



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:33 PM UTC

PDB ID : 3V94 / pdb_00003v94
Title : TcrPDEC1 catalytic domain in complex with inhibitor wyq16
Authors : Wang, H.; Kunz, S.; Chen, G.; Seebeck, T.; Wan, Y.; Robinson, H.; Martinelli, S.; Ke, H.
Deposited on : 2011-12-23
Resolution : 2.33 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:

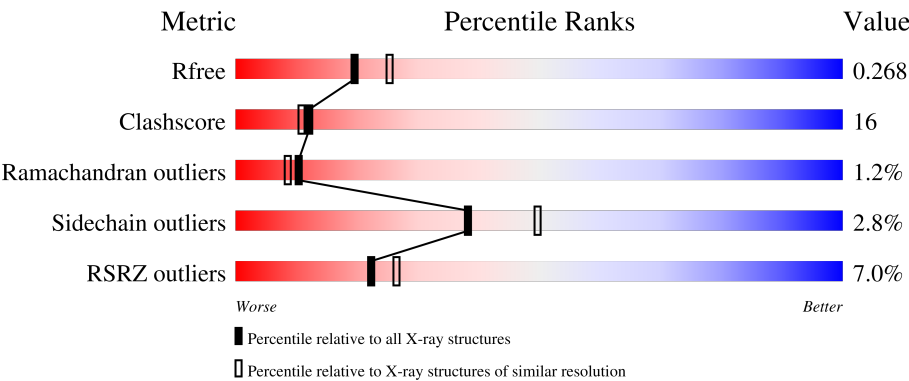
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	345	3% 77% 19% ..
1	B	345	3% 71% 23% ...
1	C	345	6% 70% 23% ..
1	D	345	7% 65% 28% ..
1	E	345	21% 60% 34% ..

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Mol	Chain	Length	Quality of chain
1	F	345	 3% 74% 19% . .
1	G	345	 5% 67% 27% . .
1	H	345	 6% 70% 23% . . .

2 Entry composition

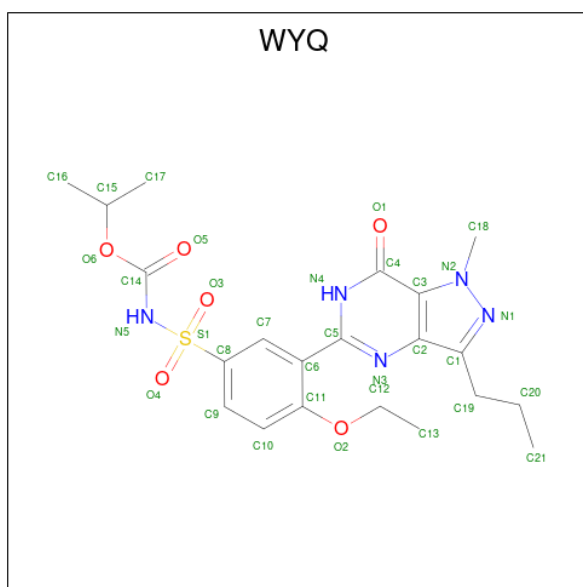
There are 5 unique types of molecules in this entry. The entry contains 21762 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cyclic nucleotide specific phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2574	1646	440	479	9			
1	B	334	Total	C	N	O	S	0	0	0
			2590	1657	442	481	10			
1	C	333	Total	C	N	O	S	0	0	0
			2582	1652	441	480	9			
1	D	331	Total	C	N	O	S	0	0	0
			2568	1643	439	477	9			
1	E	331	Total	C	N	O	S	0	0	0
			2568	1643	439	477	9			
1	F	334	Total	C	N	O	S	0	0	0
			2590	1657	442	481	10			
1	G	334	Total	C	N	O	S	0	0	0
			2590	1657	442	481	10			
1	H	330	Total	C	N	O	S	0	0	0
			2563	1640	438	476	9			

- Molecule 2 is propan-2-yl {[4-ethoxy-3-(1-methyl-7-oxo-3-propyl-6,7-dihydro-1H-pyrazolo[4,3-d]pyrimidin-5-yl)phenyl]sulfonyl}carbamate (CCD ID: WYQ) (formula: C₂₁H₂₇N₅O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			33	21	5	6	1		
2	B	1	Total	C	N	O	S	0	0
			33	21	5	6	1		
2	C	1	Total	C	N	O	S	0	0
			33	21	5	6	1		
2	D	1	Total	C	N	O	S	0	0
			33	21	5	6	1		
2	E	1	Total	C	N	O	S	0	0
			33	21	5	6	1		
2	F	1	Total	C	N	O	S	0	0
			33	21	5	6	1		
2	G	1	Total	C	N	O	S	0	0
			33	21	5	6	1		
2	H	1	Total	C	N	O	S	0	0
			33	21	5	6	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0
3	G	1	Total 1	Zn 1	0	0
3	H	1	Total 1	Zn 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0
4	G	1	Total 1	Mg 1	0	0
4	H	1	Total 1	Mg 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	169	Total 169	O 169	0	0
5	B	159	Total 159	O 159	0	0
5	C	96	Total 96	O 96	0	0
5	D	53	Total 53	O 53	0	0
5	E	45	Total 45	O 45	0	0

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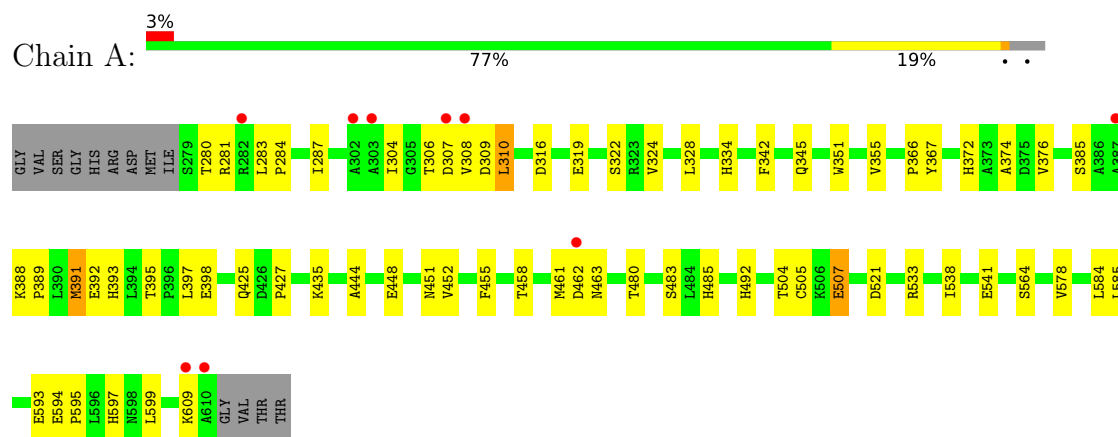
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	129	Total 129	O 129	0	0
5	G	132	Total 132	O 132	0	0
5	H	74	Total 74	O 74	0	0

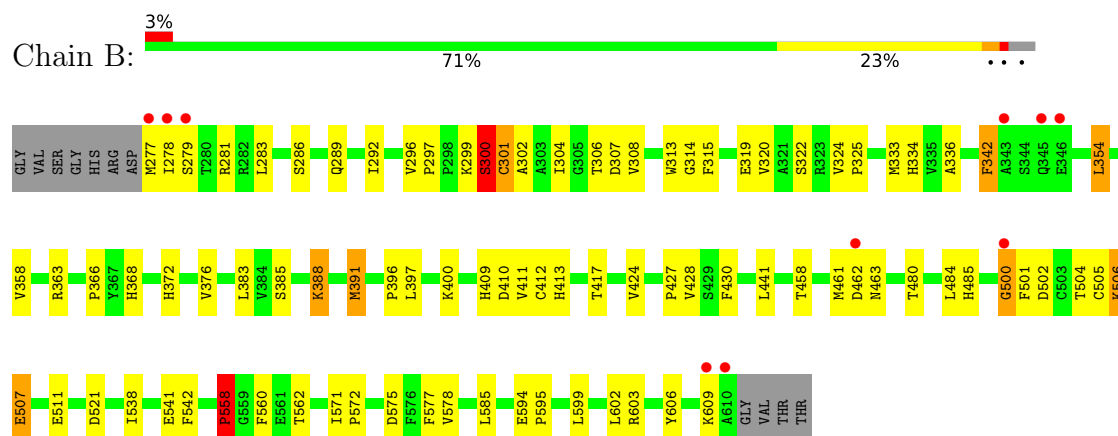
3 Residue-property plots [i](#)

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.

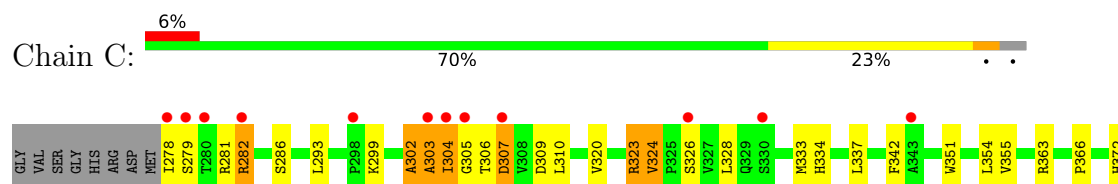
- Molecule 1: Cyclic nucleotide specific phosphodiesterase

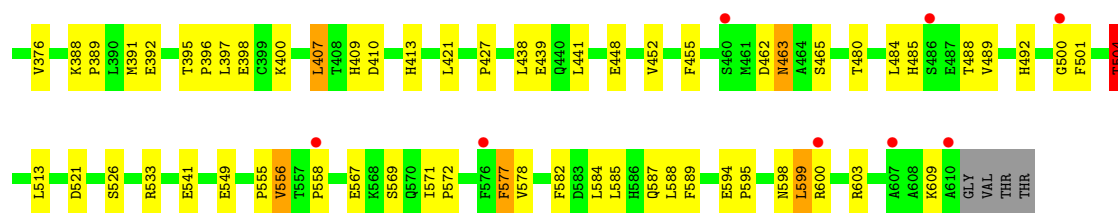


- Molecule 1: Cyclic nucleotide specific phosphodiesterase

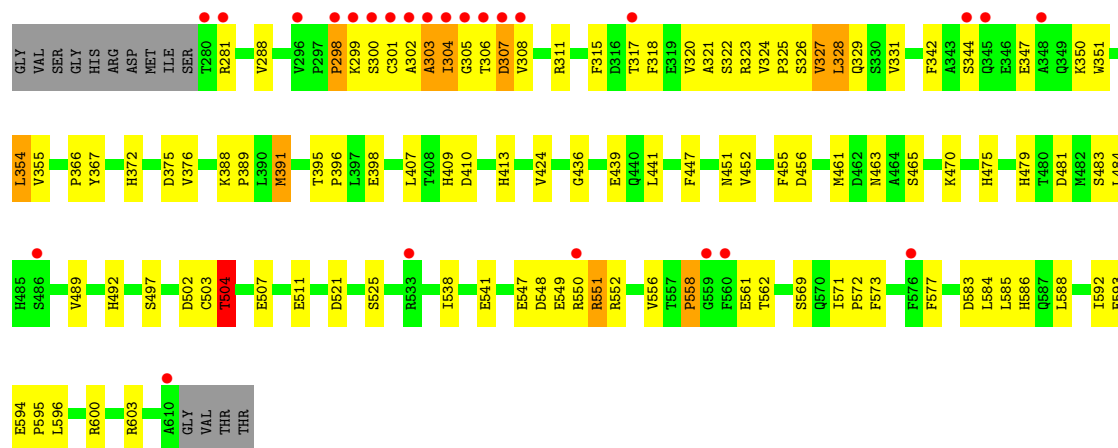


- Molecule 1: Cyclic nucleotide specific phosphodiesterase

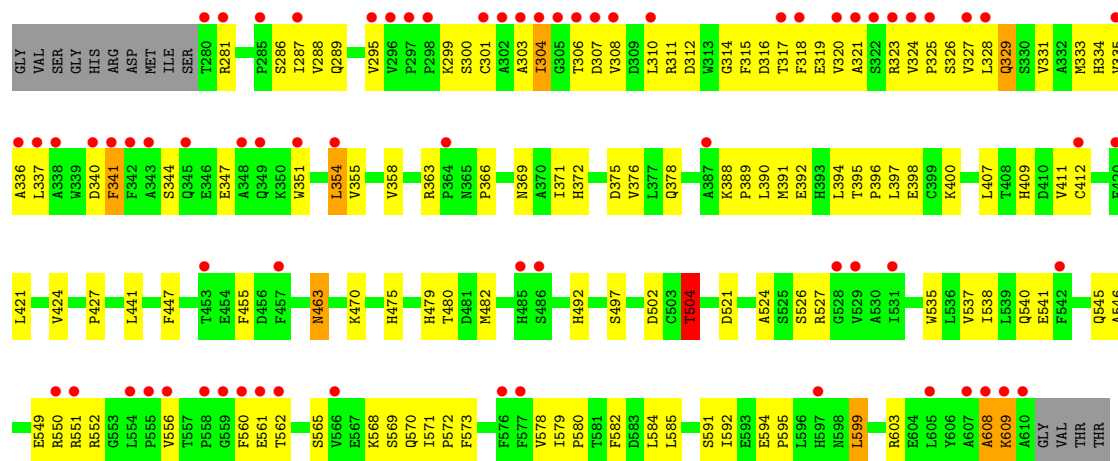




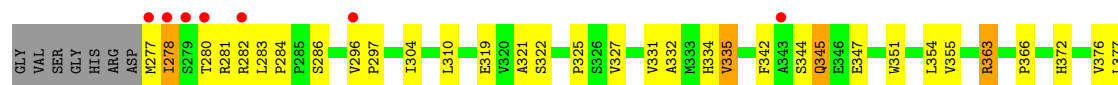
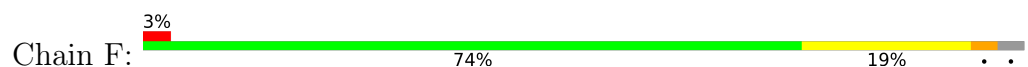
• Molecule 1: Cyclic nucleotide specific phosphodiesterase

