Type	Atoms
3	A	719	GOL	O2-C2-C3-O3
5	B	713	CDP	O4'-C4'-C5'-O5'
3	B	709	GOL	O2-C2-C3-O3

There are no ring outliers.

15 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	708	GOL	3	0
3	A	712	GOL	1	0
3	A	716	GOL	3	0
5	B	713	CDP	10	0
5	A	721	CDP	7	0
2	A	707	SO4	4	0
3	B	711	GOL	1	0
3	A	711	GOL	2	1
3	B	712	GOL	3	0
3	A	713	GOL	1	0
3	B	707	GOL	1	0
3	B	706	GOL	2	0
3	A	710	GOL	2	0
3	A	719	GOL	1	0
3	A	714	GOL	1	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 than 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.



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

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	663/705 (94%)	-0.24	6 (0%) 84 86	16, 26, 53, 103	0
1	B	665/705 (94%)	-0.23	18 (2%) 54 60	17, 29, 56, 101	0
All	All	1328/1410 (94%)	-0.24	24 (1%) 68 72	16, 27, 54, 103	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	548	TYR	6.8
1	A	548	TYR	5.4
1	A	550	SER	5.0
1	B	54	ARG	4.0
1	B	126	VAL	4.0
1	B	128	THR	3.9
1	B	549	ARG	3.9
1	B	550	SER	3.8
1	B	551	LYS	3.5
1	B	127	ASN	3.5
1	A	551	LYS	3.5
1	B	553	THR	3.5
1	B	11	THR	2.8
1	B	552	GLU	2.8
1	B	556	MET	2.6
1	A	643	PRO	2.4
1	A	549	ARG	2.4
1	B	674	GLU	2.4
1	B	10	PRO	2.3
1	A	619	VAL	2.3
1	B	38	ALA	2.3
1	B	643	PRO	2.3
1	B	547	LYS	2.1
1	B	600	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

