



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:53 PM UTC

PDB ID : 7PPG / pdb_00007ppg
Title : CRYSTAL STRUCTURE OF NAMPT IN COMPLEX WITH COMPOUND
9
Authors : Hillig, R.C.
Deposited on : 2021-09-13
Resolution : 2.13 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

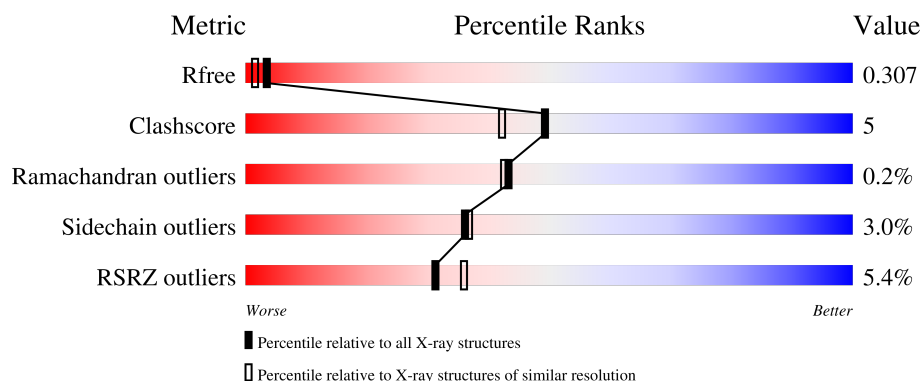
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	492	5% 85% 8% • 5%
1	B	492	3% 85% 10% 5%
1	C	492	6% 82% 12% • 5%
1	D	492	7% 86% 9% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16462 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 Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	1	0
			3744	2409	619	709	7			
1	B	466	Total	C	N	O	S	0	1	0
			3738	2405	618	708	7			
1	C	467	Total	C	N	O	S	0	0	0
			3736	2405	618	706	7			
1	D	467	Total	C	N	O	S	0	2	0
			3753	2416	620	710	7			

There are 4 discrepancies between the modelled and reference sequences:

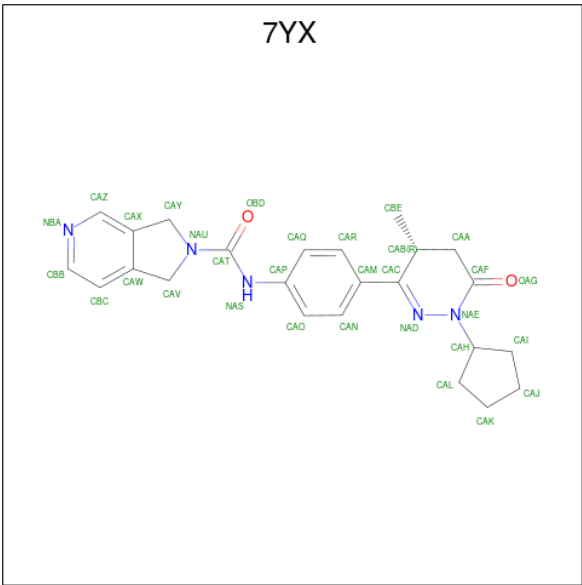
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P43490
B	0	GLY	-	expression tag	UNP P43490
C	0	GLY	-	expression tag	UNP P43490
D	0	GLY	-	expression tag	UNP P43490

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



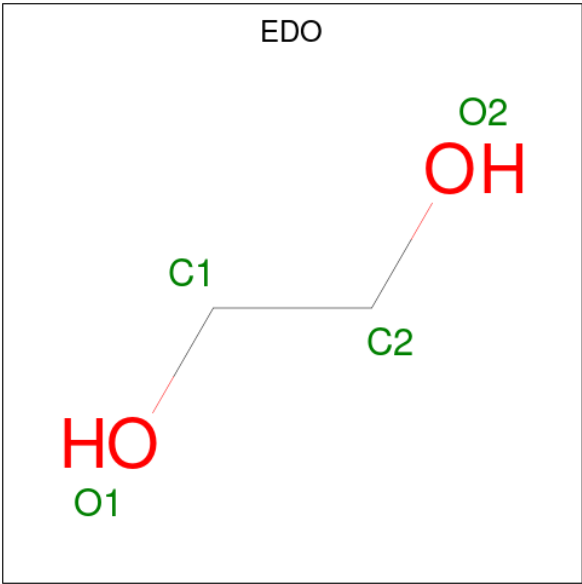
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is N-[4-[(4R)-1-cyclopentyl-4-methyl-6-oxidanylidene-4,5-dihydropyridazin-3-yl]phenyl]-1,3-dihydropyrrolo[3,4-c]pyridine-2-carboxamide (CCD ID: 7YX) (formula: C₂₄H₂₇N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			31	24	5	2		
3	B	1	Total	C	N	O	0	0
			31	24	5	2		
3	C	1	Total	C	N	O	0	0
			31	24	5	2		
3	D	1	Total	C	N	O	0	0
			31	24	5	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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	B	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

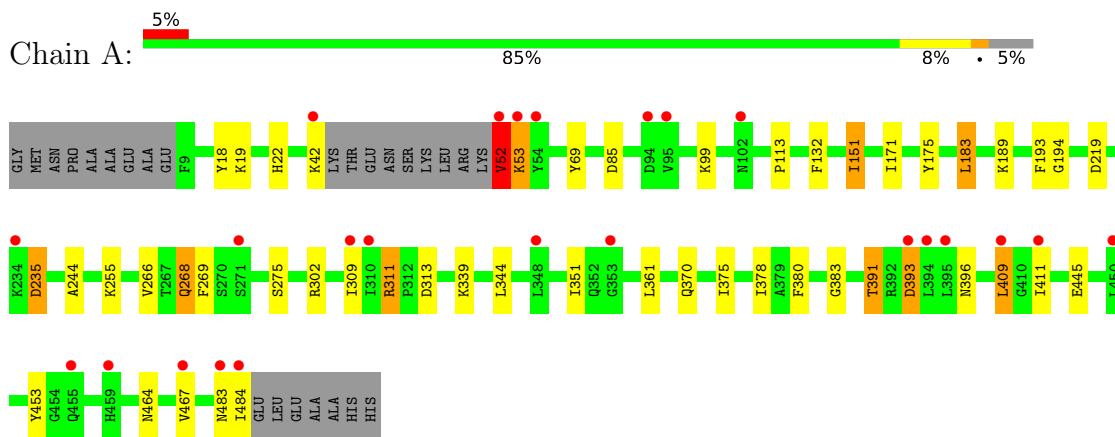
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	325	Total O 325 325	0	0
5	B	334	Total O 334 334	0	0
5	C	336	Total O 336 336	0	0
5	D	321	Total O 321 321	0	0

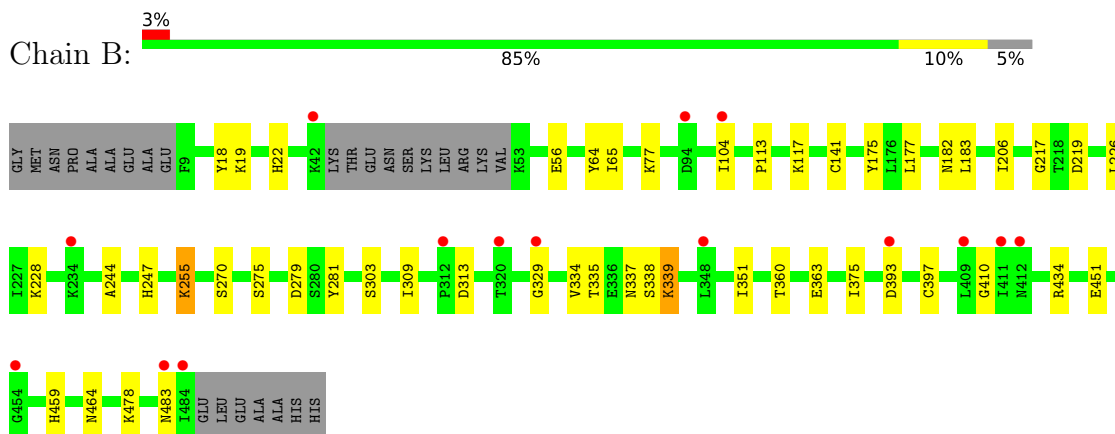
3 Residue-property plots [i](#)

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.