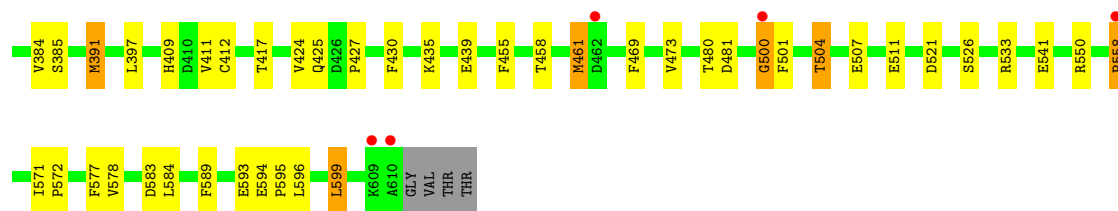


• Molecule 1: Cyclic nucleotide specific phosphodiesterase

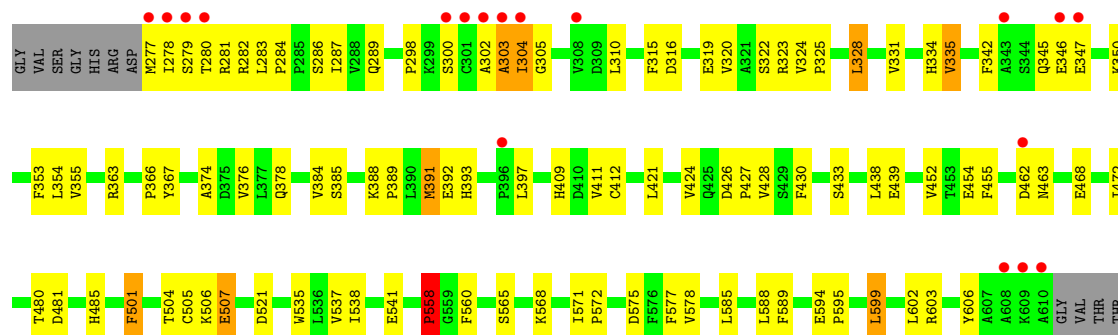


• Molecule 1: Cyclic nucleotide specific phosphodiesterase

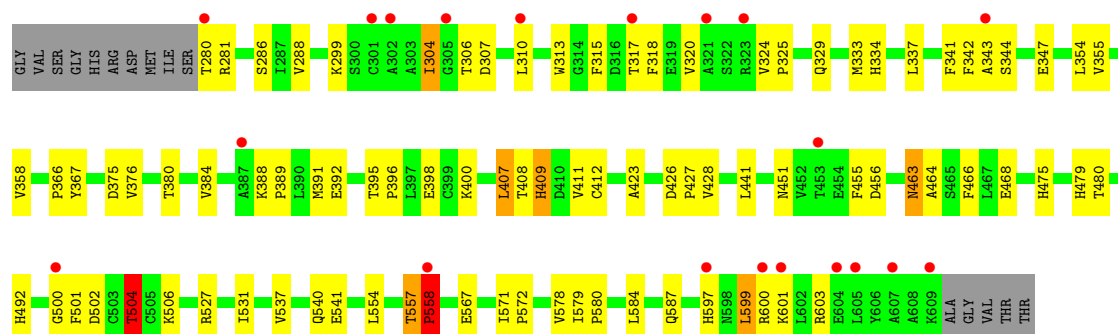




● Molecule 1: Cyclic nucleotide specific phosphodiesterase



● Molecule 1: Cyclic nucleotide specific phosphodiesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	131.15Å 131.15Å 394.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.33 30.00 – 2.33	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.33) 95.1 (30.00-2.33)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.69 (at 2.34Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.268 0.224 , 0.268	Depositor DCC
R_{free} test set	14467 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21762	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 34.07 % 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 7.2322e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: WYQ, MG, ZN

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	0.47	0/2639	0.94	6/3592 (0.2%)
1	B	0.47	0/2655	0.92	12/3613 (0.3%)
1	C	0.42	0/2647	0.90	10/3603 (0.3%)
1	D	0.39	0/2633	0.86	4/3584 (0.1%)
1	E	0.37	0/2633	0.84	3/3584 (0.1%)
1	F	0.45	0/2655	0.90	10/3613 (0.3%)
1	G	0.44	0/2655	0.93	12/3613 (0.3%)
1	H	0.39	0/2628	0.88	7/3577 (0.2%)
All	All	0.43	0/21145	0.90	64/28779 (0.2%)

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	PHE	N-CA-C	8.41	123.11	109.40
1	C	305	GLY	N-CA-C	8.12	120.97	111.63
1	G	578	VAL	N-CA-C	8.07	118.00	110.42
1	A	578	VAL	N-CA-C	8.01	117.94	110.42
1	B	578	VAL	N-CA-C	7.72	117.79	110.53
1	F	578	VAL	N-CA-C	7.35	117.33	110.42
1	H	557	THR	CA-C-N	7.08	128.69	119.84
1	H	557	THR	C-N-CA	7.08	128.69	119.84
1	G	342	PHE	N-CA-C	6.77	120.49	109.59
1	G	305	GLY	N-CA-C	6.71	118.97	111.85
1	G	480	THR	N-CA-C	-6.53	105.34	113.38
1	A	480	THR	N-CA-C	-6.53	104.94	113.17
1	B	409	HIS	N-CA-C	6.53	120.11	111.75
1	F	342	PHE	N-CA-C	6.51	119.85	109.24
1	C	342	PHE	N-CA-C	6.49	120.27	109.95
1	B	577	PHE	N-CA-C	6.43	120.94	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	THR	N-CA-C	-6.32	105.55	113.20
1	B	342	PHE	N-CA-C	6.29	119.95	109.95
1	B	560	PHE	N-CA-C	6.23	120.08	112.23
1	G	462	ASP	N-CA-C	-6.19	102.80	110.41
1	D	489	VAL	N-CA-C	-6.16	104.74	110.53
1	C	578	VAL	N-CA-C	6.12	116.30	110.42
1	G	501	PHE	N-CA-C	6.05	119.14	110.24
1	G	560	PHE	N-CA-C	6.05	119.85	112.23
1	E	480	THR	N-CA-C	-5.95	106.07	113.38
1	F	480	THR	N-CA-C	-5.88	105.87	113.16
1	F	345	GLN	N-CA-C	-5.83	106.79	114.31
1	E	578	VAL	N-CA-C	5.82	115.95	110.30
1	H	504	THR	N-CA-C	-5.81	105.28	112.90
1	G	589	PHE	CA-C-N	5.75	127.03	119.84
1	G	589	PHE	C-N-CA	5.75	127.03	119.84
1	B	562	THR	CA-C-N	5.75	125.94	120.31
1	B	562	THR	C-N-CA	5.75	125.94	120.31
1	A	287	ILE	N-CA-C	-5.51	107.37	112.83
1	B	500	GLY	N-CA-C	5.51	126.24	113.18
1	C	504	THR	N-CA-C	-5.49	106.42	113.23
1	C	589	PHE	CA-C-N	5.49	125.83	119.47
1	C	589	PHE	C-N-CA	5.49	125.83	119.47
1	F	409	HIS	N-CA-C	5.46	118.74	111.75
1	G	504	THR	N-CA-C	-5.45	106.58	113.18
1	F	504	THR	N-CA-C	-5.44	106.14	112.89
1	D	504	THR	N-CA-C	-5.41	106.52	113.23
1	A	485	HIS	N-CA-C	5.39	117.59	111.02
1	B	558	PRO	CA-C-N	-5.38	114.13	122.30
1	B	558	PRO	C-N-CA	-5.38	114.13	122.30
1	F	589	PHE	CA-C-N	5.37	125.70	119.47
1	F	589	PHE	C-N-CA	5.37	125.70	119.47
1	G	485	HIS	N-CA-C	5.36	116.81	110.97
1	C	577	PHE	N-CA-C	5.30	119.22	112.12
1	D	307	ASP	N-CA-C	-5.29	105.63	111.71
1	B	480	THR	N-CA-C	-5.18	106.65	113.17
1	G	287	ILE	N-CA-C	-5.16	107.72	112.83
1	H	409	HIS	N-CA-C	5.15	119.04	112.34
1	C	480	THR	N-CA-C	-5.10	106.74	113.17
1	F	577	PHE	N-CA-C	5.10	119.12	112.13
1	H	343	ALA	N-CA-C	-5.10	106.75	113.17
1	D	342	PHE	N-CA-C	5.08	118.03	109.95
1	H	342	PHE	N-CA-C	5.08	118.50	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
1	F	500	GLY	N-CA-C	5.07	125.19	113.18
1	H	480	THR	N-CA-C	-5.04	106.82	113.17
1	E	504	THR	N-CA-C	-5.04	106.65	112.89
1	C	324	VAL	CA-C-N	5.03	124.64	119.05
1	C	324	VAL	C-N-CA	5.03	124.64	119.05
1	B	300	SER	N-CA-C	5.03	121.50	110.80

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	2574	0	2531	56	0
1	B	2590	0	2551	100	0
1	C	2582	0	2542	74	0
1	D	2568	0	2526	102	0
1	E	2568	0	2526	104	0
1	F	2590	0	2551	65	0
1	G	2590	0	2551	90	0
1	H	2563	0	2521	81	0
2	A	33	0	27	3	0
2	B	33	0	27	15	0
2	C	33	0	27	4	0
2	D	33	0	27	4	0
2	E	33	0	27	4	0
2	F	33	0	27	3	0
2	G	33	0	27	5	0
2	H	33	0	27	3	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
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	169	0	0	4	0
5	B	159	0	0	9	0
5	C	96	0	0	4	0
5	D	53	0	0	4	0
5	E	45	0	0	3	0
5	F	129	0	0	7	0
5	G	132	0	0	5	0
5	H	74	0	0	5	0
All	All	21762	0	20515	646	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 16.

