



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:22 AM UTC

PDB ID : 6PD2 / pdb_00006pd2
Title : PntC-AEPT: fusion protein of phosphonate-specific cytidyltransferase and 2-aminoethylphosphonate (AEP) transaminase from *Treponema denticola* in complex with cytidine monophosphate-AEP
Authors : Suits, M.D.L.; Whiteside, J.
Deposited on : 2019-06-18
Resolution : 1.95 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

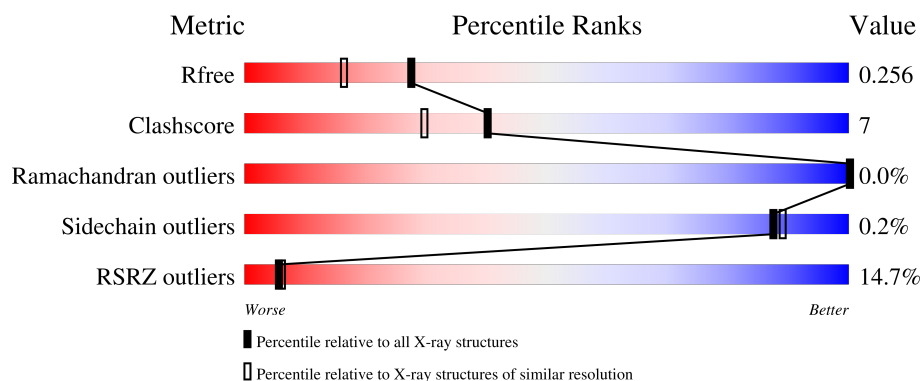
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 $\leq 5\%$. 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	624	14% 86% 12%
1	B	624	17% 82% 16%
1	C	624	9% 86% 13%
1	D	624	17% 88% 9%

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	PO4	D	709	-	-	X	-
6	EDO	A	709	-	-	X	-
6	EDO	A	716	-	-	X	-
6	EDO	B	706	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21090 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 Nucleotidyl transferase/aminotransferase, class V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	615	Total	C	N	O	S	0	0	0
			4831	3084	798	914	35			
1	B	615	Total	C	N	O	S	0	0	0
			4831	3084	798	914	35			
1	C	616	Total	C	N	O	S	0	0	0
			4838	3089	799	915	35			
1	D	608	Total	C	N	O	S	0	0	0
			4776	3051	786	904	35			

There are 32 discrepancies between the modelled and reference sequences:

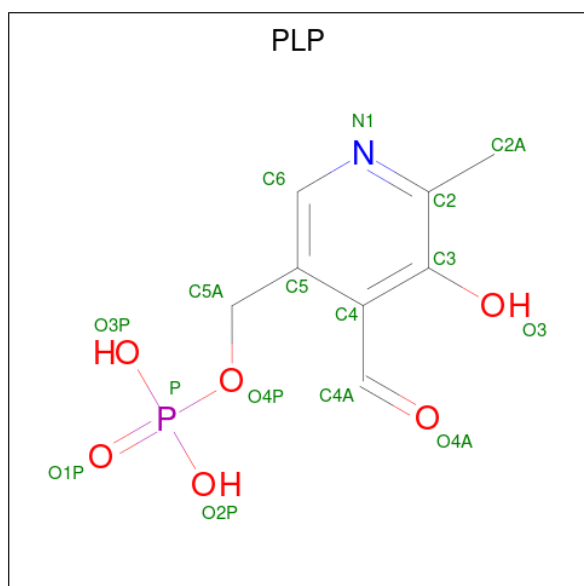
Chain	Residue	Modelled	Actual	Comment	Reference
A	617	LEU	-	expression tag	UNP Q73MU2
A	618	GLU	-	expression tag	UNP Q73MU2
A	619	HIS	-	expression tag	UNP Q73MU2
A	620	HIS	-	expression tag	UNP Q73MU2
A	621	HIS	-	expression tag	UNP Q73MU2
A	622	HIS	-	expression tag	UNP Q73MU2
A	623	HIS	-	expression tag	UNP Q73MU2
A	624	HIS	-	expression tag	UNP Q73MU2
B	617	LEU	-	expression tag	UNP Q73MU2
B	618	GLU	-	expression tag	UNP Q73MU2
B	619	HIS	-	expression tag	UNP Q73MU2
B	620	HIS	-	expression tag	UNP Q73MU2
B	621	HIS	-	expression tag	UNP Q73MU2
B	622	HIS	-	expression tag	UNP Q73MU2
B	623	HIS	-	expression tag	UNP Q73MU2
B	624	HIS	-	expression tag	UNP Q73MU2
C	617	LEU	-	expression tag	UNP Q73MU2
C	618	GLU	-	expression tag	UNP Q73MU2
C	619	HIS	-	expression tag	UNP Q73MU2
C	620	HIS	-	expression tag	UNP Q73MU2
C	621	HIS	-	expression tag	UNP Q73MU2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	622	HIS	-	expression tag	UNP Q73MU2
C	623	HIS	-	expression tag	UNP Q73MU2
C	624	HIS	-	expression tag	UNP Q73MU2
D	617	LEU	-	expression tag	UNP Q73MU2
D	618	GLU	-	expression tag	UNP Q73MU2
D	619	HIS	-	expression tag	UNP Q73MU2
D	620	HIS	-	expression tag	UNP Q73MU2
D	621	HIS	-	expression tag	UNP Q73MU2
D	622	HIS	-	expression tag	UNP Q73MU2
D	623	HIS	-	expression tag	UNP Q73MU2
D	624	HIS	-	expression tag	UNP Q73MU2

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).

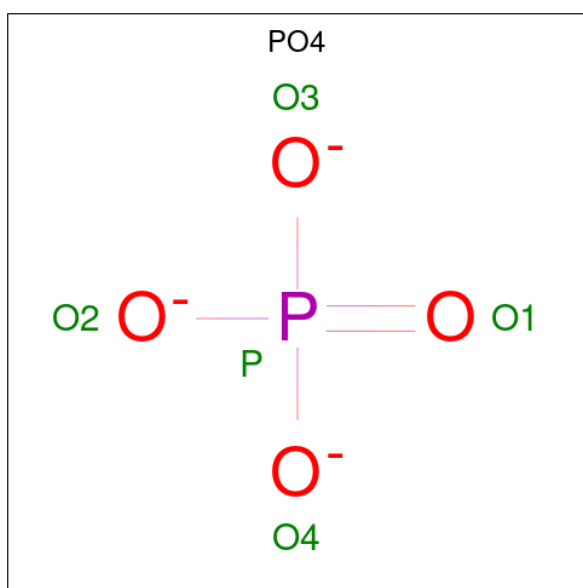


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0
3	D	2	Total Mg 2 2	0	0

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



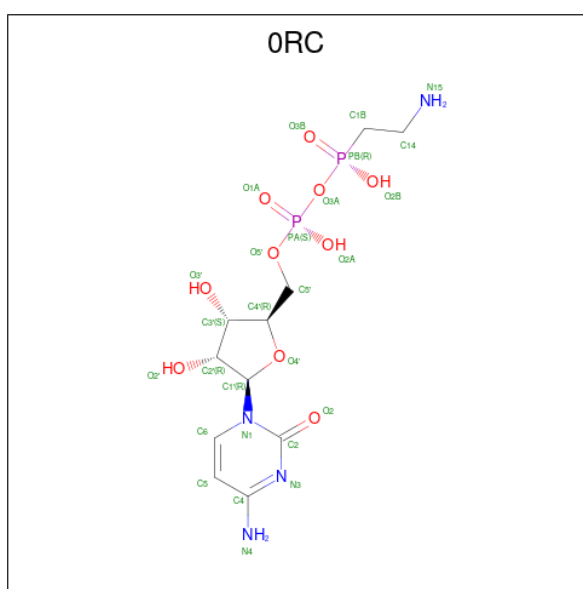
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0

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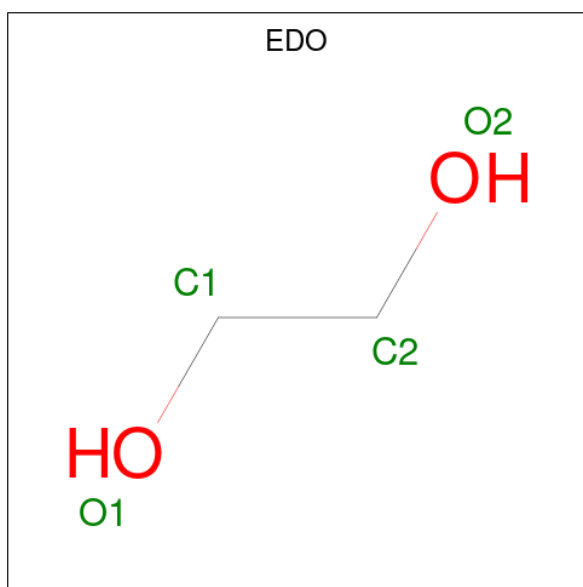
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 5'-O-[(S)-{[(R)-(2-aminoethyl)(hydroxy)phosphoryl]oxy}(hydroxy)phosphoryl]cytidine (CCD ID: 0RC) (formula: C₁₁H₂₀N₄O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	11	4	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	11	4	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	11	4	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	11	4	10	2		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



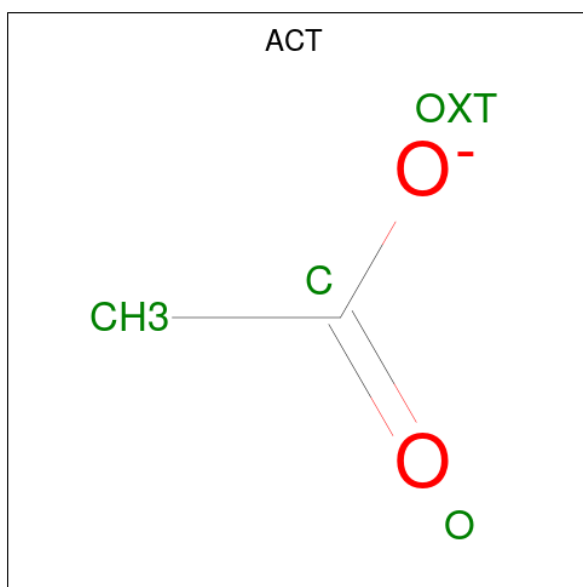
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total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

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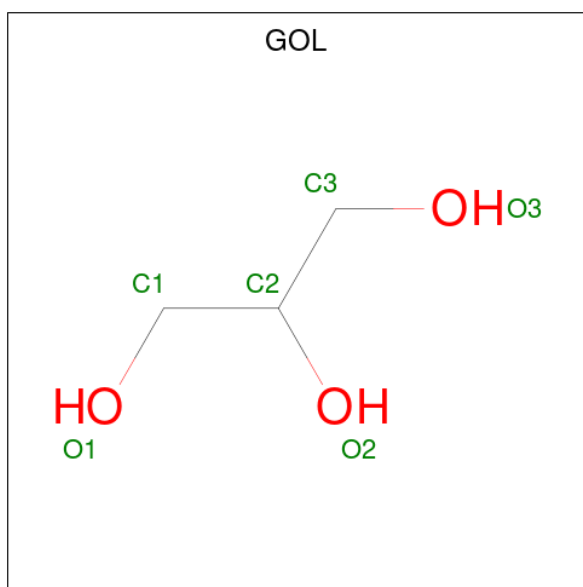
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total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

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

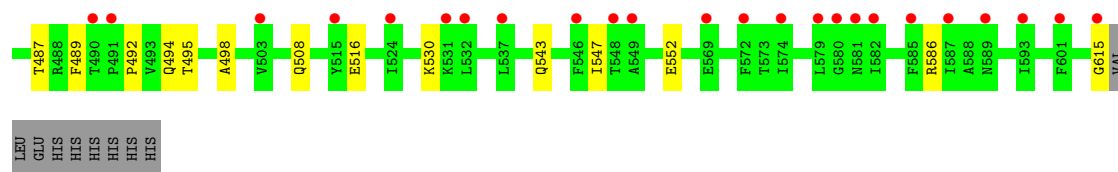
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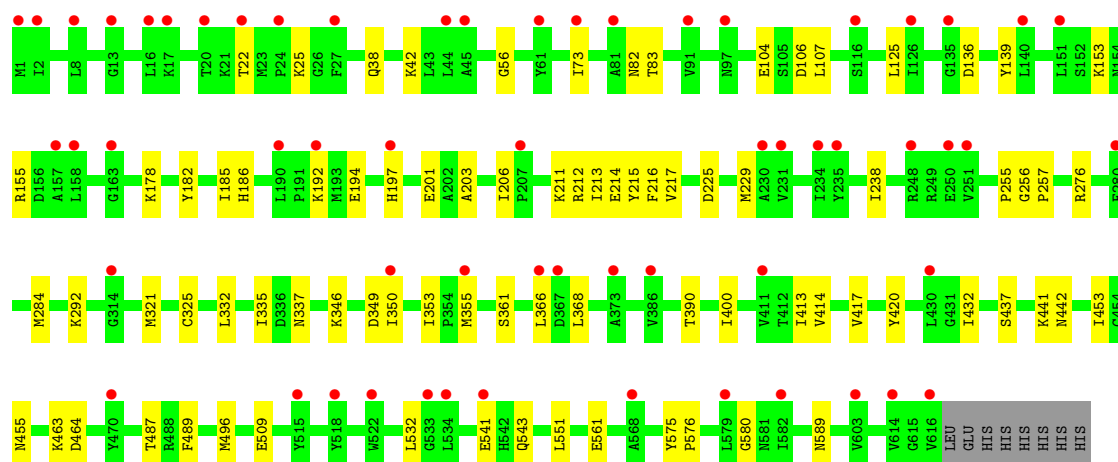
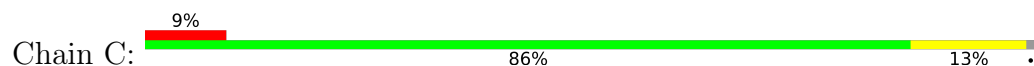
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is water.

