



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:18 AM UTC

PDB ID : 4G1N / pdb_00004g1n
Title : PKM2 in complex with an activator
Authors : Kung, C.; Hixon, J.; Dang, L.; DeLaBarre, B.; Qian, K.C.
Deposited on : 2012-07-10
Resolution : 2.30 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

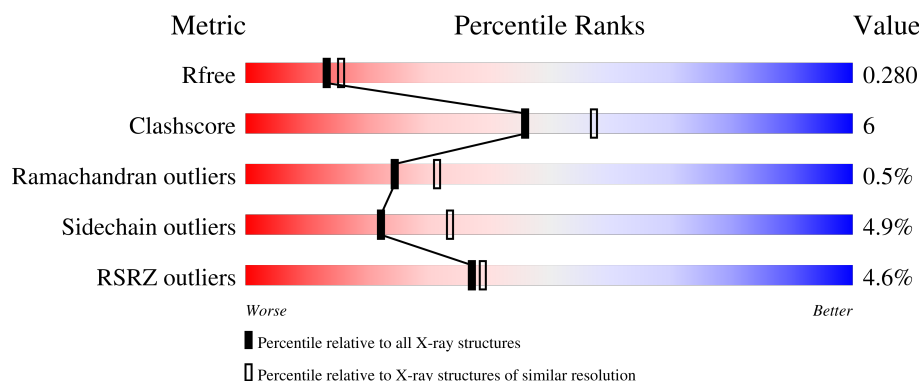
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	518	3% 86% 13% .
1	B	518	10% 83% 15% .
1	C	518	3% 83% 15% .
1	D	518	3% 84% 15% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OXL	B	601	-	X	-	-
2	OXL	D	601	-	X	-	-

2 Entry composition [i](#)

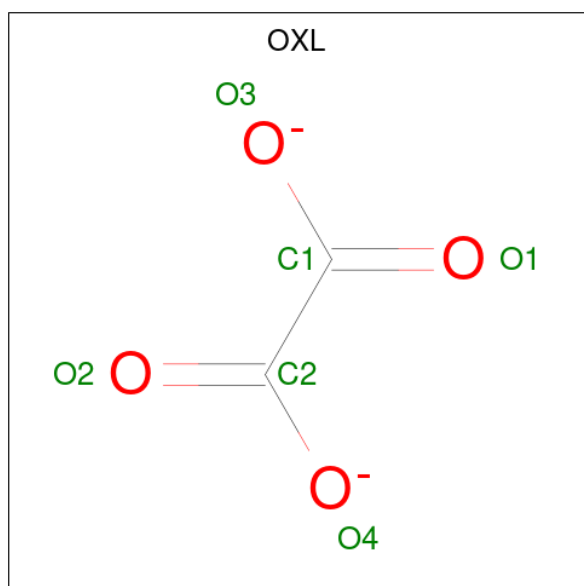
There are 5 unique types of molecules in this entry. The entry contains 16230 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyruvate kinase isozymes M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			3965	2492	704	744	25			
1	B	518	Total	C	N	O	S	0	2	0
			3978	2501	707	744	26			
1	C	518	Total	C	N	O	S	0	1	0
			3970	2496	704	744	26			
1	D	518	Total	C	N	O	S	0	0	0
			3965	2492	704	744	25			

- Molecule 2 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



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

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

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3 | A | 1 | Total Mg
1 1 | 0 | 0 |
| 3 | B | 1 | Total Mg
1 1 | 0 | 0 |
| 3 | C | 1 | Total Mg
1 1 | 0 | 0 |
| 3 | D | 1 | Total Mg
1 1 | 0 | 0 |

-

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 34	C 24	N 6	O 3	S 1	0	1
4	D	1	Total 68	C 48	N 12	O 6	S 2	0	1

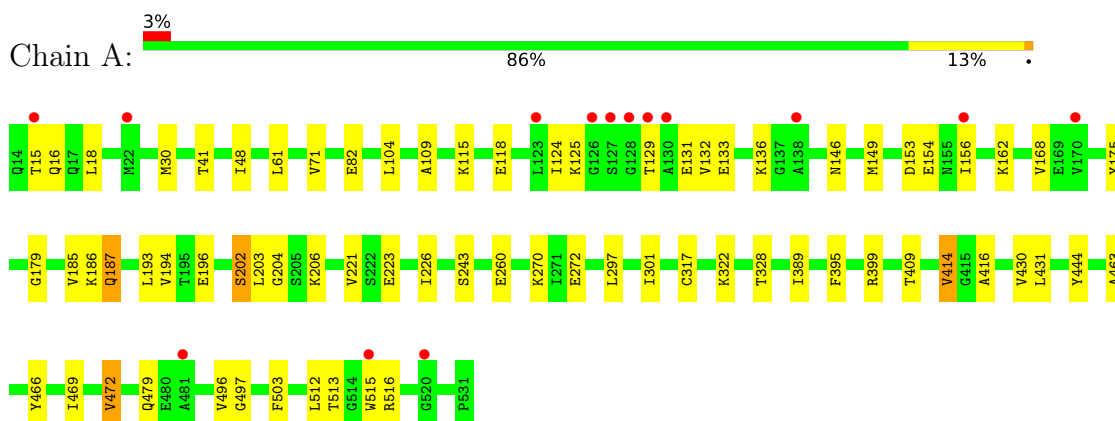
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- WORLD WIDE
PDB
PROTEIN DATA BANK

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	66	Total 66	O 66	0	0
5	B	71	Total 71	O 71	0	0
5	C	48	Total 48	O 48	0	0
5	D	37	Total 37	O 37	0	0

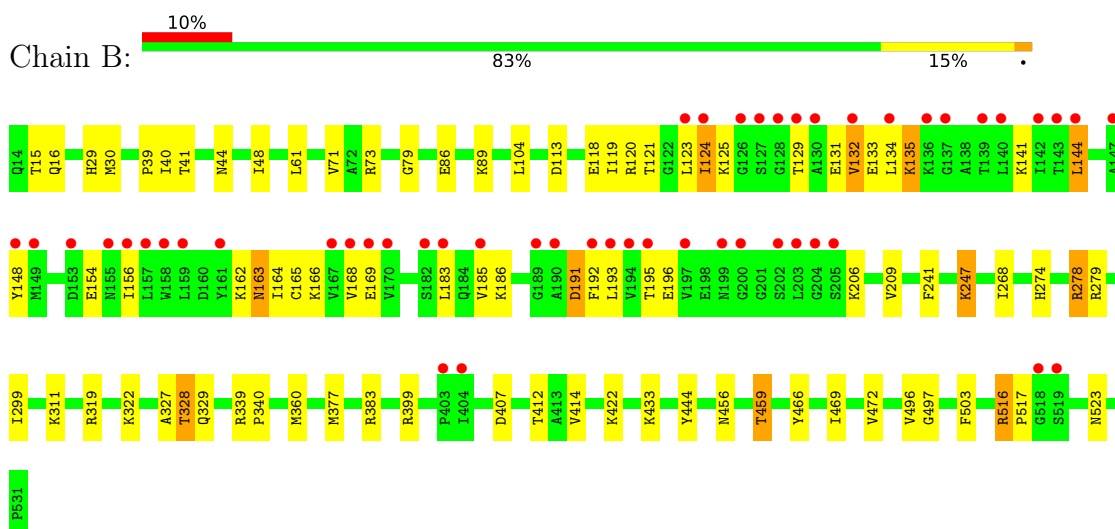
3 Residue-property plots [i](#)

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.