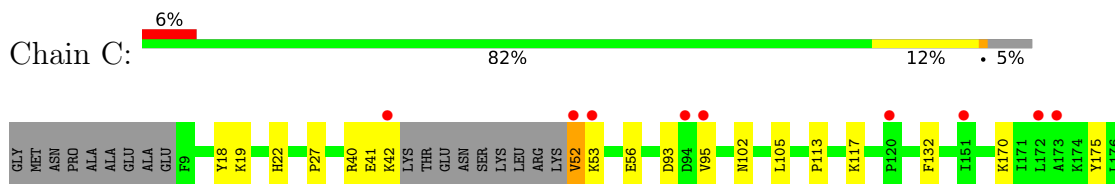
- Molecule 1: Nicotinamide phosphoribosyltransferase

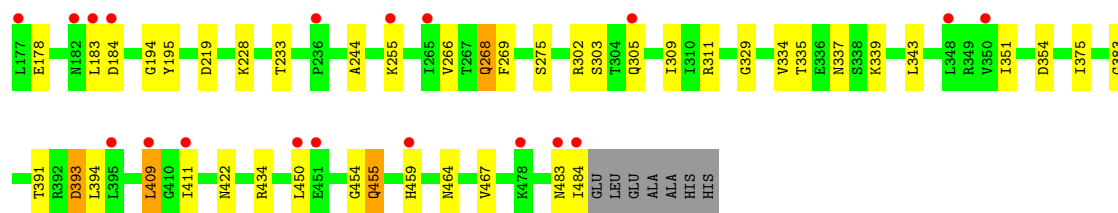


- Molecule 1: Nicotinamide phosphoribosyltransferase

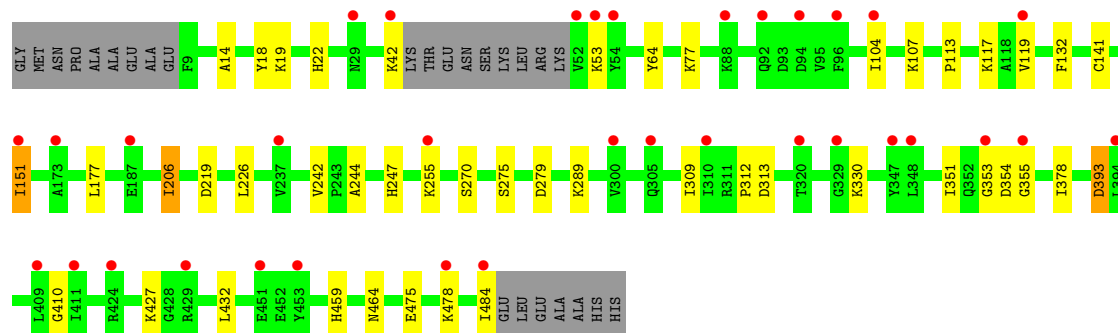
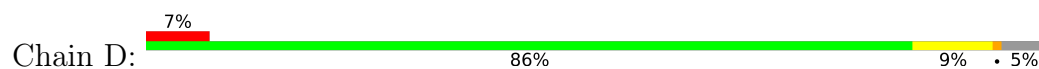


- Molecule 1: Nicotinamide phosphoribosyltransferase





● Molecule 1: Nicotinamide phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.96Å 106.18Å 121.34Å 90.00° 96.53° 90.00°	Depositor
Resolution (Å)	48.59 – 2.13 48.59 – 2.13	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.59-2.13) 98.3 (48.59-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.253 , 0.302 0.259 , 0.307	Depositor DCC
R_{free} test set	5747 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16462	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 79.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.2121e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PO4, 7YX, EDO

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	1.03	0/3832	1.32	3/5192 (0.1%)
1	B	1.03	1/3826 (0.0%)	1.31	1/5183 (0.0%)
1	C	1.03	0/3824	1.31	3/5181 (0.1%)
1	D	1.02	0/3841	1.30	2/5204 (0.0%)
All	All	1.02	1/15323 (0.0%)	1.31	9/20760 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	397	CYS	C-O	5.05	1.29	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	VAL	CA-C-N	6.29	133.56	121.54
1	A	52	VAL	C-N-CA	6.29	133.56	121.54
1	B	410	GLY	CA-C-O	-6.13	116.06	121.58
1	D	410	GLY	CA-C-O	-5.96	116.22	121.58
1	D	132	PHE	CA-CB-CG	5.44	119.24	113.80
1	A	132	PHE	CA-CB-CG	5.35	119.15	113.80
1	C	132	PHE	CA-CB-CG	5.12	118.92	113.80
1	C	233	THR	CA-C-N	5.05	127.01	120.44
1	C	233	THR	C-N-CA	5.05	127.01	120.44

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	3744	0	3724	39	0
1	B	3738	0	3717	39	0
1	C	3736	0	3721	42	0
1	D	3753	0	3736	38	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	1	0
2	D	10	0	0	1	0
3	A	31	0	0	0	0
3	B	31	0	0	0	0
3	C	31	0	0	0	0
3	D	31	0	0	3	0
4	A	8	0	12	2	0
4	B	4	0	5	2	0
4	D	4	0	5	1	0
5	A	325	0	0	14	0
5	B	334	0	0	13	0
5	C	336	0	0	19	0
5	D	321	0	0	13	0
All	All	16462	0	14920	161	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 5.