All (646) 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:F:278:ILE:HG21	1:F:430:PHE:HB3	1.34	1.08
1:B:300:SER:HB3	1:B:325:PRO:HG3	1.37	1.06
1:B:278:ILE:HG12	1:B:430:PHE:HB3	1.44	0.97
1:G:571:ILE:HG23	1:G:603:ARG:NH1	1.85	0.91
1:C:571:ILE:HG23	1:C:603:ARG:NH1	1.86	0.90
1:C:571:ILE:HG23	1:C:603:ARG:HH12	1.35	0.90
1:G:577:PHE:CE2	2:G:701:WYQ:H2	2.08	0.88
1:B:542:PHE:HE1	2:B:701:WYQ:H2	1.38	0.87
1:F:286:SER:HB2	1:F:427:PRO:HG2	1.55	0.87
1:B:278:ILE:HG21	1:B:283:LEU:HD11	1.54	0.87
1:C:303:ALA:O	1:C:304:ILE:HG12	1.76	0.85
1:C:286:SER:HB2	1:C:427:PRO:HG2	1.57	0.84
1:B:278:ILE:HD11	1:D:470:LYS:NZ	1.92	0.84
1:E:463:ASN:HD22	1:G:281:ARG:HH11	1.21	0.84
1:H:304:ILE:HD13	1:H:304:ILE:H	1.43	0.84
1:H:317:THR:HG21	1:H:375:ASP:HA	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:319:GLU:HG2	1:G:323:ARG:HH22	1.42	0.83
1:E:463:ASN:ND2	1:G:281:ARG:HH11	1.77	0.83
1:A:281:ARG:HH11	1:C:463:ASN:HD22	1.26	0.83
1:B:558:PRO:O	1:C:587:GLN:O	1.96	0.83
1:B:286:SER:HB2	1:B:427:PRO:HG2	1.62	0.82
1:G:303:ALA:O	1:G:304:ILE:HG12	1.80	0.82
1:H:286:SER:HB2	1:H:427:PRO:HG2	1.62	0.81
1:B:417:THR:HG22	2:B:701:WYQ:H8	1.45	0.81
1:B:463:ASN:ND2	1:D:281:ARG:HD3	1.96	0.80
1:D:321:ALA:HA	1:D:327:VAL:HG22	1.61	0.80
1:A:310:LEU:HD22	1:A:334:HIS:ND1	1.97	0.80
1:F:277:MET:HB2	1:H:451:ASN:HB2	1.64	0.80
1:B:502:ASP:OD2	1:B:504:THR:HG22	1.82	0.79
1:F:278:ILE:HG21	1:F:430:PHE:CB	2.13	0.79
1:E:308:VAL:HG22	1:E:311:ARG:HH21	1.48	0.79
1:H:603:ARG:HG3	1:H:603:ARG:HH11	1.47	0.79
1:B:417:THR:HG22	2:B:701:WYQ:H4	1.66	0.78
1:B:300:SER:O	1:B:301:CYS:HB2	1.84	0.78
1:B:300:SER:HB3	1:B:325:PRO:CG	2.12	0.77
1:G:320:VAL:HA	1:G:323:ARG:NH1	2.00	0.77
1:B:278:ILE:HD11	1:D:470:LYS:HZ3	1.46	0.77
1:E:497:SER:HB2	5:E:822:HOH:O	1.83	0.77
1:B:388:LYS:H	1:B:388:LYS:HD2	1.49	0.76
1:D:547:GLU:HG3	1:D:551:ARG:NH1	2.00	0.76
1:A:281:ARG:HH11	1:C:463:ASN:ND2	1.82	0.76
1:D:317:THR:HG21	1:D:375:ASP:HA	1.65	0.76
1:E:571:ILE:HB	1:E:572:PRO:HD3	1.65	0.76
1:B:385:SER:HA	1:B:391:MET:HG3	1.68	0.76
1:G:278:ILE:HD12	1:G:283:LEU:HD12	1.68	0.76
1:G:302:ALA:HB3	1:G:324:VAL:HG12	1.68	0.76
1:B:281:ARG:HH21	1:D:463:ASN:HD22	1.34	0.75
1:D:603:ARG:HG3	1:D:603:ARG:HH11	1.51	0.75
1:D:571:ILE:HG23	1:D:603:ARG:NH1	2.02	0.75
1:D:547:GLU:HG3	1:D:551:ARG:HH12	1.52	0.74
1:H:468:GLU:OE2	1:H:506:LYS:HE3	1.87	0.74
1:G:286:SER:HB2	1:G:427:PRO:HG2	1.68	0.74
1:C:571:ILE:CG2	1:C:603:ARG:HH12	2.00	0.73
1:E:366:PRO:HD2	1:E:541:GLU:HG2	1.70	0.73
1:B:542:PHE:HE1	2:B:701:WYQ:C16	2.01	0.73
1:H:501:PHE:N	5:H:817:HOH:O	2.20	0.73
1:F:366:PRO:HD2	1:F:541:GLU:HG2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:PRO:O	1:C:556:VAL:HB	1.89	0.72
1:A:463:ASN:HD22	1:C:281:ARG:HH21	1.38	0.72
1:H:492:HIS:HB2	1:H:584:LEU:HD21	1.71	0.72
1:E:571:ILE:HG23	1:E:603:ARG:NH1	2.06	0.71
1:G:571:ILE:HG23	1:G:603:ARG:HH12	1.52	0.71
1:E:376:VAL:HG22	1:E:521:ASP:HA	1.73	0.71
1:B:500:GLY:O	1:B:501:PHE:HB2	1.89	0.70
1:E:396:PRO:O	1:E:400:LYS:HG3	1.91	0.70
1:C:567:GLU:HG2	1:C:609:LYS:HD2	1.73	0.70
1:E:504:THR:HG21	5:H:858:HOH:O	1.90	0.70
1:C:372:HIS:CE1	1:C:521:ASP:OD2	2.43	0.70
1:C:302:ALA:HB3	1:C:324:VAL:HG12	1.73	0.69
1:G:278:ILE:HD12	1:G:283:LEU:CD1	2.21	0.69
1:E:310:LEU:HD22	1:E:334:HIS:CD2	2.27	0.69
1:B:289:GLN:NE2	1:B:292:ILE:HD11	2.06	0.69
1:C:577:PHE:CZ	2:C:701:WYQ:H2	2.27	0.69
1:G:319:GLU:HG2	1:G:323:ARG:NH2	2.06	0.69
1:B:542:PHE:CE1	2:B:701:WYQ:H2	2.24	0.69
1:D:366:PRO:HD2	1:D:541:GLU:HG2	1.75	0.69
1:E:289:GLN:HB2	1:E:363:ARG:HH21	1.58	0.69
1:A:319:GLU:O	1:A:322:SER:HB3	1.93	0.69
1:D:324:VAL:HG22	1:D:325:PRO:HD2	1.75	0.69
1:E:463:ASN:HD22	1:G:281:ARG:NH1	1.90	0.69
1:F:376:VAL:HG22	1:F:521:ASP:HA	1.74	0.69
1:E:569:SER:O	1:E:572:PRO:HD2	1.93	0.68
1:B:278:ILE:HG23	1:B:281:ARG:HB2	1.75	0.68
1:F:278:ILE:HD13	1:F:430:PHE:HB2	1.75	0.68
1:E:603:ARG:HG3	1:E:603:ARG:HH11	1.58	0.68
1:G:505:CYS:SG	1:G:507:GLU:HG2	2.33	0.68
1:E:317:THR:HG21	1:E:375:ASP:HA	1.75	0.68
1:G:366:PRO:HD2	1:G:541:GLU:HG2	1.76	0.68
1:A:310:LEU:HD22	1:A:334:HIS:CG	2.29	0.68
1:G:320:VAL:HA	1:G:323:ARG:HH12	1.58	0.68
1:A:393:HIS:HE1	1:G:393:HIS:HE1	1.42	0.68
1:C:571:ILE:HB	1:C:572:PRO:HD3	1.75	0.68
1:D:324:VAL:CG2	1:D:325:PRO:HD2	2.24	0.68
1:G:388:LYS:O	1:G:392:GLU:HG2	1.94	0.68
1:E:288:VAL:HG11	1:E:441:LEU:HD21	1.76	0.67
1:E:482:MET:HG3	2:E:701:WYQ:O3	1.94	0.67
1:H:358:VAL:HG11	1:H:407:LEU:CD2	2.24	0.67
1:B:333:MET:HG2	5:B:898:HOH:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:407:LEU:HD22	1:H:408:THR:HG23	1.75	0.67
1:B:306:THR:HG22	1:B:308:VAL:H	1.59	0.66
1:B:385:SER:HA	1:B:391:MET:CG	2.25	0.66
1:E:304:ILE:HD11	1:E:310:LEU:HD21	1.75	0.66
1:A:451:ASN:HD21	1:C:278:ILE:HG12	1.60	0.66
1:F:458:THR:O	1:F:461:MET:HB2	1.95	0.66
1:G:577:PHE:HE2	2:G:701:WYQ:H2	1.56	0.66
1:E:286:SER:HB2	1:E:427:PRO:HG2	1.78	0.65
1:E:447:PHE:CZ	1:E:470:LYS:HG3	2.31	0.65
1:E:538:ILE:HG12	2:E:701:WYQ:H12	1.77	0.65
1:F:500:GLY:O	1:F:501:PHE:HB2	1.96	0.65
1:G:595:PRO:O	1:G:599:LEU:HD22	1.94	0.65
1:H:578:VAL:HG12	1:H:599:LEU:HD21	1.78	0.65
1:B:366:PRO:HD2	1:B:541:GLU:HG2	1.77	0.65
2:D:701:WYQ:H1	2:D:701:WYQ:O3	1.96	0.64
1:A:306:THR:HG22	1:A:307:ASP:N	2.11	0.64
1:B:278:ILE:N	1:B:278:ILE:HD12	2.13	0.64
1:B:300:SER:CB	1:B:325:PRO:HG3	2.22	0.64
1:G:603:ARG:NE	5:G:926:HOH:O	2.30	0.64
1:B:278:ILE:CD1	1:D:470:LYS:NZ	2.60	0.64
1:H:358:VAL:HG11	1:H:407:LEU:HD23	1.78	0.64
1:A:505:CYS:SG	1:A:507:GLU:HG2	2.38	0.64
1:F:278:ILE:HD13	1:F:430:PHE:CB	2.28	0.64
1:G:558:PRO:O	1:H:587:GLN:O	2.16	0.63
1:H:344:SER:OG	1:H:347:GLU:HG3	1.98	0.63
1:G:571:ILE:HB	1:G:572:PRO:HD3	1.80	0.63
1:C:396:PRO:O	1:C:400:LYS:HG3	1.98	0.63
1:G:331:VAL:O	1:G:335:VAL:HG13	1.99	0.63
1:H:310:LEU:HD12	1:H:334:HIS:CE1	2.34	0.63
1:B:296:VAL:HG13	1:B:297:PRO:HD2	1.81	0.63
1:C:594:GLU:HB3	1:C:595:PRO:HD3	1.81	0.62
1:D:327:VAL:O	1:D:331:VAL:HG23	1.99	0.62
1:H:571:ILE:HB	1:H:572:PRO:HD3	1.82	0.62
1:B:575:ASP:OD1	1:B:603:ARG:NH1	2.32	0.62
1:D:525:SER:HB3	5:D:851:HOH:O	2.00	0.62
1:F:281:ARG:HH11	1:H:463:ASN:HD22	1.48	0.62
1:D:321:ALA:HA	1:D:327:VAL:CG2	2.29	0.62
1:B:279:SER:HB3	1:D:451:ASN:HD21	1.65	0.61
1:B:458:THR:O	1:B:461:MET:HB2	2.00	0.61
1:E:550:ARG:C	1:E:552:ARG:H	2.07	0.61
1:F:281:ARG:HH11	1:H:463:ASN:ND2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:469:PHE:O	1:F:473:VAL:HG23	2.01	0.61
1:B:278:ILE:CG1	1:B:430:PHE:HB3	2.23	0.61
1:B:376:VAL:HG22	1:B:521:ASP:HA	1.83	0.61
1:E:324:VAL:CG2	1:E:325:PRO:HD2	2.30	0.61
1:C:504:THR:HG21	5:D:840:HOH:O	2.01	0.61
1:E:354:LEU:HG	1:E:455:PHE:HB3	1.83	0.61
1:A:366:PRO:HD2	1:A:541:GLU:HG2	1.83	0.61
1:H:280:THR:HG22	1:H:281:ARG:H	1.65	0.61
1:A:308:VAL:HG23	5:A:934:HOH:O	2.00	0.61
1:G:571:ILE:CG2	1:G:603:ARG:HH12	2.13	0.61
1:F:571:ILE:HB	1:F:572:PRO:HD3	1.82	0.60
1:B:277:MET:CB	1:D:451:ASN:HB2	2.30	0.60
1:F:372:HIS:CE1	1:F:521:ASP:OD2	2.55	0.60
1:G:505:CYS:HG	1:G:507:GLU:HG2	1.65	0.60
1:H:500:GLY:O	1:H:501:PHE:HB2	2.01	0.60
1:B:278:ILE:CD1	1:D:470:LYS:HZ3	2.13	0.60
1:H:388:LYS:HE3	1:H:392:GLU:OE2	2.01	0.60
2:A:701:WYQ:H5	2:A:701:WYQ:O5	2.00	0.60
1:E:470:LYS:HG2	1:G:433:SER:OG	2.01	0.60
1:B:289:GLN:HE21	1:B:292:ILE:HD11	1.65	0.60
1:E:327:VAL:O	1:E:331:VAL:HG23	2.02	0.60
1:E:424:VAL:HG12	1:E:424:VAL:O	2.02	0.60
1:A:280:THR:HB	5:A:937:HOH:O	2.01	0.60
1:H:320:VAL:O	1:H:324:VAL:HG22	2.02	0.59
1:B:502:ASP:CG	1:B:504:THR:HG22	2.27	0.59
1:F:278:ILE:CG2	1:F:430:PHE:HB3	2.22	0.59
1:H:376:VAL:HG21	1:H:409:HIS:CE1	2.37	0.59
1:D:571:ILE:HB	1:D:572:PRO:HD3	1.83	0.59
1:H:304:ILE:HG12	1:H:310:LEU:HD21	1.84	0.59
1:D:376:VAL:HG21	1:D:409:HIS:CE1	2.38	0.59
1:E:328:LEU:HD21	1:E:407:LEU:CD1	2.32	0.59
1:E:492:HIS:HB3	1:E:584:LEU:HD11	1.84	0.59
1:E:376:VAL:HG21	1:E:409:HIS:CE1	2.37	0.58
1:D:584:LEU:HD13	1:D:588:LEU:HD12	1.85	0.58
1:E:591:SER:HB3	5:E:819:HOH:O	2.04	0.58
1:A:505:CYS:HG	1:A:507:GLU:HG2	1.69	0.58
1:D:424:VAL:HG12	1:D:424:VAL:O	2.03	0.58
1:E:608:ALA:O	1:E:609:LYS:C	2.46	0.58
1:F:584:LEU:C	1:F:584:LEU:HD13	2.29	0.57
1:G:506:LYS:HG3	5:G:902:HOH:O	2.03	0.57
1:D:344:SER:HB2	1:D:347:GLU:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:280:THR:HG22	1:H:281:ARG:N	2.19	0.57
1:D:327:VAL:HG23	5:D:826:HOH:O	2.04	0.57
1:D:441:LEU:HD23	1:D:441:LEU:C	2.29	0.57
1:F:397:LEU:O	1:F:397:LEU:HD23	2.04	0.57
1:B:277:MET:HB3	1:D:451:ASN:HB2	1.86	0.57
1:E:524:ALA:HA	1:E:527:ARG:HD2	1.85	0.57
1:G:319:GLU:O	1:G:322:SER:HB2	2.05	0.57
1:H:571:ILE:HG23	1:H:603:ARG:NH1	2.20	0.57
1:A:393:HIS:HE1	1:G:393:HIS:CE1	2.21	0.57
1:B:363:ARG:HA	1:B:363:ARG:HH11	1.68	0.57
1:C:302:ALA:HB3	1:C:324:VAL:CG1	2.34	0.57
1:C:584:LEU:HD13	1:C:588:LEU:HD12	1.87	0.57
1:F:363:ARG:HH11	1:F:363:ARG:HA	1.68	0.57
1:F:550:ARG:HB2	1:F:550:ARG:NH1	2.20	0.57
1:D:548:ASP:O	1:D:552:ARG:HG3	2.04	0.57
1:E:526:SER:HB2	1:E:599:LEU:CD2	2.34	0.57
1:G:283:LEU:HB3	1:G:284:PRO:HD2	1.86	0.57
1:B:505:CYS:SG	1:B:507:GLU:HG2	2.45	0.56
1:E:397:LEU:HB2	5:E:839:HOH:O	2.04	0.56
1:F:282:ARG:NH2	5:F:870:HOH:O	2.37	0.56
1:E:526:SER:HB2	1:E:599:LEU:HD22	1.86	0.56
1:H:537:VAL:HG12	1:H:540:GLN:NE2	2.20	0.56
1:C:555:PRO:O	1:C:556:VAL:CB	2.53	0.56
1:F:282:ARG:HA	5:F:849:HOH:O	2.04	0.56
1:G:354:LEU:HD23	1:G:455:PHE:HB3	1.87	0.56
1:H:304:ILE:HD13	1:H:304:ILE:N	2.17	0.56
1:H:396:PRO:O	1:H:400:LYS:HG3	2.05	0.56
1:C:306:THR:HG22	1:C:307:ASP:N	2.20	0.56
1:A:593:GLU:OE1	1:F:593:GLU:HG3	2.06	0.56
1:E:369:ASN:OD1	1:E:371:ILE:HB	2.06	0.56
1:F:283:LEU:HB3	1:F:284:PRO:HD2	1.88	0.56
1:G:298:PRO:HD3	1:G:353:PHE:CE1	2.41	0.56
1:D:372:HIS:O	1:D:376:VAL:HG23	2.06	0.56
1:E:312:ASP:CG	1:E:314:GLY:H	2.14	0.56
1:A:395:THR:OG1	1:A:398:GLU:HG3	2.05	0.56
1:F:354:LEU:HD23	1:F:455:PHE:HB3	1.87	0.56
1:E:299:LYS:HD2	1:E:326:SER:HB2	1.87	0.56
