



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:47 AM UTC

PDB ID : 8TC9 / pdb_00008tc9
Title : Human asparaginyl-tRNA synthetase bound to OSM-S-106
Authors : Dogovski, C.; Metcalfe, R.D.; Xie, S.C.; Morton, C.J.; Tilley, L.; Griffin, M.D.W.
Deposited on : 2023-06-30
Resolution : 2.00 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

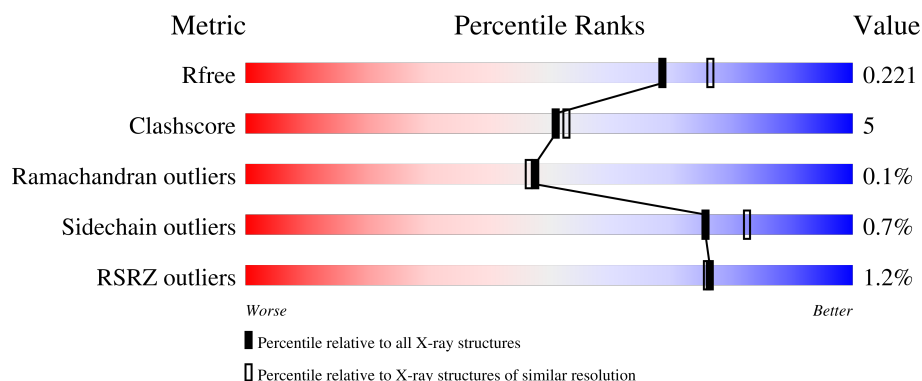
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	548	% 71% 8% 21%
1	B	548	% 68% 11% 21%
1	C	548	% 72% 7% 21%
1	D	548	% 70% 9% 21%

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
3	GOL	D	604	-	-	X	-

2 Entry composition [i](#)

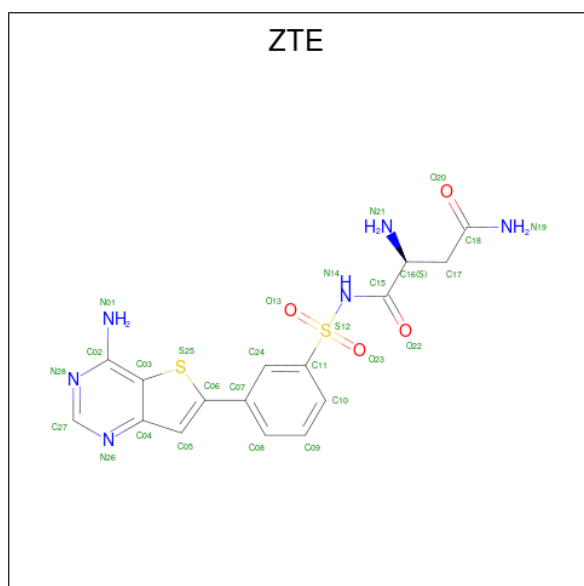
There are 4 unique types of molecules in this entry. The entry contains 15513 atoms, of which 60 are hydrogens and 0 are deuteriums.

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 Asparagine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	1	0
			3514	2234	606	648	26			
1	B	434	Total	C	N	O	S	0	1	0
			3518	2238	606	648	26			
1	C	433	Total	C	N	O	S	0	2	0
			3520	2238	608	648	26			
1	D	434	Total	C	N	O	S	0	2	0
			3524	2240	609	649	26			

- Molecule 2 is N 1 -[(3M)-3-(4-aminothieno[3,2-d]pyrimidin-6-yl)benzene-1-sulfonyl]-L-aspartamide (CCD ID: ZTE) (formula: C₁₆H₁₆N₆O₄S₂) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	S	
			43	16	15	6	4	2	0
2	C	1	Total	C	H	N	O	S	
			43	16	15	6	4	2	0
2	D	1	Total	C	H	N	O	S	
			43	16	15	6	4	2	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

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

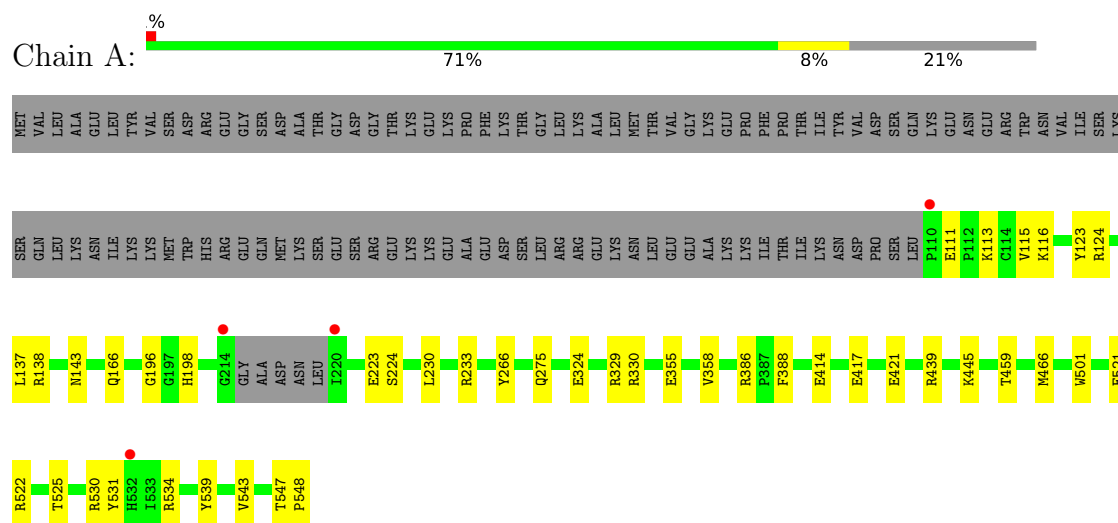
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	295	Total	O	0	0
			295	295		
4	B	310	Total	O	0	0
			310	310		
4	C	178	Total	O	0	0
			178	178		
4	D	248	Total	O	0	0
			248	248		

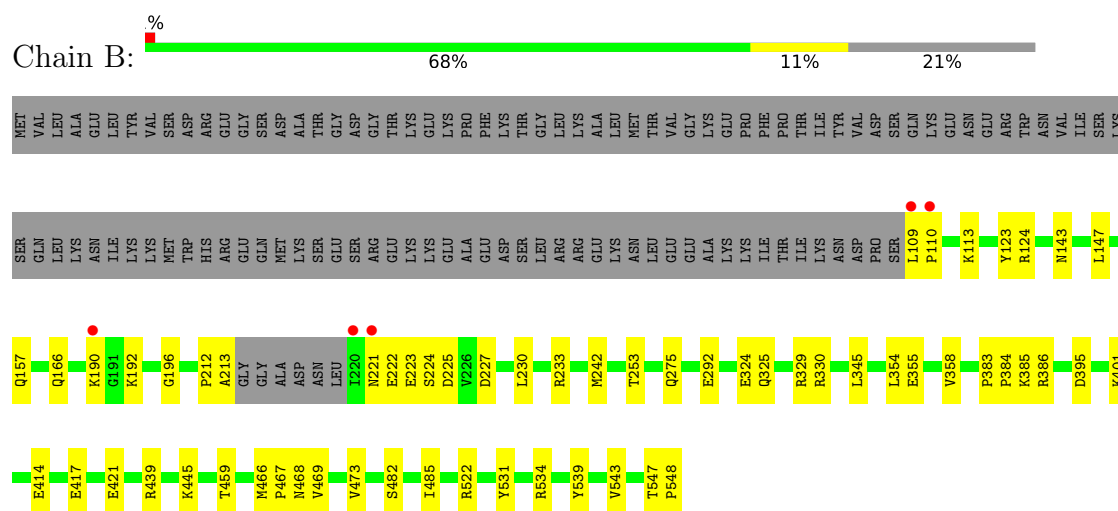
3 Residue-property plots [i](#)

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: Asparagine-tRNA ligase, cytoplasmic