All (161) 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:B:64:TYR:CE2	1:B:206:ILE:HD11	1.92	1.03
1:D:206[A]:ILE:HD12	1:D:226:LEU:HD11	1.48	0.95
1:C:40:ARG:HD3	1:C:422:ASN:O	1.66	0.94
1:D:206[A]:ILE:CD1	1:D:226:LEU:HD11	2.07	0.84
1:A:183:LEU:HD11	5:A:834:HOH:O	1.79	0.83
1:C:343:LEU:HB3	5:C:601:HOH:O	1.78	0.82
1:D:104:ILE:HD11	1:D:141:CYS:SG	2.19	0.81
1:A:171:ILE:HD13	5:A:751:HOH:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206[A]:ILE:CD1	1:D:226:LEU:CD1	2.61	0.79
1:C:40:ARG:CD	1:C:422:ASN:O	2.31	0.77
1:B:65:ILE:HD11	5:B:760:HOH:O	1.84	0.77
1:C:391:THR:HG22	5:C:739:HOH:O	1.85	0.76
1:A:445:GLU:CD	5:A:611:HOH:O	2.28	0.76
1:B:104:ILE:HD11	1:B:141:CYS:SG	2.27	0.75
1:B:64:TYR:CD2	1:B:206:ILE:HD11	2.24	0.72
1:D:247:HIS:HE1	1:D:279:ASP:OD1	1.73	0.72
1:B:363:GLU:HG3	5:B:797:HOH:O	1.89	0.71
1:D:393:ASP:OD2	5:D:601:HOH:O	2.07	0.71
1:B:247:HIS:HE1	1:B:279:ASP:OD1	1.74	0.70
1:C:170:LYS:HE3	5:C:736:HOH:O	1.92	0.70
1:A:467:VAL:HG21	5:A:843:HOH:O	1.93	0.69
1:D:206[A]:ILE:HD12	1:D:226:LEU:CD1	2.20	0.69
1:C:268:GLN:HE21	1:C:268:GLN:HA	1.57	0.69
2:D:503:PO4:O3	5:D:602:HOH:O	2.11	0.68
1:B:64:TYR:CZ	1:B:206:ILE:HD11	2.28	0.68
1:A:339:LYS:O	5:A:602:HOH:O	2.12	0.67
1:A:311:ARG:CG	1:A:351:ILE:HG23	2.25	0.67
1:C:184:ASP:OD1	5:C:603:HOH:O	2.12	0.67
1:B:182:ASN:C	1:B:183:LEU:HD12	2.22	0.65
1:C:450:LEU:O	5:C:604:HOH:O	2.14	0.65
1:A:42:LYS:O	5:A:603:HOH:O	2.14	0.65
1:D:353:GLY:O	5:D:603:HOH:O	2.14	0.65
1:A:85:ASP:OD2	5:A:604:HOH:O	2.14	0.64
4:A:504:EDO:H22	5:A:864:HOH:O	1.96	0.64
1:D:151:ILE:HG13	5:D:719:HOH:O	1.97	0.64
1:A:268:GLN:HE21	1:A:268:GLN:HA	1.61	0.64
1:D:206[A]:ILE:HD13	1:D:206[A]:ILE:N	2.12	0.63
1:A:235:ASP:HA	5:A:881:HOH:O	1.98	0.62
1:D:484:ILE:C	5:D:730:HOH:O	2.42	0.62
1:D:270:SER:N	5:D:605:HOH:O	2.32	0.62
1:B:177:LEU:HD13	1:B:183:LEU:CD1	2.30	0.61
1:D:64:TYR:CZ	1:D:206[A]:ILE:HD11	2.35	0.61
1:A:311:ARG:HG2	1:A:351:ILE:HG23	1.83	0.61
1:D:355:GLY:N	5:D:612:HOH:O	2.34	0.61
1:B:177:LEU:HD13	1:B:183:LEU:HD11	1.82	0.60
1:D:177:LEU:CD1	1:D:484:ILE:HD11	2.31	0.60
1:C:105:LEU:HD11	5:C:703:HOH:O	2.03	0.59
1:D:104:ILE:CD1	1:D:141:CYS:SG	2.91	0.58
1:B:255:LYS:HD3	1:B:281:TYR:CD1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:THR:HG23	1:C:393:ASP:H	1.67	0.58
1:C:178:GLU:HG3	5:C:711:HOH:O	2.01	0.58
1:D:177:LEU:HD13	1:D:484:ILE:HD11	1.87	0.57
1:C:455:GLN:HG3	5:C:841:HOH:O	2.05	0.57
1:A:311:ARG:HG3	1:A:351:ILE:HG23	1.86	0.57
5:A:755:HOH:O	4:B:501:EDO:H21	2.03	0.57
1:D:354:ASP:OD1	5:D:604:HOH:O	2.18	0.56
1:D:247:HIS:CE1	1:D:279:ASP:OD1	2.57	0.56
1:C:335:THR:C	5:C:601:HOH:O	2.48	0.55
1:A:361:LEU:HD21	1:A:380:PHE:CD2	2.42	0.55
1:B:247:HIS:CE1	1:B:279:ASP:OD1	2.59	0.54
1:D:312:PRO:HB2	5:D:786:HOH:O	2.08	0.54
1:D:355:GLY:CA	5:D:612:HOH:O	2.55	0.53
1:A:344:LEU:HD21	5:A:692:HOH:O	2.07	0.53
1:B:255:LYS:NZ	5:B:617:HOH:O	2.41	0.53
1:C:178:GLU:O	1:C:339:LYS:HD3	2.09	0.53
1:B:104:ILE:CD1	1:B:141:CYS:SG	2.97	0.52
1:B:335:THR:HG23	5:B:712:HOH:O	2.09	0.51
1:C:467:VAL:HG22	5:C:811:HOH:O	2.09	0.51
1:A:391:THR:CG2	1:A:393[B]:ASP:H	2.25	0.50
1:A:391:THR:HG22	1:A:393[B]:ASP:H	1.77	0.50
1:A:370:GLN:NE2	5:A:613:HOH:O	2.38	0.50
1:D:206[A]:ILE:HD13	1:D:226:LEU:CD1	2.40	0.50
1:A:391:THR:CG2	1:A:393[A]:ASP:H	2.25	0.49
1:B:451:GLU:HB3	5:B:827:HOH:O	2.12	0.49
1:B:360:THR:HG21	5:B:649:HOH:O	2.12	0.49
1:A:391:THR:HG22	1:A:393[A]:ASP:H	1.78	0.49
5:C:745:HOH:O	4:D:501:EDO:H21	2.13	0.49
1:A:52:VAL:N	5:A:623:HOH:O	2.46	0.49
1:B:339:LYS:HA	1:B:339:LYS:CE	2.43	0.48
1:B:183:LEU:HD12	1:B:183:LEU:N	2.29	0.48
1:C:183:LEU:HD11	1:C:484:ILE:HG12	1.96	0.48
1:A:175:TYR:HB3	1:A:375:ILE:HG13	1.95	0.47
1:B:64:TYR:CD2	1:B:206:ILE:CD1	2.95	0.47
1:D:242:VAL:HG13	3:D:504:7YX:CAK	2.44	0.47
1:D:427:LYS:NZ	5:D:631:HOH:O	2.48	0.47
1:A:193:PHE:HB3	4:A:504:EDO:H11	1.96	0.47
1:C:337:ASN:HB2	5:C:890:HOH:O	2.14	0.47
1:C:56:GLU:HG2	5:C:680:HOH:O	2.15	0.47
1:A:309:ILE:HG22	1:A:351:ILE:HG22	1.96	0.46
1:D:242:VAL:CG1	3:D:504:7YX:CAK	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ASP:OD2	1:C:95:VAL:HG22	2.14	0.46
1:C:27:PRO:HG2	5:C:615:HOH:O	2.13	0.46
1:C:266:VAL:O	1:C:302:ARG:NH2	2.48	0.46
1:A:266:VAL:O	1:A:302:ARG:NH2	2.49	0.46
1:A:19:LYS:HA	1:A:22:HIS:ND1	2.31	0.46
1:C:41:GLU:HG2	1:C:42:LYS:H	1.81	0.45
1:B:206:ILE:HD13	1:B:226:LEU:HD11	1.97	0.45
1:B:255:LYS:HB2	5:B:610:HOH:O	2.16	0.45
1:B:19:LYS:HA	1:B:22:HIS:ND1	2.32	0.45
1:C:117:LYS:NZ	5:C:627:HOH:O	2.46	0.45
1:C:354:ASP:OD1	5:C:606:HOH:O	2.20	0.45
1:D:19:LYS:HA	1:D:22:HIS:ND1	2.32	0.45
1:D:177:LEU:O	1:D:177:LEU:HD23	2.17	0.45
1:A:113:PRO:HA	1:A:464:ASN:HD22	1.82	0.44
1:C:40:ARG:HD2	1:C:422:ASN:O	2.16	0.44
1:C:244:ALA:HA	1:C:275:SER:O	2.17	0.44
1:B:113:PRO:HA	1:B:464:ASN:HD22	1.82	0.44
1:C:309:ILE:HG22	1:C:351:ILE:HG22	1.98	0.44
1:C:409:LEU:CD1	1:C:411:ILE:HD11	2.48	0.44
1:A:311:ARG:HG3	1:A:351:ILE:CG2	2.46	0.44
1:B:339:LYS:HA	1:B:339:LYS:HE2	2.00	0.44
1:C:391:THR:HG23	1:C:393:ASP:N	2.33	0.44
1:D:309:ILE:HG22	1:D:351:ILE:HG22	1.99	0.44
1:B:309:ILE:HG22	1:B:351:ILE:HG22	1.99	0.44
1:A:244:ALA:HA	1:A:275:SER:O	2.17	0.44
1:A:269:PHE:O	1:A:302:ARG:NH2	2.34	0.44
1:A:453:TYR:HB2	5:A:855:HOH:O	2.18	0.44
1:B:77:LYS:HE2	5:B:911:HOH:O	2.18	0.44
1:C:19:LYS:HA	1:C:22:HIS:ND1	2.32	0.44
1:C:195:TYR:OH	1:D:14:ALA:HA	2.18	0.44
1:C:113:PRO:HA	1:C:464:ASN:HD22	1.83	0.43
1:D:244:ALA:HA	1:D:275:SER:O	2.17	0.43
1:C:269:PHE:O	1:C:302:ARG:NH2	2.35	0.43
1:C:311:ARG:NH1	2:C:502:PO4:O4	2.45	0.43
1:C:394:LEU:HB2	5:C:739:HOH:O	2.19	0.43
1:D:113:PRO:HA	1:D:464:ASN:HD22	1.83	0.43
1:D:242:VAL:HG13	3:D:504:7YX:CAL	2.48	0.43
1:B:228:LYS:HE2	5:B:880:HOH:O	2.17	0.43
1:C:52:VAL:HG23	1:C:53:LYS:H	1.83	0.43
1:B:175:TYR:HB3	1:B:375:ILE:HG13	2.00	0.43
1:A:361:LEU:CD2	1:A:380:PHE:CD2	3.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ALA:HA	1:B:275:SER:O	2.19	0.42
1:B:270:SER:HB2	5:B:890:HOH:O	2.19	0.42
1:C:329:GLY:HA2	1:C:334:VAL:CG2	2.49	0.42
1:A:69:TYR:CD2	1:A:151:ILE:HD11	2.54	0.42
1:A:483:ASN:O	1:A:484:ILE:C	2.62	0.42
1:B:217:GLY:HA3	5:B:769:HOH:O	2.20	0.42
1:B:247:HIS:HD2	4:B:501:EDO:O2	2.02	0.42
1:C:175:TYR:HB3	1:C:375:ILE:HG13	2.01	0.42
1:A:409:LEU:CD1	1:A:411:ILE:HD11	2.50	0.41
1:B:313:ASP:O	1:B:313:ASP:CG	2.64	0.41
1:C:194:GLY:CA	1:C:383:GLY:HA2	2.50	0.41
1:A:393[A]:ASP:O	1:A:393[A]:ASP:OD1	2.37	0.41
1:A:391:THR:CG2	1:A:393[A]:ASP:HB3	2.50	0.41
1:D:355:GLY:HA2	5:D:612:HOH:O	2.19	0.41
1:B:337:ASN:HB2	5:B:875:HOH:O	2.21	0.41
1:D:117:LYS:HA	1:D:459:HIS:O	2.21	0.41
1:A:194:GLY:CA	1:A:383:GLY:HA2	2.51	0.41
1:B:56:GLU:HG3	5:B:801:HOH:O	2.19	0.41
1:D:313:ASP:CG	1:D:313:ASP:O	2.64	0.41
1:B:117:LYS:HA	1:B:459:HIS:O	2.21	0.41
1:C:467:VAL:HG21	5:C:881:HOH:O	2.20	0.41
1:D:475[A]:GLU:OE1	5:D:607:HOH:O	2.22	0.41
1:D:104:ILE:HD12	1:D:113:PRO:CD	2.51	0.41
1:D:119:VAL:HG12	1:D:432:LEU:CD2	2.51	0.41
1:C:117:LYS:HA	1:C:459:HIS:O	2.21	0.40
1:C:102:ASN:ND2	5:C:646:HOH:O	2.54	0.40
1:A:313:ASP:O	1:A:313:ASP:CG	2.64	0.40
1:B:329:GLY:HA2	1:B:334:VAL:CG2	2.51	0.40
1:B:434:ARG:HD3	1:B:434:ARG:HA	1.96	0.40
1:A:42:LYS:HE3	1:A:396:ASN:HD21	1.86	0.40