1:E:316:ASP:O	1:E:320:VAL:HG23	2.06	0.56
1:B:278:ILE:CG2	1:B:283:LEU:HD11	2.32	0.55
1:E:585:LEU:HD23	1:E:585:LEU:O	2.06	0.55
1:B:571:ILE:HB	1:B:572:PRO:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:389:PRO:O	1:G:393:HIS:HD2	1.90	0.55
1:H:354:LEU:HD23	1:H:455:PHE:HB3	1.88	0.55
1:B:283:LEU:HD13	1:B:427:PRO:HA	1.88	0.55
1:C:286:SER:HB2	1:C:427:PRO:CG	2.31	0.55
1:C:333:MET:O	1:C:337:LEU:HG	2.05	0.55
1:B:299:LYS:HG3	5:B:856:HOH:O	2.06	0.55
1:C:395:THR:OG1	1:C:398:GLU:HG3	2.06	0.55
1:B:306:THR:HG22	1:B:307:ASP:N	2.21	0.55
1:F:296:VAL:HG13	1:F:297:PRO:HD2	1.88	0.55
1:E:324:VAL:HG23	1:E:325:PRO:HD2	1.87	0.55
1:B:277:MET:HG2	1:B:278:ILE:H	1.72	0.54
1:B:388:LYS:H	1:B:388:LYS:CD	2.20	0.54
1:E:565:SER:OG	1:E:568:LYS:HG2	2.07	0.54
1:D:320:VAL:O	1:D:324:VAL:HG12	2.07	0.54
1:E:463:ASN:ND2	1:G:281:ARG:NH1	2.50	0.54
1:E:502:ASP:OD2	1:E:504:THR:HB	2.07	0.54
1:G:388:LYS:N	1:G:389:PRO:HD2	2.22	0.54
1:D:372:HIS:CE1	1:D:521:ASP:OD2	2.60	0.54
1:G:575:ASP:OD1	1:G:603:ARG:NH1	2.40	0.54
1:A:389:PRO:O	1:A:393:HIS:HD2	1.90	0.54
1:D:396:PRO:HG2	5:D:820:HOH:O	2.07	0.54
1:D:461:MET:HG2	1:D:465:SER:HB2	1.89	0.54
1:A:281:ARG:HD3	1:C:463:ASN:ND2	2.22	0.54
1:B:278:ILE:HG12	1:B:430:PHE:CB	2.29	0.54
1:B:277:MET:HB2	1:D:447:PHE:O	2.07	0.54
1:H:395:THR:OG1	1:H:398:GLU:HG3	2.08	0.54
1:D:395:THR:OG1	1:D:398:GLU:HG3	2.07	0.53
1:E:336:ALA:O	1:E:341:PHE:HB2	2.07	0.53
1:H:358:VAL:HG21	1:H:407:LEU:HD21	1.90	0.53
1:G:421:LEU:HD11	1:G:438:LEU:HD21	1.91	0.53
1:F:304:ILE:HG13	1:F:310:LEU:HD21	1.89	0.53
1:G:384:VAL:CG1	1:G:391:MET:HE3	2.38	0.53
1:C:500:GLY:O	1:C:501:PHE:HB2	2.08	0.53
2:C:701:WYQ:H5	2:C:701:WYQ:O5	2.09	0.53
1:H:603:ARG:HG3	1:H:603:ARG:NH1	2.21	0.53
1:D:585:LEU:C	1:D:585:LEU:HD23	2.34	0.53
1:E:328:LEU:HD23	1:E:328:LEU:O	2.08	0.53
1:G:385:SER:HA	1:G:391:MET:HG3	1.90	0.53
1:H:306:THR:HG22	1:H:307:ASP:N	2.23	0.53
1:B:463:ASN:HD21	1:D:281:ARG:HD3	1.73	0.53
1:B:585:LEU:C	1:B:585:LEU:HD23	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:VAL:HG21	1:C:409:HIS:CE1	2.44	0.53
1:E:585:LEU:HD23	1:E:585:LEU:C	2.34	0.52
1:G:320:VAL:O	1:G:324:VAL:HG22	2.09	0.52
1:D:306:THR:HG22	1:D:308:VAL:H	1.73	0.52
1:G:391:MET:HE2	1:G:391:MET:HA	1.91	0.52
1:H:504:THR:HG22	5:H:827:HOH:O	2.10	0.52
1:F:321:ALA:HB2	1:F:327:VAL:HG21	1.91	0.52
1:B:278:ILE:HA	1:B:281:ARG:HG2	1.92	0.52
1:B:397:LEU:HD23	1:B:397:LEU:C	2.35	0.52
1:G:397:LEU:HD23	1:G:397:LEU:C	2.34	0.52
1:A:458:THR:O	1:A:461:MET:HB2	2.09	0.52
1:F:344:SER:OG	1:F:347:GLU:HG3	2.10	0.52
1:A:593:GLU:HG2	1:A:597:HIS:CD2	2.44	0.52
1:A:391:MET:HE2	1:A:391:MET:HA	1.92	0.52
1:B:441:LEU:C	1:B:441:LEU:HD13	2.35	0.52
1:H:407:LEU:HD23	1:H:407:LEU:C	2.35	0.52
1:B:278:ILE:HG22	1:B:278:ILE:O	2.08	0.51
1:C:366:PRO:HD2	1:C:541:GLU:HG2	1.93	0.51
1:C:388:LYS:O	1:C:392:GLU:HG3	2.09	0.51
1:C:598:ASN:HB3	5:C:874:HOH:O	2.11	0.51
1:D:328:LEU:HD21	1:D:407:LEU:HD13	1.91	0.51
1:G:603:ARG:CZ	5:G:926:HOH:O	2.58	0.51
1:A:393:HIS:CE1	1:G:393:HIS:HE1	2.25	0.51
1:F:593:GLU:HB3	5:F:842:HOH:O	2.11	0.51
1:A:388:LYS:O	1:A:392:GLU:HG3	2.11	0.51
1:B:424:VAL:HG12	1:B:424:VAL:O	2.10	0.51
1:C:567:GLU:HG2	1:C:609:LYS:CD	2.40	0.51
1:G:354:LEU:HD13	1:G:354:LEU:C	2.36	0.51
1:H:317:THR:HG21	1:H:375:ASP:CA	2.37	0.51
1:B:417:THR:CG2	2:B:701:WYQ:H8	2.19	0.51
1:A:334:HIS:HE1	5:A:933:HOH:O	1.93	0.51
1:D:306:THR:HG22	1:D:307:ASP:N	2.26	0.51
1:B:278:ILE:CG2	1:B:281:ARG:HB2	2.40	0.51
1:F:281:ARG:O	1:F:282:ARG:HB2	2.10	0.51
1:B:396:PRO:O	1:B:400:LYS:HG3	2.11	0.51
1:F:310:LEU:HG	1:F:334:HIS:CD2	2.45	0.51
1:F:385:SER:HA	1:F:391:MET:HG3	1.93	0.51
1:H:531:ILE:HD12	1:H:531:ILE:H	1.76	0.51
1:E:344:SER:OG	1:E:347:GLU:HG3	2.11	0.51
1:G:376:VAL:HG22	1:G:521:ASP:HA	1.92	0.51
1:B:462:ASP:OD1	1:B:463:ASN:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:584:LEU:HD13	1:D:584:LEU:C	2.36	0.50
1:D:603:ARG:HG3	1:D:603:ARG:NH1	2.23	0.50
1:A:597:HIS:HB3	5:F:862:HOH:O	2.11	0.50
1:G:289:GLN:HB3	1:G:363:ARG:HH21	1.76	0.50
2:G:701:WYQ:O2	2:G:701:WYQ:N4	2.44	0.50
1:E:304:ILE:CD1	1:E:310:LEU:HD21	2.39	0.50
1:E:354:LEU:O	1:E:358:VAL:HG23	2.11	0.50
1:F:332:ALA:HA	1:F:377:LEU:HD21	1.93	0.50
1:E:549:GLU:OE2	1:E:556:VAL:HA	2.11	0.50
1:H:315:PHE:CE2	1:H:317:THR:HG22	2.46	0.50
1:A:397:LEU:C	1:A:397:LEU:HD23	2.37	0.50
1:E:538:ILE:HG21	2:E:701:WYQ:C13	2.41	0.50
1:G:602:LEU:HD11	1:G:606:TYR:CZ	2.47	0.50
1:C:310:LEU:HG	1:C:334:HIS:CD2	2.47	0.50
1:C:569:SER:O	1:C:572:PRO:HD2	2.12	0.50
1:E:308:VAL:HG22	1:E:311:ARG:NH2	2.22	0.50
1:F:397:LEU:HD23	1:F:397:LEU:C	2.37	0.50
1:G:304:ILE:HG13	1:G:310:LEU:HD21	1.93	0.50
1:A:306:THR:HG22	1:A:307:ASP:H	1.74	0.50
1:C:492:HIS:HB3	1:C:584:LEU:HD11	1.94	0.50
1:D:502:ASP:OD2	1:D:504:THR:HB	2.12	0.50
1:A:372:HIS:CE1	1:A:521:ASP:OD2	2.65	0.49
1:A:388:LYS:N	1:A:389:PRO:HD2	2.27	0.49
1:B:304:ILE:N	5:B:943:HOH:O	2.45	0.49
1:D:323:ARG:NH1	1:D:323:ARG:HB2	2.26	0.49
1:F:321:ALA:HA	1:F:327:VAL:CG2	2.42	0.49
1:B:368:HIS:CE1	2:B:701:WYQ:H6	2.47	0.49
1:E:545:GLN:NE2	1:E:560:PHE:HE1	2.10	0.49
1:C:584:LEU:CD1	1:C:588:LEU:HD12	2.42	0.49
1:C:320:VAL:O	1:C:324:VAL:HG22	2.10	0.49
1:D:300:SER:O	1:D:301:CYS:HB2	2.12	0.49
1:H:329:GLN:HA	1:H:355:VAL:HG11	1.95	0.49
1:G:452:VAL:HB	1:G:455:PHE:CD2	2.48	0.49
1:D:569:SER:O	1:D:572:PRO:HD2	2.13	0.49
1:G:468:GLU:O	1:G:472:ILE:HG13	2.13	0.49
1:H:603:ARG:HH11	1:H:603:ARG:CG	2.21	0.49
1:G:565:SER:OG	1:G:568:LYS:HG2	2.12	0.49
1:C:302:ALA:CB	1:C:324:VAL:HG12	2.42	0.49
1:G:346:GLU:OE2	1:G:350:LYS:HE3	2.13	0.49
1:D:594:GLU:N	1:D:595:PRO:HD2	2.28	0.49
1:H:310:LEU:HD12	1:H:334:HIS:ND1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:585:LEU:HD21	1:D:592:ILE:HD12	1.94	0.48
1:F:277:MET:O	1:H:466:PHE:HE2	1.96	0.48
1:B:585:LEU:HD23	1:B:585:LEU:O	2.14	0.48
1:F:278:ILE:C	1:F:280:THR:H	2.21	0.48
1:H:358:VAL:HG11	1:H:407:LEU:HD21	1.95	0.48
1:B:417:THR:HG22	2:B:701:WYQ:N5	2.23	0.48
1:C:293:LEU:HD21	1:C:448:GLU:HG2	1.95	0.48
1:C:282:ARG:HD2	1:C:282:ARG:O	2.14	0.48
1:D:571:ILE:CG2	1:D:603:ARG:HH12	2.27	0.48
1:C:388:LYS:N	1:C:389:PRO:HD2	2.29	0.48
1:A:393:HIS:CE1	1:G:393:HIS:CE1	3.00	0.48
1:B:306:THR:HG23	5:B:854:HOH:O	2.14	0.48
1:F:384:VAL:O	1:F:391:MET:HG2	2.14	0.48
1:A:306:THR:CG2	1:A:307:ASP:N	2.77	0.47
1:C:549:GLU:OE2	1:C:556:VAL:HA	2.14	0.47
1:D:302:ALA:O	1:D:304:ILE:N	2.47	0.47
1:D:571:ILE:CG2	1:D:603:ARG:NH1	2.74	0.47
1:A:507:GLU:CD	1:A:507:GLU:H	2.22	0.47
1:C:410:ASP:O	1:C:413:HIS:HB2	2.14	0.47
1:E:299:LYS:HD3	1:E:325:PRO:HB2	1.95	0.47
1:E:411:VAL:O	1:E:412:CYS:HB2	2.14	0.47
1:H:475:HIS:O	1:H:479:HIS:HD2	1.98	0.47
1:G:506:LYS:HG2	1:G:507:GLU:OE2	2.14	0.47
1:G:603:ARG:NH2	5:G:926:HOH:O	2.47	0.47
1:H:500:GLY:N	5:H:817:HOH:O	2.47	0.47
1:A:452:VAL:HB	1:A:455:PHE:CD2	2.48	0.47
1:C:299:LYS:HG3	5:C:853:HOH:O	2.14	0.47
1:D:299:LYS:HD2	1:D:326:SER:HB2	1.96	0.47
1:D:308:VAL:HA	1:D:311:ARG:HH21	1.78	0.47
1:C:299:LYS:HD2	1:C:326:SER:OG	2.15	0.47
1:E:582:PHE:CD2	1:E:595:PRO:HB2	2.49	0.47
1:A:462:ASP:HB2	5:A:891:HOH:O	2.14	0.47
1:E:310:LEU:HD22	1:E:334:HIS:HD2	1.80	0.47
1:G:280:THR:HG22	1:G:280:THR:O	2.14	0.47
1:A:451:ASN:ND2	1:C:278:ILE:HG12	2.27	0.47
2:B:701:WYQ:H10	2:B:701:WYQ:C14	2.45	0.47
1:C:278:ILE:HG13	1:C:279:SER:N	2.30	0.47
1:C:376:VAL:HG22	1:C:521:ASP:HA	1.97	0.47
1:C:397:LEU:C	1:C:397:LEU:HD23	2.39	0.47
1:E:538:ILE:CG1	2:E:701:WYQ:H12	2.45	0.47
1:E:447:PHE:CE1	1:E:470:LYS:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:701:WYQ:H13	2:G:701:WYQ:H11	1.56	0.46
1:H:315:PHE:HE2	1:H:317:THR:HG22	1.79	0.46
1:H:388:LYS:HE3	1:H:392:GLU:CD	2.39	0.46
1:A:492:HIS:HB2	1:A:584:LEU:HD21	1.97	0.46
1:B:306:THR:CG2	1:B:307:ASP:N	2.78	0.46
1:C:363:ARG:NH2	5:C:829:HOH:O	2.48	0.46
1:D:586:HIS:NE2	1:D:593:GLU:HG2	2.30	0.46
1:G:347:GLU:HG2	5:G:830:HOH:O	2.14	0.46
1:H:288:VAL:HG11	1:H:441:LEU:HD11	1.98	0.46
1:H:380:THR:O	1:H:384:VAL:HG23	2.15	0.46
1:G:454:GLU:N	1:G:454:GLU:OE1	2.49	0.46
1:B:325:PRO:HG2	5:B:930:HOH:O	2.15	0.46
1:B:507:GLU:O	1:B:511:GLU:HG3	2.15	0.46
1:D:304:ILE:HD12	1:D:315:PHE:HZ	1.80	0.46
1:D:410:ASP:O	1:D:413:HIS:HB2	2.14	0.46
1:E:306:THR:HG22	1:E:307:ASP:N	2.30	0.46
1:G:397:LEU:HD23	1:G:397:LEU:O	2.16	0.46
1:H:388:LYS:O	1:H:392:GLU:HG3	2.16	0.46
1:C:304:ILE:HG13	1:C:310:LEU:HD21	1.96	0.46
1:H:299:LYS:HD3	1:H:325:PRO:HB2	1.97	0.46
1:A:281:ARG:NH1	1:C:463:ASN:HD22	2.05	0.46
1:C:463:ASN:HD22	1:C:463:ASN:HA	1.54	0.46
1:D:492:HIS:HB3	1:D:584:LEU:HD11	1.97	0.46
1:E:331:VAL:O	1:E:335:VAL:HG22	2.16	0.46
1:H:306:THR:HG22	1:H:307:ASP:H	1.81	0.46
1:A:564:SER:HB2	1:D:600:ARG:HH21	1.81	0.46
1:B:372:HIS:CE1	1:B:521:ASP:OD2	2.69	0.46
1:E:315:PHE:HE2	1:E:317:THR:HG22	1.81	0.46
1:A:391:MET:HA	1:A:391:MET:CE	2.46	0.46
1:B:538:ILE:HD11	2:B:701:WYQ:H3	1.97	0.46
1:D:320:VAL:C	1:D:322:SER:H	2.24	0.46
1:D:583:ASP:HA	1:D:596:LEU:HD22	1.97	0.46
1:F:376:VAL:HG21	1:F:521:ASP:OD2	2.16	0.46
1:H:600:ARG:NE	5:H:836:HOH:O	2.44	0.46
1:E:329:GLN:HE21	1:E:329:GLN:HB2	1.52	0.46
1:F:277:MET:O	1:F:278:ILE:HG23	2.15	0.46
1:C:577:PHE:CE2	2:C:701:WYQ:H2	2.51	0.45
1:D:350:LYS:HD3	1:D:456:ASP:O	2.16	0.45
1:B:319:GLU:O	1:B:322:SER:HB2	2.16	0.45
1:B:396:PRO:HG2	5:B:858:HOH:O	2.16	0.45
1:D:315:PHE:HE2	1:D:317:THR:HG22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:585:LEU:HD23	1:D:585:LEU:O	2.17	0.45
1:E:281:ARG:HH11	1:G:463:ASN:HD22	1.63	0.45
1:F:351:TRP:O	1:F:355:VAL:HG23	2.16	0.45
1:G:316:ASP:CG	1:G:319:GLU:HB2	2.41	0.45
1:C:452:VAL:HB	1:C:455:PHE:CD2	2.52	0.45
1:E:351:TRP:O	1:E:355:VAL:HG23	2.15	0.45
1:E:571:ILE:CB	1:E:572:PRO:HD3	2.39	0.45
1:B:521:ASP:OD2	1:B:521:ASP:O	2.34	0.45
1:D:481:ASP:CG	1:D:483:SER:HB3	2.42	0.45
1:B:278:ILE:HG23	1:B:281:ARG:CB	2.44	0.45