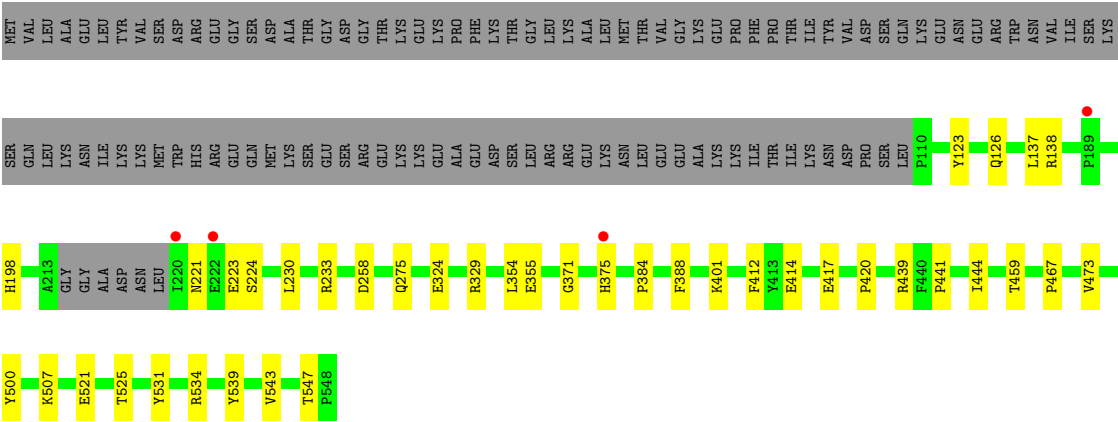


- Molecule 1: Asparagine-tRNA ligase, cytoplasmic

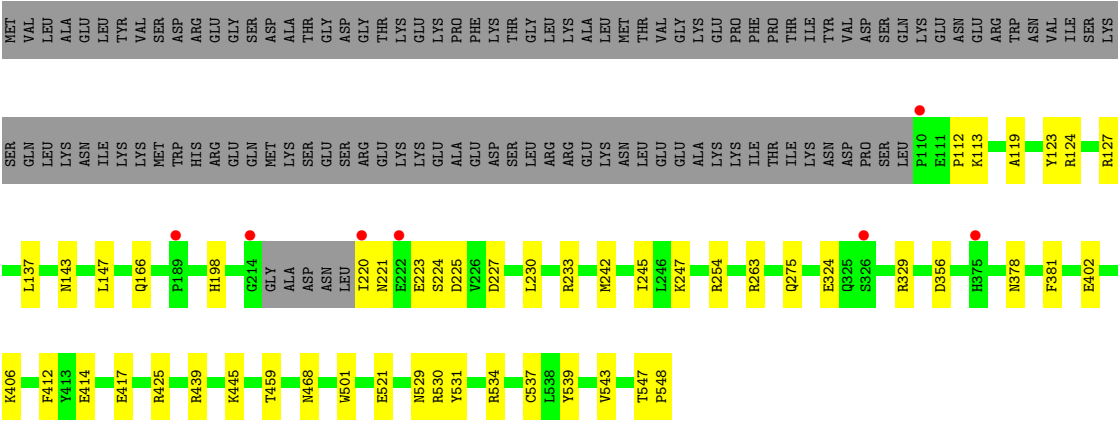


- Molecule 1: Asparagine-tRNA ligase, cytoplasmic





• Molecule 1: Asparagine–tRNA ligase, cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.09Å 126.81Å 161.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.46 – 2.00 49.46 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.46-2.00) 99.8 (49.46-2.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.182 , 0.221 0.182 , 0.221	Depositor DCC
R_{free} test set	7965 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtrriage
Anisotropy	0.492	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15513	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.31 % 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 1.0107e-04. 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.29	0/3600	0.49	0/4871
1	B	0.30	0/3604	0.50	0/4878
1	C	0.25	0/3607	0.45	0/4881
1	D	0.28	0/3611	0.47	0/4886
All	All	0.28	0/14422	0.48	0/19516