There are no symmetry-related clashes.

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	464/492 (94%)	447 (96%)	16 (3%)	1 (0%)	43	42
1	B	463/492 (94%)	450 (97%)	12 (3%)	1 (0%)	43	42
1	C	463/492 (94%)	447 (96%)	14 (3%)	2 (0%)	30	26
1	D	465/492 (94%)	450 (97%)	15 (3%)	0	100	100
All	All	1855/1968 (94%)	1794 (97%)	57 (3%)	4 (0%)	43	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	LYS
1	C	483	ASN
1	B	483	ASN
1	C	454	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	412/430 (96%)	395 (96%)	17 (4%)	27	24
1	B	411/430 (96%)	403 (98%)	8 (2%)	50	55
1	C	411/430 (96%)	399 (97%)	12 (3%)	37	38
1	D	413/430 (96%)	398 (96%)	15 (4%)	31	30
All	All	1647/1720 (96%)	1595 (97%)	52 (3%)	36	35

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	TYR
1	A	52	VAL
1	A	53	LYS
1	A	99	LYS

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Mol	Chain	Res	Type
1	A	151	ILE
1	A	183	LEU
1	A	189	LYS
1	A	219	ASP
1	A	235	ASP
1	A	255	LYS
1	A	268	GLN
1	A	311	ARG
1	A	378	ILE
1	A	391	THR
1	A	393[A]	ASP
1	A	393[B]	ASP
1	A	409	LEU
1	B	18	TYR
1	B	219	ASP
1	B	255	LYS
1	B	303	SER
1	B	338	SER
1	B	339	LYS
1	B	393	ASP
1	B	478	LYS
1	C	18	TYR
1	C	52	VAL
1	C	219	ASP
1	C	228	LYS
1	C	255	LYS
1	C	268	GLN
1	C	303	SER
1	C	305	GLN
1	C	393	ASP
1	C	409	LEU
1	C	434	ARG
1	C	455	GLN
1	D	18	TYR
1	D	42	LYS
1	D	53	LYS
1	D	77	LYS
1	D	107	LYS
1	D	151	ILE
1	D	206[A]	ILE
1	D	206[B]	ILE
1	D	219	ASP

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Mol	Chain	Res	Type
1	D	255	LYS
1	D	289	LYS
1	D	330	LYS
1	D	378	ILE
1	D	393	ASP
1	D	478	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	154	GLN
1	A	201	GLN
1	A	268	GLN
1	A	285	ASN
1	A	396	ASN
1	A	407	ASN
1	A	464	ASN
1	A	481	GLN
1	B	92	GLN
1	B	201	GLN
1	B	247	HIS
1	B	305	GLN
1	B	396	ASN
1	B	412	ASN
1	B	459	HIS
1	B	464	ASN
1	B	481	GLN
1	C	29	ASN
1	C	154	GLN
1	C	201	GLN
1	C	268	GLN
1	C	285	ASN
1	C	305	GLN
1	C	407	ASN
1	C	412	ASN
1	C	464	ASN
1	C	481	GLN
1	D	154	GLN
1	D	201	GLN
1	D	247	HIS
1	D	396	ASN

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Mol	Chain	Res	Type
1	D	464	ASN
1	D	481	GLN

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 ⓘ

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	C	502	-	4,4,4	1.05	0	6,6,6	0.83	0
2	PO4	B	502	-	4,4,4	0.93	0	6,6,6	0.46	0
3	7YX	D	504	-	34,35,35	3.06	12 (35%)	42,50,50	2.51	16 (38%)
4	EDO	A	504	-	3,3,3	0.06	0	2,2,2	0.26	0
3	7YX	A	503	-	34,35,35	3.15	11 (32%)	42,50,50	2.55	17 (40%)
2	PO4	A	502	-	4,4,4	0.96	0	6,6,6	0.60	0
2	PO4	C	501	-	4,4,4	1.12	0	6,6,6	0.68	0
3	7YX	C	503	-	34,35,35	3.13	14 (41%)	42,50,50	2.79	17 (40%)
4	EDO	A	505	-	3,3,3	0.32	0	2,2,2	0.27	0
4	EDO	B	501	-	3,3,3	0.73	0	2,2,2	0.13	0
4	EDO	D	501	-	3,3,3	0.77	0	2,2,2	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	A	501	-	4,4,4	0.95	0	6,6,6	0.84	0
2	PO4	D	503	-	4,4,4	1.39	1 (25%)	6,6,6	0.48	0
3	7YX	B	503	-	34,35,35	3.15	11 (32%)	42,50,50	3.15	18 (42%)
2	PO4	D	502	-	4,4,4	0.60	0	6,6,6	0.57	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	7YX	D	504	-	-	3/16/47/47	0/5/5/5
4	EDO	A	504	-	-	1/1/1/1	-
3	7YX	A	503	-	-	3/16/47/47	0/5/5/5
4	EDO	A	505	-	-	1/1/1/1	-
4	EDO	B	501	-	-	1/1/1/1	-
4	EDO	D	501	-	-	1/1/1/1	-
3	7YX	C	503	-	-	3/16/47/47	0/5/5/5
3	7YX	B	503	-	-	3/16/47/47	0/5/5/5