1:B:320:VAL:O	1:B:324:VAL:HG12	2.17	0.45
1:E:286:SER:HB2	1:E:427:PRO:CG	2.45	0.45
1:F:439:GLU:HG2	1:F:481:ASP:HB2	1.98	0.45
1:G:585:LEU:C	1:G:585:LEU:HD23	2.41	0.45
1:A:594:GLU:HB3	1:A:595:PRO:HD3	1.99	0.45
1:D:351:TRP:O	1:D:355:VAL:HG23	2.16	0.45
1:G:585:LEU:HD23	1:G:585:LEU:O	2.16	0.45
1:C:421:LEU:HD11	1:C:438:LEU:HD21	1.99	0.45
1:E:561:GLU:O	1:E:562:THR:C	2.59	0.45
1:H:411:VAL:O	1:H:412:CYS:HB2	2.17	0.45
1:E:287:ILE:HD11	1:E:421:LEU:HD21	1.98	0.45
1:G:367:TYR:CD1	1:G:538:ILE:HB	2.51	0.45
1:D:354:LEU:HG	1:D:455:PHE:HB3	1.98	0.45
1:G:376:VAL:HG21	1:G:409:HIS:CE1	2.52	0.45
1:H:537:VAL:O	1:H:540:GLN:HB2	2.16	0.45
2:H:701:WYQ:H11	2:H:701:WYQ:H13	1.54	0.45
1:D:388:LYS:N	1:D:389:PRO:HD2	2.32	0.45
1:D:550:ARG:C	1:D:552:ARG:H	2.25	0.45
1:C:484:LEU:O	1:C:488:THR:HG23	2.17	0.44
1:D:317:THR:HG21	1:D:375:ASP:CA	2.40	0.44
1:D:436:GLY:HA2	1:D:439:GLU:OE1	2.17	0.44
1:E:395:THR:OG1	1:E:398:GLU:HG3	2.17	0.44
1:F:354:LEU:HD13	1:F:354:LEU:C	2.43	0.44
1:G:278:ILE:CD1	1:G:430:PHE:HB2	2.46	0.44
1:H:341:PHE:CZ	1:H:400:LYS:HA	2.53	0.44
1:A:585:LEU:C	1:A:585:LEU:HD23	2.41	0.44
1:E:320:VAL:HG12	1:E:320:VAL:O	2.17	0.44
1:E:340:ASP:OD1	1:E:340:ASP:O	2.35	0.44
1:B:278:ILE:HD11	1:D:470:LYS:HZ2	1.79	0.44
1:C:323:ARG:HB2	1:C:324:VAL:H	1.62	0.44
1:C:354:LEU:HD13	1:C:455:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:701:WYQ:H11	2:C:701:WYQ:H12	1.70	0.44
1:D:502:ASP:C	1:D:504:THR:H	2.25	0.44
1:E:463:ASN:HD22	1:E:463:ASN:HA	1.56	0.44
1:E:546:ALA:HA	1:E:549:GLU:OE2	2.17	0.44
1:G:354:LEU:HD23	1:G:455:PHE:CB	2.48	0.44
1:D:367:TYR:CD1	1:D:538:ILE:HB	2.52	0.44
1:F:331:VAL:O	1:F:335:VAL:HG13	2.17	0.44
1:F:385:SER:HA	1:F:391:MET:CG	2.48	0.44
1:G:300:SER:HB3	1:G:325:PRO:HG3	1.99	0.44
1:D:328:LEU:HD21	1:D:407:LEU:CD1	2.47	0.44
1:E:594:GLU:N	1:E:595:PRO:HD2	2.33	0.44
1:E:603:ARG:HH11	1:E:603:ARG:CG	2.27	0.44
1:F:417:THR:HG21	2:F:701:WYQ:O5	2.18	0.44
1:F:425:GLN:HE21	1:H:464:ALA:HB2	1.83	0.44
1:G:594:GLU:HB3	1:G:595:PRO:HD3	1.99	0.44
1:H:310:LEU:HD12	1:H:334:HIS:CG	2.53	0.44
2:H:701:WYQ:O2	2:H:701:WYQ:N4	2.48	0.44
1:F:345:GLN:O	1:F:345:GLN:NE2	2.49	0.44
1:G:501:PHE:CE1	1:G:588:LEU:HD13	2.52	0.44
1:G:521:ASP:OD2	1:G:521:ASP:C	2.60	0.44
1:B:410:ASP:O	1:B:413:HIS:HB2	2.17	0.44
1:D:318:PHE:O	1:D:321:ALA:HB3	2.17	0.44
1:E:281:ARG:HH11	1:G:463:ASN:ND2	2.16	0.44
1:H:441:LEU:C	1:H:441:LEU:HD23	2.43	0.44
1:A:376:VAL:HG22	1:A:521:ASP:HA	2.00	0.44
1:D:324:VAL:HG22	1:D:325:PRO:CD	2.44	0.44
1:E:319:GLU:OE1	1:E:323:ARG:NH2	2.51	0.44
1:E:328:LEU:HD22	1:E:355:VAL:CG1	2.48	0.44
1:F:278:ILE:C	1:F:280:THR:N	2.75	0.44
1:F:281:ARG:HD3	1:H:463:ASN:ND2	2.32	0.44
1:G:281:ARG:HG2	1:G:283:LEU:HD21	2.00	0.44
1:H:603:ARG:NH1	1:H:603:ARG:CG	2.81	0.44
1:B:334:HIS:HE1	5:B:847:HOH:O	2.01	0.43
1:B:313:TRP:CZ3	1:B:383:LEU:HG	2.53	0.43
1:D:475:HIS:O	1:D:479:HIS:HD2	2.02	0.43
1:B:277:MET:HB2	1:D:451:ASN:HB2	2.00	0.43
1:D:298:PRO:O	1:D:299:LYS:HG3	2.17	0.43
1:A:304:ILE:HG22	1:A:324:VAL:HG11	2.00	0.43
1:B:278:ILE:CD1	1:D:470:LYS:HZ2	2.29	0.43
1:E:315:PHE:CD2	1:E:378:GLN:HG3	2.53	0.43
1:H:333:MET:O	1:H:337:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ILE:HG23	1:B:281:ARG:HG3	1.99	0.43
1:B:302:ALA:HB3	1:B:324:VAL:HG23	2.01	0.43
1:D:303:ALA:C	1:D:305:GLY:H	2.27	0.43
1:E:319:GLU:C	1:E:321:ALA:H	2.26	0.43
1:E:326:SER:OG	1:E:329:GLN:HB2	2.17	0.43
1:E:570:GLN:O	1:E:571:ILE:C	2.62	0.43
1:G:310:LEU:HG	1:G:334:HIS:CD2	2.53	0.43
1:B:507:GLU:CD	1:B:507:GLU:H	2.26	0.43
1:D:561:GLU:O	1:D:562:THR:C	2.61	0.43
1:E:388:LYS:HE3	1:E:392:GLU:OE2	2.18	0.43
1:C:533:ARG:HH22	1:C:567:GLU:HG3	1.84	0.43
1:F:277:MET:HB3	1:F:278:ILE:H	1.50	0.43
1:F:411:VAL:O	1:F:412:CYS:HB2	2.18	0.43
1:C:585:LEU:C	1:C:585:LEU:HD23	2.44	0.43
1:D:304:ILE:HD12	1:D:315:PHE:CZ	2.54	0.43
1:F:594:GLU:HB3	1:F:595:PRO:HD3	2.01	0.43
1:H:426:ASP:OD1	1:H:428:VAL:HG22	2.19	0.43
1:A:316:ASP:CG	1:A:319:GLU:HB2	2.44	0.43
1:B:500:GLY:O	1:B:501:PHE:CB	2.63	0.43
1:B:506:LYS:NZ	1:B:506:LYS:HB3	2.34	0.43
1:C:485:HIS:O	1:C:489:VAL:HG23	2.19	0.43
1:E:579:ILE:N	1:E:580:PRO:HD2	2.33	0.43
1:F:277:MET:O	1:H:466:PHE:CE2	2.72	0.43
1:H:366:PRO:HD2	1:H:541:GLU:HG2	2.01	0.43
1:C:438:LEU:O	1:C:441:LEU:HB3	2.19	0.42
1:E:295:VAL:HG22	1:E:455:PHE:CZ	2.54	0.42
1:E:463:ASN:OD1	1:G:283:LEU:HD23	2.19	0.42
2:G:701:WYQ:H22	2:G:701:WYQ:H3	2.00	0.42
1:H:599:LEU:HD12	1:H:599:LEU:HA	1.91	0.42
1:B:417:THR:CG2	2:B:701:WYQ:H4	2.42	0.42
1:B:424:VAL:O	1:B:424:VAL:CG1	2.67	0.42
1:D:288:VAL:HG11	1:D:441:LEU:HD11	2.00	0.42
1:B:314:GLY:O	1:B:315:PHE:C	2.62	0.42
1:C:306:THR:O	1:C:309:ASP:HB2	2.19	0.42
1:E:328:LEU:HD21	1:E:407:LEU:HD13	2.01	0.42
1:E:390:LEU:O	1:E:394:LEU:HG	2.20	0.42
1:F:319:GLU:O	1:F:322:SER:HB2	2.19	0.42
1:A:385:SER:HA	1:A:391:MET:HG3	2.01	0.42
1:D:323:ARG:NH1	1:D:323:ARG:CB	2.83	0.42
2:F:701:WYQ:O2	2:F:701:WYQ:N4	2.48	0.42
1:G:535:TRP:C	1:G:537:VAL:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:423:ALA:HB1	1:H:554:LEU:HD13	2.00	0.42
1:B:278:ILE:HG23	1:B:281:ARG:CG	2.49	0.42
1:B:363:ARG:HH11	1:B:363:ARG:CA	2.32	0.42
1:B:575:ASP:CG	1:B:603:ARG:NH1	2.77	0.42
1:F:296:VAL:CG1	1:F:297:PRO:HD2	2.50	0.42
1:F:435:LYS:HD3	5:F:905:HOH:O	2.19	0.42
1:H:531:ILE:HD12	1:H:531:ILE:N	2.35	0.42
2:B:701:WYQ:H14	5:B:872:HOH:O	2.20	0.42
1:D:549:GLU:OE2	1:D:556:VAL:HA	2.19	0.42
1:E:372:HIS:HA	1:E:535:TRP:CH2	2.55	0.42
1:E:447:PHE:CD2	1:E:470:LYS:HE3	2.55	0.42
1:G:424:VAL:O	1:G:424:VAL:HG12	2.19	0.42
1:G:439:GLU:HG2	1:G:481:ASP:HB2	2.01	0.42
1:A:351:TRP:O	1:A:355:VAL:HG23	2.18	0.42
1:G:277:MET:O	1:G:278:ILE:HG13	2.19	0.42
1:H:557:THR:HG23	1:H:558:PRO:HD2	2.02	0.42
2:B:701:WYQ:O2	2:B:701:WYQ:N4	2.51	0.42
1:E:537:VAL:O	1:E:540:GLN:HB3	2.20	0.42
1:G:411:VAL:O	1:G:412:CYS:HB2	2.20	0.42
1:D:366:PRO:HD2	1:D:541:GLU:CG	2.48	0.42
1:D:461:MET:HG2	1:D:465:SER:CB	2.49	0.42
1:E:333:MET:O	1:E:337:LEU:HB2	2.20	0.42
1:F:321:ALA:CA	1:F:327:VAL:CG2	2.97	0.42
1:H:354:LEU:O	1:H:358:VAL:HG23	2.20	0.42
1:H:567:GLU:CD	1:H:567:GLU:H	2.27	0.42
1:A:372:HIS:O	1:A:376:VAL:HG23	2.20	0.42
1:B:354:LEU:O	1:B:358:VAL:HG23	2.19	0.42
2:B:701:WYQ:H10	2:B:701:WYQ:O5	2.20	0.42
1:C:351:TRP:O	1:C:355:VAL:HG23	2.19	0.42
1:C:600:ARG:NE	5:C:834:HOH:O	2.52	0.42
1:E:475:HIS:O	1:E:479:HIS:HD2	2.02	0.42
1:G:328:LEU:HD23	1:G:374:ALA:HA	2.01	0.42
1:H:502:ASP:OD2	1:H:504:THR:HB	2.18	0.42
1:C:439:GLU:H	1:C:439:GLU:CD	2.28	0.41
1:D:304:ILE:HB	1:D:320:VAL:HG11	2.02	0.41
1:D:320:VAL:HG22	1:D:323:ARG:HH21	1.85	0.41
1:G:426:ASP:OD1	1:G:428:VAL:HG23	2.20	0.41
1:H:388:LYS:N	1:H:389:PRO:HD2	2.34	0.41
2:A:701:WYQ:H21	1:D:497:SER:HA	2.02	0.41
1:D:439:GLU:CD	1:D:439:GLU:H	2.28	0.41
1:G:281:ARG:O	1:G:282:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:315:PHE:CD2	1:G:378:GLN:HG3	2.55	0.41
1:H:367:TYR:OH	2:H:701:WYQ:H14	2.20	0.41
1:H:463:ASN:HD22	1:H:463:ASN:HA	1.59	0.41
1:A:367:TYR:OH	2:A:701:WYQ:H14	2.21	0.41
1:D:452:VAL:HB	1:D:455:PHE:CD2	2.56	0.41
1:F:325:PRO:HG2	5:F:917:HOH:O	2.19	0.41
1:D:367:TYR:OH	2:D:701:WYQ:H14	2.20	0.41
1:D:376:VAL:HG21	1:D:409:HIS:HE1	1.85	0.41
1:H:313:TRP:O	1:H:527:ARG:HG2	2.20	0.41
1:A:367:TYR:CD1	1:A:538:ILE:HB	2.55	0.41
1:B:424:VAL:CG1	5:B:822:HOH:O	2.68	0.41
2:B:701:WYQ:H11	2:B:701:WYQ:H13	1.62	0.41
1:C:407:LEU:HD12	1:C:407:LEU:O	2.19	0.41
1:D:573:PHE:O	1:D:577:PHE:HB2	2.21	0.41
1:E:546:ALA:HB2	1:E:560:PHE:HB3	2.02	0.41
1:F:533:ARG:HG2	5:F:907:HOH:O	2.20	0.41
1:F:583:ASP:HA	1:F:596:LEU:HD22	2.03	0.41
1:D:329:GLN:HA	1:D:355:VAL:HG11	2.02	0.41
2:F:701:WYQ:O5	2:F:701:WYQ:H5	2.20	0.41
1:H:407:LEU:HD22	1:H:408:THR:CG2	2.45	0.41
1:A:306:THR:CG2	1:A:307:ASP:H	2.34	0.41
1:C:513:LEU:HD23	1:C:513:LEU:HA	1.95	0.41
1:D:315:PHE:CE2	1:D:317:THR:HG22	2.55	0.41
1:E:524:ALA:HB1	1:E:535:TRP:CD1	2.56	0.41
1:B:594:GLU:HB3	1:B:595:PRO:HD3	2.02	0.41
1:D:507:GLU:O	1:D:511:GLU:HG3	2.21	0.41
1:E:319:GLU:C	1:E:321:ALA:N	2.78	0.41
1:A:283:LEU:HB3	1:A:284:PRO:HD2	2.03	0.41
1:A:435:LYS:HE2	1:A:483:SER:OG	2.21	0.41
1:G:310:LEU:HG	1:G:334:HIS:CE1	2.56	0.41
1:H:579:ILE:N	1:H:580:PRO:HD2	2.35	0.41
1:H:597:HIS:O	1:H:601:LYS:HG3	2.21	0.41
1:E:570:GLN:O	1:E:573:PHE:N	2.53	0.41
1:F:507:GLU:O	1:F:511:GLU:HG3	2.20	0.41
1:B:336:ALA:HB1	1:B:342:PHE:CE2	2.56	0.40
1:F:319:GLU:OE2	1:F:319:GLU:C	2.63	0.40
1:G:328:LEU:HD13	1:G:355:VAL:HG13	2.03	0.40
1:H:571:ILE:CG2	1:H:603:ARG:NH1	2.83	0.40
1:B:602:LEU:HD11	1:B:606:TYR:CZ	2.57	0.40
1:G:389:PRO:HA	1:G:392:GLU:CG	2.51	0.40
1:A:328:LEU:HA	1:A:374:ALA:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:VAL:O	1:B:412:CYS:HB2	2.21	0.40
1:C:363:ARG:HA	1:C:363:ARG:HD3	1.87	0.40
1:C:526:SER:HB3	1:C:599:LEU:HD21	2.03	0.40
1:C:582:PHE:CD2	1:C:595:PRO:HB3	2.56	0.40
1:D:391:MET:HA	1:D:391:MET:HE2	2.03	0.40
1:A:306:THR:O	1:A:309:ASP:HB2	2.21	0.40
1:D:320:VAL:C	1:D:322:SER:N	2.79	0.40
2:D:701:WYQ:H1	2:D:701:WYQ:S1	2.62	0.40
2:D:701:WYQ:O2	2:D:701:WYQ:N4	2.51	0.40
1:E:388:LYS:N	1:E:389:PRO:HD2	2.36	0.40
1:E:585:LEU:HD21	1:E:592:ILE:HD12	2.03	0.40
1:F:526:SER:HA	1:F:599:LEU:HD13	2.03	0.40
1:A:444:ALA:O	1:A:448:GLU:HG3	2.21	0.40
1:C:462:ASP:HB3	1:C:465:SER:H	1.87	0.40
1:E:289:GLN:CB	1:E:363:ARG:HH21	2.30	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	330/345 (96%)	325 (98%)	4 (1%)	1 (0%)	36	41
1	B	332/345 (96%)	319 (96%)	9 (3%)	4 (1%)	10	8
1	C	331/345 (96%)	308 (93%)	18 (5%)	5 (2%)	8	6
1	D	329/345 (95%)	309 (94%)	14 (4%)	6 (2%)	6	4
1	E	329/345 (95%)	302 (92%)	19 (6%)	8 (2%)	4	2
1	F	332/345 (96%)	319 (96%)	11 (3%)	2 (1%)	21	22
1	G	332/345 (96%)	315 (95%)	13 (4%)	4 (1%)	10	8
1	H	328/345 (95%)	308 (94%)	18 (6%)	2 (1%)	21	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2643/2760 (96%)	2505 (95%)	106 (4%)	32 (1%)	10 8