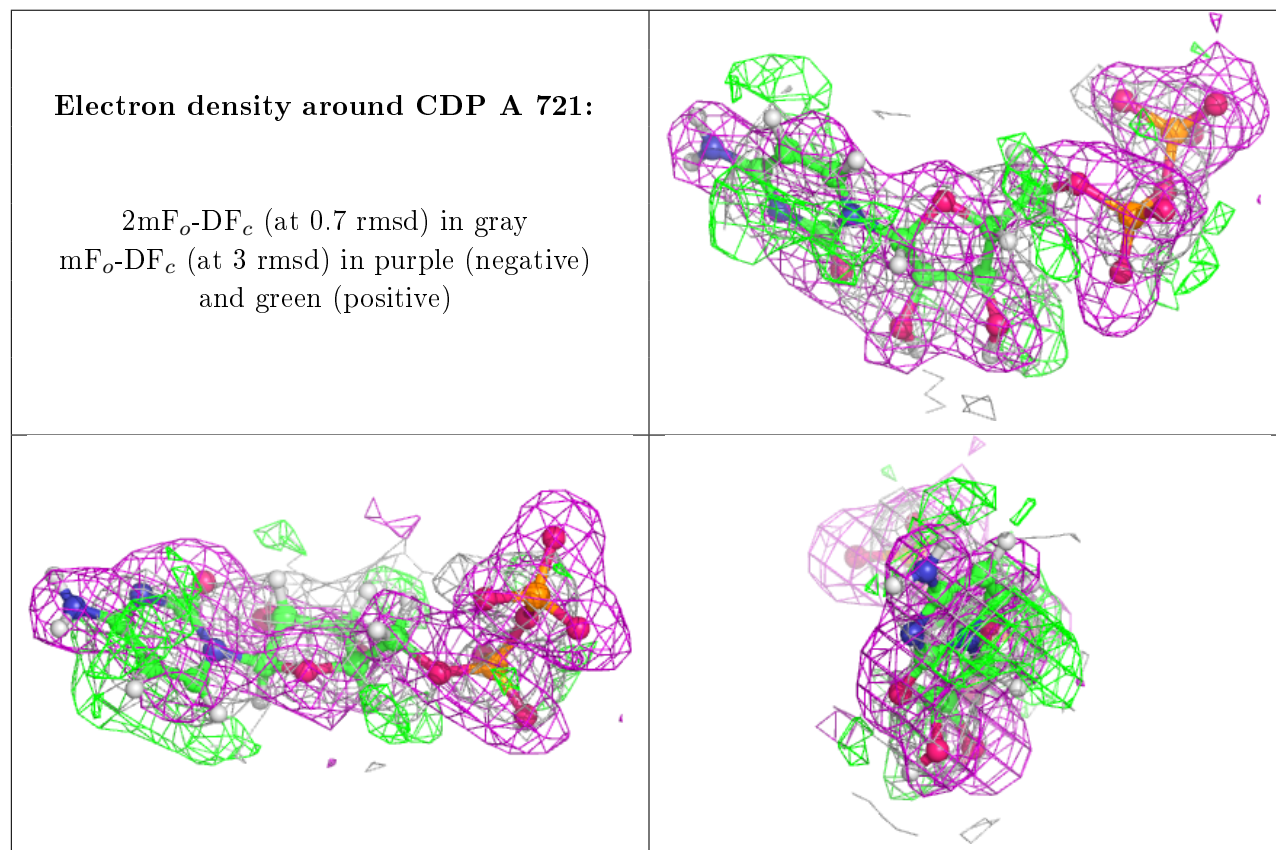
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	710	6/6	0.56	0.28	60,78,78,84	0
3	GOL	A	715	6/6	0.65	0.21	57,60,64,65	0
3	GOL	B	708	6/6	0.66	0.23	40,44,58,61	0
5	CDP	A	721	25/25	0.69	0.60	20,20,20,20	0
5	CDP	B	713	21/25	0.70	0.57	20,20,20,20	0
3	GOL	B	706	6/6	0.73	0.19	40,49,55,56	0
3	GOL	B	712	6/6	0.76	0.29	43,53,54,59	0
3	GOL	B	711	6/6	0.76	0.24	36,52,55,57	0
3	GOL	A	712	6/6	0.80	0.20	29,61,63,66	0
3	GOL	B	707	6/6	0.81	0.20	30,43,56,59	0
3	GOL	A	716	6/6	0.84	0.20	44,50,56,62	0
3	GOL	A	717	6/6	0.84	0.27	36,42,64,69	0
3	GOL	A	718	6/6	0.88	0.16	61,65,69,74	0
3	GOL	A	711	6/6	0.89	0.20	58,63,66,71	0
3	GOL	A	719	6/6	0.91	0.17	41,54,59,60	0
3	GOL	B	709	6/6	0.92	0.14	45,51,54,55	0
3	GOL	A	709	6/6	0.93	0.18	36,39,44,50	0
2	SO4	B	705	5/5	0.93	0.14	81,82,85,86	0
3	GOL	A	708	6/6	0.93	0.17	37,52,54,57	0
3	GOL	A	714	6/6	0.93	0.12	59,61,61,66	0
4	MG	A	720	1/1	0.94	0.08	40,40,40,40	0
3	GOL	B	710	6/6	0.94	0.10	46,58,60,60	0
2	SO4	A	706	5/5	0.96	0.10	78,81,85,87	0
2	SO4	A	707	5/5	0.97	0.13	57,60,68,69	0
3	GOL	A	713	6/6	0.97	0.12	26,36,38,38	0
2	SO4	B	701	5/5	0.98	0.13	47,48,49,51	0
2	SO4	B	703	5/5	0.98	0.11	49,49,54,56	0