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3514	0	3436	32	0
1	B	3518	0	3443	45	0
1	C	3520	0	3439	28	0
1	D	3524	0	3442	43	0
2	A	28	15	0	1	0
2	B	28	15	0	0	0
2	C	28	15	0	0	0
2	D	28	15	0	0	0
3	A	48	0	64	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	72	0	95	6	0
3	C	48	0	64	6	0
3	D	66	0	86	9	0
4	A	295	0	0	6	0
4	B	310	0	0	11	0
4	C	178	0	0	8	0
4	D	248	0	0	10	0
All	All	15453	60	14069	148	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 (148) 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:358:VAL:HG11	1:B:466:MET:HE3	1.50	0.92
1:D:529:ASN:OD1	3:D:604:GOL:H12	1.77	0.85
1:B:522:ARG:HH12	3:B:611:GOL:H32	1.43	0.83
1:B:230:LEU:HD21	1:B:534:ARG:HD2	1.62	0.80
1:A:522:ARG:HH22	3:A:609:GOL:H32	1.48	0.79
1:B:395:ASP:OD2	4:B:701:HOH:O	2.01	0.77
1:A:143:ASN:OD1	1:A:166:GLN:NE2	2.17	0.76
4:B:784:HOH:O	3:C:606:GOL:H2	1.85	0.76
4:B:866:HOH:O	3:C:607:GOL:H12	1.87	0.75
1:B:358:VAL:HG11	1:B:466:MET:CE	2.16	0.73
1:D:242:MET:SD	4:D:808:HOH:O	2.49	0.70
1:B:522:ARG:NH1	3:B:611:GOL:H32	2.07	0.70
1:B:547:THR:HG23	1:C:275:GLN:OE1	1.92	0.70
1:D:521:GLU:OE2	3:D:607:GOL:H12	1.92	0.70
1:A:329:ARG:HH21	3:A:604:GOL:H32	1.55	0.69
1:A:358:VAL:HG11	1:A:466:MET:HE3	1.75	0.69
1:D:402:GLU:OE2	4:D:701:HOH:O	2.11	0.69
1:B:221:ASN:C	1:B:223:GLU:H	2.00	0.69
1:C:221:ASN:C	1:C:223:GLU:H	2.01	0.68
1:B:222:GLU:OE2	4:B:702:HOH:O	2.11	0.66
1:B:329:ARG:HD2	1:B:531:TYR:CZ	2.29	0.66
1:D:468:ASN:O	3:D:604:GOL:H2	1.95	0.66
1:A:230:LEU:HD21	1:A:534:ARG:HD2	1.76	0.66
1:B:414:GLU:O	1:B:417:GLU:HG2	1.96	0.66
1:D:221:ASN:C	1:D:223:GLU:H	2.03	0.66
1:A:522:ARG:HH12	3:A:609:GOL:H11	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ARG:NH2	4:A:704:HOH:O	2.28	0.64
1:D:220:ILE:HG23	4:D:929:HOH:O	1.97	0.64
1:D:324:GLU:O	1:D:543:VAL:HG22	1.98	0.64
4:B:908:HOH:O	1:C:547:THR:HG22	1.98	0.62
1:B:324:GLU:O	1:B:543:VAL:HG22	2.00	0.62
1:B:242:MET:HG3	4:B:829:HOH:O	1.98	0.62
1:A:414:GLU:O	1:A:417:GLU:HG2	1.99	0.61
1:D:414:GLU:O	1:D:417:GLU:HG2	1.99	0.61
1:B:275:GLN:OE1	1:C:547:THR:HG23	2.00	0.61
1:C:324:GLU:O	1:C:543:VAL:HG22	2.00	0.61
1:B:330:ARG:CZ	1:B:421:GLU:HG3	2.31	0.61
1:D:529:ASN:HA	3:D:604:GOL:H11	1.82	0.60
1:A:324:GLU:O	1:A:543:VAL:HG22	2.01	0.60
1:B:109:LEU:N	1:B:110:PRO:HD2	2.17	0.60
1:D:113:LYS:HE3	4:D:755:HOH:O	2.01	0.60
1:D:537:CYS:HB3	3:D:607:GOL:O2	2.01	0.59
1:D:329:ARG:HD2	1:D:531:TYR:CZ	2.36	0.59
1:D:127:ARG:HH12	3:D:605:GOL:H12	1.66	0.59
1:B:385:LYS:HG2	4:B:733:HOH:O	2.01	0.59
1:A:358:VAL:HG11	1:A:466:MET:CE	2.33	0.59
1:B:522:ARG:HH12	3:B:611:GOL:C3	2.17	0.58
1:B:253:THR:HB	4:B:835:HOH:O	2.04	0.57
1:A:113:LYS:HD3	1:A:123:TYR:HE2	1.70	0.57
1:C:467:PRO:O	4:C:701:HOH:O	2.17	0.57
1:A:329:ARG:NH2	3:A:604:GOL:H32	2.19	0.57
1:C:500:TYR:CE2	3:C:601:GOL:H12	2.39	0.57
1:A:329:ARG:HD2	1:A:531:TYR:CZ	2.39	0.56
3:A:608:GOL:H32	4:A:716:HOH:O	2.06	0.56
1:B:292:GLU:HG2	4:B:844:HOH:O	2.05	0.56
1:D:529:ASN:HA	3:D:604:GOL:C1	2.36	0.55
1:A:330:ARG:NH1	1:A:421:GLU:HG3	2.21	0.55
1:A:275:GLN:OE1	1:D:547:THR:HG23	2.06	0.54
1:B:325:GLN:NE2	4:B:707:HOH:O	2.37	0.54
3:C:603:GOL:H31	4:C:740:HOH:O	2.07	0.54
1:B:225:ASP:OD2	1:B:227:ASP:HB2	2.07	0.54
1:B:190:LYS:HE2	1:D:119:ALA:HB2	1.90	0.53
1:B:221:ASN:C	1:B:223:GLU:N	2.67	0.53
1:D:242:MET:HG3	4:D:808:HOH:O	2.08	0.53
1:C:221:ASN:HB2	1:C:224:SER:HB2	1.90	0.52
1:B:233:ARG:HG3	1:B:539:TYR:CE1	2.44	0.52
1:A:530:ARG:O	3:A:604:GOL:H31	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ARG:HD3	4:A:904:HOH:O	2.10	0.51
1:C:414:GLU:O	1:C:417:GLU:HG2	2.11	0.51
1:D:143:ASN:OD1	1:D:166:GLN:NE2	2.40	0.51
1:C:137:LEU:C	1:C:137:LEU:HD23	2.36	0.51
1:B:213:ALA:HB2	3:B:602:GOL:H2	1.91	0.50
1:D:378:ASN:ND2	1:D:381:PHE:HB2	2.25	0.50
1:D:230:LEU:HD21	1:D:534:ARG:HD2	1.94	0.50
1:A:115:VAL:HG12	1:A:116:LYS:O	2.12	0.50
1:A:547:THR:HG23	1:D:275:GLN:OE1	2.12	0.49
1:B:113:LYS:HD3	1:B:123:TYR:HE2	1.77	0.49
1:C:355:GLU:CD	1:C:388:PHE:H	2.20	0.49
1:B:157:GLN:OE1	1:B:192:LYS:HE2	2.13	0.48
1:C:329:ARG:HD2	1:C:531:TYR:CZ	2.48	0.48
1:B:143:ASN:OD1	1:B:166:GLN:NE2	2.39	0.48
1:C:230:LEU:HD21	1:C:534:ARG:HD2	1.95	0.47
3:C:607:GOL:H11	4:C:743:HOH:O	2.14	0.47
1:D:137:LEU:C	1:D:137:LEU:HD23	2.39	0.47
1:D:225:ASP:OD2	1:D:227:ASP:HB2	2.14	0.47
1:B:439:ARG:HA	1:B:459:THR:O	2.15	0.47
1:B:482:SER:O	1:B:485:ILE:HG22	2.14	0.47
1:D:242:MET:CG	4:D:808:HOH:O	2.62	0.47
1:B:345:LEU:H	1:B:345:LEU:HD23	1.80	0.47
1:B:213:ALA:N	3:B:602:GOL:O1	2.44	0.46
4:A:878:HOH:O	1:D:547:THR:HG22	2.15	0.46
1:B:547:THR:HA	1:B:548:PRO:C	2.40	0.46
1:C:384:PRO:O	4:C:702:HOH:O	2.20	0.46
1:A:116:LYS:HE2	4:A:945:HOH:O	2.16	0.46
1:B:401:LYS:NZ	4:B:714:HOH:O	2.45	0.46
1:B:124:ARG:NH2	1:B:196:GLY:O	2.49	0.46
1:A:233:ARG:HG3	1:A:539:TYR:CE1	2.51	0.46
1:C:233:ARG:HG3	1:C:539:TYR:CE1	2.51	0.45
1:D:112:PRO:HD2	4:D:930:HOH:O	2.16	0.45
1:D:439:ARG:HA	1:D:459:THR:O	2.17	0.45
1:D:406:LYS:HG2	1:D:412:PHE:CD1	2.51	0.45
1:B:233:ARG:O	1:B:233:ARG:HD3	2.17	0.45
1:D:530:ARG:O	3:D:604:GOL:H32	2.17	0.45
1:A:355:GLU:HG2	1:A:388:PHE:CD2	2.52	0.45
1:C:439:ARG:HA	1:C:459:THR:O	2.17	0.45
1:A:386:ARG:NH1	4:A:716:HOH:O	2.49	0.45
1:A:439:ARG:HA	1:A:459:THR:O	2.17	0.45
1:D:113:LYS:HD3	1:D:123:TYR:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:GLU:OE1	1:B:386:ARG:HB3	2.17	0.44
1:A:548:PRO:HB3	1:D:501:TRP:CD1	2.52	0.44
1:D:547:THR:HA	1:D:548:PRO:C	2.42	0.44
1:D:445:LYS:NZ	4:D:710:HOH:O	2.49	0.44
1:A:266:TYR:CE1	3:A:606:GOL:H31	2.53	0.44
1:C:138:ARG:NH1	4:C:716:HOH:O	2.47	0.44
1:C:354:LEU:HD22	1:C:473:VAL:HG11	2.01	0.43
1:D:221:ASN:C	1:D:223:GLU:N	2.71	0.43
1:A:547:THR:HA	1:A:548:PRO:C	2.44	0.43
3:A:606:GOL:H12	1:D:254:ARG:HH12	1.84	0.43
1:C:401:LYS:HG3	1:C:412:PHE:CD1	2.54	0.43
1:D:233:ARG:HG3	1:D:539:TYR:CE1	2.53	0.43
1:A:521:GLU:O	1:A:525:THR:HG23	2.19	0.43
1:C:521:GLU:O	1:C:525:THR:HG23	2.18	0.43
1:D:247:LYS:NZ	4:D:709:HOH:O	2.49	0.43
1:A:501:TRP:CD1	1:D:548:PRO:HB3	2.54	0.43
1:C:355:GLU:HG2	1:C:388:PHE:CD2	2.54	0.42
1:C:371:GLY:O	1:C:375[B]:HIS:ND1	2.51	0.42
1:C:441:PRO:HD2	1:C:444:ILE:HD11	2.01	0.42
1:C:123:TYR:HA	1:C:126:GLN:NE2	2.34	0.42
1:B:109:LEU:N	1:B:110:PRO:CD	2.82	0.42
1:C:507:LYS:NZ	4:C:718:HOH:O	2.52	0.42
1:B:212:PRO:HA	3:B:602:GOL:O1	2.19	0.42
1:B:445:LYS:HA	1:B:445:LYS:HD2	1.88	0.42
1:D:425:ARG:NH2	1:D:468:ASN:C	2.78	0.42
1:B:467:PRO:O	1:B:468:ASN:HB2	2.20	0.41
1:C:221:ASN:C	1:C:223:GLU:N	2.70	0.41
1:C:258:ASP:OD2	3:C:603:GOL:H11	2.21	0.41
1:D:221:ASN:HB2	1:D:224:SER:HB2	2.01	0.41
1:D:263:ARG:HH21	1:D:356:ASP:CG	2.24	0.41
3:D:607:GOL:H2	4:D:704:HOH:O	2.19	0.41
1:A:124:ARG:NH2	1:A:196:GLY:O	2.54	0.41
2:A:601:ZTE:S25	3:A:609:GOL:H2	2.61	0.41
1:A:137:LEU:HD23	1:A:137:LEU:C	2.46	0.40
1:A:445:LYS:HA	1:A:445:LYS:HD2	1.88	0.40
1:B:354:LEU:HD22	1:B:473:VAL:HG11	2.04	0.40
1:B:547:THR:HG22	4:C:813:HOH:O	2.20	0.40
1:C:420:PRO:HG3	4:C:708:HOH:O	2.22	0.40
1:D:245:ILE:HD11	1:D:530:ARG:HD2	2.04	0.40
1:B:383:PRO:HA	1:B:384:PRO:HD3	1.95	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	431/548 (79%)	415 (96%)	16 (4%)	0	100	100
1	B	431/548 (79%)	416 (96%)	14 (3%)	1 (0%)	43	42
1	C	431/548 (79%)	419 (97%)	12 (3%)	0	100	100
1	D	432/548 (79%)	417 (96%)	15 (4%)	0	100	100
All	All	1725/2192 (79%)	1667 (97%)	57 (3%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	469	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	384/485 (79%)	380 (99%)	4 (1%)	68	75
1	B	385/485 (79%)	383 (100%)	2 (0%)	81	87
1	C	385/485 (79%)	384 (100%)	1 (0%)	86	91
1	D	385/485 (79%)	382 (99%)	3 (1%)	73	80
All	All	1539/1940 (79%)	1529 (99%)	10 (1%)	76	85

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	GLU
1	A	198	HIS
1	A	223	GLU
1	A	224	SER
1	B	147	LEU
1	B	224	SER
1	C	198	HIS
1	D	124	ARG
1	D	147	LEU
1	D	198	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	GLN
1	B	277	GLN
1	C	277	GLN
1	D	277	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](#)