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	609	LYS
1	C	304	ILE
1	D	298	PRO
1	D	558	PRO
1	E	300	SER
1	E	301	CYS
1	E	303	ALA
1	E	341	PHE
1	F	558	PRO
1	G	279	SER
1	G	304	ILE
1	C	302	ALA
1	C	556	VAL
1	D	303	ALA
1	E	609	LYS
1	G	303	ALA
1	A	609	LYS
1	B	301	CYS
1	B	485	HIS
1	C	303	ALA
1	C	323	ARG
1	D	503	CYS
1	E	551	ARG
1	E	608	ALA
1	F	278	ILE
1	B	300	SER
1	D	551	ARG
1	E	304	ILE
1	H	456	ASP
1	H	558	PRO
1	D	304	ILE
1	G	558	PRO

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	276/286 (96%)	268 (97%)	8 (3%)	37	48
1	B	278/286 (97%)	269 (97%)	9 (3%)	34	44
1	C	277/286 (97%)	268 (97%)	9 (3%)	34	44
1	D	275/286 (96%)	268 (98%)	7 (2%)	42	54
1	E	275/286 (96%)	268 (98%)	7 (2%)	42	54
1	F	278/286 (97%)	270 (97%)	8 (3%)	37	48
1	G	278/286 (97%)	271 (98%)	7 (2%)	42	54
1	H	275/286 (96%)	267 (97%)	8 (3%)	37	48
All	All	2212/2288 (97%)	2149 (97%)	63 (3%)	38	50