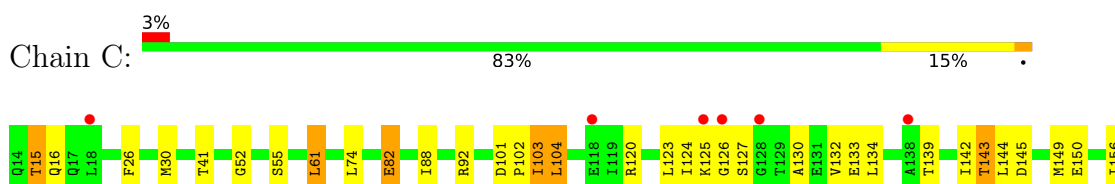
• Molecule 1: Pyruvate kinase isozymes M1/M2

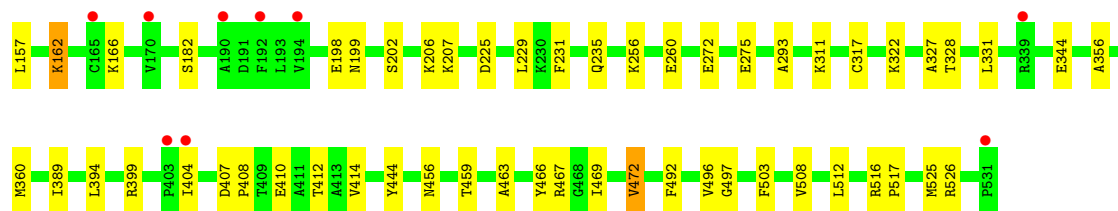


• Molecule 1: Pyruvate kinase isozymes M1/M2

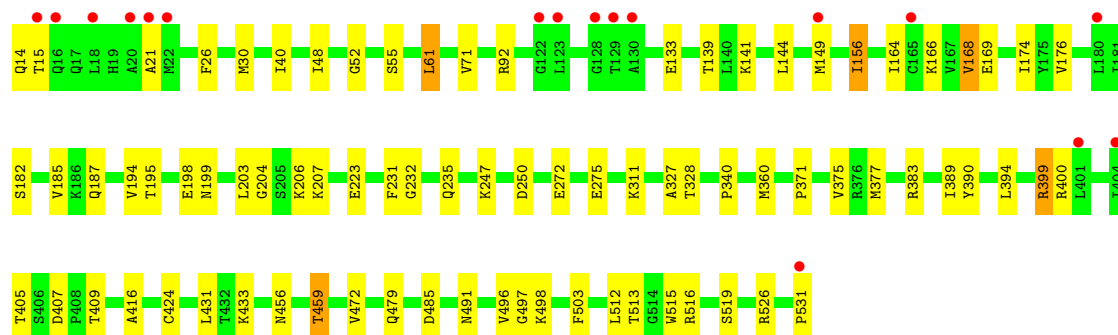
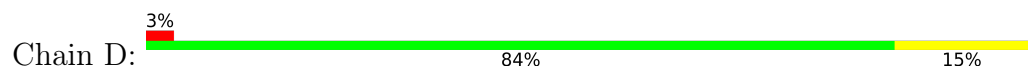


• Molecule 1: Pyruvate kinase isozymes M1/M2





● Molecule 1: Pyruvate kinase isozymes M1/M2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.12Å 94.14Å 146.15Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	40.24 – 2.30 40.24 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.24-2.30) 99.0 (40.24-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.211 , 0.266 (Not available) , 0.280	Depositor DCC
R_{free} test set	5068 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 25.7	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	0.95	EDS
Total number of atoms	16230	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: MG, NZT, OXL

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	0.68	0/4029	0.90	0/5441
1	B	0.70	0/4048	0.94	8/5465 (0.1%)
1	C	0.66	0/4037	0.90	2/5451 (0.0%)
1	D	0.64	0/4029	0.91	4/5441 (0.1%)
All	All	0.67	0/16143	0.91	14/21798 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	LYS	CA-C-N	7.68	127.67	119.76
1	B	322	LYS	C-N-CA	7.68	127.67	119.76
1	B	299	ILE	N-CA-C	-6.53	106.61	111.90
1	B	407	ASP	CA-C-N	6.05	125.77	119.05
1	B	407	ASP	C-N-CA	6.05	125.77	119.05
1	B	193	LEU	N-CA-C	6.00	119.32	108.69
1	B	124	ILE	N-CA-C	5.84	116.41	107.77
1	C	52	GLY	CA-C-N	5.62	125.08	119.24
1	C	52	GLY	C-N-CA	5.62	125.08	119.24
1	D	407	ASP	CA-C-N	5.52	125.17	119.05
1	D	407	ASP	C-N-CA	5.52	125.17	119.05
1	D	52	GLY	CA-C-N	5.28	124.73	119.24
1	D	52	GLY	C-N-CA	5.28	124.73	119.24
1	B	44	ASN	N-CA-C	5.02	117.64	111.82

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	3965	0	4049	34	0
1	B	3978	0	4071	64	0
1	C	3970	0	4058	54	0
1	D	3965	0	4049	45	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	34	0	22	1	0
4	D	68	0	44	14	0
5	A	66	0	0	0	0
5	B	71	0	0	2	0
5	C	48	0	0	2	0
5	D	37	0	0	1	0
All	All	16230	0	16293	188	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 6.