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	7YX	CAA-CAF	-10.12	1.35	1.51
3	C	503	7YX	CAA-CAF	-8.80	1.37	1.51
3	A	503	7YX	CAC-NAD	8.51	1.35	1.29
3	A	503	7YX	CAA-CAF	-8.10	1.38	1.51
3	D	504	7YX	CAA-CAF	-7.52	1.39	1.51
3	A	503	7YX	CAY-CAX	-7.42	1.40	1.50
3	D	504	7YX	CAC-NAD	7.19	1.34	1.29
3	B	503	7YX	CAB-CAC	-6.92	1.41	1.51
3	D	504	7YX	CAV-CAW	-6.78	1.41	1.50
3	C	503	7YX	CAB-CAC	-6.51	1.42	1.51
3	C	503	7YX	CAY-CAX	-6.43	1.42	1.50
3	C	503	7YX	CAV-CAW	-6.35	1.42	1.50
3	B	503	7YX	CAV-CAW	-6.34	1.42	1.50
3	D	504	7YX	CAM-CAC	-6.05	1.39	1.48
3	D	504	7YX	CAY-CAX	-5.76	1.42	1.50
3	C	503	7YX	CAC-NAD	5.65	1.33	1.29
3	B	503	7YX	CAY-CAX	-5.48	1.43	1.50
3	A	503	7YX	CAB-CAC	-5.33	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	7YX	CAC-NAD	4.96	1.32	1.29
3	A	503	7YX	CAV-CAW	-4.93	1.43	1.50
3	B	503	7YX	CAZ-NBA	4.61	1.44	1.34
3	A	503	7YX	CAP-NAS	-4.52	1.32	1.41
3	A	503	7YX	CAM-CAC	-4.40	1.41	1.48
3	C	503	7YX	CAM-CAC	-4.38	1.41	1.48
3	D	504	7YX	CAB-CAC	-4.29	1.45	1.51
3	D	504	7YX	CAP-NAS	-3.99	1.33	1.41
3	D	504	7YX	CAZ-NBA	3.98	1.42	1.34
3	B	503	7YX	CAV-NAU	3.91	1.52	1.46
3	B	503	7YX	CAM-CAC	-3.85	1.42	1.48
3	C	503	7YX	CBB-NBA	3.33	1.43	1.33
3	C	503	7YX	CAP-NAS	-3.25	1.35	1.41
3	A	503	7YX	CAZ-NBA	3.24	1.41	1.34
3	C	503	7YX	CAV-NAU	3.13	1.51	1.46
3	A	503	7YX	CBC-CAW	-3.11	1.34	1.39
3	C	503	7YX	CAZ-NBA	3.11	1.40	1.34
3	C	503	7YX	CBC-CAW	-2.95	1.34	1.39
3	B	503	7YX	CAL-CAH	2.88	1.60	1.53
3	A	503	7YX	NAE-NAD	-2.53	1.32	1.37
3	B	503	7YX	CBB-NBA	2.47	1.40	1.33
3	C	503	7YX	CAY-NAU	-2.35	1.43	1.46
3	A	503	7YX	CAX-CAW	-2.31	1.35	1.39
3	D	504	7YX	CAJ-CAI	-2.30	1.42	1.51
3	D	504	7YX	CBC-CAW	-2.28	1.35	1.39
2	D	503	PO4	P-O1	2.25	1.55	1.50
3	D	504	7YX	CBB-NBA	2.24	1.40	1.33
3	C	503	7YX	CAT-NAS	2.21	1.41	1.37
3	C	503	7YX	CAO-CAN	2.18	1.42	1.38
3	B	503	7YX	CAY-NAU	-2.04	1.44	1.46
3	D	504	7YX	NAE-NAD	-2.03	1.33	1.37

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	7YX	CAX-CAY-NAU	10.63	107.42	102.42
3	C	503	7YX	CAA-CAF-NAE	8.17	124.71	114.24
3	A	503	7YX	CAA-CAF-NAE	7.71	124.12	114.24
3	B	503	7YX	CAA-CAB-CAC	7.61	118.28	108.13
3	B	503	7YX	CAA-CAF-NAE	7.33	123.63	114.24
3	D	504	7YX	CAA-CAF-NAE	7.28	123.56	114.24
3	C	503	7YX	CAX-CAY-NAU	7.08	105.75	102.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	7YX	CAA-CAB-CAC	6.67	117.03	108.13
3	A	503	7YX	CAA-CAB-CAC	5.62	115.64	108.13
3	B	503	7YX	CAW-CAV-NAU	5.34	104.93	102.42
3	C	503	7YX	CAC-NAD-NAE	5.22	124.44	118.97
3	D	504	7YX	CAH-NAE-CAF	5.02	126.33	120.31
3	B	503	7YX	CAC-NAD-NAE	4.87	124.08	118.97
3	D	504	7YX	CAA-CAB-CAC	4.67	114.36	108.13
3	D	504	7YX	CAC-NAD-NAE	4.64	123.83	118.97
3	A	503	7YX	CAC-NAD-NAE	4.60	123.80	118.97
3	D	504	7YX	CAF-NAE-NAD	-4.27	120.15	125.19
3	A	503	7YX	CAW-CAV-NAU	-4.22	100.44	102.42
3	A	503	7YX	CBB-CBC-CAW	4.17	123.49	119.58
3	C	503	7YX	OAG-CAF-NAE	-4.16	116.15	120.83
3	C	503	7YX	CAF-NAE-NAD	-3.99	120.48	125.19
3	B	503	7YX	CAB-CAC-NAD	-3.81	118.00	122.84
3	A	503	7YX	CBC-CBB-NBA	-3.67	117.34	123.60
3	D	504	7YX	CBC-CBB-NBA	-3.58	117.48	123.60
3	C	503	7YX	CAN-CAM-CAC	3.58	125.02	120.74
3	B	503	7YX	CAF-NAE-NAD	-3.53	121.02	125.19
3	D	504	7YX	CBB-CBC-CAW	3.51	122.87	119.58
3	D	504	7YX	CAX-CAY-NAU	-3.45	100.80	102.42
3	A	503	7YX	CAF-NAE-NAD	-3.43	121.15	125.19
3	A	503	7YX	CAJ-CAI-CAH	-3.42	96.92	104.61
3	D	504	7YX	OAG-CAF-CAA	-3.31	115.81	122.04
3	B	503	7YX	CAR-CAQ-CAP	3.31	124.11	120.30
3	B	503	7YX	OAG-CAF-CAA	-3.27	115.89	122.04
3	D	504	7YX	CAM-CAC-NAD	-3.26	112.04	115.98
3	C	503	7YX	CAJ-CAI-CAH	-3.14	97.55	104.61
3	A	503	7YX	CAN-CAM-CAC	3.09	124.44	120.74
3	B	503	7YX	CBE-CAB-CAA	-3.06	102.10	112.50
3	A	503	7YX	CAK-CAJ-CAI	-3.06	95.80	105.97
3	B	503	7YX	CAJ-CAI-CAH	-3.04	97.78	104.61
3	C	503	7YX	CAB-CAC-NAD	-3.04	118.99	122.84
3	B	503	7YX	CBB-CBC-CAW	3.02	122.42	119.58
3	A	503	7YX	OAG-CAF-NAE	-2.95	117.51	120.83
3	B	503	7YX	CAO-CAP-CAQ	-2.94	115.14	119.04
3	D	504	7YX	CAW-CAV-NAU	-2.87	101.07	102.42
3	D	504	7YX	CAK-CAJ-CAI	-2.85	96.48	105.97
3	C	503	7YX	CAO-CAP-CAQ	-2.69	115.47	119.04
3	D	504	7YX	OBD-CAT-NAU	-2.53	118.14	121.67
3	C	503	7YX	CAR-CAQ-CAP	2.52	123.20	120.30
3	B	503	7YX	CBC-CBB-NBA	-2.51	119.32	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	7YX	CBE-CAB-CAA	-2.48	104.07	112.50
3	D	504	7YX	CAB-CAA-CAF	2.48	116.06	111.77
3	D	504	7YX	CBE-CAB-CAC	2.45	113.58	109.70
3	A	503	7YX	CAP-NAS-CAT	-2.38	121.22	126.04
3	D	504	7YX	CAJ-CAK-CAL	-2.37	98.07	105.97
3	C	503	7YX	OBD-CAT-NAU	-2.31	118.44	121.67
3	B	503	7YX	CAK-CAJ-CAI	-2.31	98.30	105.97
3	C	503	7YX	CAK-CAJ-CAI	-2.28	98.38	105.97
3	B	503	7YX	CAO-CAP-NAS	2.28	128.06	120.41
3	B	503	7YX	CBE-CAB-CAC	-2.26	106.11	109.70
3	A	503	7YX	OBD-CAT-NAU	-2.25	118.52	121.67
3	C	503	7YX	CAW-CAV-NAU	2.20	103.46	102.42
3	A	503	7YX	CAQ-CAR-CAM	2.16	123.11	120.80
3	C	503	7YX	CAO-CAP-NAS	2.16	127.65	120.41
3	B	503	7YX	CAN-CAM-CAC	2.14	123.30	120.74
3	A	503	7YX	CAV-CAW-CAX	2.12	112.30	110.07
3	C	503	7YX	CAX-CAZ-NBA	-2.11	121.78	124.58
3	A	503	7YX	CAR-CAM-CAC	-2.02	118.33	120.74
3	A	503	7YX	OAG-CAF-CAA	-2.00	118.27	122.04