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	LEU
1	A	345	GLN
1	A	391	MET
1	A	425	GLN
1	A	427	PRO
1	A	507	GLU
1	A	533	ARG
1	A	599	LEU
1	B	354	LEU
1	B	388	LYS
1	B	391	MET
1	B	428	VAL
1	B	484	LEU
1	B	506	LYS
1	B	507	GLU
1	B	558	PRO
1	B	599	LEU
1	C	282	ARG
1	C	307	ASP
1	C	328	LEU
1	C	391	MET
1	C	407	LEU
1	C	463	ASN

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Mol	Chain	Res	Type
1	C	504	THR
1	C	558	PRO
1	C	599	LEU
1	D	327	VAL
1	D	328	LEU
1	D	354	LEU
1	D	391	MET
1	D	484	LEU
1	D	504	THR
1	D	558	PRO
1	E	318	PHE
1	E	329	GLN
1	E	354	LEU
1	E	391	MET
1	E	463	ASN
1	E	504	THR
1	E	599	LEU
1	F	335	VAL
1	F	363	ARG
1	F	391	MET
1	F	424	VAL
1	F	461	MET
1	F	504	THR
1	F	558	PRO
1	F	599	LEU
1	G	328	LEU
1	G	335	VAL
1	G	345	GLN
1	G	391	MET
1	G	507	GLU
1	G	558	PRO
1	G	599	LEU
1	H	304	ILE
1	H	318	PHE
1	H	391	MET
1	H	407	LEU
1	H	463	ASN
1	H	504	THR
1	H	558	PRO
1	H	599	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	GLN
1	A	360	ASN
1	A	393	HIS
1	A	451	ASN
1	A	463	ASN
1	A	492	HIS
1	B	289	GLN
1	B	334	HIS
1	B	345	GLN
1	B	360	ASN
1	B	365	ASN
1	B	425	GLN
1	B	451	ASN
1	B	463	ASN
1	B	479	HIS
1	B	570	GLN
1	B	587	GLN
1	B	597	HIS
1	C	360	ASN
1	C	365	ASN
1	C	451	ASN
1	C	463	ASN
1	C	479	HIS
1	C	485	HIS
1	C	587	GLN
1	D	345	GLN
1	D	360	ASN
1	D	393	HIS
1	D	425	GLN
1	D	451	ASN
1	D	463	ASN
1	D	479	HIS
1	D	492	HIS
1	D	540	GLN
1	E	329	GLN
1	E	334	HIS
1	E	360	ASN
1	E	365	ASN
1	E	451	ASN
1	E	463	ASN
1	E	475	HIS
1	E	479	HIS
1	F	289	GLN

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Mol	Chain	Res	Type
1	F	345	GLN
1	F	360	ASN
1	F	365	ASN
1	F	425	GLN
1	F	451	ASN
1	F	463	ASN
1	F	485	HIS
1	F	492	HIS
1	F	597	HIS
1	G	289	GLN
1	G	345	GLN
1	G	349	GLN
1	G	393	HIS
1	G	463	ASN
1	G	475	HIS
1	H	345	GLN
1	H	360	ASN
1	H	365	ASN
1	H	425	GLN
1	H	451	ASN
1	H	463	ASN
1	H	475	HIS
1	H	479	HIS
1	H	540	GLN
1	H	587	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

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	WYQ	E	701	-	35,35,35	2.43	5 (14%)	49,51,51	2.52	17 (34%)
2	WYQ	D	701	-	35,35,35	2.42	5 (14%)	49,51,51	2.58	19 (38%)
2	WYQ	H	701	-	35,35,35	2.42	5 (14%)	49,51,51	2.56	19 (38%)
2	WYQ	G	701	-	35,35,35	2.43	5 (14%)	49,51,51	2.52	19 (38%)
2	WYQ	C	701	-	35,35,35	2.41	5 (14%)	49,51,51	2.55	20 (40%)
2	WYQ	B	701	-	35,35,35	2.45	5 (14%)	49,51,51	2.61	20 (40%)
2	WYQ	A	701	-	35,35,35	2.43	5 (14%)	49,51,51	2.53	19 (38%)
2	WYQ	F	701	-	35,35,35	2.42	5 (14%)	49,51,51	2.51	18 (36%)

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	WYQ	E	701	-	-	13/25/25/25	0/3/3/3
2	WYQ	D	701	-	-	9/25/25/25	0/3/3/3
2	WYQ	H	701	-	-	10/25/25/25	0/3/3/3
2	WYQ	G	701	-	-	8/25/25/25	0/3/3/3
2	WYQ	C	701	-	-	10/25/25/25	0/3/3/3
2	WYQ	B	701	-	-	7/25/25/25	0/3/3/3
2	WYQ	A	701	-	-	13/25/25/25	0/3/3/3
2	WYQ	F	701	-	-	10/25/25/25	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	WYQ	C18-N2	-7.32	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	701	WYQ	C18-N2	-7.32	1.33	1.46
2	D	701	WYQ	C18-N2	-7.29	1.33	1.46
2	F	701	WYQ	C18-N2	-7.27	1.33	1.46
2	C	701	WYQ	C18-N2	-7.27	1.33	1.46
2	H	701	WYQ	C18-N2	-7.26	1.33	1.46
2	E	701	WYQ	C18-N2	-7.25	1.33	1.46
2	A	701	WYQ	C18-N2	-7.24	1.33	1.46
2	A	701	WYQ	N2-N1	-6.86	1.23	1.36
2	D	701	WYQ	N2-N1	-6.81	1.23	1.36
2	E	701	WYQ	N2-N1	-6.81	1.23	1.36
2	F	701	WYQ	N2-N1	-6.79	1.23	1.36
2	C	701	WYQ	N2-N1	-6.79	1.23	1.36
2	B	701	WYQ	N2-N1	-6.77	1.23	1.36
2	H	701	WYQ	N2-N1	-6.76	1.23	1.36
2	G	701	WYQ	N2-N1	-6.76	1.23	1.36
2	B	701	WYQ	O3-S1	6.06	1.50	1.43
2	F	701	WYQ	O3-S1	6.02	1.50	1.43
2	H	701	WYQ	O3-S1	6.00	1.50	1.43
2	E	701	WYQ	O3-S1	5.96	1.50	1.43
2	C	701	WYQ	O3-S1	5.95	1.50	1.43
2	A	701	WYQ	O3-S1	5.95	1.50	1.43
2	D	701	WYQ	O3-S1	5.91	1.50	1.43
2	G	701	WYQ	O3-S1	5.89	1.50	1.43
2	B	701	WYQ	C14-N5	-5.35	1.33	1.38
2	E	701	WYQ	C14-N5	-5.25	1.33	1.38
2	H	701	WYQ	C14-N5	-5.23	1.33	1.38
2	G	701	WYQ	C14-N5	-5.23	1.33	1.38
2	A	701	WYQ	C14-N5	-5.22	1.33	1.38
2	D	701	WYQ	C14-N5	-5.17	1.33	1.38
2	C	701	WYQ	C14-N5	-5.10	1.33	1.38
2	F	701	WYQ	C14-N5	-5.10	1.33	1.38
2	B	701	WYQ	C6-C5	-4.64	1.39	1.47
2	E	701	WYQ	C6-C5	-4.54	1.39	1.47
2	F	701	WYQ	C6-C5	-4.54	1.39	1.47
2	D	701	WYQ	C6-C5	-4.54	1.39	1.47
2	G	701	WYQ	C6-C5	-4.53	1.39	1.47
2	A	701	WYQ	C6-C5	-4.52	1.39	1.47
2	C	701	WYQ	C6-C5	-4.50	1.39	1.47
2	H	701	WYQ	C6-C5	-4.47	1.39	1.47

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	WYQ	O3-S1-O4	-8.71	108.94	119.52
2	C	701	WYQ	O3-S1-O4	-8.67	108.99	119.52
2	D	701	WYQ	O3-S1-O4	-8.64	109.02	119.52
2	B	701	WYQ	O3-S1-O4	-8.64	109.03	119.52
2	H	701	WYQ	O3-S1-O4	-8.64	109.03	119.52
2	G	701	WYQ	O3-S1-O4	-8.61	109.06	119.52
2	E	701	WYQ	O3-S1-O4	-8.03	109.77	119.52
2	F	701	WYQ	O3-S1-O4	-7.62	110.26	119.52
2	F	701	WYQ	C2-N3-C5	6.05	121.08	114.57
2	B	701	WYQ	C2-N3-C5	6.04	121.07	114.57
2	C	701	WYQ	C2-N3-C5	6.02	121.05	114.57
2	D	701	WYQ	C2-N3-C5	5.96	120.99	114.57
2	E	701	WYQ	C2-N3-C5	5.91	120.94	114.57
2	H	701	WYQ	C2-N3-C5	5.79	120.80	114.57
2	G	701	WYQ	C2-N3-C5	5.70	120.71	114.57
2	A	701	WYQ	C2-N3-C5	5.67	120.68	114.57
2	D	701	WYQ	O6-C14-O5	-4.80	117.49	124.55
2	H	701	WYQ	O6-C14-O5	-4.49	117.94	124.55
2	B	701	WYQ	C3-C4-N4	4.39	118.67	110.94
2	F	701	WYQ	C3-C4-N4	4.39	118.66	110.94
2	B	701	WYQ	C4-C3-N2	4.35	135.11	131.24
2	F	701	WYQ	C4-N4-C5	-4.35	119.30	125.86
2	C	701	WYQ	C3-C4-N4	4.35	118.59	110.94
2	E	701	WYQ	C3-C4-N4	4.34	118.58	110.94
2	E	701	WYQ	C4-N4-C5	-4.34	119.31	125.86
2	B	701	WYQ	C4-N4-C5	-4.28	119.41	125.86
2	H	701	WYQ	C4-N4-C5	-4.25	119.45	125.86
2	F	701	WYQ	O6-C14-O5	-4.25	118.30	124.55
2	D	701	WYQ	C3-C4-N4	4.25	118.41	110.94
2	H	701	WYQ	C3-C4-N4	4.24	118.39	110.94
2	C	701	WYQ	C4-N4-C5	-4.21	119.51	125.86
2	D	701	WYQ	C4-N4-C5	-4.20	119.52	125.86
2	G	701	WYQ	C3-C4-N4	4.20	118.33	110.94
2	F	701	WYQ	C4-C3-N2	4.18	134.95	131.24
2	C	701	WYQ	C4-C3-N2	4.17	134.94	131.24
2	A	701	WYQ	C4-N4-C5	-4.16	119.58	125.86
2	A	701	WYQ	C3-C4-N4	4.15	118.25	110.94
2	G	701	WYQ	C4-N4-C5	-4.13	119.64	125.86
2	E	701	WYQ	C3-C2-N3	-3.99	121.19	124.87
2	E	701	WYQ	C18-N2-C3	-3.97	123.87	129.21
2	A	701	WYQ	C18-N2-C3	-3.92	123.94	129.21
2	G	701	WYQ	C18-N2-C3	-3.91	123.96	129.21
2	B	701	WYQ	O6-C14-O5	-3.86	118.87	124.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	WYQ	C3-C2-N3	-3.86	121.31	124.87
2	E	701	WYQ	O6-C14-O5	-3.85	118.89	124.55
2	F	701	WYQ	C3-C2-N3	-3.84	121.32	124.87
2	H	701	WYQ	C18-N2-C3	-3.84	124.05	129.21
2	D	701	WYQ	C18-N2-C3	-3.83	124.06	129.21
2	H	701	WYQ	C4-C3-N2	3.81	134.62	131.24
2	C	701	WYQ	C18-N2-C3	-3.77	124.14	129.21
2	H	701	WYQ	C3-C2-N3	-3.76	121.40	124.87
2	A	701	WYQ	C3-C2-N3	-3.76	121.41	124.87
2	D	701	WYQ	C4-C3-N2	3.72	134.54	131.24
2	B	701	WYQ	C15-O6-C14	-3.72	109.61	116.56
2	C	701	WYQ	C3-C2-N3	-3.70	121.45	124.87
2	A	701	WYQ	O6-C14-O5	-3.69	119.12	124.55
2	E	701	WYQ	C1-C2-N3	3.69	134.35	129.76
2	A	701	WYQ	C4-C3-N2	3.68	134.51	131.24
2	E	701	WYQ	C4-C3-N2	3.67	134.50	131.24
2	B	701	WYQ	C3-C2-N3	-3.66	121.49	124.87
2	B	701	WYQ	C18-N2-C3	-3.63	124.33	129.21
2	F	701	WYQ	C18-N2-C3	-3.63	124.33	129.21
2	G	701	WYQ	C3-C2-N3	-3.62	121.53	124.87
2	G	701	WYQ	C4-C3-N2	3.62	134.45	131.24
2	E	701	WYQ	C12-O2-C11	-3.59	110.75	118.08
2	D	701	WYQ	C12-O2-C11	-3.52	110.88	118.08
2	D	701	WYQ	C1-C2-N3	3.52	134.14	129.76
2	A	701	WYQ	C1-C2-N3	3.49	134.10	129.76
2	G	701	WYQ	C1-C2-N3	3.48	134.10	129.76
2	F	701	WYQ	C15-O6-C14	-3.47	110.08	116.56
2	C	701	WYQ	O6-C14-O5	-3.44	119.48	124.55
2	G	701	WYQ	O6-C14-O5	-3.42	119.51	124.55
2	H	701	WYQ	C1-C2-N3	3.40	134.00	129.76
2	F	701	WYQ	C1-C2-N3	3.40	133.99	129.76
2	C	701	WYQ	C1-C2-N3	3.33	133.91	129.76
2	G	701	WYQ	C12-O2-C11	-3.28	111.38	118.08
2	H	701	WYQ	C12-O2-C11	-3.27	111.39	118.08
2	A	701	WYQ	C12-O2-C11	-3.27	111.39	118.08
2	B	701	WYQ	C1-C2-N3	3.24	133.80	129.76
2	C	701	WYQ	C12-O2-C11	-3.23	111.49	118.08
2	B	701	WYQ	C12-O2-C11	-3.16	111.63	118.08
2	F	701	WYQ	C12-O2-C11	-3.13	111.69	118.08
2	D	701	WYQ	C8-S1-N5	3.04	110.91	106.06
2	E	701	WYQ	C15-O6-C14	-3.04	110.87	116.56
2	E	701	WYQ	C18-N2-N1	3.00	123.78	119.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	701	WYQ	C18-N2-N1	3.00	123.77	119.29
2	C	701	WYQ	C8-S1-N5	2.98	110.81	106.06
2	B	701	WYQ	C8-S1-N5	2.96	110.78	106.06
2	A	701	WYQ	C18-N2-N1	2.95	123.71	119.29
2	G	701	WYQ	C8-S1-N5	2.92	110.72	106.06
2	A	701	WYQ	C11-C6-C5	-2.92	119.27	124.48
2	H	701	WYQ	C18-N2-N1	2.91	123.65	119.29
2	D	701	WYQ	C18-N2-N1	2.91	123.64	119.29
2	B	701	WYQ	C19-C1-N1	2.83	126.76	121.89
2	G	701	WYQ	O1-C4-C3	-2.79	120.78	127.62
2	B	701	WYQ	O1-C4-C3	-2.78	120.80	127.62
2	H	701	WYQ	C19-C1-N1	2.78	126.67	121.89
2	H	701	WYQ	O1-C4-C3	-2.77	120.82	127.62
2	C	701	WYQ	C19-C1-N1	2.77	126.65	121.89
2	F	701	WYQ	O1-C4-C3	-2.77	120.83	127.62
2	D	701	WYQ	O1-C4-C3	-2.76	120.84	127.62
2	C	701	WYQ	C18-N2-N1	2.76	123.42	119.29
2	B	701	WYQ	C2-C3-C4	-2.71	119.17	121.36
2	E	701	WYQ	O1-C4-C3	-2.71	120.98	127.62
2	C	701	WYQ	O1-C4-C3	-2.70	120.99	127.62
2	H	701	WYQ	C8-S1-N5	2.70	110.36	106.06
2	C	701	WYQ	C2-C3-C4	-2.65	119.22	121.36
2	G	701	WYQ	C11-C6-C5	-2.65	119.75	124.48
2	H	701	WYQ	C15-O6-C14	-2.64	111.62	116.56
2	F	701	WYQ	C19-C1-N1	2.64	126.43	121.89
2	G	701	WYQ	C19-C1-N1	2.64	126.43	121.89
2	F	701	WYQ	C18-N2-N1	2.62	123.21	119.29
2	B	701	WYQ	C18-N2-N1	2.62	123.20	119.29
2	A	701	WYQ	C8-S1-N5	2.59	110.19	106.06
2	C	701	WYQ	N4-C5-N3	-2.58	120.15	122.85
2	D	701	WYQ	C19-C1-N1	2.58	126.34	121.89
2	F	701	WYQ	C2-C3-C4	-2.57	119.29	121.36
2	H	701	WYQ	C1-N1-N2	2.56	110.19	106.63
2	B	701	WYQ	N4-C5-N3	-2.55	120.19	122.85
2	A	701	WYQ	C19-C1-N1	2.55	126.28	121.89
2	A	701	WYQ	C1-N1-N2	2.55	110.18	106.63
2	E	701	WYQ	C1-N1-N2	2.54	110.17	106.63
2	D	701	WYQ	C1-N1-N2	2.52	110.14	106.63
2	A	701	WYQ	O1-C4-C3	-2.51	121.45	127.62
2	E	701	WYQ	C19-C1-N1	2.49	126.18	121.89
2	B	701	WYQ	C1-N1-N2	2.47	110.07	106.63
2	G	701	WYQ	C15-O6-C14	-2.46	111.95	116.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	WYQ	N4-C5-N3	-2.46	120.28	122.85
2	C	701	WYQ	C1-N1-N2	2.45	110.05	106.63
2	A	701	WYQ	C15-O6-C14	-2.45	111.98	116.56
2	F	701	WYQ	C1-N1-N2	2.45	110.04	106.63
2	G	701	WYQ	C1-N1-N2	2.43	110.02	106.63
2	F	701	WYQ	N4-C5-N3	-2.41	120.34	122.85
2	H	701	WYQ	C2-C3-C4	-2.40	119.43	121.36
2	G	701	WYQ	N4-C5-N3	-2.40	120.35	122.85
2	H	701	WYQ	C11-C6-C5	-2.39	120.22	124.48
2	G	701	WYQ	C2-C3-C4	-2.37	119.45	121.36
2	C	701	WYQ	C15-O6-C14	-2.37	112.13	116.56
2	D	701	WYQ	C2-C3-C4	-2.33	119.48	121.36
2	E	701	WYQ	C2-C3-C4	-2.30	119.51	121.36
2	E	701	WYQ	N4-C5-N3	-2.28	120.47	122.85
2	B	701	WYQ	C2-C3-N2	-2.28	105.71	107.25
2	A	701	WYQ	C2-C3-C4	-2.26	119.54	121.36
2	D	701	WYQ	C15-O6-C14	-2.25	112.35	116.56
2	H	701	WYQ	N4-C5-N3	-2.23	120.52	122.85
2	F	701	WYQ	C2-C3-N2	-2.21	105.76	107.25
2	A	701	WYQ	N4-C5-N3	-2.21	120.55	122.85
2	C	701	WYQ	C11-C6-C5	-2.20	120.55	124.48
2	C	701	WYQ	C2-C3-N2	-2.11	105.83	107.25
2	B	701	WYQ	C6-C5-N4	2.07	121.15	118.14
2	D	701	WYQ	C11-C6-C5	-2.07	120.78	124.48