All (188) 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:30[B]:MET:SD	4:D:603[B]:NZT:H17	1.80	1.23
1:D:48:ILE:HB	1:D:360:MET:HG3	1.58	0.84
1:B:516:ARG:HB2	1:B:517:PRO:HD2	1.63	0.78
1:B:73:ARG:NH1	1:B:113:ASP:OD1	2.18	0.77
1:B:414:VAL:HG12	1:B:444:TYR:CE2	2.20	0.77
1:C:55:SER:O	1:C:61:LEU:HD13	1.84	0.76
1:A:414:VAL:HG12	1:A:444:TYR:CE2	2.21	0.75
1:C:327:ALA:HB1	1:C:360:MET:HE2	1.69	0.74
1:C:389:ILE:HD11	1:C:467:ARG:HH21	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:HIS:HD2	1:B:30[B]:MET:HE2	1.55	0.71
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.71	0.71
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.77	0.67
1:B:29:HIS:HD2	1:B:30[B]:MET:CE	2.09	0.65
1:A:15:THR:HG23	1:A:16:GLN:HG2	1.78	0.65
4:D:603[B]:NZT:H10	4:D:603[B]:NZT:OAB	1.96	0.65
1:B:29:HIS:CD2	1:B:30[B]:MET:HE2	2.31	0.64
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.79	0.64
1:D:55:SER:O	1:D:61:LEU:HD13	1.98	0.64
1:D:231:PHE:CE2	1:D:235:GLN:HG3	2.33	0.63
1:C:394:LEU:HD13	4:D:603[A]:NZT:CAG	2.29	0.62
1:B:133:GLU:HG2	1:B:134:LEU:N	2.14	0.62
1:D:390:TYR:HB3	4:D:603[A]:NZT:H1	1.81	0.62
1:C:389:ILE:HD11	1:C:467:ARG:NH2	2.15	0.62
1:B:185:VAL:HA	1:B:195:THR:HG22	1.81	0.62
1:B:48:ILE:HG12	1:B:71:VAL:HB	1.81	0.61
1:A:203:LEU:HD23	1:A:204:GLY:O	2.01	0.61
1:D:185:VAL:HA	1:D:195:THR:HG22	1.83	0.61
1:B:399:ARG:HH21	1:D:399:ARG:NH2	1.98	0.60
1:B:183:LEU:HD13	1:B:195:THR:HG21	1.82	0.60
1:D:141:LYS:HE3	1:D:156:ILE:HD12	1.84	0.60
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.83	0.60
1:B:121:THR:O	1:B:206:LYS:HD3	2.02	0.59
1:C:389:ILE:HG23	4:D:603[B]:NZT:OAC	2.02	0.59
1:C:127:SER:HB2	1:C:130:ALA:HB2	1.84	0.59
1:B:132:VAL:HG13	1:B:133:GLU:N	2.16	0.59
1:A:515:TRP:CE3	1:C:526:ARG:HD3	2.37	0.58
1:C:124:ILE:C	1:C:126:GLY:H	2.12	0.58
1:C:30[A]:MET:HE3	1:D:311:LYS:HB3	1.85	0.58
1:C:82:GLU:HG3	5:C:724:HOH:O	2.03	0.58
1:A:131:GLU:OE1	1:A:202:SER:HB2	2.03	0.57
1:A:146:ASN:O	1:A:149:MET:HB3	2.04	0.57
1:D:231:PHE:CZ	1:D:235:GLN:HG3	2.39	0.57
4:D:603[B]:NZT:H18	4:D:603[B]:NZT:CAM	2.33	0.57
1:B:132:VAL:HG13	1:B:133:GLU:H	1.69	0.57
1:B:133:GLU:O	1:B:154:GLU:HB3	2.04	0.57
4:D:603[B]:NZT:OAB	4:D:603[B]:NZT:CAJ	2.52	0.56
1:D:433:LYS:O	1:D:459:THR:HG21	2.04	0.56
1:C:123:LEU:HD12	1:C:150:GLU:HG2	1.87	0.56
1:D:247:LYS:O	1:D:250:ASP:HB2	2.05	0.56
1:C:143:THR:HG22	1:C:145:ASP:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:VAL:HG21	1:C:496:VAL:HG11	1.87	0.56
1:C:456:ASN:CG	1:C:459:THR:HG23	2.32	0.55
1:B:39:PRO:HB2	1:B:383:ARG:HG2	1.89	0.55
1:B:124:ILE:HD12	1:B:132:VAL:HG12	1.88	0.55
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.43	0.54
1:C:356:ALA:O	1:C:467:ARG:NH1	2.36	0.54
1:C:231:PHE:CE2	1:C:235:GLN:HG3	2.43	0.54
1:B:168:VAL:HG12	1:B:169:GLU:N	2.21	0.54
1:B:399:ARG:HH21	1:D:399:ARG:HH21	1.56	0.54
1:D:479:GLN:HB2	1:D:485:ASP:HB2	1.91	0.53
1:D:174:ILE:CD1	1:D:185:VAL:HG23	2.39	0.53
1:C:389:ILE:CD1	1:C:467:ARG:HH21	2.19	0.53
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.44	0.53
1:A:223:GLU:HA	1:A:226:ILE:HD12	1.90	0.52
1:B:433:LYS:O	1:B:459:THR:HG21	2.09	0.52
1:B:134:LEU:HD13	1:B:154:GLU:HB2	1.91	0.52
1:B:186:LYS:H	1:B:195:THR:HA	1.74	0.52
1:D:431:LEU:HD22	1:D:513:THR:HG22	1.92	0.52
1:A:431:LEU:HD22	1:A:513:THR:HG22	1.90	0.52
1:C:103:ILE:HG22	1:C:104:LEU:HD13	1.90	0.52
1:B:144:LEU:HD22	1:B:191:ASP:HB2	1.92	0.52
1:B:340:PRO:HG3	1:B:377:MET:HG2	1.92	0.52
1:C:311:LYS:HB3	1:D:30:MET:HE3	1.92	0.51
1:D:456:ASN:HB3	1:D:459:THR:HG23	1.91	0.51
1:C:327:ALA:CB	1:C:360:MET:HE2	2.39	0.51
1:B:399:ARG:NH2	1:D:399:ARG:HH21	2.09	0.51
1:C:516:ARG:HB2	1:C:517:PRO:HD2	1.93	0.51
1:A:472:VAL:HG21	1:A:496:VAL:HG11	1.93	0.51
1:C:26:PHE:O	1:C:30[A]:MET:HG2	2.11	0.51
1:B:516:ARG:C	1:B:516:ARG:HD3	2.34	0.50
1:C:225:ASP:O	1:C:229:LEU:HG	2.10	0.50
1:C:410:GLU:O	1:C:414:VAL:HG23	2.11	0.50
1:B:164:ILE:O	1:B:168:VAL:HG23	2.12	0.50
1:A:71:VAL:HG22	1:A:109:ALA:HB3	1.94	0.50
1:A:395:PHE:CZ	1:A:399:ARG:HD2	2.47	0.49
1:A:175:TYR:HB3	1:A:179:GLY:HA2	1.94	0.49
1:C:15:THR:HG23	1:C:16:GLN:HG2	1.92	0.49
1:B:456:ASN:CG	1:B:459:THR:HG23	2.37	0.49
1:C:414:VAL:HG22	1:C:444:TYR:CZ	2.48	0.49
1:A:146:ASN:HB3	1:A:149:MET:HE2	1.95	0.49
1:A:515:TRP:CD2	1:C:526:ARG:HD3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:LEU:CD1	4:D:603[A]:NZT:H23	2.41	0.49
1:D:456:ASN:CG	1:D:459:THR:HG23	2.38	0.49
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.48	0.49
1:D:204:GLY:HA3	1:D:207:LYS:HE2	1.93	0.49
1:C:124:ILE:O	1:C:126:GLY:N	2.45	0.49
1:D:182:SER:HB3	1:D:198:GLU:HB2	1.94	0.48
1:B:40:ILE:O	1:B:383:ARG:HD2	2.12	0.48
1:C:394:LEU:HD13	4:D:603[A]:NZT:H23	1.95	0.48
1:C:414:VAL:HG22	1:C:444:TYR:CE2	2.49	0.48
1:C:182:SER:HB3	1:C:198:GLU:HB2	1.94	0.48
1:C:272:GLU:HB3	1:C:293:ALA:HB3	1.96	0.48
1:C:463:ALA:HB1	1:C:469:ILE:HG21	1.94	0.48
1:B:241:PHE:HD1	1:B:268:ILE:HB	1.79	0.48
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.95	0.48
1:B:168:VAL:CG1	1:B:169:GLU:N	2.77	0.48
1:B:247:LYS:HD2	1:B:279:ARG:NH2	2.28	0.48
1:B:274:HIS:CD2	1:B:278:ARG:HD3	2.49	0.48
1:D:144:LEU:HD21	1:D:164:ILE:HG22	1.95	0.48
4:D:603[A]:NZT:H18	4:D:603[A]:NZT:CAM	2.42	0.48
1:B:123:LEU:HB3	1:B:129:THR:HB	1.95	0.47
1:D:389:ILE:HG23	4:D:603[A]:NZT:OAC	2.14	0.47
1:B:414:VAL:HG12	1:B:444:TYR:CZ	2.49	0.47
1:C:472:VAL:CG1	1:C:492:PHE:CE2	2.97	0.47
1:D:327:ALA:HB1	1:D:360:MET:HE2	1.96	0.47
1:A:389:ILE:HG23	4:A:603[A]:NZT:OAC	2.14	0.47
1:B:422:LYS:HE3	1:D:405:THR:HG22	1.96	0.47
1:A:30:MET:CE	1:B:311:LYS:HB3	2.45	0.47
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.49	0.47
1:B:516:ARG:HB2	1:B:517:PRO:CD	2.40	0.47
1:B:29:HIS:CD2	1:B:30[B]:MET:CE	2.93	0.46
1:B:274:HIS:HD2	1:B:278:ARG:HD3	1.80	0.46
1:A:16:GLN:HG3	1:A:18:LEU:HG	1.98	0.46
1:B:119:ILE:HG22	1:B:209:VAL:HB	1.97	0.46
1:C:162:LYS:H	1:C:162:LYS:CD	2.28	0.46
1:B:164:ILE:HG23	1:B:165:CYS:N	2.30	0.46
1:C:142:ILE:HA	1:C:157:LEU:O	2.16	0.46
1:C:256:LYS:NZ	5:C:715:HOH:O	2.48	0.46
1:D:394:LEU:HD13	4:D:603[B]:NZT:CAG	2.46	0.45
1:A:463:ALA:HB1	1:A:469:ILE:HG21	1.98	0.45
1:B:162:LYS:O	1:B:164:ILE:N	2.42	0.45
1:C:412:THR:HG22	1:C:512:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ILE:O	1:D:383:ARG:HD2	2.17	0.45
1:C:120:ARG:HA	1:C:207:LYS:O	2.17	0.45
1:B:16:GLN:HA	5:B:762:HOH:O	2.16	0.45
1:A:430:VAL:HG22	1:A:512:LEU:HD12	1.99	0.45
1:C:88:ILE:O	1:C:92:ARG:HG3	2.17	0.44
1:C:407:ASP:HA	1:C:408:PRO:HD3	1.88	0.44
1:A:416:ALA:HB2	1:A:512:LEU:HD21	2.00	0.44
1:D:187:GLN:HB3	1:D:194:VAL:HB	1.99	0.43
1:A:317:CYS:HB3	1:A:322:LYS:O	2.18	0.43
1:D:498:LYS:NZ	1:D:531:PRO:O	2.51	0.43
1:B:123:LEU:HB3	1:B:124:ILE:H	1.75	0.43
1:A:162:LYS:HD2	1:A:162:LYS:HA	1.73	0.43
1:A:153:ASP:HB2	1:A:154:GLU:OE1	2.18	0.43
1:B:141:LYS:O	1:B:156:ILE:HA	2.18	0.43
1:B:144:LEU:HD11	1:B:164:ILE:HG21	1.99	0.43
1:A:243:SER:HA	1:A:270:LYS:HD3	2.01	0.43
4:D:603[B]:NZT:CAM	4:D:603[B]:NZT:CAR	2.97	0.42
1:B:134:LEU:HD12	1:B:135:LYS:H	1.84	0.42
1:C:317:CYS:HB3	1:C:322:LYS:O	2.19	0.42
1:A:186:LYS:HD2	1:A:196:GLU:HB2	2.00	0.42
1:B:144:LEU:HD21	1:B:164:ILE:HG22	2.01	0.42
1:A:48:ILE:HG12	1:A:71:VAL:HB	2.01	0.42
1:B:121:THR:O	1:B:206:LYS:HA	2.19	0.42
1:C:166:LYS:HE2	1:C:166:LYS:HB3	1.79	0.42
1:A:30:MET:HE3	1:B:311:LYS:HB3	2.02	0.42
1:A:297:LEU:O	1:A:301:ILE:HG12	2.20	0.42
1:B:328:THR:HG22	1:B:329:GLN:HG3	2.01	0.42
1:D:176:VAL:HG11	1:D:203:LEU:HD11	2.02	0.42
1:D:340:PRO:HG3	1:D:377:MET:HG2	2.02	0.42
1:C:466:TYR:HB2	1:C:469:ILE:HD12	2.02	0.41
1:A:115:LYS:O	1:A:118:GLU:HG3	2.19	0.41
1:B:15:THR:HG23	1:B:16:GLN:HG2	2.02	0.41
1:B:162:LYS:C	1:B:164:ILE:H	2.25	0.41
1:D:515:TRP:CH2	1:D:516:ARG:HD2	2.56	0.41
1:B:327:ALA:HB1	1:B:360:MET:HE2	2.02	0.41
1:B:79:GLY:HA2	5:B:754:HOH:O	2.21	0.41
1:D:371:PRO:O	1:D:375:VAL:HG23	2.21	0.41
1:A:187:GLN:HB2	1:A:194:VAL:HB	2.02	0.41
1:C:101:ASP:HA	1:C:102:PRO:HD2	1.95	0.41
1:D:399:ARG:O	1:D:400:ARG:C	2.64	0.41
1:C:74:LEU:HD11	1:C:88:ILE:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ILE:C	1:C:126:GLY:N	2.78	0.40
1:D:14:GLN:HB3	1:D:15:THR:H	1.60	0.40
1:D:21:ALA:HB1	5:D:711:HOH:O	2.20	0.40
1:B:118:GLU:OE2	1:B:120:ARG:HD2	2.20	0.40
1:B:399:ARG:NH2	1:D:399:ARG:HE	2.18	0.40
1:D:26:PHE:CE2	4:D:603[A]:NZT:H2O	2.56	0.40
1:D:168:VAL:CG1	1:D:169:GLU:N	2.84	0.40
1:A:399:ARG:CZ	1:C:399:ARG:HH21	2.34	0.40
1:D:48:ILE:HG12	1:D:71:VAL:HB	2.03	0.40
1:B:86:GLU:O	1:B:89:LYS:HB3	2.20	0.40
1:A:399:ARG:NH2	1:C:399:ARG:NH2	2.69	0.40
1:B:456:ASN:OD1	1:B:456:ASN:C	2.65	0.40
1:B:523:ASN:O	1:D:526:ARG:HA	2.22	0.40
1:C:331:LEU:HD23	1:C:344:GLU:HB3	2.04	0.40
1:D:231:PHE:O	1:D:232:GLY:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	516/518 (100%)	499 (97%)	15 (3%)	2 (0%)	30	38
1	B	518/518 (100%)	493 (95%)	20 (4%)	5 (1%)	12	15
1	C	517/518 (100%)	497 (96%)	18 (4%)	2 (0%)	30	38
1	D	516/518 (100%)	492 (95%)	22 (4%)	2 (0%)	30	38
All	All	2067/2072 (100%)	1981 (96%)	75 (4%)	11 (0%)	24	31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	163	ASN
1	A	328	THR
1	A	125	LYS
1	B	328	THR
1	C	125	LYS
1	C	328	THR
1	D	328	THR
1	B	125	LYS
1	B	191	ASP
1	D	399	ARG
1	B	132	VAL