There are no chirality outliers.

All (16) torsion outliers are listed below:

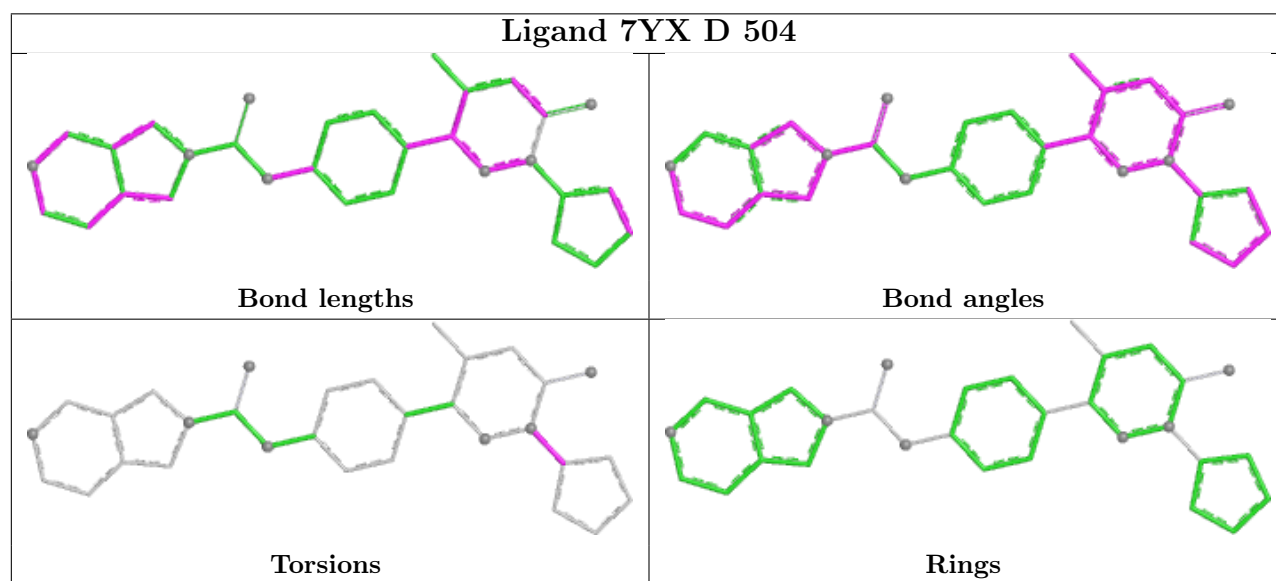
Mol	Chain	Res	Type	Atoms
3	A	503	7YX	CAI-CAH-NAE-NAD
3	A	503	7YX	CAL-CAH-NAE-NAD
3	A	503	7YX	CAL-CAH-NAE-CAF
3	B	503	7YX	CAI-CAH-NAE-NAD
3	B	503	7YX	CAI-CAH-NAE-CAF
3	B	503	7YX	CAL-CAH-NAE-CAF
3	C	503	7YX	CAI-CAH-NAE-NAD
3	C	503	7YX	CAL-CAH-NAE-CAF
3	D	504	7YX	CAI-CAH-NAE-NAD
4	A	505	EDO	O1-C1-C2-O2
4	A	504	EDO	O1-C1-C2-O2
4	B	501	EDO	O1-C1-C2-O2
4	D	501	EDO	O1-C1-C2-O2
3	C	503	7YX	CAI-CAH-NAE-CAF
3	D	504	7YX	CAI-CAH-NAE-CAF
3	D	504	7YX	CAL-CAH-NAE-CAF

There are no ring outliers.

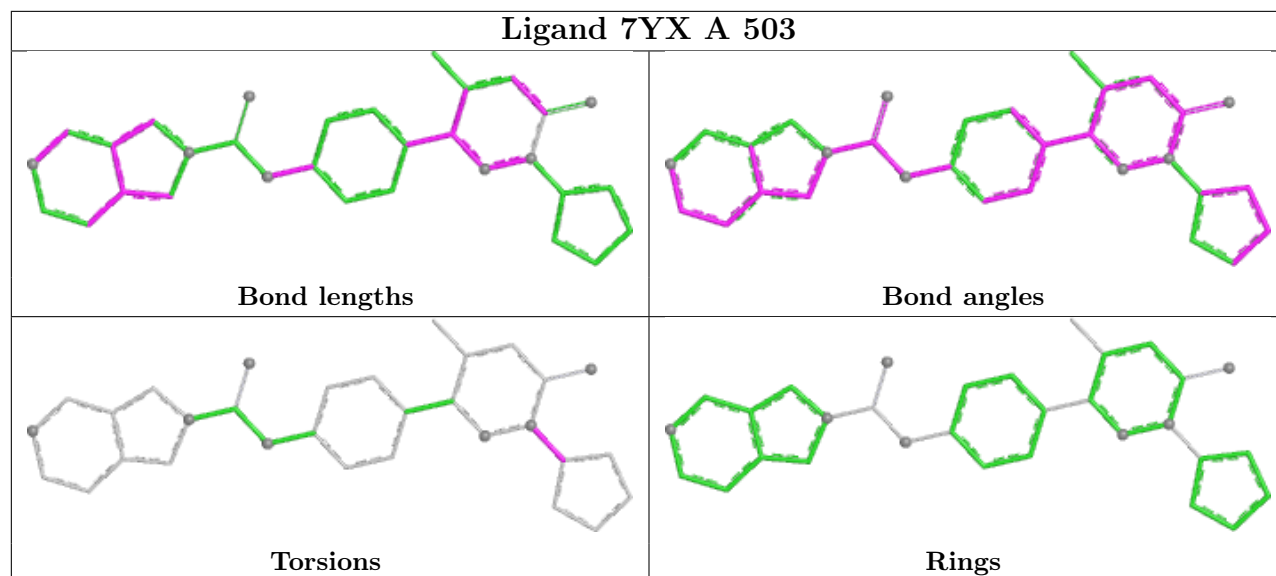
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	502	PO4	1	0
3	D	504	7YX	3	0
4	A	504	EDO	2	0
4	B	501	EDO	2	0
4	D	501	EDO	1	0
2	D	503	PO4	1	0