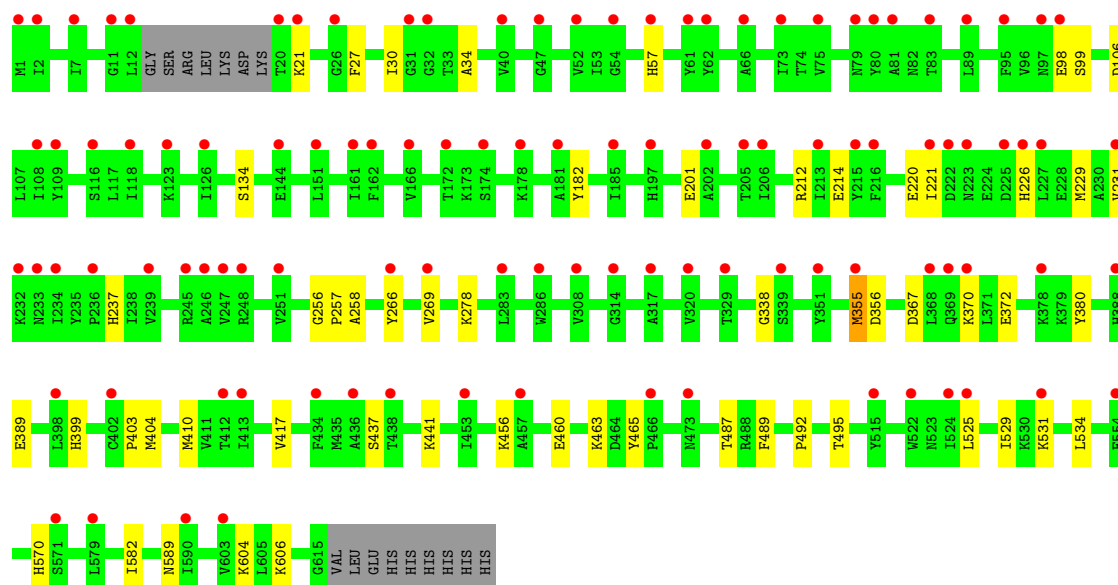
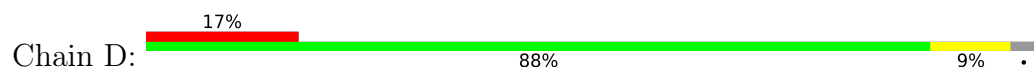
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	354	Total	O	0	0
			354	354		
9	B	352	Total	O	0	0
			352	352		
9	C	411	Total	O	0	0
			411	411		
9	D	330	Total	O	0	0
			330	330		



- Molecule 1: Nucleotidyl transferase/aminotransferase, class V



- Molecule 1: Nucleotidyl transferase/aminotransferase, class V



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.45Å 154.05Å 134.58Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	47.98 – 1.95 47.98 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.98-1.95) 98.1 (47.98-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.220 , 0.254 0.222 , 0.256	Depositor DCC
R_{free} test set	10992 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.768	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21090	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: ORC, MG, GOL, ACT, EDO, PLP, PO4

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	0.49	0/4925	0.64	0/6655
1	B	0.48	0/4925	0.63	0/6655
1	C	0.53	0/4932	0.66	4/6665 (0.1%)
1	D	0.49	0/4869	0.64	0/6581
All	All	0.50	0/19651	0.64	4/26556 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	276	ARG	NE-CZ-NH1	-5.93	115.57	121.50
1	C	276	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	C	509	GLU	CA-C-N	5.09	131.25	121.54
1	C	509	GLU	C-N-CA	5.09	131.25	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4831	0	4866	68	0
1	B	4831	0	4866	80	0
1	C	4838	0	4875	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4776	0	4803	43	0
2	A	16	0	7	1	0
2	B	16	0	8	0	0
2	C	16	0	7	1	0
2	D	16	0	7	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0
4	C	15	0	0	0	0
4	D	15	0	0	3	0
5	A	27	0	0	2	0
5	B	27	0	0	2	0
5	C	27	0	0	0	0
5	D	27	0	0	0	0
6	A	40	0	58	16	0
6	B	12	0	18	9	0
6	C	28	0	42	9	0
6	D	28	0	42	2	0
7	A	8	0	6	0	0
7	C	4	0	3	0	0
8	B	12	0	14	3	0
9	A	354	0	0	7	1
9	B	352	0	0	13	1
9	C	411	0	0	15	0
9	D	330	0	0	9	0
All	All	21090	0	19622	259	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 7.