43 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	$\# Z > 2$
3	GOL	D	606	-	5,5,5	0.82	0	5,5,5	1.18	0
3	GOL	D	612	-	5,5,5	1.23	0	5,5,5	0.94	0
3	GOL	A	602	-	5,5,5	0.83	0	5,5,5	1.08	0
3	GOL	D	608	-	5,5,5	0.93	0	5,5,5	1.03	0
3	GOL	A	603	-	5,5,5	0.95	0	5,5,5	1.26	0
3	GOL	C	605	-	5,5,5	1.03	0	5,5,5	0.90	0
3	GOL	D	604	-	5,5,5	0.98	0	5,5,5	1.11	0
3	GOL	C	608	-	5,5,5	1.00	0	5,5,5	1.01	0
3	GOL	D	611	-	5,5,5	0.86	0	5,5,5	1.10	0
3	GOL	B	610	-	5,5,5	0.86	0	5,5,5	1.07	0
2	ZTE	D	601	-	29,30,30	2.97	13 (44%)	39,44,44	2.67	11 (28%)
3	GOL	C	606	-	5,5,5	0.88	0	5,5,5	1.13	1 (20%)
3	GOL	C	609	-	5,5,5	1.00	0	5,5,5	1.05	0
3	GOL	D	603	-	5,5,5	0.83	0	5,5,5	1.04	0
3	GOL	C	601	-	5,5,5	0.89	0	5,5,5	0.94	0
3	GOL	D	607	-	5,5,5	1.17	0	5,5,5	1.19	1 (20%)
2	ZTE	C	602	-	29,30,30	2.98	13 (44%)	39,44,44	2.82	10 (25%)
3	GOL	C	603	-	5,5,5	0.79	0	5,5,5	1.06	1 (20%)
3	GOL	B	608	-	5,5,5	0.92	0	5,5,5	1.03	0
3	GOL	A	604	-	5,5,5	1.03	0	5,5,5	1.05	0
3	GOL	B	604	-	5,5,5	0.93	0	5,5,5	1.22	0
3	GOL	B	612	-	5,5,5	0.95	0	5,5,5	1.20	1 (20%)
3	GOL	D	602	-	5,5,5	1.21	1 (20%)	5,5,5	1.35	1 (20%)
2	ZTE	A	601	-	29,30,30	2.80	13 (44%)	39,44,44	2.67	13 (33%)
3	GOL	D	609	-	5,5,5	1.07	0	5,5,5	1.02	1 (20%)
3	GOL	A	606	-	5,5,5	0.83	0	5,5,5	1.42	1 (20%)
3	GOL	B	607	-	5,5,5	0.72	0	5,5,5	1.25	1 (20%)
3	GOL	B	602	-	5,5,5	1.04	1 (20%)	5,5,5	1.18	0
3	GOL	B	611	-	5,5,5	0.95	0	5,5,5	0.95	0
3	GOL	B	606	-	5,5,5	1.37	1 (20%)	5,5,5	1.00	0
2	ZTE	B	601	-	29,30,30	2.73	14 (48%)	39,44,44	2.97	13 (33%)
3	GOL	B	603	-	5,5,5	0.83	0	5,5,5	1.25	1 (20%)
3	GOL	C	607	-	5,5,5	0.87	0	5,5,5	1.14	1 (20%)
3	GOL	D	610	-	5,5,5	1.05	0	5,5,5	1.07	0
3	GOL	A	605	-	5,5,5	0.79	0	5,5,5	1.12	1 (20%)
3	GOL	B	613	-	5,5,5	0.93	0	5,5,5	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	C	604	-	5,5,5	0.82	0	5,5,5	1.45	1 (20%)
3	GOL	B	605	-	5,5,5	0.85	0	5,5,5	1.24	1 (20%)
3	GOL	A	607	-	5,5,5	0.98	0	5,5,5	1.29	1 (20%)
3	GOL	A	608	-	5,5,5	0.87	0	5,5,5	1.27	1 (20%)
3	GOL	A	609	-	5,5,5	1.11	0	5,5,5	1.15	0
3	GOL	D	605	-	5,5,5	1.09	0	5,5,5	0.95	0
3	GOL	B	609	-	5,5,5	1.05	0	5,5,5	1.01	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	606	-	-	0/4/4/4	-
3	GOL	D	612	-	-	4/4/4/4	-
3	GOL	A	602	-	-	2/4/4/4	-
3	GOL	D	608	-	-	2/4/4/4	-
3	GOL	A	603	-	-	1/4/4/4	-
3	GOL	C	605	-	-	4/4/4/4	-
3	GOL	D	604	-	-	2/4/4/4	-
3	GOL	C	608	-	-	4/4/4/4	-
3	GOL	D	611	-	-	2/4/4/4	-
3	GOL	B	610	-	-	1/4/4/4	-
2	ZTE	D	601	-	-	4/23/23/23	0/3/3/3
3	GOL	C	606	-	-	2/4/4/4	-
3	GOL	C	609	-	-	2/4/4/4	-
3	GOL	D	603	-	-	3/4/4/4	-
3	GOL	C	601	-	-	0/4/4/4	-
3	GOL	D	607	-	-	0/4/4/4	-
2	ZTE	C	602	-	-	4/23/23/23	0/3/3/3
3	GOL	C	603	-	-	0/4/4/4	-
3	GOL	B	608	-	-	1/4/4/4	-
3	GOL	A	604	-	-	4/4/4/4	-
3	GOL	B	604	-	-	1/4/4/4	-
3	GOL	B	612	-	-	0/4/4/4	-
3	GOL	D	602	-	-	2/4/4/4	-
2	ZTE	A	601	-	-	4/23/23/23	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	609	-	-	2/4/4/4	-
3	GOL	A	606	-	-	4/4/4/4	-
3	GOL	B	607	-	-	0/4/4/4	-
3	GOL	B	602	-	-	0/4/4/4	-
3	GOL	B	611	-	-	4/4/4/4	-
3	GOL	B	606	-	-	0/4/4/4	-
2	ZTE	B	601	-	-	4/23/23/23	0/3/3/3
3	GOL	B	603	-	-	3/4/4/4	-
3	GOL	C	607	-	-	0/4/4/4	-
3	GOL	D	610	-	-	0/4/4/4	-
3	GOL	A	605	-	-	2/4/4/4	-
3	GOL	B	613	-	-	4/4/4/4	-
3	GOL	C	604	-	-	3/4/4/4	-
3	GOL	B	605	-	-	0/4/4/4	-
3	GOL	A	607	-	-	0/4/4/4	-
3	GOL	A	608	-	-	2/4/4/4	-
3	GOL	A	609	-	-	2/4/4/4	-
3	GOL	D	605	-	-	2/4/4/4	-
3	GOL	B	609	-	-	0/4/4/4	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	602	ZTE	C04-C05	6.85	1.53	1.42
2	D	601	ZTE	C04-C05	6.64	1.53	1.42
2	D	601	ZTE	C11-S12	6.23	1.86	1.76
2	A	601	ZTE	C04-C05	6.05	1.52	1.42
2	C	602	ZTE	C11-S12	6.01	1.85	1.76
2	B	601	ZTE	C04-C05	5.94	1.52	1.42
2	C	602	ZTE	O13-S12	5.73	1.50	1.43
2	D	601	ZTE	O13-S12	5.68	1.50	1.43
2	A	601	ZTE	O13-S12	5.63	1.50	1.43
2	D	601	ZTE	C15-N14	5.53	1.47	1.37
2	A	601	ZTE	C11-S12	5.44	1.84	1.76
2	C	602	ZTE	C15-N14	5.43	1.47	1.37
2	B	601	ZTE	C11-S12	5.37	1.84	1.76
2	A	601	ZTE	C15-N14	5.35	1.47	1.37
2	B	601	ZTE	O13-S12	5.07	1.49	1.43
2	B	601	ZTE	C15-N14	4.83	1.46	1.37
2	D	601	ZTE	S12-N14	4.50	1.75	1.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	602	ZTE	S12-N14	4.32	1.74	1.64
2	C	602	ZTE	C18-N19	4.13	1.46	1.32
2	A	601	ZTE	S12-N14	3.98	1.73	1.64
2	A	601	ZTE	C18-N19	3.96	1.45	1.32
2	B	601	ZTE	C18-N19	3.93	1.45	1.32
2	B	601	ZTE	S12-N14	3.92	1.73	1.64
2	D	601	ZTE	C18-N19	3.91	1.45	1.32
2	D	601	ZTE	O23-S12	3.60	1.47	1.43
2	C	602	ZTE	O23-S12	3.42	1.47	1.43
2	C	602	ZTE	C06-S25	-3.40	1.67	1.75
2	D	601	ZTE	C02-N01	3.34	1.42	1.34
2	B	601	ZTE	C02-N01	3.31	1.42	1.34
2	D	601	ZTE	C06-S25	-3.30	1.67	1.75
2	C	602	ZTE	C02-N01	3.29	1.42	1.34
2	A	601	ZTE	C06-S25	-3.22	1.68	1.75
2	D	601	ZTE	C07-C06	3.14	1.53	1.47
2	B	601	ZTE	C06-S25	-3.13	1.68	1.75
2	C	602	ZTE	C07-C06	3.11	1.53	1.47
2	A	601	ZTE	C02-N01	3.05	1.42	1.34
2	B	601	ZTE	O23-S12	3.04	1.47	1.43
2	A	601	ZTE	C24-C07	-2.97	1.35	1.39
2	D	601	ZTE	C24-C07	-2.86	1.35	1.39
2	B	601	ZTE	C24-C07	-2.79	1.35	1.39
2	A	601	ZTE	O23-S12	2.78	1.46	1.43
3	B	606	GOL	O2-C2	-2.78	1.35	1.43
2	C	602	ZTE	C24-C07	-2.63	1.35	1.39
2	B	601	ZTE	C07-C06	2.59	1.52	1.47
2	A	601	ZTE	C07-C06	2.43	1.52	1.47
3	D	602	GOL	O2-C2	-2.27	1.36	1.43
2	B	601	ZTE	O20-C18	-2.25	1.17	1.23
2	C	602	ZTE	O20-C18	-2.18	1.17	1.23
2	B	601	ZTE	C09-C10	-2.16	1.35	1.38
2	D	601	ZTE	C09-C10	-2.13	1.35	1.38
2	B	601	ZTE	C09-C08	2.12	1.42	1.38
2	A	601	ZTE	O20-C18	-2.11	1.17	1.23
2	A	601	ZTE	C09-C08	2.10	1.42	1.38
3	B	602	GOL	O2-C2	-2.08	1.37	1.43
2	C	602	ZTE	C09-C08	2.08	1.42	1.38
2	D	601	ZTE	O20-C18	-2.07	1.17	1.23