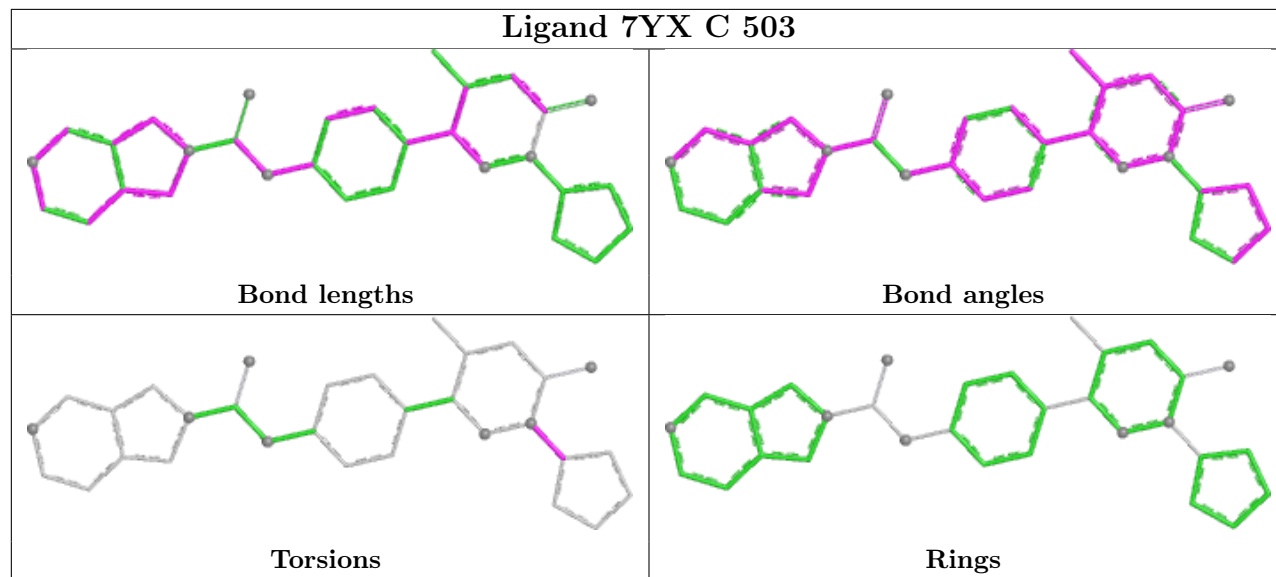
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



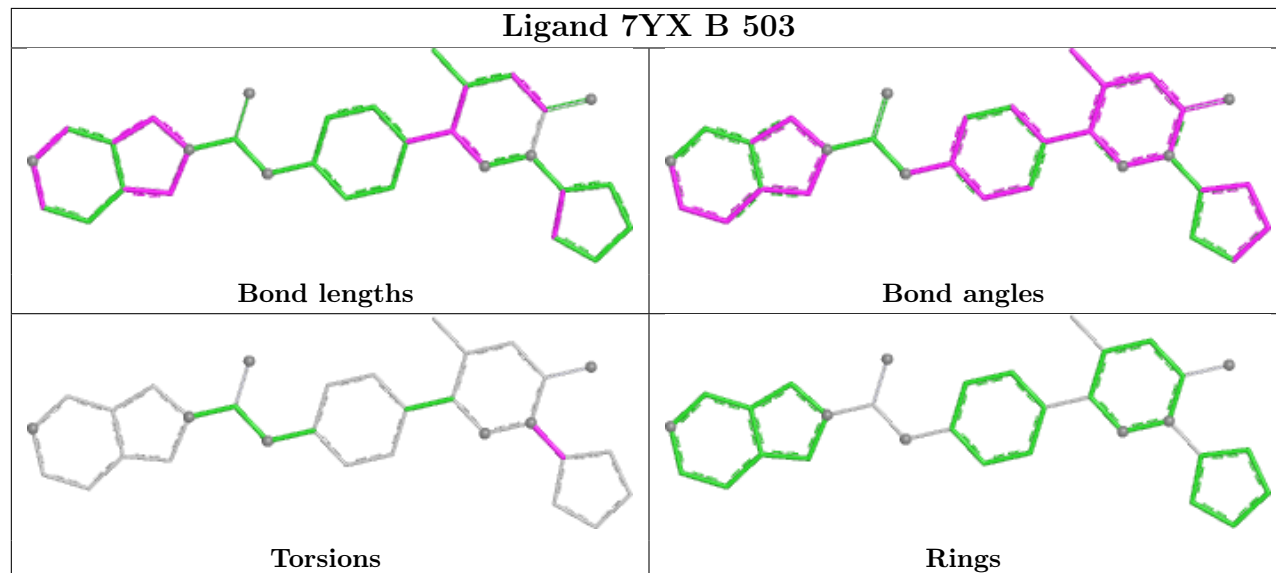
Ligand 7YX A 503



Ligand 7YX C 503



Ligand 7YX B 503



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	467/492 (94%)	0.63	24 (5%)	33	38	9, 19, 36, 58	1 (0%)
1	B	466/492 (94%)	0.51	15 (3%)	50	54	8, 18, 33, 64	1 (0%)
1	C	467/492 (94%)	0.70	28 (5%)	27	32	8, 20, 35, 80	0
1	D	467/492 (94%)	0.64	34 (7%)	21	24	5, 19, 38, 69	2 (0%)
All	All	1867/1968 (94%)	0.62	101 (5%)	31	36	5, 19, 36, 80	4 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	52	VAL	6.4
1	C	411	ILE	5.4
1	C	484	ILE	5.1
1	C	52	VAL	4.8
1	A	409	LEU	4.6
1	A	394	LEU	4.3
1	B	348	LEU	4.1
1	D	42	LYS	4.1
1	C	265	ILE	3.7
1	C	94	ASP	3.7
1	A	52	VAL	3.7
1	C	42	LYS	3.7
1	D	104	ILE	3.7
1	A	450	LEU	3.6
1	B	484	ILE	3.6
1	D	329	GLY	3.6
1	A	484	ILE	3.5
1	A	94	ASP	3.5
1	B	104	ILE	3.5
1	A	102	ASN	3.5
1	B	42	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	393[A]	ASP	3.4
1	A	395	LEU	3.4
1	D	305	GLN	3.4
1	A	483	ASN	3.3
1	C	483	ASN	3.3
1	C	177	LEU	3.3
1	D	394	LEU	3.3
1	A	271	SER	3.2
1	C	450	LEU	3.2
1	B	234	LYS	3.2
1	C	348	LEU	3.2
1	A	234	LYS	3.1
1	D	187	GLU	3.1
1	D	54	TYR	3.0
1	D	347	TYR	3.0
1	D	255	LYS	3.0
1	D	29	ASN	3.0
1	C	172	LEU	3.0
1	C	184	ASP	2.9
1	A	411	ILE	2.9
1	B	393	ASP	2.8
1	D	348	LEU	2.8
1	D	424	ARG	2.8
1	A	95	VAL	2.8
1	B	329	GLY	2.8
1	A	53	LYS	2.8
1	C	53	LYS	2.8
1	D	237	VAL	2.8
1	B	320	THR	2.7
1	C	395	LEU	2.7
1	D	409	LEU	2.7
1	D	173	ALA	2.7
1	A	348	LEU	2.7
1	A	54	TYR	2.7
1	B	483	ASN	2.7
1	B	411	ILE	2.7
1	D	300	VAL	2.7
1	D	310	ILE	2.6
1	D	94	ASP	2.6
1	A	353	GLY	2.6
1	D	451	GLU	2.5
1	D	484	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	42	LYS	2.5
1	D	429	ARG	2.5
1	C	173	ALA	2.5
1	C	95	VAL	2.4
1	C	183	LEU	2.4
1	C	459	HIS	2.4
1	B	94	ASP	2.4
1	B	312	PRO	2.4
1	D	355	GLY	2.4
1	D	453	TYR	2.3
1	C	255	LYS	2.3
1	C	409	LEU	2.3
1	D	119	VAL	2.3
1	D	96	PHE	2.3
1	B	454	GLY	2.3
1	C	182	ASN	2.2
1	A	309	ILE	2.2
1	D	478	LYS	2.2
1	D	88	LYS	2.2
1	D	151	ILE	2.2
1	A	467	VAL	2.2
1	C	305	GLN	2.2
1	C	350	VAL	2.1
1	A	459	HIS	2.1
1	B	409	LEU	2.1
1	C	151	ILE	2.1
1	D	53	LYS	2.1
1	B	412	ASN	2.1
1	C	451	GLU	2.1
1	C	120	PRO	2.1
1	A	455	GLN	2.1
1	A	310	ILE	2.1
1	D	92	GLN	2.0
1	C	478	LYS	2.0
1	D	411	ILE	2.0
1	C	236	PRO	2.0
1	D	320	THR	2.0
1	D	353	GLY	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 oligosaccharides in this entry.