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	426/426 (100%)	402 (94%)	24 (6%)	19	28
1	B	428/426 (100%)	410 (96%)	18 (4%)	26	40
1	C	427/426 (100%)	403 (94%)	24 (6%)	19	28
1	D	426/426 (100%)	408 (96%)	18 (4%)	26	40
All	All	1707/1704 (100%)	1623 (95%)	84 (5%)	22	34

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	61	LEU
1	A	82	GLU
1	A	104	LEU
1	A	124	ILE
1	A	129	THR
1	A	132	VAL
1	A	133	GLU
1	A	136	LYS
1	A	156	ILE
1	A	168	VAL

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Mol	Chain	Res	Type
1	A	185	VAL
1	A	187	GLN
1	A	193	LEU
1	A	202	SER
1	A	206	LYS
1	A	221	VAL
1	A	260	GLU
1	A	272	GLU
1	A	409	THR
1	A	414	VAL
1	A	472	VAL
1	A	479	GLN
1	A	516	ARG
1	B	41	THR
1	B	61	LEU
1	B	104	LEU
1	B	131	GLU
1	B	135	LYS
1	B	144	LEU
1	B	148	TYR
1	B	163	ASN
1	B	166	LYS
1	B	192	PHE
1	B	196	GLU
1	B	247	LYS
1	B	278	ARG
1	B	319	ARG
1	B	339	ARG
1	B	412	THR
1	B	459	THR
1	B	516	ARG
1	C	15	THR
1	C	41	THR
1	C	61	LEU
1	C	82	GLU
1	C	103	ILE
1	C	104	LEU
1	C	132	VAL
1	C	133	GLU
1	C	134	LEU
1	C	139	THR
1	C	143	THR

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Mol	Chain	Res	Type
1	C	144	LEU
1	C	149	MET
1	C	156	ILE
1	C	162	LYS
1	C	199	ASN
1	C	202	SER
1	C	206	LYS
1	C	260	GLU
1	C	275	GLU
1	C	404	ILE
1	C	472	VAL
1	C	508	VAL
1	C	525	MET
1	D	61	LEU
1	D	92	ARG
1	D	133	GLU
1	D	139	THR
1	D	149	MET
1	D	156	ILE
1	D	166	LYS
1	D	168	VAL
1	D	199	ASN
1	D	206	LYS
1	D	223	GLU
1	D	272	GLU
1	D	275	GLU
1	D	409	THR
1	D	424	CYS
1	D	459	THR
1	D	491	ASN
1	D	519	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	187	GLN
1	A	235	GLN
1	A	393	GLN
1	A	458	GLN
1	A	479	GLN
1	B	155	ASN