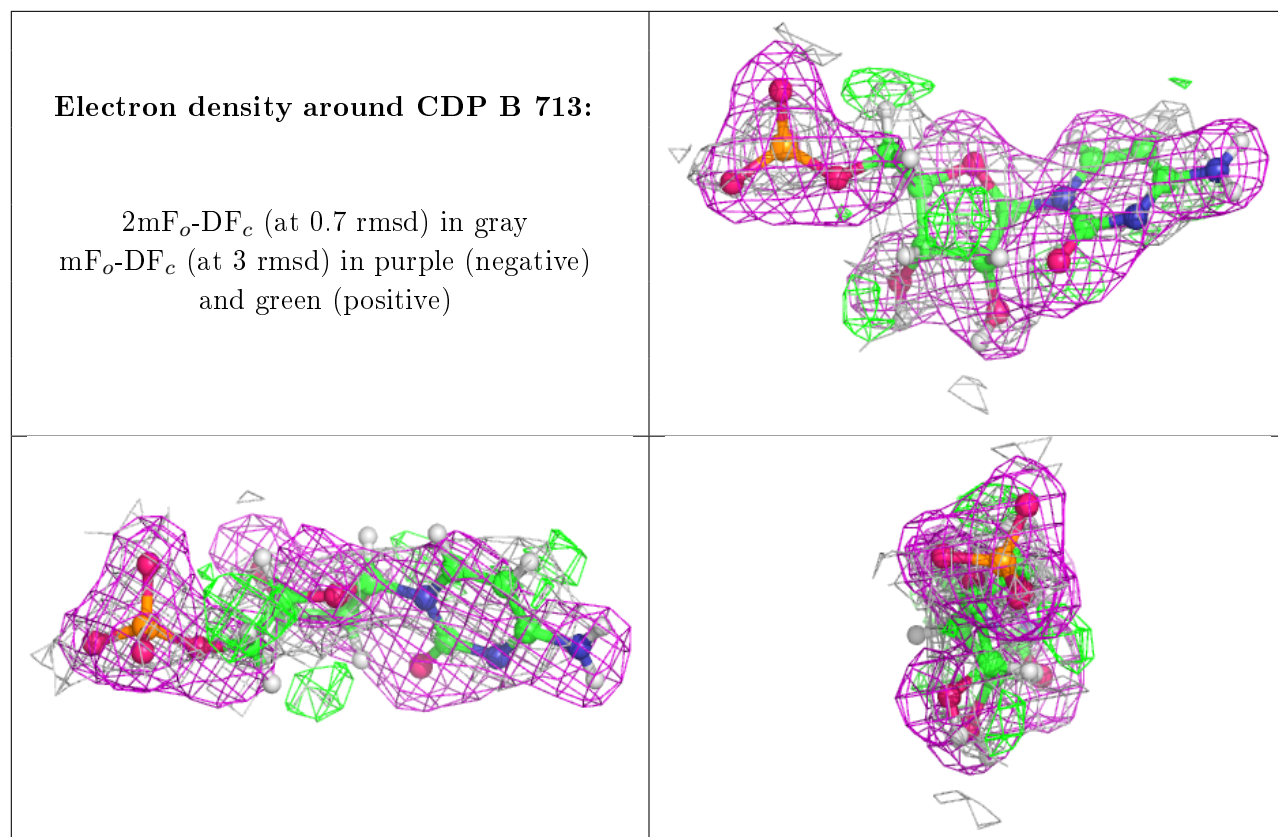
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	B	704	5/5	0.98	0.12	33,35,41,49	0
2	SO4	A	703	5/5	0.98	0.10	41,42,46,48	0
2	SO4	A	701	5/5	0.98	0.10	41,44,45,48	0
2	SO4	A	705	5/5	0.99	0.10	31,39,42,46	0
2	SO4	A	704	5/5	0.99	0.12	32,36,44,46	0
2	SO4	B	702	5/5	0.99	0.12	39,40,49,49	0
2	SO4	A	702	5/5	0.99	0.12	38,40,47,48	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.