All (259) 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:C:337:ASN:ND2	1:C:366:LEU:HD11	1.77	0.99
1:A:321:MET:HE2	1:A:413:ILE:HG23	1.45	0.99
1:B:1:MET:SD	9:B:1144:HOH:O	2.30	0.89
1:C:83:THR:O	1:C:192:LYS:NZ	2.05	0.88
1:D:417:VAL:HG12	1:D:441:LYS:HD2	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ALA:HA	1:B:193:MET:HE1	1.55	0.88
1:B:178:LYS:NZ	9:B:804:HOH:O	2.07	0.86
1:C:82:ASN:C	1:C:192:LYS:HE2	2.05	0.82
4:D:709:PO4:O2	9:D:801:HOH:O	1.96	0.82
1:A:481:PHE:HB3	6:A:709:EDO:H22	1.63	0.81
1:C:321:MET:O	9:C:2301:HOH:O	1.99	0.79
1:D:21:LYS:H	1:D:21:LYS:HD2	1.46	0.79
1:C:335:ILE:O	9:C:2302:HOH:O	2.02	0.78
1:B:552:GLU:OE2	9:B:801:HOH:O	2.03	0.77
1:D:367:ASP:CG	1:D:370:LYS:HE3	2.09	0.77
1:A:437:SER:OG	6:A:716:EDO:H22	1.85	0.77
4:D:714:PO4:O1	9:D:802:HOH:O	2.04	0.76
1:C:455:ASN:HD22	6:C:2208:EDO:H22	1.50	0.76
1:B:615:GLY:O	9:B:802:HOH:O	2.05	0.75
1:A:456:LYS:O	1:A:460:GLU:HG2	1.87	0.75
1:C:212:ARG:NH1	1:C:214:GLU:OE2	2.21	0.73
1:B:292:LYS:O	9:B:803:HOH:O	2.06	0.72
1:B:172:THR:HG23	1:B:175:THR:H	1.52	0.72
1:D:98:GLU:CD	1:D:99:SER:H	1.99	0.70
1:B:276:ARG:NH2	4:D:709:PO4:O4	2.23	0.70
1:D:266:TYR:O	1:D:269:VAL:HG22	1.93	0.69
1:B:221:ILE:HD11	1:B:230:ALA:HB2	1.74	0.68
1:A:256:GLY:HA2	1:A:257:PRO:C	2.18	0.67
1:C:325:CYS:HB2	9:C:2301:HOH:O	1.94	0.67
1:A:250:GLU:OE2	9:A:801:HOH:O	2.13	0.67
1:D:226:HIS:HA	1:D:229:MET:HE3	1.78	0.66
1:D:256:GLY:HA2	1:D:257:PRO:C	2.21	0.66
1:B:516:GLU:OE1	9:B:805:HOH:O	2.14	0.66
1:C:349:ASP:OD2	9:C:2303:HOH:O	2.14	0.66
1:C:361:SER:H	6:C:2209:EDO:H21	1.61	0.65
1:A:64:ASN:HA	1:A:67:LYS:HD2	1.79	0.65
1:A:321:MET:CE	1:A:413:ILE:HG23	2.25	0.65
1:A:7:ILE:HD12	1:A:103:LEU:HB2	1.79	0.65
1:B:477:GLN:HE22	8:B:711:GOL:H32	1.62	0.64
1:A:478:TYR:HA	6:A:709:EDO:H11	1.78	0.63
6:B:706:EDO:H11	9:D:1034:HOH:O	1.98	0.63
1:B:417:VAL:HG12	1:B:441:LYS:HD2	1.81	0.62
1:C:561:GLU:HG2	9:C:2677:HOH:O	1.98	0.62
1:B:477:GLN:HE22	8:B:711:GOL:C3	2.12	0.62
1:A:441:LYS:HG2	9:A:810:HOH:O	1.98	0.61
1:D:531:LYS:NZ	1:D:606:LYS:HD2	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:ASN:HD22	1:C:366:LEU:HD11	1.61	0.61
1:B:25:LYS:HE3	1:B:106:ASP:HB3	1.81	0.61
1:B:483:LYS:HA	1:B:483:LYS:HE2	1.81	0.60
1:A:443:ILE:H	6:A:716:EDO:H11	1.66	0.60
1:D:570:HIS:ND1	1:D:604:LYS:HE3	2.17	0.59
1:A:222:ASP:CG	5:A:705:0RC:O3B	2.44	0.59
1:C:292:LYS:HA	1:C:453:ILE:HD13	1.85	0.59
1:C:455:ASN:ND2	6:C:2208:EDO:H22	2.17	0.59
1:C:368:LEU:HD13	1:C:400:ILE:HG21	1.85	0.58
1:A:184:LYS:NZ	9:A:813:HOH:O	2.30	0.58
1:A:138:VAL:H	6:A:717:EDO:H12	1.69	0.57
1:A:262:ASP:CG	6:A:712:EDO:H22	2.30	0.57
1:A:443:ILE:N	6:A:716:EDO:H11	2.19	0.57
1:D:182:TYR:CD1	1:D:201:GLU:HG2	2.39	0.57
1:B:144:GLU:H	1:B:144:GLU:CD	2.13	0.56
1:D:456:LYS:NZ	9:D:806:HOH:O	2.38	0.56
1:A:481:PHE:HB3	6:A:709:EDO:C2	2.35	0.56
1:C:256:GLY:HA2	1:C:257:PRO:C	2.31	0.56
1:B:222:ASP:OD1	5:B:705:0RC:O3B	2.23	0.56
1:A:182:TYR:CD1	1:A:201:GLU:HG2	2.41	0.55
1:A:117:LEU:HD11	1:A:127:LEU:HB2	1.89	0.54
1:C:346:LYS:HG3	6:C:2210:EDO:H21	1.89	0.54
1:A:441:LYS:NZ	2:A:701:PLP:O4A	2.39	0.54
1:C:541:GLU:HG3	9:C:2673:HOH:O	2.08	0.54
1:B:226:HIS:HA	1:B:229:MET:HE3	1.90	0.54
1:A:321:MET:HE3	1:A:434:PHE:CB	2.37	0.54
1:B:212:ARG:NH1	1:B:214:GLU:OE1	2.24	0.54
1:B:295:ALA:HB3	9:B:803:HOH:O	2.06	0.54
6:B:706:EDO:H11	1:D:257:PRO:HB3	1.91	0.53
1:C:580:GLY:O	9:C:2304:HOH:O	2.19	0.52
1:D:465:TYR:HB3	6:D:706:EDO:O2	2.10	0.52
1:A:141:GLU:OE1	1:A:159:LYS:HE3	2.10	0.52
1:C:353:ILE:O	1:C:355:MET:HG2	2.10	0.52
1:D:465:TYR:HB3	6:D:706:EDO:H12	1.92	0.52
1:C:284:MET:HE1	1:C:487:THR:HG21	1.91	0.52
1:A:110:ASP:OD1	1:A:245:ARG:NH2	2.43	0.52
1:A:522:TRP:O	1:A:526:VAL:HG22	2.09	0.52
1:A:141:GLU:OE2	1:A:159:LYS:HG3	2.09	0.52
1:A:321:MET:HE3	1:A:434:PHE:HB2	1.92	0.52
1:C:82:ASN:C	1:C:192:LYS:CE	2.82	0.51
1:C:104:GLU:HB2	1:C:107:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:PRO:HD3	1:A:430:LEU:O	2.11	0.51
1:C:284:MET:HE2	1:C:496:MET:HE1	1.92	0.51
1:B:530:LYS:O	9:B:806:HOH:O	2.19	0.50
1:C:350:ILE:HG13	6:C:2210:EDO:H11	1.93	0.50
1:C:25:LYS:HE3	1:C:106:ASP:HB3	1.93	0.50
1:B:427:LEU:HD22	1:B:432:ILE:HB	1.94	0.50
1:A:414:VAL:HG21	1:A:432:ILE:HG12	1.94	0.50
1:B:273:ILE:H	6:B:706:EDO:C2	2.24	0.50
1:C:366:LEU:HD12	1:C:366:LEU:N	2.27	0.49
1:D:278:LYS:NZ	9:D:817:HOH:O	2.45	0.49
1:A:466:PRO:HA	6:A:714:EDO:H12	1.93	0.49
1:B:273:ILE:H	6:B:706:EDO:H21	1.77	0.49
1:B:346:LYS:NZ	9:B:822:HOH:O	2.39	0.49
1:B:222:ASP:CG	5:B:705:0RC:O3B	2.54	0.49
1:B:256:GLY:HA2	1:B:257:PRO:C	2.38	0.49
1:C:178:LYS:NZ	9:C:2305:HOH:O	2.22	0.49
1:D:212:ARG:NH1	1:D:214:GLU:OE1	2.46	0.49
1:A:529:ILE:HG23	1:A:534:LEU:HB2	1.95	0.49
1:C:487:THR:HG23	1:C:489:PHE:O	2.13	0.49
1:B:213:ILE:HB	1:B:216:PHE:HB2	1.94	0.48
1:C:185:ILE:HG22	1:C:186:HIS:CD2	2.48	0.48
1:D:182:TYR:CG	1:D:201:GLU:HG2	2.48	0.48
1:B:27:PHE:CE2	1:B:61:TYR:HB3	2.48	0.48
1:B:417:VAL:HG12	1:B:441:LYS:CD	2.41	0.48
1:D:531:LYS:HZ1	1:D:606:LYS:HD2	1.76	0.48
1:C:413:ILE:HD13	9:C:2301:HOH:O	2.13	0.48
1:B:382:HIS:CD2	1:B:411:VAL:HB	2.49	0.48
1:C:284:MET:HE3	1:C:496:MET:SD	2.54	0.48
1:C:217:VAL:HG12	1:C:238:ILE:HG13	1.96	0.48
1:B:23:MET:HB2	9:B:832:HOH:O	2.14	0.48
1:B:228:GLU:HG3	1:B:232:LYS:NZ	2.29	0.48
1:C:211:LYS:NZ	9:C:2333:HOH:O	2.43	0.48
1:A:7:ILE:CD1	1:A:103:LEU:HB2	2.44	0.48
1:A:1:MET:HE3	1:A:3:LYS:HD3	1.96	0.47
1:B:70:PRO:HD2	1:B:508:GLN:OE1	2.14	0.47
1:C:213:ILE:HB	1:C:216:PHE:HB2	1.94	0.47
1:C:337:ASN:ND2	1:C:366:LEU:CD1	2.64	0.47
1:D:460:GLU:O	1:D:463:LYS:HG2	2.14	0.47
1:A:25:LYS:HE2	9:A:1093:HOH:O	2.13	0.47
1:D:212:ARG:NH2	1:D:214:GLU:OE1	2.47	0.47
1:C:22:THR:HG22	1:C:22:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:706:EDO:O1	1:D:258:ALA:O	2.32	0.47
1:D:338:GLY:HA3	1:D:389:GLU:CD	2.40	0.47
1:A:12:LEU:HD13	1:A:57:HIS:CG	2.50	0.47
1:B:367:ASP:OD2	1:B:370:LYS:HD2	2.14	0.47
1:D:417:VAL:HA	1:D:437:SER:HA	1.96	0.47
1:B:489:PHE:HB2	8:B:711:GOL:H2	1.96	0.47
1:C:182:TYR:CD1	1:C:201:GLU:HG2	2.50	0.47
1:C:390:THR:HG21	2:C:2202:PLP:O3	2.15	0.47
1:B:178:LYS:HE3	1:B:206:ILE:HD11	1.96	0.46
1:D:367:ASP:OD2	1:D:370:LYS:HE3	2.16	0.46
1:C:420:TYR:O	1:C:442:ASN:HB2	2.15	0.46
1:D:487:THR:HG23	1:D:489:PHE:O	2.15	0.46
1:A:212:ARG:HH12	1:A:214:GLU:CD	2.23	0.46
1:D:582:ILE:HD11	9:D:999:HOH:O	2.15	0.46
1:A:57:HIS:CE1	1:A:58:CYS:HG	2.33	0.46
1:A:443:ILE:H	6:A:716:EDO:C1	2.29	0.46
1:B:463:LYS:HD2	1:B:464:ASP:OD1	2.16	0.46
1:A:481:PHE:CD2	6:A:709:EDO:H21	2.50	0.46
1:C:463:LYS:HG3	1:C:464:ASP:N	2.30	0.46
1:A:138:VAL:H	6:A:717:EDO:C1	2.28	0.46
1:B:406:LYS:NZ	1:B:433:ASP:OD2	2.42	0.46
1:D:226:HIS:HD2	1:D:229:MET:CE	2.28	0.46
1:B:221:ILE:HA	1:B:226:HIS:HB3	1.97	0.46
1:D:98:GLU:CG	1:D:99:SER:H	2.29	0.45
1:A:547:ILE:HA	1:A:588:ALA:HA	1.98	0.45
1:B:21:LYS:HG2	1:B:22:THR:HG23	1.98	0.45
1:B:155:ARG:NH2	1:B:161:ILE:HD13	2.31	0.45
1:A:332:LEU:O	1:A:355:MET:HA	2.16	0.45
1:C:139:TYR:CE2	1:C:155:ARG:HG2	2.51	0.45
1:D:372:GLU:HB2	1:D:404:MET:SD	2.56	0.45
1:A:512:GLN:NE2	9:A:802:HOH:O	2.17	0.45
1:A:526:VAL:HG21	9:A:1105:HOH:O	2.16	0.45
1:C:284:MET:CE	1:C:496:MET:HE1	2.47	0.45
1:B:203:ALA:HA	1:B:206:ILE:O	2.17	0.45
1:B:268:GLN:HG2	1:B:498:ALA:HB2	1.99	0.45
1:D:355:MET:HG2	1:D:356:ASP:N	2.32	0.44
1:A:481:PHE:HD2	6:A:709:EDO:H21	1.82	0.44
1:B:417:VAL:HA	1:B:437:SER:HA	1.98	0.44
1:B:384:ALA:HA	1:B:413:ILE:O	2.17	0.44
1:A:3:LYS:HE3	1:A:98:GLU:OE1	2.18	0.44
1:C:194:GLU:HB2	1:C:197:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:PHE:O	1:B:212:ARG:NE	2.48	0.44
1:C:215:TYR:O	6:C:2206:EDO:H11	2.18	0.44
1:C:361:SER:CB	6:C:2209:EDO:H21	2.48	0.44
1:C:575:TYR:CD1	1:C:576:PRO:HD2	2.53	0.44
1:A:321:MET:HE2	1:A:321:MET:HB3	1.72	0.44
1:A:321:MET:HE3	1:A:434:PHE:HB3	1.99	0.44
1:A:518:TYR:CE1	1:A:590:ILE:HA	2.52	0.44
1:C:543:GLN:HB3	9:C:2419:HOH:O	2.16	0.44
6:C:2209:EDO:H22	9:C:2448:HOH:O	2.18	0.44
1:A:441:LYS:HB2	6:A:716:EDO:O2	2.18	0.43
1:A:221:ILE:HA	1:A:226:HIS:HB3	2.00	0.43
1:B:332:LEU:O	1:B:355:MET:HA	2.18	0.43
1:B:543:GLN:HB3	9:B:933:HOH:O	2.18	0.43
1:C:203:ALA:HA	1:C:206:ILE:O	2.17	0.43
1:D:57:HIS:HD2	9:D:814:HOH:O	2.00	0.43
1:A:75:VAL:HG21	1:A:95:PHE:CE2	2.54	0.43
1:D:30:ILE:HG12	1:D:231:VAL:HG22	2.01	0.43
1:D:134:SER:HB2	1:D:229:MET:HE1	2.00	0.43
1:A:420:TYR:O	6:A:716:EDO:H21	2.18	0.43
1:B:292:LYS:HA	1:B:453:ILE:HD13	2.00	0.43
1:D:492:PRO:HB2	1:D:495:THR:HB	2.00	0.43
1:A:529:ILE:HD11	1:A:550:ILE:HD11	2.01	0.43
1:B:57:HIS:HA	1:B:80:TYR:CE1	2.54	0.43
1:C:532:LEU:HD23	9:C:2320:HOH:O	2.18	0.43
1:A:22:THR:HG22	1:A:22:THR:O	2.18	0.43
1:A:182:TYR:CE1	1:A:201:GLU:HG2	2.53	0.43
1:B:487:THR:HG23	1:B:489:PHE:O	2.19	0.43
1:B:25:LYS:HE2	9:B:1101:HOH:O	2.18	0.43
1:B:230:ALA:HA	1:B:234:ILE:HB	2.01	0.43
1:C:255:PRO:O	1:C:441:LYS:NZ	2.51	0.43
1:B:494:GLN:HE22	6:B:706:EDO:H12	1.84	0.43
1:C:125:LEU:HD11	1:C:211:LYS:HB2	2.01	0.43
1:A:283:LEU:CD1	1:A:500:ARG:HD2	2.50	0.42
1:A:441:LYS:HE2	9:C:2385:HOH:O	2.19	0.42
1:B:226:HIS:HD2	1:B:229:MET:CE	2.32	0.42
1:B:494:GLN:NE2	6:B:706:EDO:H12	2.33	0.42
1:C:417:VAL:HA	1:C:437:SER:HA	2.00	0.42
1:D:525:LEU:O	1:D:529:ILE:HG13	2.19	0.42
1:A:615:GLY:O	9:A:803:HOH:O	2.21	0.42
1:B:143:ASP:OD1	1:B:145:LYS:N	2.47	0.42
1:B:272:ASP:CA	6:B:706:EDO:H21	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LYS:HE3	1:A:106:ASP:HB3	2.00	0.42
1:C:366:LEU:HD12	1:C:366:LEU:H	1.85	0.42
1:D:237:HIS:HD2	9:D:1079:HOH:O	2.01	0.42
1:B:276:ARG:HD3	9:B:1078:HOH:O	2.19	0.42
1:B:492:PRO:HB2	1:B:495:THR:HB	2.01	0.42
1:D:529:ILE:HG23	1:D:534:LEU:HB2	2.00	0.42
1:B:219:ARG:HG3	1:B:220:GLU:O	2.20	0.42
1:B:316:GLY:O	1:B:320:VAL:HG23	2.20	0.42
1:B:337:ASN:HB2	1:B:361:SER:O	2.19	0.42
1:B:457:ALA:O	1:B:461:LYS:HG3	2.19	0.42
1:B:25:LYS:HE3	1:B:106:ASP:CB	2.50	0.42
1:C:225:ASP:O	1:C:229:MET:HG3	2.19	0.42
1:B:68:LYS:HD3	1:B:69:TYR:CE2	2.54	0.42
1:C:346:LYS:HG3	6:C:2210:EDO:C2	2.50	0.42
1:D:106:ASP:O	1:D:220:GLU:HA	2.20	0.42
1:B:228:GLU:HG3	1:B:232:LYS:HD2	2.01	0.42
1:B:272:ASP:HA	6:B:706:EDO:H21	2.01	0.42
1:A:299:GLU:CD	1:A:299:GLU:H	2.28	0.41
1:B:172:THR:HG22	1:B:175:THR:OG1	2.21	0.41
1:B:327:PRO:HD3	1:B:465:TYR:CE2	2.55	0.41
1:B:372:GLU:HB2	1:B:404:MET:SD	2.61	0.41
1:B:145:LYS:HA	1:B:145:LYS:HD2	1.74	0.41
1:B:184:LYS:HE3	1:B:184:LYS:HB2	1.85	0.41
1:B:547:ILE:HD11	1:B:586:ARG:HB3	2.02	0.41
1:C:417:VAL:HG12	1:C:441:LYS:HD2	2.02	0.41
1:C:551:LEU:HD23	1:C:551:LEU:HA	1.87	0.41
1:A:40:VAL:O	1:A:44:LEU:HG	2.21	0.41
1:D:399:HIS:O	1:D:403:PRO:HG2	2.21	0.41
1:A:360:SER:CB	1:A:366:LEU:HD23	2.51	0.41
1:C:332:LEU:O	1:C:355:MET:HA	2.21	0.41
1:D:221:ILE:HA	1:D:226:HIS:HB3	2.01	0.41
1:A:6:VAL:HG22	1:A:52:VAL:HB	2.03	0.41
1:B:186:HIS:HA	1:B:189:ASP:OD1	2.20	0.41
1:C:73:ILE:HD12	9:C:2639:HOH:O	2.21	0.41
1:D:27:PHE:HA	1:D:34:ALA:HB1	2.03	0.41
1:B:182:TYR:CD1	1:B:201:GLU:HG2	2.56	0.41
1:B:415:ASP:OD1	1:B:415:ASP:C	2.63	0.41
1:D:380:TYR:O	1:D:410:MET:HG2	2.21	0.41
1:A:321:MET:CE	1:A:434:PHE:HB2	2.51	0.40
1:A:213:ILE:HB	1:A:216:PHE:HB2	2.03	0.40
1:A:579:LEU:HD23	1:A:582:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:GLU:CD	1:B:144:GLU:N	2.79	0.40
1:C:136:ASP:OD1	1:C:153:LYS:NZ	2.46	0.40
1:C:414:VAL:HG21	1:C:432:ILE:HG12	2.02	0.40
5:A:705:ORC:N15	6:A:717:EDO:O2	2.55	0.40
1:B:134:SER:HB2	1:B:229:MET:HE1	2.02	0.40
1:D:441:LYS:NZ	9:D:801:HOH:O	2.33	0.40
1:C:38:GLN:O	1:C:42:LYS:HG3	2.21	0.40
1:A:12:LEU:HD13	1:A:57:HIS:CD2	2.56	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)
9:A:813:HOH:O	9:B:832:HOH:O[1_554]	2.18	0.02