6.4 Ligands

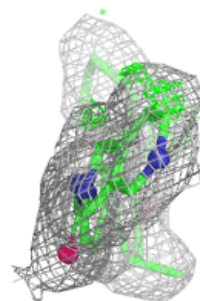
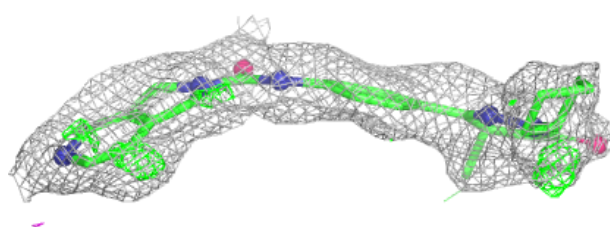
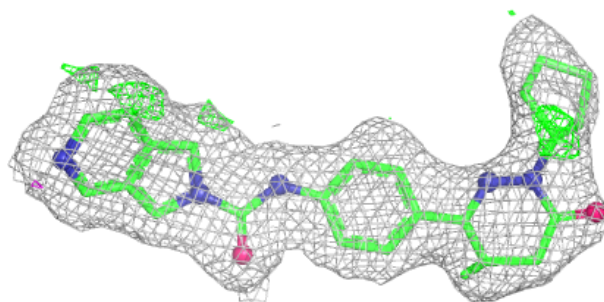
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	505	4/4	0.78	0.13	16,23,23,27	0
4	EDO	A	504	4/4	0.82	0.14	27,34,35,48	0
2	PO4	D	502	5/5	0.87	0.14	47,51,54,65	0
3	7YX	C	503	31/31	0.88	0.11	10,19,31,42	0
3	7YX	B	503	31/31	0.91	0.10	7,15,32,41	0
3	7YX	D	504	31/31	0.91	0.10	12,16,34,44	0
3	7YX	A	503	31/31	0.92	0.12	11,21,50,55	0
2	PO4	C	502	5/5	0.92	0.14	19,19,36,37	0
2	PO4	A	502	5/5	0.92	0.11	27,32,36,39	0
2	PO4	B	502	5/5	0.93	0.12	27,29,36,59	0
4	EDO	B	501	4/4	0.93	0.10	6,9,14,21	0
4	EDO	D	501	4/4	0.94	0.09	6,10,17,18	0
2	PO4	C	501	5/5	0.95	0.12	23,27,36,57	0
2	PO4	D	503	5/5	0.95	0.08	22,23,27,28	0
2	PO4	A	501	5/5	0.96	0.10	14,20,26,28	0

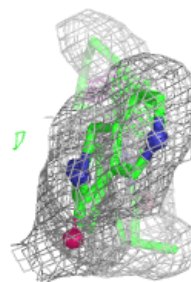
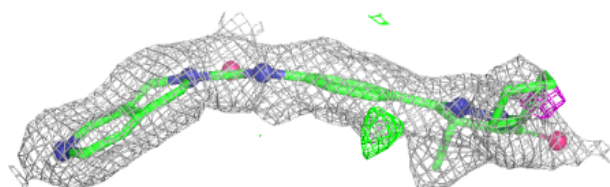
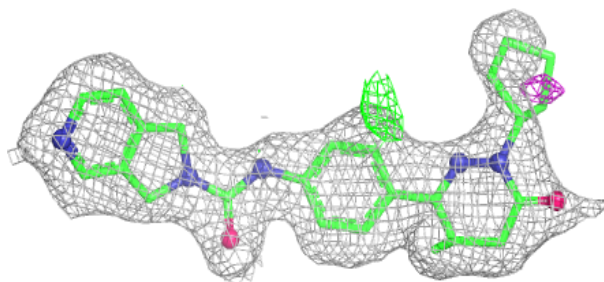
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7YX C 503:

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

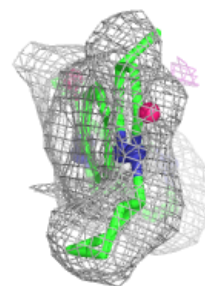
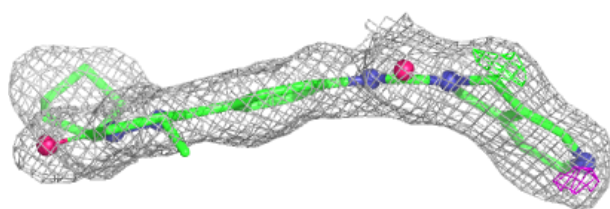
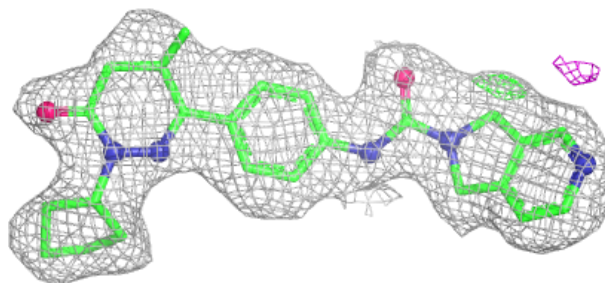
**Electron density around 7YX B 503:**

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

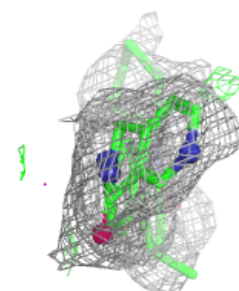
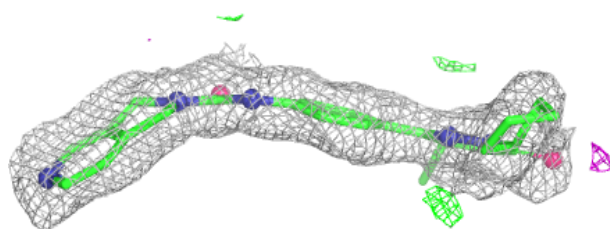
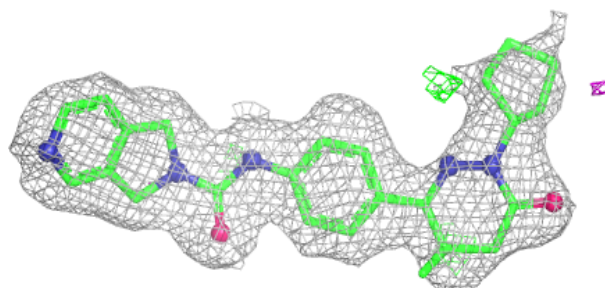


Electron density around 7YX D 504:

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

**Electron density around 7YX A 503:**

$2mF_o-DF_c$ (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.