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Mol	Chain	Res	Type
1	B	163	ASN
1	B	378	GLN
1	B	393	GLN
1	B	439	HIS
1	B	458	GLN
1	C	393	GLN
1	C	458	GLN
1	C	491	ASN
1	D	146	ASN
1	D	252	HIS
1	D	391	HIS
1	D	393	GLN
1	D	440	GLN
1	D	458	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OXL	B	601	3	5,5,5	1.88	2 (40%)	6,6,6	1.99	2 (33%)
2	OXL	A	601	3	5,5,5	2.10	1 (20%)	6,6,6	2.39	2 (33%)
4	NZT	D	603[B]	-	38,38,38	3.06	11 (28%)	53,54,54	1.93	12 (22%)
2	OXL	C	601	3	5,5,5	2.39	1 (20%)	6,6,6	1.98	2 (33%)
2	OXL	D	601	3	5,5,5	2.31	1 (20%)	6,6,6	1.90	2 (33%)
4	NZT	D	603[A]	-	38,38,38	2.90	10 (26%)	53,54,54	2.05	11 (20%)
4	NZT	A	603[A]	-	38,38,38	2.81	14 (36%)	53,54,54	2.03	14 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OXL	B	601	3	-	4/4/4/4	-
2	OXL	A	601	3	-	1/4/4/4	-
4	NZT	D	603[B]	-	-	7/23/33/33	0/5/5/5
2	OXL	C	601	3	-	0/4/4/4	-
2	OXL	D	601	3	-	4/4/4/4	-
4	NZT	D	603[A]	-	-	4/23/33/33	0/5/5/5
4	NZT	A	603[A]	-	-	4/23/33/33	0/5/5/5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603[B]	NZT	OAB-S1	8.88	1.53	1.43
4	A	603[A]	NZT	OAB-S1	8.60	1.53	1.43
4	D	603[A]	NZT	OAB-S1	8.13	1.53	1.43
4	D	603[B]	NZT	OAC-S1	8.12	1.52	1.43
4	D	603[A]	NZT	OAC-S1	6.89	1.51	1.43
4	A	603[A]	NZT	CBC-CBE	-6.75	1.38	1.42
4	D	603[B]	NZT	CAZ-NAX	-6.46	1.33	1.43
4	A	603[A]	NZT	OAC-S1	6.45	1.51	1.43
4	D	603[A]	NZT	CBA-CAY	-5.76	1.40	1.50
4	D	603[A]	NZT	CAZ-NAX	-5.68	1.34	1.43
4	D	603[B]	NZT	CBA-CAY	-5.55	1.40	1.50
4	D	603[A]	NZT	CBC-CBE	-5.49	1.39	1.42
4	D	603[A]	NZT	CBC-S1	-5.20	1.72	1.77
4	D	603[A]	NZT	CAF-NAW	5.17	1.42	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603[B]	NZT	CBC-S1	-4.97	1.72	1.77
4	A	603[A]	NZT	CAZ-NAX	-4.75	1.36	1.43
4	D	603[B]	NZT	S1-NAX	-4.72	1.56	1.63
4	D	603[B]	NZT	CBC-CBE	-4.55	1.39	1.42
4	D	603[B]	NZT	CAF-NAW	4.52	1.41	1.32
4	A	603[A]	NZT	CAF-NAW	4.35	1.40	1.32
4	A	603[A]	NZT	CBA-CAY	-4.24	1.42	1.50
2	C	601	OXL	C2-C1	-4.22	1.47	1.54
2	D	601	OXL	C2-C1	-3.98	1.47	1.54
4	A	603[A]	NZT	CAP-NAU	3.60	1.41	1.34
2	A	601	OXL	C2-C1	-3.58	1.48	1.54
4	D	603[A]	NZT	CAH-NAV	3.10	1.41	1.34
4	D	603[B]	NZT	CAP-NAU	2.99	1.40	1.34
4	D	603[B]	NZT	CAH-NAV	2.97	1.40	1.34
4	A	603[A]	NZT	CAR-NBF	2.85	1.52	1.47
4	D	603[A]	NZT	CAP-NAU	2.81	1.40	1.34
2	B	601	OXL	C2-C1	-2.76	1.49	1.54
4	D	603[A]	NZT	CAG-NAU	2.65	1.41	1.33
4	D	603[B]	NZT	CAG-NAU	2.63	1.41	1.33
4	A	603[A]	NZT	CAH-NAV	2.46	1.39	1.34
4	A	603[A]	NZT	CBE-NAW	-2.37	1.33	1.37
4	A	603[A]	NZT	CAS-NBG	2.33	1.50	1.46
4	A	603[A]	NZT	CAG-NAU	2.33	1.40	1.33
4	A	603[A]	NZT	S1-NAX	2.28	1.67	1.63
4	A	603[A]	NZT	CAQ-NBF	2.02	1.50	1.47
2	B	601	OXL	O2-C2	2.01	1.27	1.22

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	603[A]	NZT	OAC-S1-OAB	-8.84	108.78	119.52
4	A	603[A]	NZT	OAC-S1-OAB	-7.71	110.15	119.52
4	D	603[B]	NZT	OAC-S1-OAB	-7.15	110.84	119.52
4	A	603[A]	NZT	CBC-CBE-CBD	4.85	120.36	117.70
4	D	603[A]	NZT	CAT-NBG-CAS	4.71	122.17	111.57
4	D	603[B]	NZT	CAT-NBG-CAS	4.56	121.82	111.57
4	D	603[B]	NZT	CBC-CBE-CBD	4.53	120.19	117.70
2	A	601	OXL	O3-C1-C2	4.27	121.12	112.83
4	D	603[A]	NZT	CAI-CBC-S1	4.11	121.70	116.92
2	C	601	OXL	O4-C2-C1	3.95	120.50	112.83
2	D	601	OXL	O4-C2-C1	3.62	119.86	112.83
4	D	603[B]	NZT	CAI-CBC-S1	3.62	121.14	116.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603[A]	NZT	CAR-NBF-CAQ	3.55	119.92	112.68
4	A	603[A]	NZT	CBC-S1-NAX	3.49	112.84	107.33
4	D	603[A]	NZT	CBC-CBE-CBD	3.37	119.55	117.70
2	A	601	OXL	O4-C2-C1	3.30	119.22	112.83
2	B	601	OXL	O3-C1-C2	3.28	119.19	112.83
4	A	603[A]	NZT	CAI-CBC-S1	3.23	120.68	116.92
4	A	603[A]	NZT	CAH-NAV-CBB	3.14	121.37	116.81
4	D	603[A]	NZT	CAH-NAV-CBB	3.08	121.28	116.81
4	A	603[A]	NZT	CAT-CAR-NBF	3.06	116.50	110.42
4	D	603[B]	NZT	CAH-NAV-CBB	2.95	121.09	116.81
2	B	601	OXL	O4-C2-C1	2.90	118.46	112.83
4	D	603[B]	NZT	CAF-NAW-CBE	2.87	120.70	117.31
4	D	603[A]	NZT	CAG-CAH-NAV	-2.87	118.15	122.19
4	D	603[A]	NZT	CAD-CAF-NAW	-2.76	119.92	123.97
4	A	603[A]	NZT	CAI-CBC-CBE	-2.57	119.08	121.07
4	D	603[B]	NZT	OAB-S1-CBC	2.55	112.54	108.09
4	A	603[A]	NZT	CAT-NBG-CAS	2.53	117.27	111.57
4	D	603[A]	NZT	CAF-NAW-CBE	2.51	120.27	117.31
4	A	603[A]	NZT	CBA-CAY-NBF	2.50	121.78	118.66
4	D	603[B]	NZT	CAD-CAF-NAW	-2.49	120.31	123.97
2	D	601	OXL	O3-C1-C2	2.38	117.44	112.83
4	A	603[A]	NZT	CBC-CBE-NAW	-2.37	118.64	119.54
4	D	603[A]	NZT	CBE-CBC-S1	-2.35	118.13	120.70
4	D	603[B]	NZT	CBD-CBE-NAW	-2.32	120.18	122.63
4	A	603[A]	NZT	CAG-CAH-NAV	-2.31	118.93	122.19
2	C	601	OXL	O3-C1-C2	2.24	117.17	112.83
4	D	603[A]	NZT	CBC-S1-NAX	2.21	110.82	107.33
4	D	603[B]	NZT	CAR-NBF-CAQ	2.20	117.17	112.68
4	D	603[B]	NZT	CAG-CAH-NAV	-2.19	119.10	122.19
4	A	603[A]	NZT	CAT-NBG-CBB	2.17	126.18	120.41
4	D	603[B]	NZT	CBE-CBC-S1	-2.05	118.45	120.70
4	A	603[A]	NZT	CAD-CAF-NAW	-2.03	120.98	123.97
4	D	603[A]	NZT	OAB-S1-CBC	2.01	111.59	108.09