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	613/624 (98%)	589 (96%)	24 (4%)	0	100	100
1	B	613/624 (98%)	594 (97%)	19 (3%)	0	100	100
1	C	614/624 (98%)	594 (97%)	19 (3%)	1 (0%)	43	36
1	D	604/624 (97%)	584 (97%)	20 (3%)	0	100	100
All	All	2444/2496 (98%)	2361 (97%)	82 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	56	GLY

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	524/533 (98%)	524 (100%)	0	100	100
1	B	524/533 (98%)	522 (100%)	2 (0%)	84	85
1	C	525/533 (98%)	524 (100%)	1 (0%)	87	89
1	D	518/533 (97%)	516 (100%)	2 (0%)	84	85
All	All	2091/2132 (98%)	2086 (100%)	5 (0%)	87	89

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

Mol	Chain	Res	Type
1	B	165	LEU
1	B	483	LYS
1	C	589	ASN
1	D	355	MET
1	D	589	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	97	ASN
1	B	82	ASN
1	B	223	ASN
1	B	523	ASN
1	C	64	ASN
1	C	82	ASN
1	C	285	GLN
1	C	369	GLN
1	C	589	ASN
1	D	589	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 59 ligands modelled in this entry, 8 are monoatomic - leaving 51 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	$\# Z > 2$
4	PO4	C	2215	-	4,4,4	0.99	0	6,6,6	0.87	0
6	EDO	B	707	-	3,3,3	0.37	0	2,2,2	0.46	0
8	GOL	B	709	-	5,5,5	0.55	0	5,5,5	1.13	0
4	PO4	A	718	-	4,4,4	1.10	0	6,6,6	0.65	0
2	PLP	C	2202	-	16,16,16	1.07	1 (6%)	20,23,23	1.10	1 (5%)
6	EDO	D	711	-	3,3,3	0.28	0	2,2,2	0.84	0
6	EDO	A	717	-	3,3,3	0.24	0	2,2,2	0.36	0
6	EDO	C	2209	-	3,3,3	0.77	0	2,2,2	0.10	0
4	PO4	D	714	-	4,4,4	0.45	0	6,6,6	0.74	0
6	EDO	A	706	-	3,3,3	0.70	0	2,2,2	0.17	0
6	EDO	D	707	-	3,3,3	0.49	0	2,2,2	0.57	0
4	PO4	D	709	-	4,4,4	1.11	0	6,6,6	0.82	0
2	PLP	A	701	-	16,16,16	1.13	2 (12%)	20,23,23	1.49	4 (20%)
7	ACT	A	707	-	3,3,3	2.12	1 (33%)	3,3,3	1.36	0
6	EDO	A	710	-	3,3,3	0.33	0	2,2,2	0.95	0
6	EDO	B	706	-	3,3,3	0.23	0	2,2,2	0.41	0
4	PO4	C	2204	-	4,4,4	0.65	0	6,6,6	1.30	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	714	-	3,3,3	0.40	0	2,2,2	0.45	0
6	EDO	B	710	-	3,3,3	0.61	0	2,2,2	0.56	0
6	EDO	D	713	-	3,3,3	0.58	0	2,2,2	0.42	0
8	GOL	B	711	-	5,5,5	1.87	3 (60%)	5,5,5	1.18	0
6	EDO	D	708	-	3,3,3	0.56	0	2,2,2	0.38	0
6	EDO	C	2212	-	3,3,3	0.53	0	2,2,2	0.15	0
4	PO4	C	2207	-	4,4,4	0.77	0	6,6,6	0.72	0
7	ACT	C	2201	-	3,3,3	1.51	1 (33%)	3,3,3	1.24	0
5	ORC	A	705	3	28,28,28	4.57	13 (46%)	37,42,42	1.96	7 (18%)
5	ORC	D	705	3	28,28,28	4.34	15 (53%)	37,42,42	1.40	5 (13%)
6	EDO	A	713	-	3,3,3	0.41	0	2,2,2	0.35	0
6	EDO	C	2206	-	3,3,3	0.38	0	2,2,2	0.68	0
4	PO4	B	708	-	4,4,4	0.89	0	6,6,6	0.67	0
6	EDO	A	711	-	3,3,3	0.60	0	2,2,2	1.22	0
6	EDO	C	2208	-	3,3,3	0.35	0	2,2,2	0.97	0
5	ORC	B	705	3	28,28,28	4.41	15 (53%)	37,42,42	1.76	8 (21%)
6	EDO	C	2213	-	3,3,3	0.58	0	2,2,2	0.29	0
6	EDO	D	706	-	3,3,3	0.45	0	2,2,2	0.78	0
4	PO4	B	712	-	4,4,4	0.35	0	6,6,6	0.83	0
6	EDO	C	2210	-	3,3,3	0.54	0	2,2,2	0.53	0
6	EDO	C	2214	-	3,3,3	0.52	0	2,2,2	0.62	0
4	PO4	D	704	-	4,4,4	0.67	0	6,6,6	0.73	0
6	EDO	D	712	-	3,3,3	0.56	0	2,2,2	0.58	0
6	EDO	A	712	-	3,3,3	0.29	0	2,2,2	0.93	0
2	PLP	B	701	-	16,16,16	1.28	1 (6%)	20,23,23	1.23	3 (15%)
7	ACT	A	715	-	3,3,3	1.30	0	3,3,3	1.35	0
5	ORC	C	2205	3	28,28,28	4.58	14 (50%)	37,42,42	1.51	6 (16%)
6	EDO	A	708	-	3,3,3	0.53	0	2,2,2	0.30	0
4	PO4	B	704	-	4,4,4	0.91	0	6,6,6	0.88	0
6	EDO	A	709	-	3,3,3	0.49	0	2,2,2	0.76	0
2	PLP	D	702	-	16,16,16	1.21	2 (12%)	20,23,23	1.21	2 (10%)
4	PO4	A	704	-	4,4,4	0.94	0	6,6,6	1.09	0
6	EDO	D	710	-	3,3,3	0.60	0	2,2,2	0.09	0
6	EDO	A	716	-	3,3,3	0.39	0	2,2,2	0.86	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	EDO	B	707	-	-	1/1/1/1	-
8	GOL	B	709	-	-	2/4/4/4	-
2	PLP	C	2202	-	-	2/8/8/8	0/1/1/1
6	EDO	D	711	-	-	0/1/1/1	-
6	EDO	A	717	-	-	0/1/1/1	-
6	EDO	C	2209	-	-	0/1/1/1	-
6	EDO	A	706	-	-	0/1/1/1	-
6	EDO	D	707	-	-	0/1/1/1	-
2	PLP	A	701	-	-	1/8/8/8	0/1/1/1
6	EDO	A	710	-	-	0/1/1/1	-
6	EDO	A	714	-	-	1/1/1/1	-
6	EDO	B	710	-	-	1/1/1/1	-
6	EDO	D	713	-	-	0/1/1/1	-
8	GOL	B	711	-	-	2/4/4/4	-
6	EDO	D	708	-	-	0/1/1/1	-
6	EDO	C	2212	-	-	1/1/1/1	-
5	ORC	A	705	3	-	4/17/36/36	0/2/2/2
5	ORC	D	705	3	-	3/17/36/36	0/2/2/2
6	EDO	A	713	-	-	1/1/1/1	-
6	EDO	C	2206	-	-	1/1/1/1	-
6	EDO	A	711	-	-	0/1/1/1	-
6	EDO	C	2208	-	-	0/1/1/1	-
5	ORC	B	705	3	-	3/17/36/36	0/2/2/2
6	EDO	C	2213	-	-	0/1/1/1	-
6	EDO	D	706	-	-	1/1/1/1	-
6	EDO	C	2210	-	-	0/1/1/1	-
6	EDO	C	2214	-	-	0/1/1/1	-
6	EDO	D	712	-	-	0/1/1/1	-
6	EDO	A	712	-	-	1/1/1/1	-
2	PLP	B	701	-	-	1/8/8/8	0/1/1/1
5	ORC	C	2205	3	-	2/17/36/36	0/2/2/2
6	EDO	A	708	-	-	0/1/1/1	-
6	EDO	A	709	-	-	1/1/1/1	-
2	PLP	D	702	-	-	0/8/8/8	0/1/1/1
6	EDO	B	706	-	-	1/1/1/1	-
6	EDO	D	710	-	-	0/1/1/1	-
6	EDO	A	716	-	-	0/1/1/1	-