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ZTE	O23-S12-O13	-12.23	104.67	119.52
2	C	602	ZTE	O23-S12-O13	-11.75	105.25	119.52
2	D	601	ZTE	O23-S12-O13	-10.77	106.44	119.52
2	A	601	ZTE	O23-S12-O13	-10.04	107.33	119.52
2	C	602	ZTE	C03-S25-C06	5.63	97.35	91.52
2	D	601	ZTE	C03-S25-C06	5.36	97.06	91.52
2	A	601	ZTE	C27-N26-C04	5.10	120.19	115.72
2	C	602	ZTE	O23-S12-C11	5.08	114.39	107.98
2	C	602	ZTE	C27-N26-C04	4.92	120.04	115.72
2	A	601	ZTE	N28-C27-N26	-4.89	121.18	128.58
2	B	601	ZTE	N28-C27-N26	-4.86	121.22	128.58
2	B	601	ZTE	C27-N26-C04	4.79	119.92	115.72
2	C	602	ZTE	N28-C27-N26	-4.69	121.48	128.58
2	B	601	ZTE	C03-S25-C06	4.58	96.25	91.52
2	B	601	ZTE	C07-C06-S25	4.53	126.65	119.70
2	D	601	ZTE	C07-C06-S25	4.43	126.49	119.70
2	D	601	ZTE	N28-C27-N26	-4.38	121.95	128.58
2	D	601	ZTE	C27-N26-C04	4.36	119.54	115.72
2	A	601	ZTE	C03-S25-C06	4.13	95.79	91.52
2	B	601	ZTE	C07-C24-C11	-3.86	116.81	119.71
2	A	601	ZTE	C07-C06-S25	3.83	125.57	119.70
2	B	601	ZTE	C15-N14-S12	-3.42	118.29	124.18
2	A	601	ZTE	C07-C24-C11	-3.35	117.18	119.71
2	A	601	ZTE	O23-S12-C11	3.30	112.14	107.98
2	C	602	ZTE	C07-C06-S25	3.16	124.55	119.70
2	D	601	ZTE	C15-N14-S12	-3.07	118.90	124.18
2	B	601	ZTE	C17-C16-C15	-3.04	101.19	109.27
2	D	601	ZTE	C17-C16-C15	-2.93	101.50	109.27
2	B	601	ZTE	C03-C02-N01	-2.84	119.99	122.85
2	B	601	ZTE	O23-S12-N14	2.83	114.86	106.77
2	A	601	ZTE	C03-C02-N01	-2.76	120.08	122.85
2	A	601	ZTE	C24-C07-C06	-2.74	117.11	120.97
2	B	601	ZTE	O22-C15-N14	-2.74	118.02	122.98
2	B	601	ZTE	C07-C06-C05	-2.73	121.18	128.43
2	A	601	ZTE	C07-C06-C05	-2.70	121.25	128.43
2	D	601	ZTE	C07-C24-C11	-2.69	117.68	119.71
2	C	602	ZTE	C17-C16-C15	-2.65	102.23	109.27
3	A	606	GOL	C3-C2-C1	-2.64	102.12	111.80
2	C	602	ZTE	C24-C07-C06	-2.58	117.33	120.97
2	A	601	ZTE	C08-C07-C24	2.55	122.20	119.25
2	A	601	ZTE	C17-C16-C15	-2.54	102.52	109.27
3	C	604	GOL	C3-C2-C1	-2.53	102.51	111.80
2	D	601	ZTE	C07-C06-C05	-2.49	121.81	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ZTE	C15-N14-S12	-2.43	120.00	124.18
2	D	601	ZTE	C03-C02-N01	-2.42	120.42	122.85
3	A	607	GOL	C3-C2-C1	-2.31	103.31	111.80
2	C	602	ZTE	C15-N14-S12	-2.25	120.31	124.18
3	B	605	GOL	C3-C2-C1	-2.22	103.66	111.80
3	B	603	GOL	C3-C2-C1	-2.20	103.73	111.80
3	D	607	GOL	C3-C2-C1	-2.20	103.73	111.80
3	B	607	GOL	C3-C2-C1	-2.12	104.01	111.80
2	B	601	ZTE	C10-C11-C24	2.11	123.28	120.68
3	A	608	GOL	C3-C2-C1	-2.10	104.08	111.80
3	A	605	GOL	C3-C2-C1	-2.10	104.10	111.80
3	B	612	GOL	C3-C2-C1	-2.10	104.11	111.80
3	C	603	GOL	C3-C2-C1	-2.07	104.20	111.80
2	C	602	ZTE	C03-C02-N01	-2.04	120.80	122.85
2	D	601	ZTE	O23-S12-C11	2.03	110.54	107.98
3	C	607	GOL	C3-C2-C1	-2.03	104.36	111.80
3	C	606	GOL	C3-C2-C1	-2.01	104.41	111.80
3	D	602	GOL	C3-C2-C1	-2.00	104.44	111.80
3	D	609	GOL	C3-C2-C1	-2.00	104.44	111.80

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GOL	C1-C2-C3-O3
3	A	605	GOL	O1-C1-C2-C3
3	A	606	GOL	O1-C1-C2-C3
3	A	608	GOL	C1-C2-C3-O3
3	A	608	GOL	O2-C2-C3-O3
3	B	603	GOL	C1-C2-C3-O3
3	B	611	GOL	C1-C2-C3-O3
3	B	613	GOL	C1-C2-C3-O3
3	B	613	GOL	O2-C2-C3-O3
3	C	605	GOL	C1-C2-C3-O3
3	C	608	GOL	O1-C1-C2-C3
3	C	609	GOL	O1-C1-C2-C3
3	D	602	GOL	C1-C2-C3-O3
3	D	602	GOL	O2-C2-C3-O3
3	D	603	GOL	O2-C2-C3-O3
3	D	608	GOL	C1-C2-C3-O3
3	D	609	GOL	C1-C2-C3-O3
3	D	611	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	D	612	GOL	O1-C1-C2-C3
3	D	612	GOL	C1-C2-C3-O3
3	D	612	GOL	O2-C2-C3-O3
3	A	602	GOL	O2-C2-C3-O3
3	B	611	GOL	O1-C1-C2-O2
3	B	611	GOL	O2-C2-C3-O3
3	D	608	GOL	O2-C2-C3-O3
3	D	612	GOL	O1-C1-C2-O2
3	A	604	GOL	O1-C1-C2-C3
3	A	604	GOL	C1-C2-C3-O3
3	A	606	GOL	C1-C2-C3-O3
3	A	609	GOL	C1-C2-C3-O3
3	B	611	GOL	O1-C1-C2-C3
3	B	613	GOL	O1-C1-C2-C3
3	C	604	GOL	C1-C2-C3-O3
3	C	605	GOL	O1-C1-C2-C3
3	C	606	GOL	C1-C2-C3-O3
3	C	608	GOL	C1-C2-C3-O3
3	D	603	GOL	C1-C2-C3-O3
3	D	604	GOL	O1-C1-C2-C3
3	D	605	GOL	C1-C2-C3-O3
3	A	604	GOL	O2-C2-C3-O3
3	A	605	GOL	O1-C1-C2-O2
3	A	606	GOL	O1-C1-C2-O2
3	A	609	GOL	O2-C2-C3-O3
3	B	603	GOL	O2-C2-C3-O3
3	C	604	GOL	O2-C2-C3-O3
3	C	605	GOL	O2-C2-C3-O3
3	C	609	GOL	O1-C1-C2-O2
3	D	604	GOL	O1-C1-C2-O2
3	D	605	GOL	O2-C2-C3-O3
3	D	609	GOL	O2-C2-C3-O3
3	D	611	GOL	O1-C1-C2-O2
2	A	601	ZTE	C24-C11-S12-O13
2	B	601	ZTE	C24-C11-S12-O13
2	C	602	ZTE	C24-C11-S12-O13
2	D	601	ZTE	C24-C11-S12-O13
2	A	601	ZTE	C10-C11-S12-O13
2	D	601	ZTE	C10-C11-S12-O13
2	C	602	ZTE	C10-C11-S12-O13
2	B	601	ZTE	C10-C11-S12-O13
3	B	613	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	C	606	GOL	O2-C2-C3-O3
3	C	608	GOL	O1-C1-C2-O2
3	A	604	GOL	O1-C1-C2-O2
3	B	610	GOL	O2-C2-C3-O3
2	C	602	ZTE	C24-C11-S12-N14
2	C	602	ZTE	C10-C11-S12-N14
2	B	601	ZTE	C24-C11-S12-N14
3	A	606	GOL	O2-C2-C3-O3
3	B	603	GOL	O1-C1-C2-O2
3	C	604	GOL	O1-C1-C2-O2
3	C	605	GOL	O1-C1-C2-O2
2	A	601	ZTE	C24-C11-S12-N14
2	B	601	ZTE	C10-C11-S12-N14
2	D	601	ZTE	C24-C11-S12-N14
2	A	601	ZTE	C10-C11-S12-N14
2	D	601	ZTE	C10-C11-S12-N14
3	D	603	GOL	O1-C1-C2-O2
3	A	603	GOL	O1-C1-C2-O2
3	C	608	GOL	O2-C2-C3-O3
3	B	604	GOL	O1-C1-C2-O2
3	B	608	GOL	O1-C1-C2-O2