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603[A]	NZT	CAP-CBB-NBG-CAS
4	A	603[A]	NZT	CAP-CBB-NBG-CAT
4	D	603[A]	NZT	NAV-CBB-NBG-CAS
4	D	603[A]	NZT	CAP-CBB-NBG-CAS

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Mol	Chain	Res	Type	Atoms
4	D	603[A]	NZT	NAV-CBB-NBG-CAT
4	D	603[A]	NZT	CAP-CBB-NBG-CAT
4	D	603[B]	NZT	CAP-CBB-NBG-CAS
4	D	603[B]	NZT	NAV-CBB-NBG-CAT
4	D	603[B]	NZT	CAP-CBB-NBG-CAT
4	A	603[A]	NZT	NAV-CBB-NBG-CAS
2	B	601	OXL	O1-C1-C2-O2
2	B	601	OXL	O3-C1-C2-O4
4	D	603[B]	NZT	NAV-CBB-NBG-CAS
2	B	601	OXL	O1-C1-C2-O4
2	B	601	OXL	O3-C1-C2-O2
4	D	603[B]	NZT	CAZ-NAX-S1-OAC
4	A	603[A]	NZT	NAV-CBB-NBG-CAT
2	D	601	OXL	O3-C1-C2-O4
2	D	601	OXL	O1-C1-C2-O2
4	D	603[B]	NZT	CAZ-NAX-S1-CBC
4	D	603[B]	NZT	CAZ-NAX-S1-OAB
2	D	601	OXL	O3-C1-C2-O2
2	D	601	OXL	O1-C1-C2-O4
2	A	601	OXL	O1-C1-C2-O2

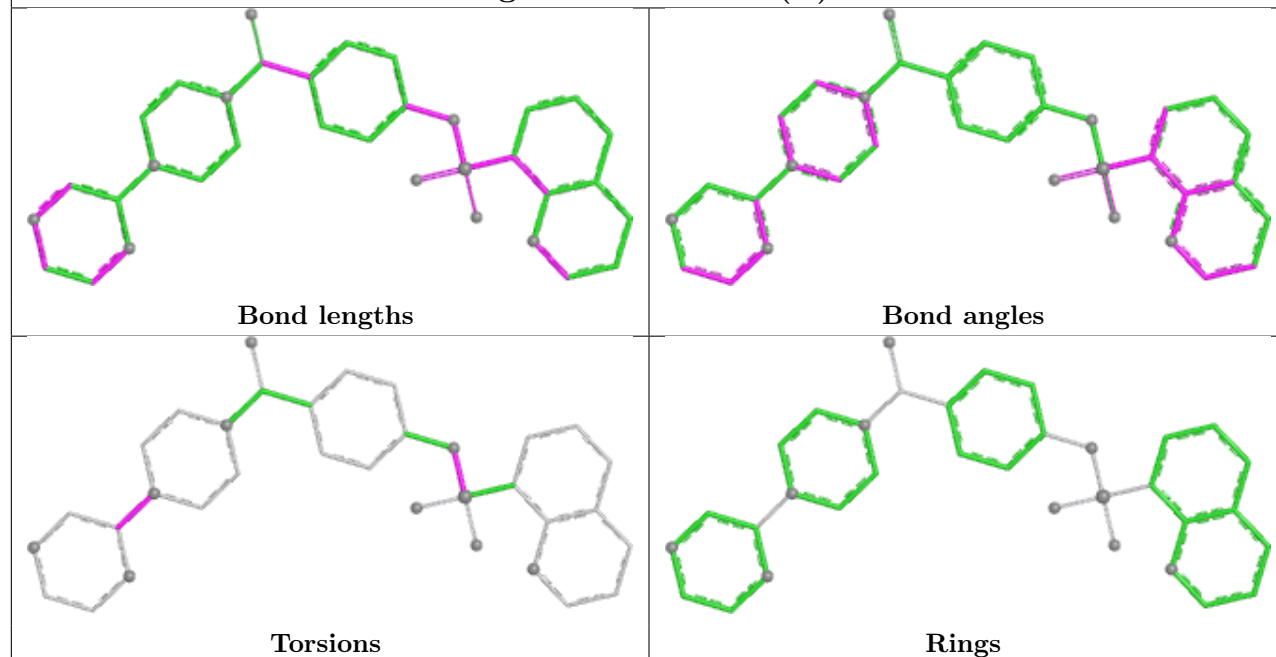
There are no ring outliers.

3 monomers are involved in 15 short contacts:

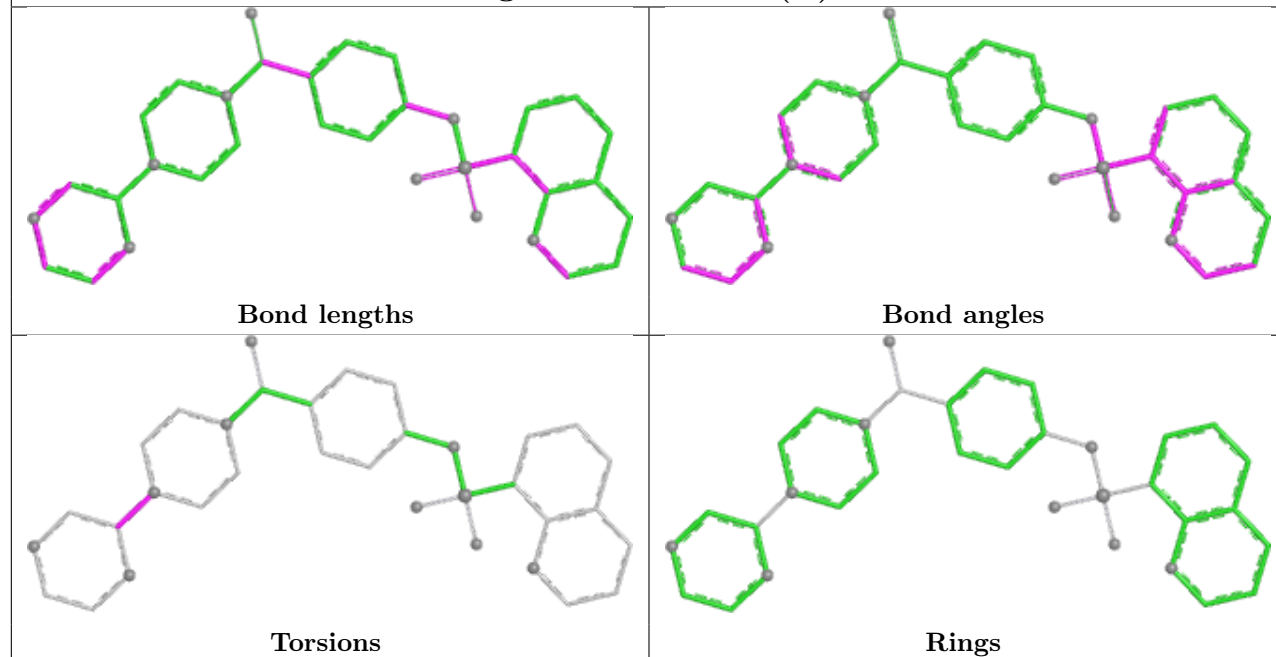
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	603[B]	NZT	7	0
4	D	603[A]	NZT	7	0
4	A	603[A]	NZT	1	0