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2205	ORC	PA-O3A	11.00	1.71	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2205	ORC	PB-O3A	10.60	1.70	1.58
5	A	705	ORC	PB-O3A	10.39	1.70	1.58
5	A	705	ORC	PA-O3A	9.96	1.70	1.59
5	B	705	ORC	PB-O3A	9.65	1.69	1.58
5	D	705	ORC	PB-O3A	9.40	1.68	1.58
5	B	705	ORC	C2'-C3'	-8.07	1.31	1.53
5	D	705	ORC	C2'-C3'	-8.07	1.31	1.53
5	A	705	ORC	O4'-C1'	8.03	1.60	1.42
5	D	705	ORC	PA-O3A	7.92	1.68	1.59
5	C	2205	ORC	C2'-C3'	-7.79	1.32	1.53
5	D	705	ORC	O4'-C1'	7.77	1.60	1.42
5	B	705	ORC	O4'-C4'	-7.73	1.27	1.45
5	B	705	ORC	O4'-C1'	7.73	1.59	1.42
5	B	705	ORC	PA-O3A	7.57	1.67	1.59
5	A	705	ORC	C2'-C3'	-7.55	1.32	1.53
5	A	705	ORC	O4'-C4'	-7.44	1.28	1.45
5	C	2205	ORC	O4'-C1'	7.35	1.59	1.42
5	D	705	ORC	C3'-C4'	7.03	1.70	1.53
5	D	705	ORC	O4'-C4'	-6.98	1.29	1.45
5	C	2205	ORC	O4'-C4'	-6.86	1.29	1.45
5	C	2205	ORC	C3'-C4'	6.85	1.70	1.53
5	A	705	ORC	C3'-C4'	6.58	1.69	1.53
5	B	705	ORC	C3'-C4'	6.34	1.69	1.53
5	D	705	ORC	C1'-N1	-5.98	1.30	1.47
5	C	2205	ORC	C1'-N1	-5.76	1.31	1.47
5	A	705	ORC	C1'-N1	-5.72	1.31	1.47
5	B	705	ORC	C1'-N1	-5.54	1.31	1.47
5	A	705	ORC	C4-N4	5.37	1.46	1.33
5	B	705	ORC	C2-N1	-5.27	1.29	1.40
5	B	705	ORC	C4-N4	5.26	1.46	1.33
5	D	705	ORC	C4-N4	5.24	1.46	1.33
5	A	705	ORC	C1B-C14	5.22	1.60	1.53
5	C	2205	ORC	C4-N4	4.92	1.45	1.33
5	A	705	ORC	C2-N1	-4.92	1.29	1.40
5	B	705	ORC	C1B-C14	4.73	1.60	1.53
5	C	2205	ORC	C2-N1	-4.26	1.31	1.40
5	B	705	ORC	O2-C2	-4.22	1.15	1.23
5	D	705	ORC	C2-N1	-4.20	1.31	1.40
5	D	705	ORC	O2-C2	-3.93	1.16	1.23
5	C	2205	ORC	C1B-C14	3.80	1.58	1.53
5	D	705	ORC	O5'-C5'	-3.67	1.30	1.44
5	B	705	ORC	O5'-C5'	-3.63	1.30	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2205	ORC	O2-C2	-3.62	1.17	1.23
5	C	2205	ORC	O5'-C5'	-3.62	1.30	1.44
7	A	707	ACT	CH3-C	3.52	1.62	1.49
5	A	705	ORC	O2-C2	-3.41	1.17	1.23
5	A	705	ORC	O5'-C5'	-3.10	1.32	1.44
2	B	701	PLP	C2-N1	3.03	1.39	1.33
5	D	705	ORC	PB-O3B	2.73	1.58	1.51
5	D	705	ORC	PA-O1A	2.66	1.60	1.50
5	D	705	ORC	C1B-C14	2.62	1.56	1.53
8	B	711	GOL	O2-C2	-2.56	1.35	1.43
5	C	2205	ORC	PA-O1A	2.50	1.59	1.50
2	A	701	PLP	C4-C5	-2.49	1.38	1.42
5	A	705	ORC	PA-O1A	2.46	1.59	1.50
8	B	711	GOL	O3-C3	-2.33	1.32	1.42
2	D	702	PLP	C2-N1	2.29	1.37	1.33
2	D	702	PLP	C3-C2	-2.27	1.38	1.41
5	B	705	ORC	C4-N3	-2.24	1.30	1.34
5	D	705	ORC	C4-N3	-2.23	1.30	1.34
5	B	705	ORC	PA-O1A	2.22	1.58	1.50
2	C	2202	PLP	C4-C4A	2.16	1.51	1.46
5	B	705	ORC	PB-O3B	2.16	1.56	1.51
8	B	711	GOL	C1-C2	2.15	1.60	1.51
5	C	2205	ORC	PA-O5'	2.13	1.67	1.59
7	C	2201	ACT	O-C	2.07	1.31	1.22
2	A	701	PLP	C4-C4A	2.06	1.51	1.46

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	705	ORC	PB-C1B-C14	-7.59	97.86	114.06
5	B	705	ORC	PB-O3A-PA	-4.23	118.57	132.37
5	B	705	ORC	C3'-C2'-C1'	4.02	109.08	101.46
5	A	705	ORC	PB-O3A-PA	-3.99	119.35	132.37
5	B	705	ORC	O4'-C1'-C2'	-3.91	98.26	106.62
5	B	705	ORC	PB-C1B-C14	-3.10	107.44	114.06
2	D	702	PLP	C5-C6-N1	-3.06	118.85	123.83
5	D	705	ORC	O2-C2-N3	-3.06	117.50	122.33
5	A	705	ORC	C3'-C2'-C1'	3.06	107.25	101.46
5	C	2205	ORC	C3'-C2'-C1'	3.02	107.17	101.46
5	D	705	ORC	PB-O3A-PA	-3.00	122.58	132.37
5	C	2205	ORC	O2B-PB-O3B	2.99	119.68	109.95
5	C	2205	ORC	O3B-PB-C1B	2.93	117.38	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	PLP	O4A-C4A-C4	-2.82	118.10	124.80
5	B	705	ORC	O4'-C1'-N1	2.69	114.45	108.36
5	D	705	ORC	O4'-C1'-C2'	-2.68	100.88	106.62
2	A	701	PLP	C4-C3-C2	2.67	121.64	120.14
5	C	2205	ORC	PB-O3A-PA	-2.59	123.92	132.37
5	A	705	ORC	O4'-C1'-N1	2.58	114.20	108.36
2	A	701	PLP	C2A-C2-C3	2.56	123.79	120.80
2	B	701	PLP	C5-C6-N1	-2.56	119.67	123.83
5	C	2205	ORC	O4'-C1'-N1	2.44	113.89	108.36
5	C	2205	ORC	O2-C2-N3	-2.42	118.51	122.33
5	A	705	ORC	C5-C4-N3	-2.40	117.28	121.32
2	C	2202	PLP	O4A-C4A-C4	-2.38	119.16	124.80
2	A	701	PLP	O2P-P-O1P	2.35	119.99	110.83
2	B	701	PLP	O4A-C4A-C4	-2.34	119.26	124.80
5	A	705	ORC	O4'-C4'-C3'	2.30	109.72	105.15
5	B	705	ORC	O2'-C2'-C1'	2.30	118.01	110.10
2	B	701	PLP	O3P-P-O4P	2.29	112.63	106.67
5	D	705	ORC	C5'-C4'-C3'	-2.24	107.14	115.21
5	B	705	ORC	O2B-PB-C1B	-2.18	100.40	105.54
5	D	705	ORC	C3'-C2'-C1'	2.16	105.55	101.46
5	B	705	ORC	C5-C4-N3	-2.16	117.68	121.32
5	A	705	ORC	O2A-PA-O3A	2.09	112.93	107.27
4	C	2204	PO4	O4-P-O1	-2.08	103.61	110.95
2	D	702	PLP	O4A-C4A-C4	-2.04	119.95	124.80

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	705	ORC	C14-C1B-PB-O3B
5	A	705	ORC	C14-C1B-PB-O3A
5	B	705	ORC	C14-C1B-PB-O3B
5	B	705	ORC	C14-C1B-PB-O2B
5	B	705	ORC	C14-C1B-PB-O3A
5	C	2205	ORC	C14-C1B-PB-O2B
5	D	705	ORC	C5'-O5'-PA-O1A
8	B	709	GOL	O1-C1-C2-C3
8	B	711	GOL	O1-C1-C2-O2
8	B	711	GOL	O1-C1-C2-C3
2	C	2202	PLP	C3-C4-C4A-O4A
8	B	709	GOL	O1-C1-C2-O2
2	B	701	PLP	C3-C4-C4A-O4A

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Mol	Chain	Res	Type	Atoms
6	A	709	EDO	O1-C1-C2-O2
6	A	712	EDO	O1-C1-C2-O2
6	C	2206	EDO	O1-C1-C2-O2
6	A	714	EDO	O1-C1-C2-O2
6	D	706	EDO	O1-C1-C2-O2
5	A	705	0RC	C14-C1B-PB-O2B
5	D	705	0RC	C3'-C4'-C5'-O5'
5	A	705	0RC	C5'-O5'-PA-O1A
5	C	2205	0RC	C5'-O5'-PA-O1A
2	C	2202	PLP	C5-C4-C4A-O4A
6	B	706	EDO	O1-C1-C2-O2
6	B	707	EDO	O1-C1-C2-O2
6	B	710	EDO	O1-C1-C2-O2
2	A	701	PLP	C5A-O4P-P-O2P
6	A	713	EDO	O1-C1-C2-O2
6	C	2212	EDO	O1-C1-C2-O2
5	D	705	0RC	O4'-C4'-C5'-O5'

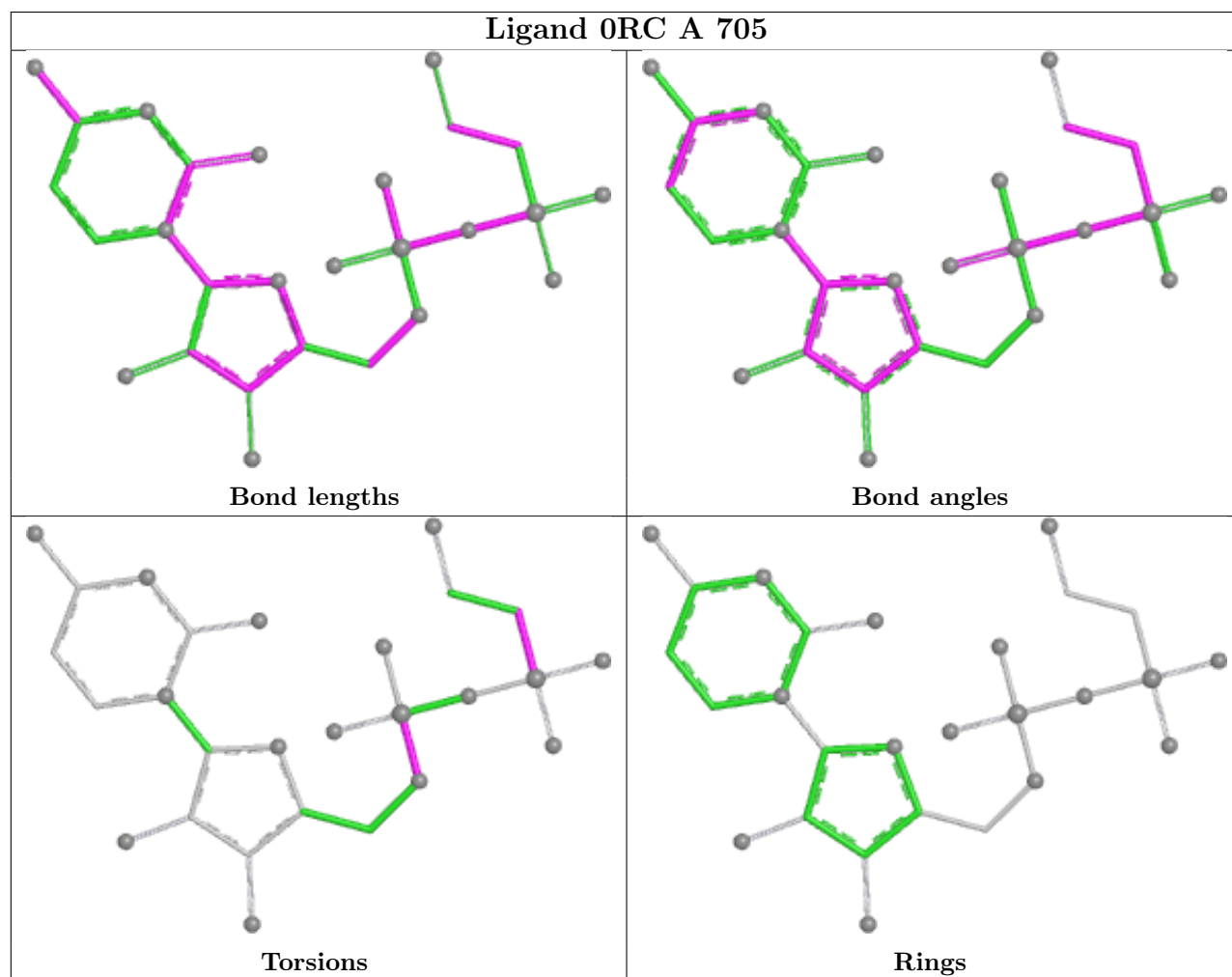
There are no ring outliers.