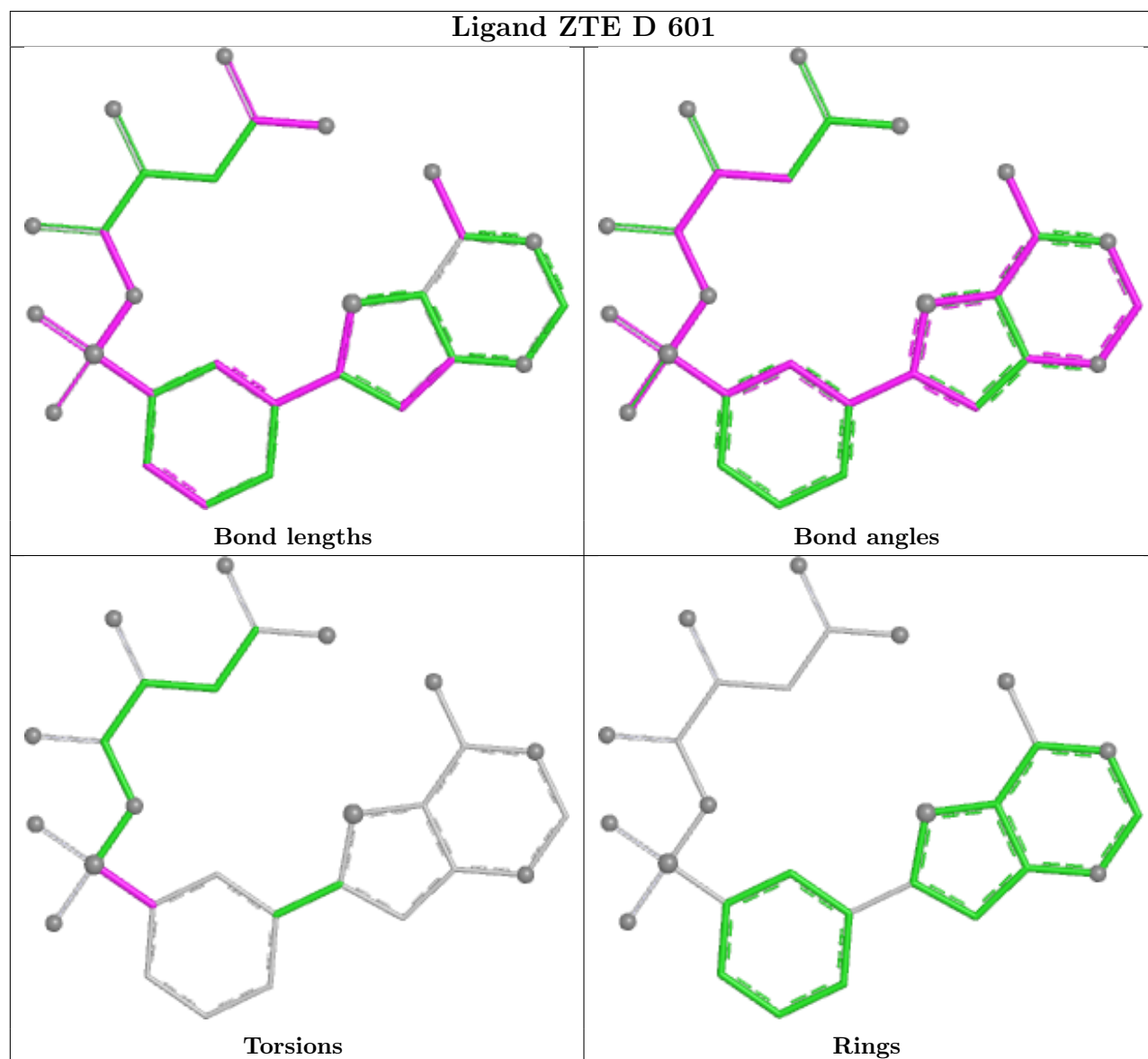
There are no ring outliers.

14 monomers are involved in 30 short contacts:

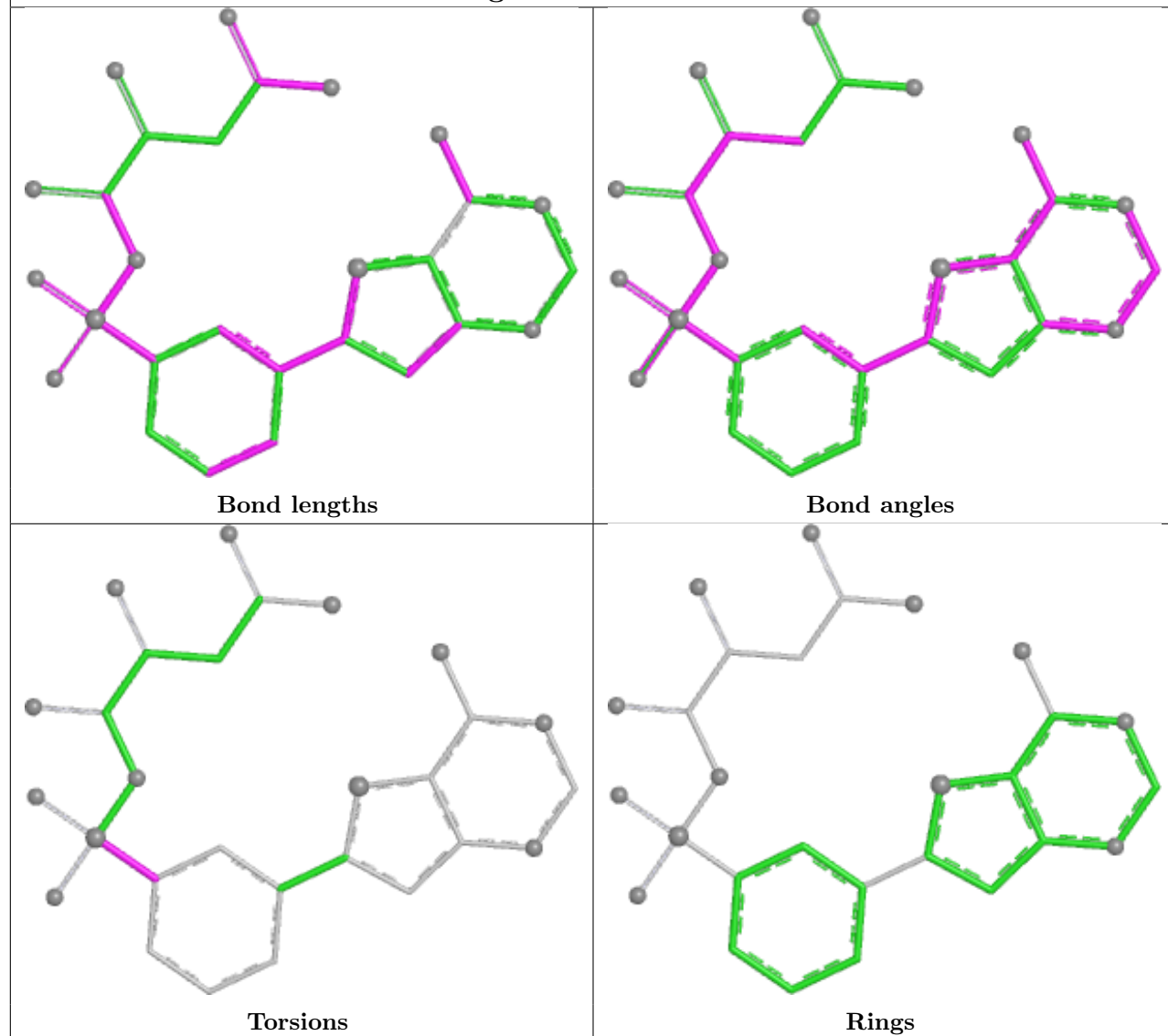
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	604	GOL	5	0
3	C	606	GOL	1	0
3	C	601	GOL	1	0
3	D	607	GOL	3	0
3	C	603	GOL	2	0
3	A	604	GOL	3	0
2	A	601	ZTE	1	0
3	A	606	GOL	2	0
3	B	602	GOL	3	0
3	B	611	GOL	3	0
3	C	607	GOL	2	0
3	A	608	GOL	1	0
3	A	609	GOL	3	0
3	D	605	GOL	1	0