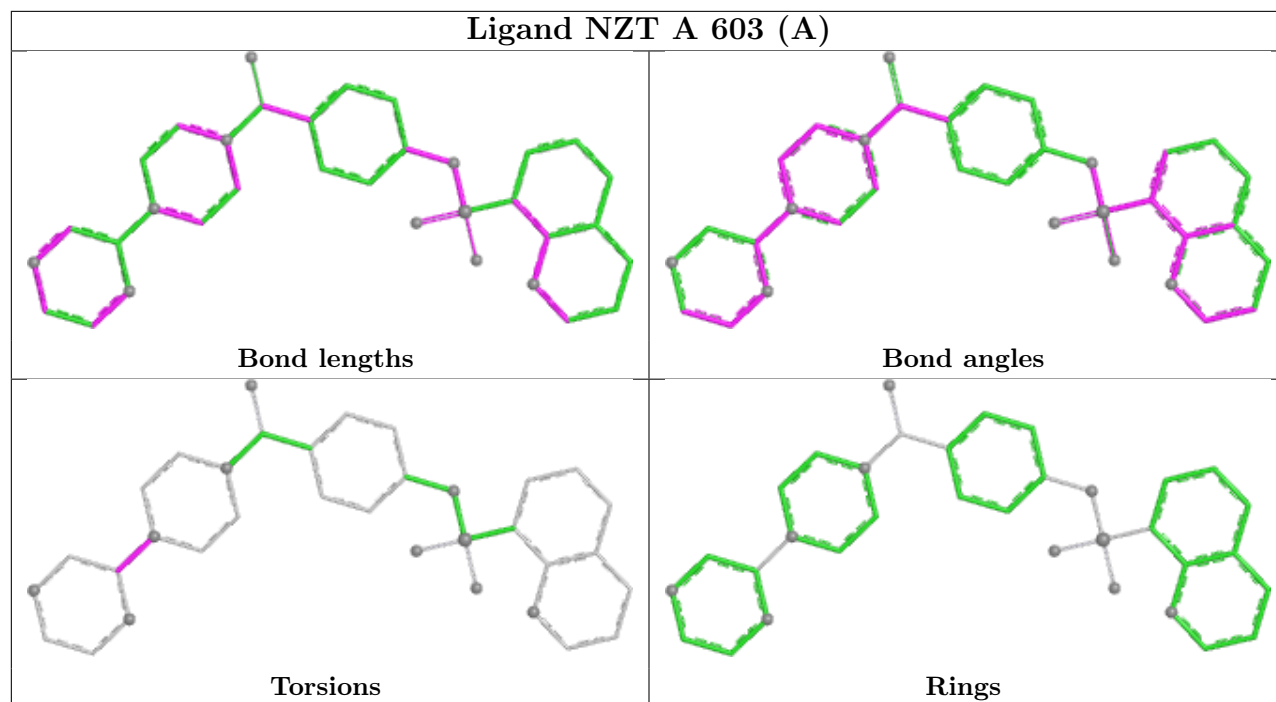
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 NZT D 603 (B)



Ligand NZT D 603 (A)





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	518/518 (100%)	0.14	14 (2%) 56 58	23, 41, 72, 114	0
1	B	518/518 (100%)	0.38	50 (9%) 13 15	18, 39, 122, 177	2 (0%)
1	C	518/518 (100%)	0.27	15 (2%) 53 56	21, 43, 77, 122	1 (0%)
1	D	518/518 (100%)	0.35	17 (3%) 49 51	27, 45, 78, 124	0
All	All	2072/2072 (100%)	0.29	96 (4%) 37 39	18, 42, 89, 177	3 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	157	LEU	7.0
1	B	170	VAL	5.6
1	B	156	ILE	5.4
1	B	140	LEU	5.3
1	B	132	VAL	4.9
1	C	404	ILE	4.9
1	B	129	THR	4.6
1	B	134	LEU	4.3
1	C	403	PRO	4.1
1	B	143	THR	4.1
1	B	153	ASP	4.1
1	B	194	VAL	3.9
1	B	159	LEU	3.7
1	B	168	VAL	3.7
1	B	192	PHE	3.7
1	B	204	GLY	3.6
1	B	123	LEU	3.6
1	C	126	GLY	3.6
1	B	202	SER	3.6
1	B	148	TYR	3.6
1	B	142	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	199	ASN	3.6
1	B	158	TRP	3.6
1	B	147	ALA	3.5
1	B	195	THR	3.5
1	D	20	ALA	3.4
1	A	156	ILE	3.4
1	D	130	ALA	3.4
1	B	144	LEU	3.3
1	A	515	TRP	3.3
1	A	126	GLY	3.2
1	B	130	ALA	3.2
1	A	22	MET	3.2
1	D	18	LEU	3.1
1	D	128	GLY	3.1
1	B	190	ALA	3.0
1	B	183	LEU	3.0
1	D	21	ALA	2.9
1	B	155	ASN	2.9
1	A	129	THR	2.9
1	B	404	ILE	2.9
1	B	197	VAL	2.8
1	C	194	VAL	2.8
1	B	149	MET	2.8
1	D	180	LEU	2.8
1	A	138	ALA	2.8
1	B	203	LEU	2.8
1	B	185	VAL	2.8
1	B	169	GLU	2.7
1	B	167	VAL	2.7
1	B	403	PRO	2.7
1	B	205	SER	2.7
1	D	129	THR	2.6
1	D	15	THR	2.6
1	B	128	GLY	2.6
1	D	149	MET	2.6
1	C	531	PRO	2.6
1	B	137	GLY	2.6
1	B	200	GLY	2.6
1	A	127	SER	2.6
1	A	520	GLY	2.5
1	D	22	MET	2.5
1	A	15	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	125	LYS	2.5
1	C	128	GLY	2.5
1	B	193	LEU	2.4
1	B	124	ILE	2.4
1	C	190	ALA	2.4
1	C	192	PHE	2.4
1	A	123	LEU	2.4
1	D	16	GLN	2.4
1	D	401	LEU	2.3
1	B	189	GLY	2.3
1	B	139	THR	2.3
1	D	404	ILE	2.3
1	A	170	VAL	2.3
1	B	136	LYS	2.3
1	A	128	GLY	2.3
1	A	481	ALA	2.3
1	C	138	ALA	2.3
1	B	127	SER	2.3
1	B	161	TYR	2.2
1	B	182	SER	2.2
1	D	123	LEU	2.2
1	D	122	GLY	2.1
1	C	165	CYS	2.1
1	C	118	GLU	2.1
1	B	126	GLY	2.1
1	B	518	GLY	2.1
1	D	165	CYS	2.1
1	C	170	VAL	2.1
1	D	531	PRO	2.1
1	C	18	LEU	2.1
1	B	519	SER	2.0
1	A	130	ALA	2.0
1	C	339	ARG	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