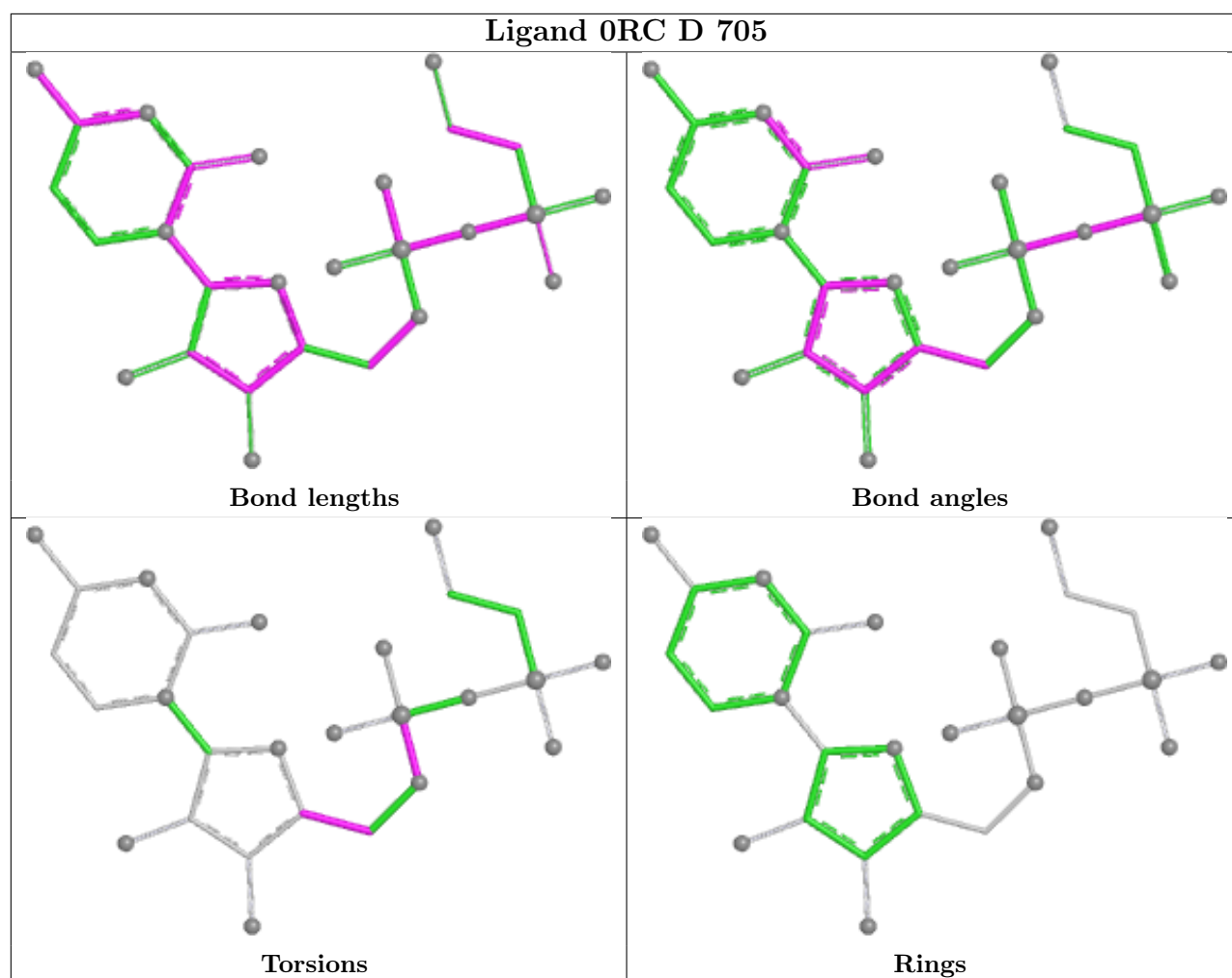
18 monomers are involved in 47 short contacts:

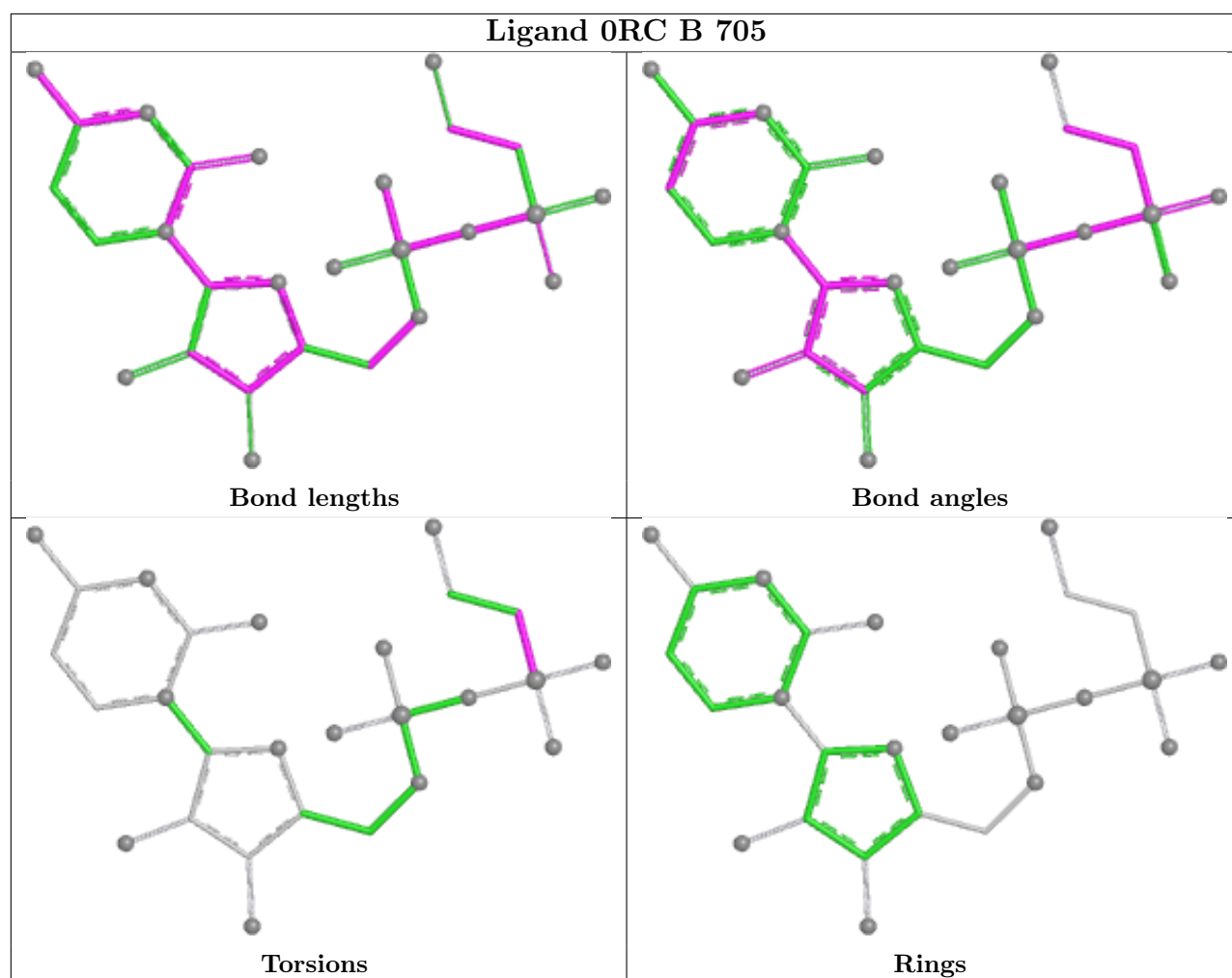
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2202	PLP	1	0
6	A	717	EDO	3	0
6	C	2209	EDO	3	0
4	D	714	PO4	1	0
4	D	709	PO4	2	0
2	A	701	PLP	1	0
6	B	706	EDO	9	0
6	A	714	EDO	1	0
8	B	711	GOL	3	0
5	A	705	0RC	2	0
6	C	2206	EDO	1	0
6	C	2208	EDO	2	0
5	B	705	0RC	2	0
6	D	706	EDO	2	0
6	C	2210	EDO	3	0
6	A	712	EDO	1	0
6	A	709	EDO	5	0
6	A	716	EDO	6	0

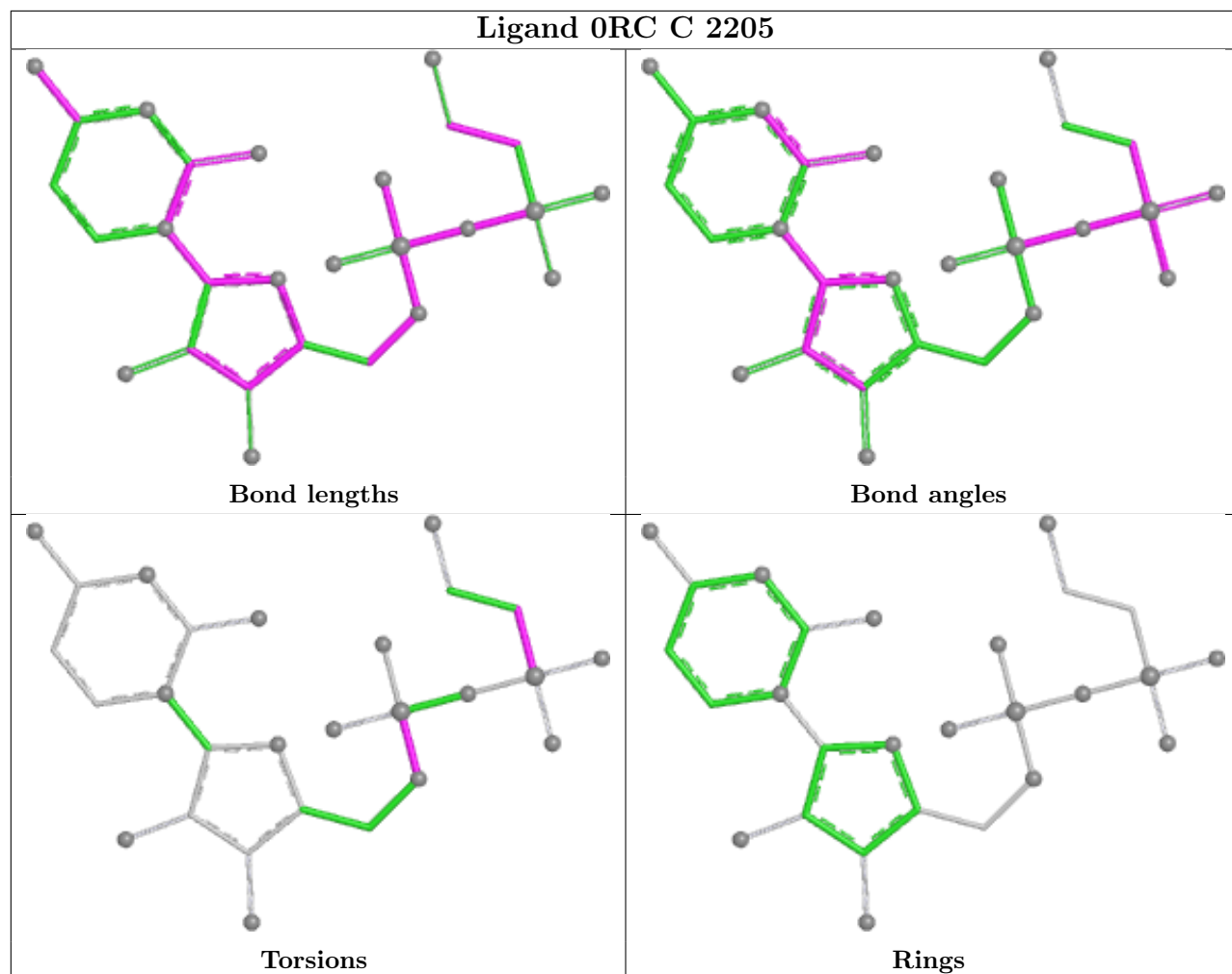
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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	615/624 (98%)	1.18	90 (14%) 6 6	15, 25, 37, 51	0
1	B	615/624 (98%)	1.27	106 (17%) 4 4	15, 26, 42, 60	0
1	C	616/624 (98%)	1.08	59 (9%) 13 15	13, 23, 36, 54	0
1	D	608/624 (97%)	1.31	106 (17%) 4 4	15, 25, 42, 51	0
All	All	2454/2496 (98%)	1.21	361 (14%) 6 6	13, 25, 40, 60	0