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

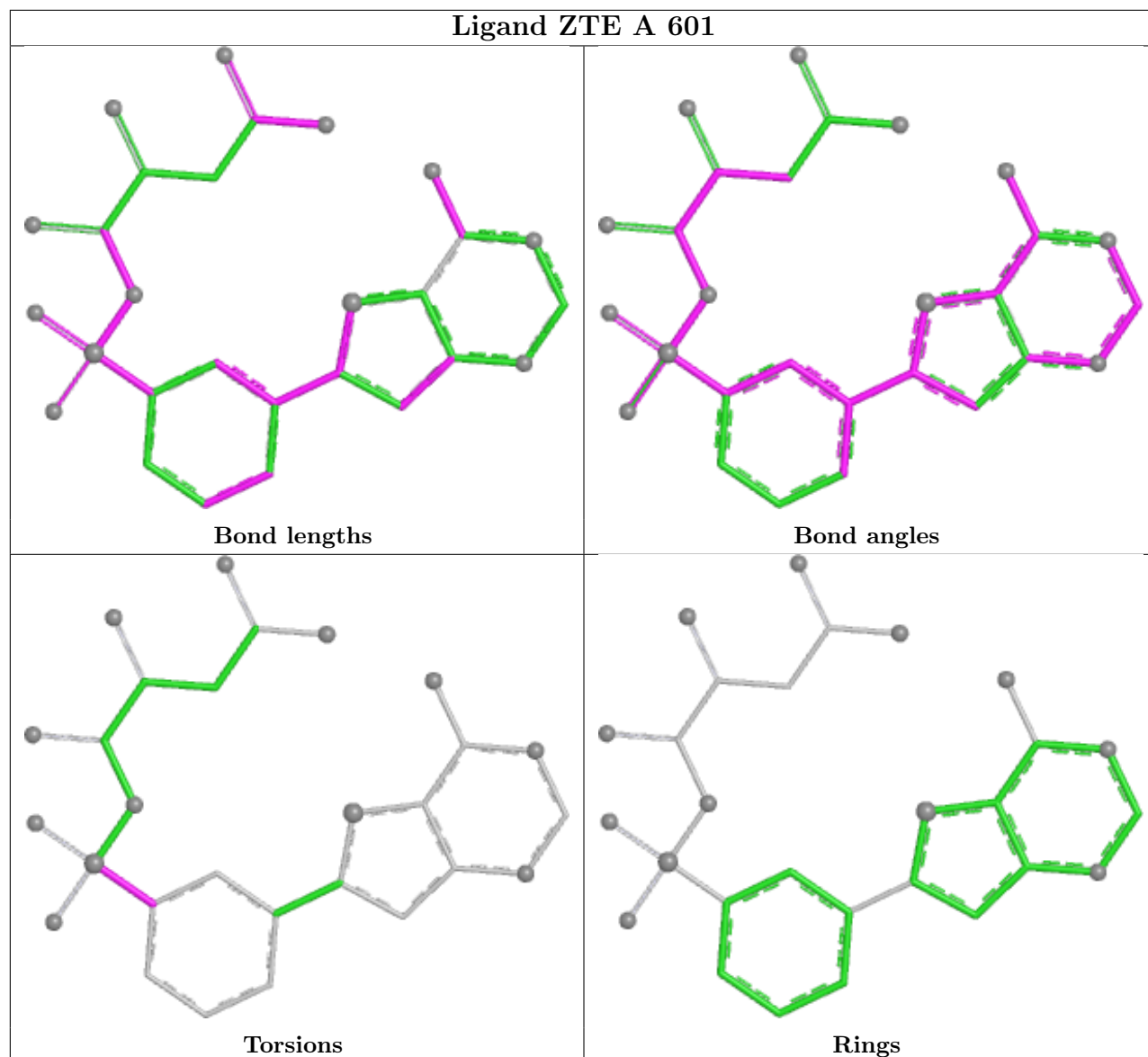
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