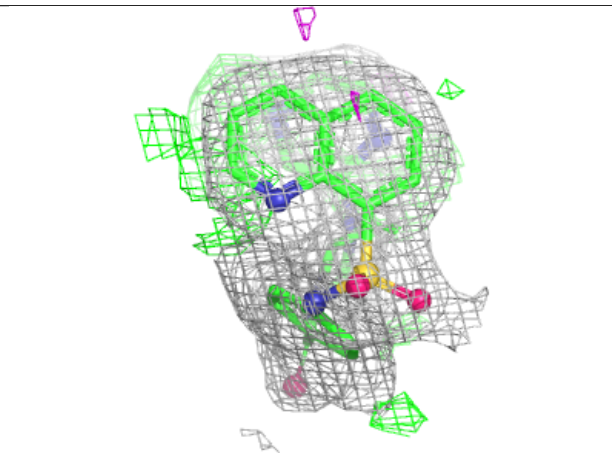
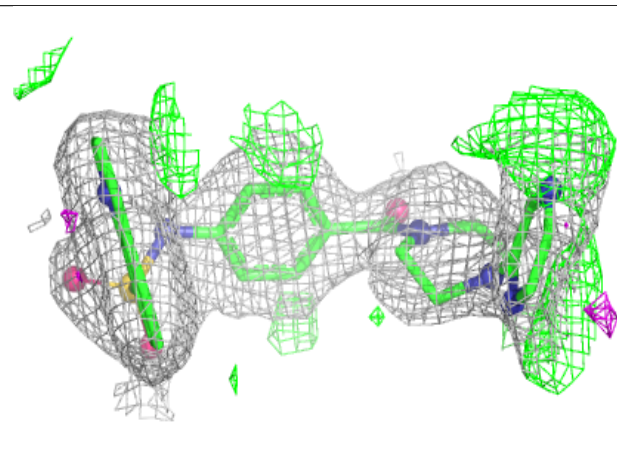
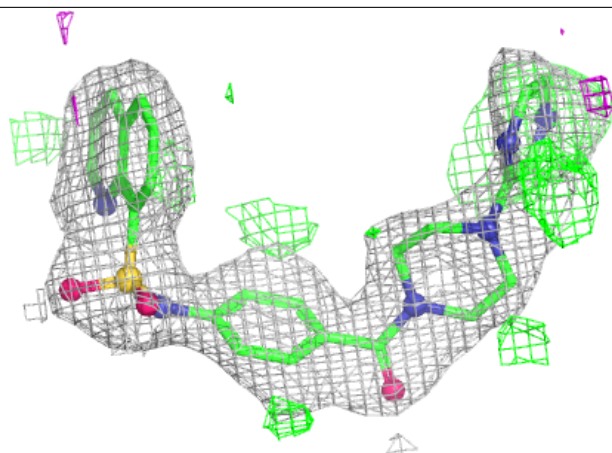
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NZT	A	603[A]	34/34	0.84	0.14	34,42,57,60	0
2	OXL	D	601	6/6	0.85	0.15	45,49,52,54	0
2	OXL	A	601	6/6	0.88	0.13	50,56,61,64	0
4	NZT	D	603[A]	34/34	0.88	0.17	31,34,47,48	34
4	NZT	D	603[B]	34/34	0.88	0.17	33,36,47,48	34
2	OXL	B	601	6/6	0.90	0.13	39,44,49,49	0
3	MG	C	602	1/1	0.93	0.05	50,50,50,50	0
2	OXL	C	601	6/6	0.94	0.12	45,47,48,49	0
3	MG	D	602	1/1	0.98	0.04	45,45,45,45	0
3	MG	B	602	1/1	0.99	0.02	39,39,39,39	0
3	MG	A	602	1/1	0.99	0.03	47,47,47,47	0

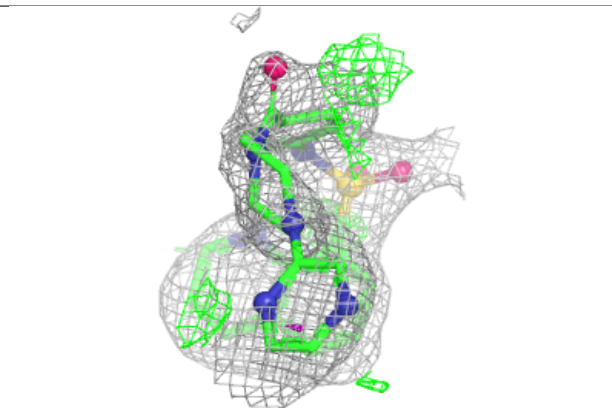
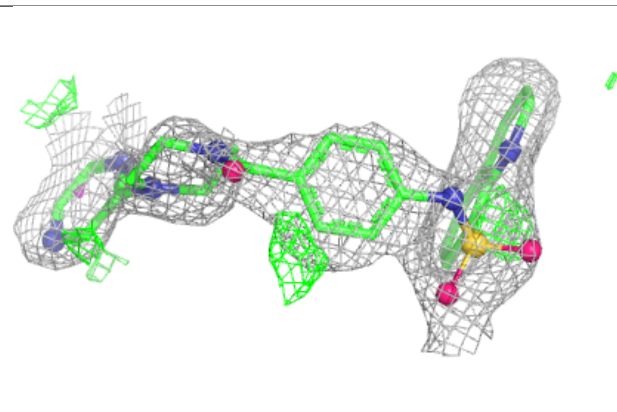
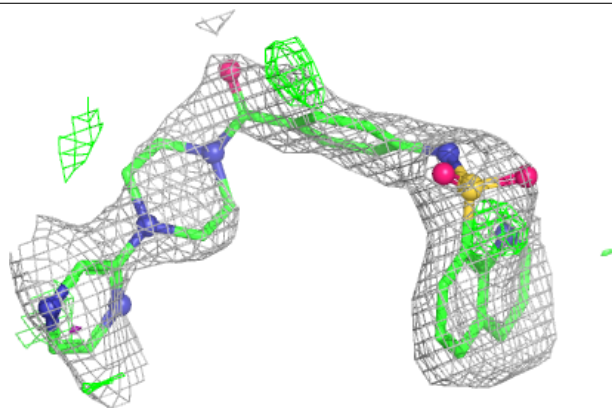
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NZT A 603 (A):

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

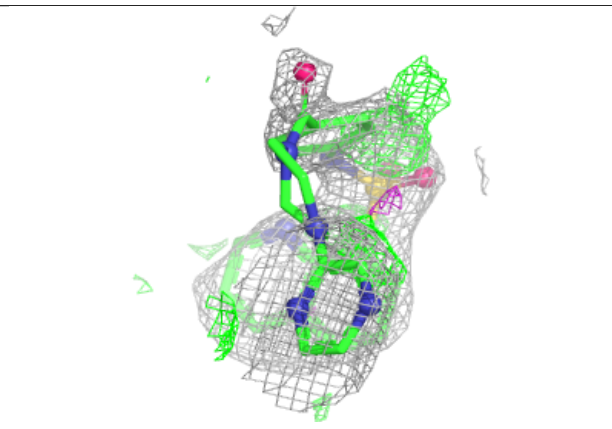
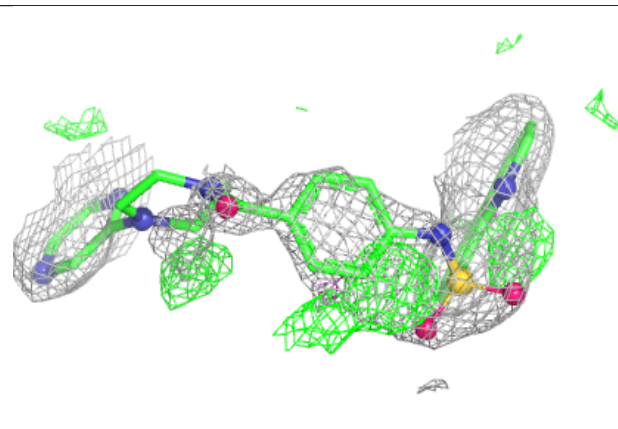
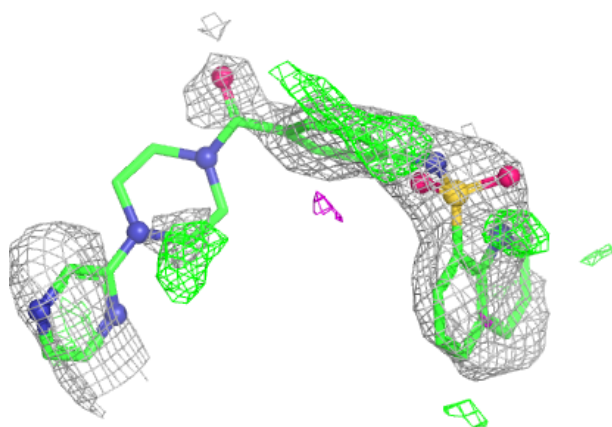
**Electron density around NZT D 603 (A):**

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



Electron density around NZT D 603 (B):

$2mF_o-DF_c$ (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.