All (361) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	580	GLY	5.7
1	C	366	LEU	5.1
1	D	185	ILE	4.8
1	C	616	VAL	4.7
1	B	181	ALA	4.5
1	D	314	GLY	4.4
1	D	21	LYS	4.3
1	D	12	LEU	4.2
1	A	350	ILE	4.2
1	C	235	TYR	4.2
1	B	1	MET	4.1
1	D	75	VAL	4.0
1	B	579	LEU	4.0
1	B	151	LEU	4.0
1	C	314	GLY	4.0
1	D	438	THR	3.9
1	B	57	HIS	3.9
1	A	1	MET	3.9
1	A	16	LEU	3.8
1	B	183	ALA	3.7
1	D	108	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	185	ILE	3.6
1	B	582	ILE	3.6
1	D	80	TYR	3.5
1	D	79	ASN	3.5
1	B	101	LEU	3.5
1	D	231	VAL	3.5
1	D	226	HIS	3.5
1	A	239	VAL	3.4
1	A	151	LEU	3.4
1	B	152	SER	3.4
1	C	430	LEU	3.4
1	D	473	ASN	3.3
1	C	1	MET	3.3
1	D	329	THR	3.3
1	A	118	ILE	3.3
1	B	239	VAL	3.3
1	D	247	VAL	3.2
1	A	95	PHE	3.2
1	B	210	ILE	3.2
1	B	447	ALA	3.2
1	C	230	ALA	3.2
1	C	568	ALA	3.2
1	A	152	SER	3.2
1	B	161	ILE	3.2
1	D	118	ILE	3.2
1	D	466	PRO	3.2
1	B	178	LYS	3.2
1	B	190	LEU	3.2
1	A	20	THR	3.1
1	A	88	THR	3.1
1	B	97	ASN	3.1
1	A	493	VAL	3.1
1	B	334	VAL	3.1
1	A	57	HIS	3.1
1	A	158	LEU	3.1
1	A	131	ALA	3.1
1	A	10	GLY	3.1
1	A	35	ILE	3.1
1	C	13	GLY	3.1
1	D	11	GLY	3.1
1	B	266	TYR	3.1
1	D	227	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	97	ASN	3.1
1	B	230	ALA	3.1
1	D	246	ALA	3.1
1	B	221	ILE	3.0
1	A	537	LEU	3.0
1	C	411	VAL	3.0
1	D	251	VAL	3.0
1	D	54	GLY	3.0
1	B	593	ILE	3.0
1	A	515	TYR	3.0
1	B	188	SER	3.0
1	A	22	THR	3.0
1	C	16	LEU	3.0
1	D	116	SER	3.0
1	B	349	ASP	3.0
1	C	116	SER	2.9
1	D	239	VAL	2.9
1	C	22	THR	2.9
1	C	24	PRO	2.9
1	D	216	PHE	2.9
1	D	161	ILE	2.9
1	B	89	LEU	2.9
1	D	571	SER	2.9
1	B	6	VAL	2.9
1	B	82	ASN	2.9
1	D	223	ASN	2.9
1	B	58	CYS	2.9
1	C	470	TYR	2.9
1	D	222	ASP	2.9
1	A	582	ILE	2.9
1	D	73	ILE	2.9
1	D	221	ILE	2.9
1	A	533	GLY	2.9
1	D	266	TYR	2.8
1	B	73	ILE	2.8
1	B	587	ILE	2.8
1	A	132	THR	2.8
1	D	83	THR	2.8
1	A	91	VAL	2.8
1	C	61	TYR	2.8
1	B	546	PHE	2.8
1	A	150	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	158	LEU	2.8
1	C	251	VAL	2.8
1	A	349	ASP	2.8
1	D	61	TYR	2.8
1	B	191	PRO	2.8
1	B	52	VAL	2.8
1	D	320	VAL	2.8
1	A	133	LYS	2.7
1	B	430	LEU	2.7
1	B	75	VAL	2.7
1	D	57	HIS	2.7
1	B	175	THR	2.7
1	B	532	LEU	2.7
1	D	368	LEU	2.7
1	B	581	ASN	2.7
1	D	123	LYS	2.7
1	A	345	ALA	2.7
1	B	32	GLY	2.7
1	B	615	GLY	2.7
1	D	20	THR	2.7
1	A	15	ARG	2.7
1	D	524	ILE	2.7
1	A	40	VAL	2.7
1	A	113	GLY	2.6
1	A	457	ALA	2.6
1	A	615	GLY	2.6
1	B	457	ALA	2.6
1	D	434	PHE	2.6
1	B	144	GLU	2.6
1	A	12	LEU	2.6
1	B	2	ILE	2.6
1	C	350	ILE	2.6
1	A	81	ALA	2.6
1	B	222	ASP	2.6
1	A	581	ASN	2.6
1	C	27	PHE	2.6
1	D	213	ILE	2.6
1	B	355	MET	2.6
1	C	157	ALA	2.6
1	A	44	LEU	2.6
1	A	248	ARG	2.6
1	C	8	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	369	GLN	2.6
1	C	2	ILE	2.6
1	D	453	ILE	2.6
1	C	603	VAL	2.6
1	B	79	ASN	2.6
1	A	518	TYR	2.5
1	B	107	LEU	2.5
1	B	394	LEU	2.5
1	C	163	GLY	2.5
1	D	206	ILE	2.5
1	A	157	ALA	2.5
1	C	231	VAL	2.5
1	C	541	GLU	2.5
1	B	441	LYS	2.5
1	A	107	LEU	2.5
1	D	398	LEU	2.5
1	D	31	GLY	2.5
1	B	51	ILE	2.5
1	D	413	ILE	2.5
1	D	233	ASN	2.5
1	D	248	ARG	2.5
1	A	271	ALA	2.5
1	C	91	VAL	2.5
1	A	255	PRO	2.5
1	C	192	LYS	2.5
1	B	162	PHE	2.5
1	B	572	PHE	2.5
1	C	579	LEU	2.5
1	A	401	ILE	2.5
1	D	174	SER	2.5
1	B	45	ALA	2.5
1	A	75	VAL	2.5
1	B	40	VAL	2.5
1	B	91	VAL	2.5
1	A	469	ASN	2.4
1	D	62	TYR	2.4
1	D	162	PHE	2.4
1	A	30	ILE	2.4
1	D	286	TRP	2.4
1	C	135	GLY	2.4
1	C	533	GLY	2.4
1	B	16	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	61	TYR	2.4
1	C	20	THR	2.4
1	B	549	ALA	2.4
1	A	247	VAL	2.4
1	D	554	GLU	2.4
1	C	151	LEU	2.4
1	D	178	LYS	2.4
1	D	525	LEU	2.4
1	A	155	ARG	2.4
1	D	412	THR	2.4
1	A	357	ILE	2.4
1	D	66	ALA	2.4
1	A	231	VAL	2.4
1	B	503	VAL	2.4
1	B	12	LEU	2.3
1	C	515	TYR	2.3
1	D	95	PHE	2.3
1	A	348	ALA	2.3
1	B	157	ALA	2.3
1	C	373	ALA	2.3
1	D	7	ILE	2.3
1	B	589	ASN	2.3
1	D	236	PRO	2.3
1	D	47	GLY	2.3
1	A	138	VAL	2.3
1	B	138	VAL	2.3
1	D	245	ARG	2.3
1	B	195	TYR	2.3
1	C	280	PHE	2.3
1	B	376	ALA	2.3
1	D	181	ALA	2.3
1	A	185	ILE	2.3
1	C	207	PRO	2.3
1	C	355	MET	2.3
1	C	582	ILE	2.3
1	D	2	ILE	2.3
1	A	145	LYS	2.3
1	A	448	GLY	2.3
1	B	231	VAL	2.3
1	D	52	VAL	2.3
1	C	250	GLU	2.3
1	C	190	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	522	TRP	2.3
1	B	205	THR	2.3
1	D	515	TYR	2.3
1	B	204	LYS	2.3
1	D	81	ALA	2.3
1	B	206	ILE	2.3
1	B	574	ILE	2.3
1	D	40	VAL	2.3
1	D	166	VAL	2.3
1	B	223	ASN	2.3
1	A	227	LEU	2.3
1	A	398	LEU	2.3
1	D	205	THR	2.3
1	A	45	ALA	2.2
1	A	242	GLU	2.2
1	B	139	TYR	2.2
1	C	518	TYR	2.2
1	D	215	TYR	2.2
1	D	126	ILE	2.2
1	D	97	ASN	2.2
1	D	197	HIS	2.2
1	D	388	HIS	2.2
1	A	193	MET	2.2
1	D	1	MET	2.2
1	B	490	THR	2.2
1	D	144	GLU	2.2
1	B	491	PRO	2.2
1	A	376	ALA	2.2
1	A	380	TYR	2.2
1	B	62	TYR	2.2
1	B	80	TYR	2.2
1	B	357	ILE	2.2
1	C	17	LYS	2.2
1	D	355	MET	2.2
1	D	531	LYS	2.2
1	D	269	VAL	2.2
1	B	83	THR	2.2
1	A	28	LEU	2.2
1	B	333	LEU	2.2
1	C	158	LEU	2.2
1	D	89	LEU	2.2
1	A	611	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	367	ASP	2.2
1	A	5	ALA	2.2
1	A	61	TYR	2.2
1	A	558	TYR	2.2
1	B	115	PHE	2.2
1	B	601	PHE	2.2
1	D	351	TYR	2.2
1	A	48	ILE	2.2
1	C	234	ILE	2.2
1	A	154	ASN	2.2
1	D	308	VAL	2.2
1	B	172	THR	2.2
1	D	26	GLY	2.2
1	D	436	ALA	2.2
1	A	80	TYR	2.1
1	B	78	GLU	2.1
1	B	340	TYR	2.1
1	B	48	ILE	2.1
1	D	590	ILE	2.1
1	B	22	THR	2.1
1	B	264	VAL	2.1
1	C	386	VAL	2.1
1	A	298	SER	2.1
1	A	236	PRO	2.1
1	A	368	LEU	2.1
1	D	283	LEU	2.1
1	D	370	LYS	2.1
1	C	197	HIS	2.1
1	B	479	ALA	2.1
1	B	585	PHE	2.1
1	A	161	ILE	2.1
1	C	73	ILE	2.1
1	D	234	ILE	2.1
1	A	205	THR	2.1
1	B	548	THR	2.1
1	C	522	TRP	2.1
1	A	208	VAL	2.1
1	A	21	LYS	2.1
1	B	483	LYS	2.1
1	D	232	LYS	2.1
1	A	299	GLU	2.1
1	A	371	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	537	LEU	2.1
1	C	534	LEU	2.1
1	D	579	LEU	2.1
1	D	457	ALA	2.1
1	A	234	ILE	2.1
1	A	356	ASP	2.1
1	D	225	ASP	2.1
1	A	123	LYS	2.1
1	B	531	LYS	2.1
1	D	172	THR	2.1
1	B	10	GLY	2.1
1	B	316	GLY	2.1
1	A	97	ASN	2.1
1	D	603	VAL	2.1
1	B	165	LEU	2.1
1	C	140	LEU	2.1
1	D	151	LEU	2.1
1	A	203	ALA	2.1
1	C	45	ALA	2.1
1	D	202	ALA	2.1
1	D	317	ALA	2.1
1	B	524	ILE	2.0
1	B	569	GLU	2.0
1	D	339	SER	2.0
1	B	182	TYR	2.0
1	B	515	TYR	2.0
1	D	109	TYR	2.0
1	A	459	LEU	2.0
1	C	44	LEU	2.0
1	D	402	CYS	2.0
1	B	384	ALA	2.0
1	C	81	ALA	2.0
1	D	98	GLU	2.0
1	D	378	LYS	2.0
1	A	27	PHE	2.0
1	A	206	ILE	2.0
1	A	601	PHE	2.0
1	C	126	ILE	2.0
1	A	82	ASN	2.0
1	B	163	GLY	2.0
1	B	235	TYR	2.0
1	B	442	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	32	GLY	2.0
1	A	322	VAL	2.0
1	C	248	ARG	2.0
1	C	614	VAL	2.0