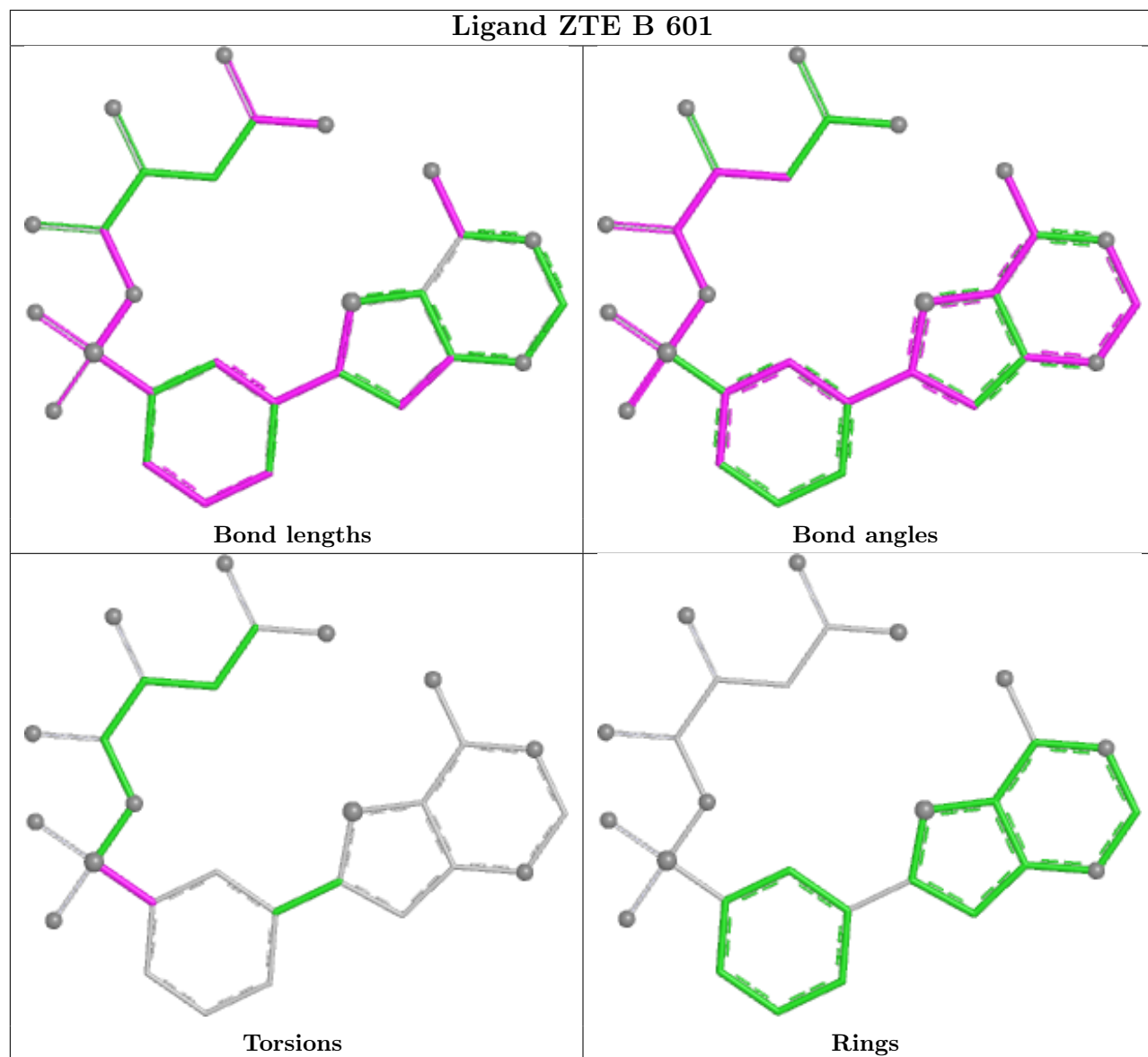


Ligand ZTE C 602



Ligand ZTE A 601





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	434/548 (79%)	-0.41	4 (0%) 81 80	20, 34, 59, 121	1 (0%)
1	B	434/548 (79%)	-0.40	5 (1%) 76 76	16, 33, 58, 124	1 (0%)
1	C	433/548 (79%)	-0.12	4 (0%) 81 80	24, 44, 88, 130	2 (0%)
1	D	434/548 (79%)	-0.29	7 (1%) 70 70	21, 36, 82, 121	2 (0%)
All	All	1735/2192 (79%)	-0.30	20 (1%) 76 76	16, 36, 74, 130	6 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	110	PRO	5.7
1	C	220	ILE	5.4
1	A	220	ILE	5.1
1	B	220	ILE	4.8
1	B	109	LEU	4.6
1	D	220	ILE	4.6
1	D	214	GLY	3.4
1	A	532[A]	HIS	3.2
1	A	110	PRO	2.8
1	C	375[A]	HIS	2.7
1	B	190	LYS	2.7
1	A	214	GLY	2.6
1	B	110	PRO	2.4
1	D	222	GLU	2.2
1	D	375[A]	HIS	2.2
1	C	189	PRO	2.2
1	D	189	PRO	2.2
1	C	222	GLU	2.1
1	B	221	ASN	2.0
1	D	326	SER	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($\text{\AA}^2$)	Q<0.9
3	GOL	D	611	6/6	0.64	0.15	63,69,76,78	0
3	GOL	A	609	6/6	0.66	0.18	52,53,63,70	0
3	GOL	B	611	6/6	0.69	0.17	46,58,64,65	0
3	GOL	D	608	6/6	0.70	0.16	53,62,73,77	0
3	GOL	C	609	6/6	0.73	0.16	59,69,74,77	0
3	GOL	B	608	6/6	0.75	0.16	52,56,65,71	0
3	GOL	A	608	6/6	0.78	0.16	49,61,69,69	0
3	GOL	D	606	6/6	0.79	0.14	48,65,71,76	0
3	GOL	C	605	6/6	0.80	0.12	66,67,73,77	0
3	GOL	C	604	6/6	0.82	0.12	68,73,75,76	0
3	GOL	C	608	6/6	0.83	0.12	54,62,68,75	0
3	GOL	D	612	6/6	0.83	0.13	55,57,66,67	0
3	GOL	D	604	6/6	0.85	0.12	55,61,63,68	0
3	GOL	B	606	6/6	0.85	0.14	40,52,58,61	0
3	GOL	A	604	6/6	0.85	0.13	54,56,62,64	0
3	GOL	A	606	6/6	0.85	0.13	39,56,64,66	0
3	GOL	C	601	6/6	0.85	0.12	56,61,64,75	0
3	GOL	B	605	6/6	0.86	0.12	49,52,54,59	0
3	GOL	C	606	6/6	0.86	0.12	49,59,63,71	0
3	GOL	B	604	6/6	0.86	0.14	39,53,63,67	0
3	GOL	A	603	6/6	0.87	0.13	32,40,49,65	0
3	GOL	B	603	6/6	0.87	0.11	42,54,64,67	0
3	GOL	A	602	6/6	0.87	0.12	37,53,53,65	0
3	GOL	D	602	6/6	0.88	0.14	42,45,51,58	0
3	GOL	D	603	6/6	0.88	0.12	50,52,56,67	0
3	GOL	D	610	6/6	0.88	0.13	55,62,65,69	0
3	GOL	C	603	6/6	0.88	0.09	44,50,56,62	0

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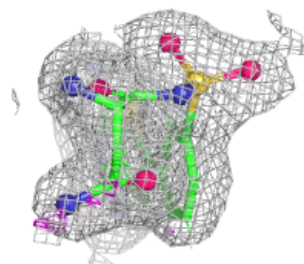
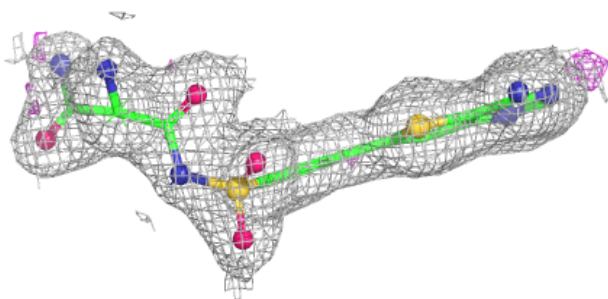
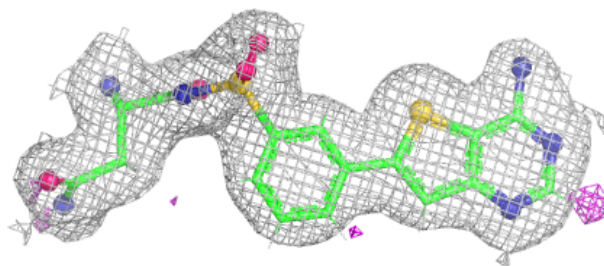
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	605	6/6	0.88	0.11	53,61,64,65	0
3	GOL	B	609	6/6	0.89	0.11	50,60,60,65	0
3	GOL	B	602	6/6	0.89	0.13	39,52,55,67	0
3	GOL	A	605	6/6	0.90	0.12	43,56,72,73	0
3	GOL	B	613	6/6	0.90	0.11	49,54,65,75	0
3	GOL	B	610	6/6	0.90	0.10	48,53,60,64	0
3	GOL	A	607	6/6	0.91	0.12	40,46,53,57	0
3	GOL	C	607	6/6	0.92	0.12	46,48,50,60	0
3	GOL	B	607	6/6	0.92	0.11	38,39,48,60	0
3	GOL	D	607	6/6	0.93	0.10	37,42,51,62	0
3	GOL	D	609	6/6	0.94	0.09	45,49,53,66	0
3	GOL	B	612	6/6	0.94	0.08	32,34,43,49	0
2	ZTE	D	601	28/28	0.97	0.06	22,32,38,44	0
2	ZTE	C	602	28/28	0.97	0.05	24,34,43,48	0
2	ZTE	B	601	28/28	0.98	0.05	22,28,36,38	0
2	ZTE	A	601	28/28	0.98	0.05	22,29,37,42	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.

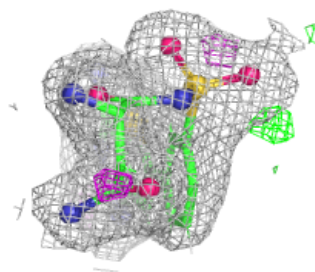
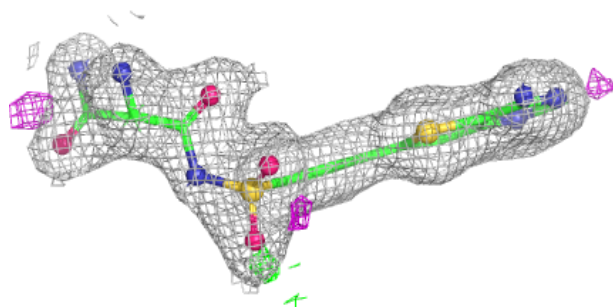
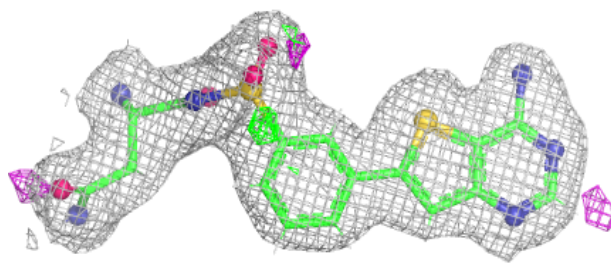
Electron density around ZTE D 601:

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

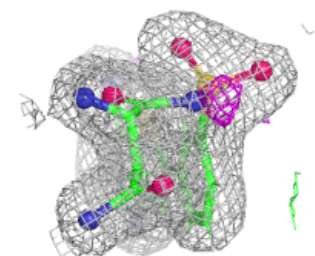
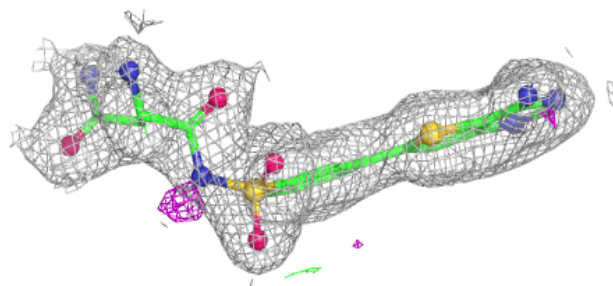
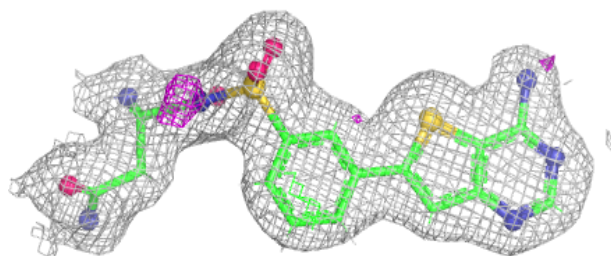


Electron density around ZTE C 602:

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

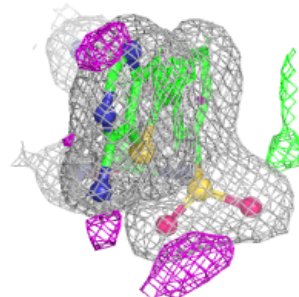
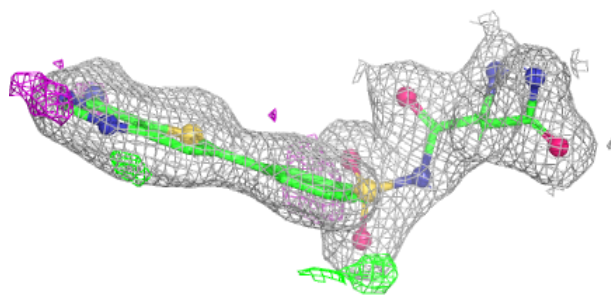
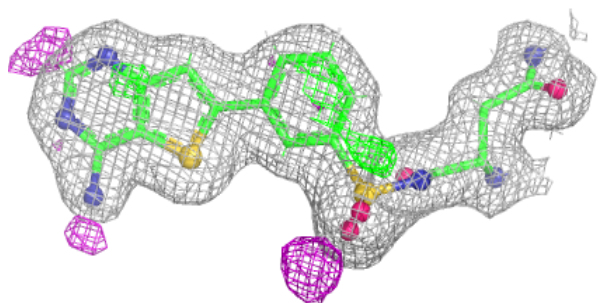
**Electron density around ZTE B 601:**

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



Electron density around ZTE A 601:

$2mF_o-DF_c$ (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.