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 oligosaccharides 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
3	MG	D	703	1/1	0.55	0.19	46,46,46,46	0
4	PO4	D	704	5/5	0.58	0.17	54,60,67,78	0
4	PO4	B	712	5/5	0.66	0.19	30,31,43,51	0
6	EDO	A	711	4/4	0.67	0.24	35,40,42,42	0
7	ACT	A	707	4/4	0.68	0.19	25,29,31,33	0
6	EDO	C	2209	4/4	0.70	0.20	22,29,31,32	0
4	PO4	C	2215	5/5	0.71	0.19	30,36,40,48	0
7	ACT	A	715	4/4	0.72	0.20	27,34,37,46	0
4	PO4	A	718	5/5	0.75	0.19	30,32,43,51	0
6	EDO	D	707	4/4	0.77	0.17	30,32,38,39	0
6	EDO	B	706	4/4	0.77	0.24	20,21,22,24	0
6	EDO	A	716	4/4	0.77	0.36	21,22,23,29	0
3	MG	B	702	1/1	0.78	0.12	34,34,34,34	0
8	GOL	B	709	6/6	0.78	0.15	24,36,38,41	0
4	PO4	B	708	5/5	0.79	0.14	36,37,48,50	0
7	ACT	C	2201	4/4	0.79	0.16	21,22,29,34	0
3	MG	A	702	1/1	0.79	0.13	31,31,31,31	0
3	MG	C	2203	1/1	0.80	0.14	28,28,28,28	0
6	EDO	B	707	4/4	0.80	0.17	22,22,25,26	0

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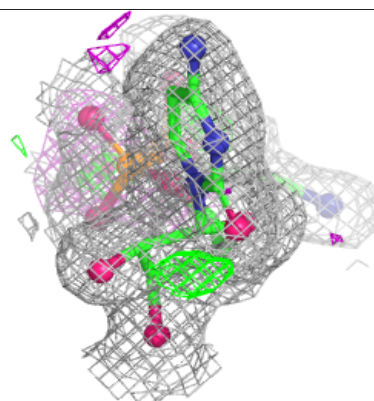
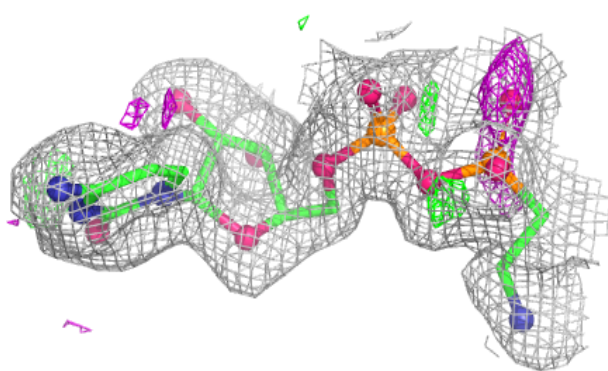
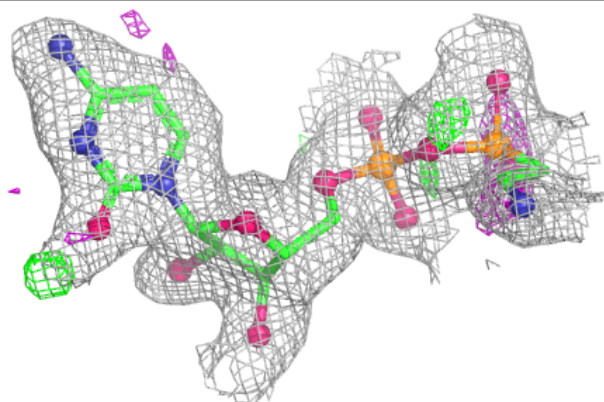
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	C	2210	4/4	0.82	0.14	23,33,33,37	0
6	EDO	A	709	4/4	0.82	0.17	20,22,25,26	0
4	PO4	D	714	5/5	0.82	0.18	28,33,38,46	0
4	PO4	C	2207	5/5	0.83	0.17	30,37,41,43	0
6	EDO	D	708	4/4	0.83	0.16	30,31,32,40	0
6	EDO	B	710	4/4	0.83	0.16	23,24,24,29	0
6	EDO	D	706	4/4	0.84	0.17	19,21,24,30	0
6	EDO	D	713	4/4	0.84	0.14	23,25,25,27	0
6	EDO	A	714	4/4	0.84	0.14	26,27,36,38	0
6	EDO	A	717	4/4	0.86	0.22	26,27,30,34	0
6	EDO	A	712	4/4	0.86	0.18	17,20,26,27	0
6	EDO	A	713	4/4	0.87	0.13	24,27,28,28	0
6	EDO	A	710	4/4	0.87	0.11	21,21,22,25	0
6	EDO	A	706	4/4	0.87	0.12	14,18,18,20	0
5	ORC	A	705	27/27	0.87	0.12	25,27,32,37	0
6	EDO	D	710	4/4	0.87	0.11	21,24,26,29	0
8	GOL	B	711	6/6	0.87	0.20	15,20,27,27	0
2	PLP	D	702	16/16	0.89	0.12	17,20,31,32	0
6	EDO	D	712	4/4	0.89	0.09	15,15,17,18	0
5	ORC	B	705	27/27	0.89	0.11	27,33,41,43	0
6	EDO	C	2212	4/4	0.89	0.12	16,17,17,22	0
5	ORC	D	705	27/27	0.90	0.11	31,35,37,40	0
2	PLP	C	2202	16/16	0.91	0.11	14,19,23,30	0
6	EDO	C	2206	4/4	0.91	0.17	24,25,28,33	0
3	MG	A	703	1/1	0.91	0.06	27,27,27,27	0
4	PO4	C	2204	5/5	0.91	0.12	24,25,26,29	0
5	ORC	C	2205	27/27	0.92	0.10	22,26,31,34	0
6	EDO	C	2208	4/4	0.92	0.12	19,24,24,25	0
6	EDO	C	2214	4/4	0.93	0.10	19,23,24,26	0
4	PO4	A	704	5/5	0.93	0.10	23,24,25,35	0
6	EDO	C	2213	4/4	0.93	0.12	17,20,21,23	0
3	MG	D	701	1/1	0.94	0.07	41,41,41,41	0
4	PO4	D	709	5/5	0.94	0.12	22,24,29,31	0
2	PLP	A	701	16/16	0.94	0.09	16,20,25,32	0
3	MG	B	703	1/1	0.94	0.06	33,33,33,33	0
2	PLP	B	701	16/16	0.94	0.11	18,23,29,36	0
4	PO4	B	704	5/5	0.94	0.11	24,27,30,33	0
6	EDO	D	711	4/4	0.94	0.09	20,24,25,26	0
6	EDO	A	708	4/4	0.95	0.07	21,21,23,29	0
3	MG	C	2211	1/1	0.97	0.04	26,26,26,26	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.

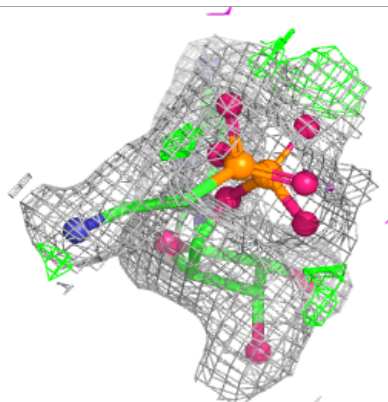
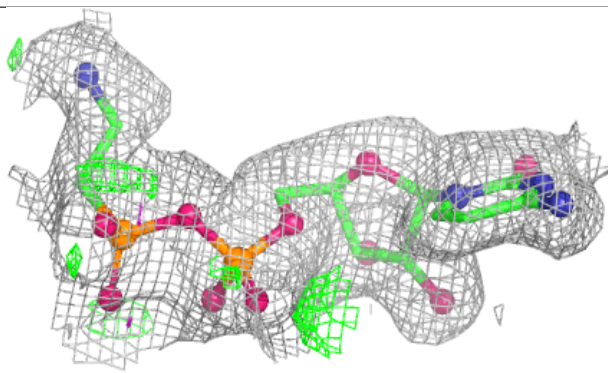
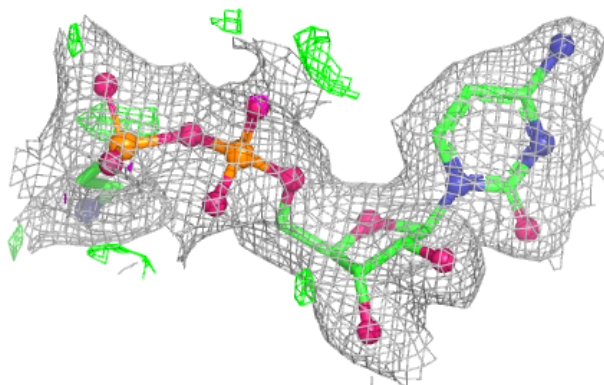
Electron density around 0RC A 705:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



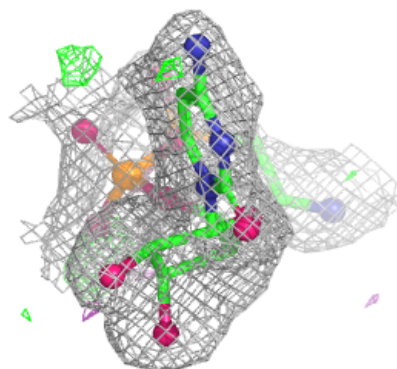
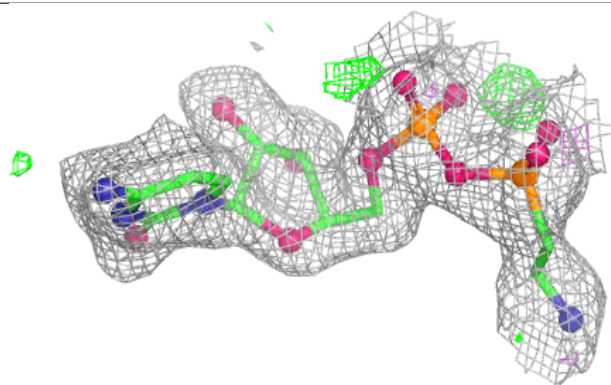
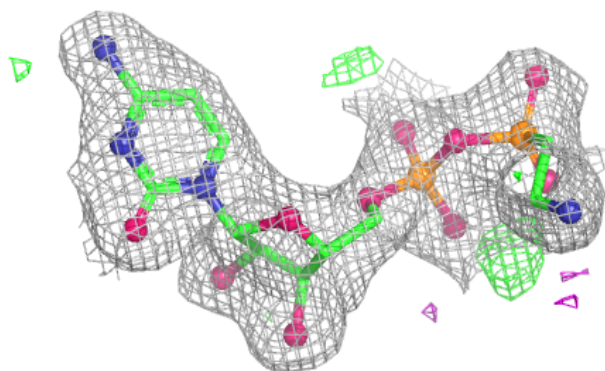
Electron density around 0RC B 705:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

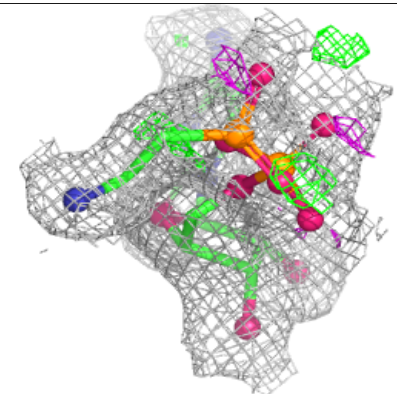
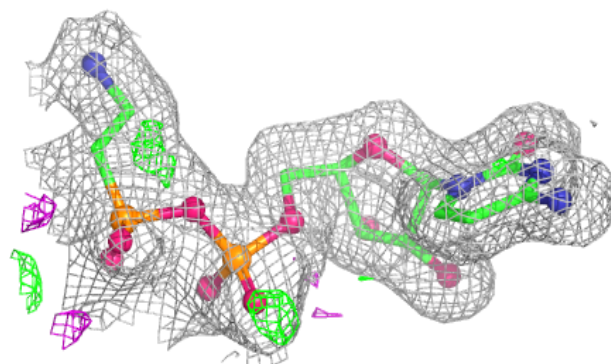
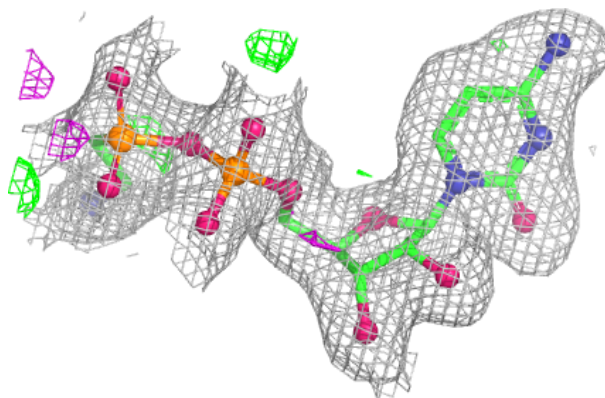


Electron density around 0RC D 705:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 0RC C 2205:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.