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	WYQ	O6-C14-N5-S1
2	A	701	WYQ	O5-C14-N5-S1
2	A	701	WYQ	C14-N5-S1-O4
2	A	701	WYQ	C1-C19-C20-C21
2	B	701	WYQ	O5-C14-O6-C15
2	B	701	WYQ	N5-C14-O6-C15
2	B	701	WYQ	O6-C14-N5-S1
2	B	701	WYQ	O5-C14-N5-S1
2	B	701	WYQ	C1-C19-C20-C21
2	C	701	WYQ	O6-C14-N5-S1
2	C	701	WYQ	O5-C14-N5-S1
2	D	701	WYQ	O5-C14-O6-C15
2	D	701	WYQ	N5-C14-O6-C15

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Mol	Chain	Res	Type	Atoms
2	D	701	WYQ	O6-C14-N5-S1
2	D	701	WYQ	O5-C14-N5-S1
2	D	701	WYQ	C1-C19-C20-C21
2	E	701	WYQ	O6-C14-N5-S1
2	E	701	WYQ	O5-C14-N5-S1
2	E	701	WYQ	C14-N5-S1-O4
2	E	701	WYQ	C14-N5-S1-C8
2	E	701	WYQ	C1-C19-C20-C21
2	F	701	WYQ	O6-C14-N5-S1
2	F	701	WYQ	O5-C14-N5-S1
2	F	701	WYQ	C14-N5-S1-O4
2	F	701	WYQ	C14-N5-S1-C8
2	F	701	WYQ	C1-C19-C20-C21
2	G	701	WYQ	O6-C14-N5-S1
2	G	701	WYQ	O5-C14-N5-S1
2	G	701	WYQ	C1-C19-C20-C21
2	H	701	WYQ	O5-C14-O6-C15
2	H	701	WYQ	N5-C14-O6-C15
2	H	701	WYQ	O6-C14-N5-S1
2	H	701	WYQ	O5-C14-N5-S1
2	E	701	WYQ	C7-C8-S1-N5
2	E	701	WYQ	C9-C8-S1-N5
2	G	701	WYQ	C9-C8-S1-N5
2	G	701	WYQ	C7-C8-S1-N5
2	A	701	WYQ	C9-C8-S1-N5
2	G	701	WYQ	C13-C12-O2-C11
2	A	701	WYQ	C7-C8-S1-N5
2	C	701	WYQ	C7-C8-S1-O4
2	D	701	WYQ	C7-C8-S1-O4
2	D	701	WYQ	C9-C8-S1-O4
2	H	701	WYQ	C9-C8-S1-O4
2	C	701	WYQ	C9-C8-S1-O4
2	F	701	WYQ	C7-C8-S1-O3
2	A	701	WYQ	C17-C15-O6-C14
2	H	701	WYQ	C7-C8-S1-O4
2	F	701	WYQ	C9-C8-S1-O3
2	C	701	WYQ	C1-C19-C20-C21
2	A	701	WYQ	C16-C15-O6-C14
2	C	701	WYQ	C9-C8-S1-N5
2	A	701	WYQ	C7-C8-S1-O4
2	A	701	WYQ	C13-C12-O2-C11
2	C	701	WYQ	C7-C8-S1-N5

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Mol	Chain	Res	Type	Atoms
2	D	701	WYQ	C9-C8-S1-N5
2	F	701	WYQ	C7-C8-S1-N5
2	D	701	WYQ	C7-C8-S1-N5
2	B	701	WYQ	C9-C8-S1-O4
2	H	701	WYQ	C7-C8-S1-N5
2	E	701	WYQ	C10-C11-O2-C12
2	H	701	WYQ	C13-C12-O2-C11
2	A	701	WYQ	C9-C8-S1-O4
2	H	701	WYQ	C9-C8-S1-N5
2	F	701	WYQ	C14-N5-S1-O3
2	C	701	WYQ	C16-C15-O6-C14
2	G	701	WYQ	C7-C8-S1-O4
2	A	701	WYQ	C14-N5-S1-C8
2	G	701	WYQ	C9-C8-S1-O4
2	E	701	WYQ	C6-C11-O2-C12
2	C	701	WYQ	C17-C15-O6-C14
2	F	701	WYQ	C9-C8-S1-N5
2	B	701	WYQ	C7-C8-S1-O4
2	E	701	WYQ	N4-C5-C6-C7
2	E	701	WYQ	C9-C8-S1-O3
2	E	701	WYQ	N1-C1-C19-C20
2	E	701	WYQ	C7-C8-S1-O3
2	C	701	WYQ	N4-C5-C6-C11
2	H	701	WYQ	C2-C1-C19-C20
2	A	701	WYQ	N4-C5-C6-C7

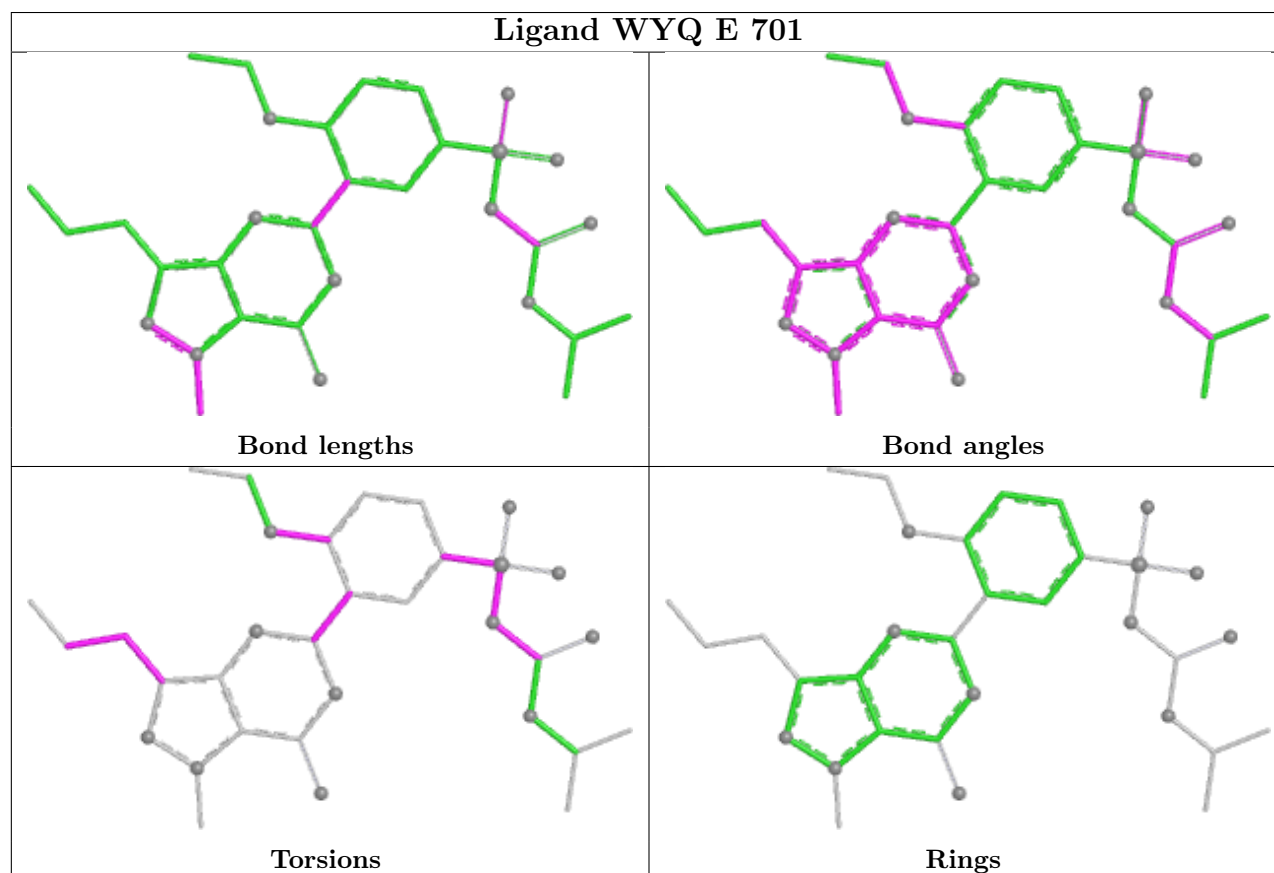
There are no ring outliers.

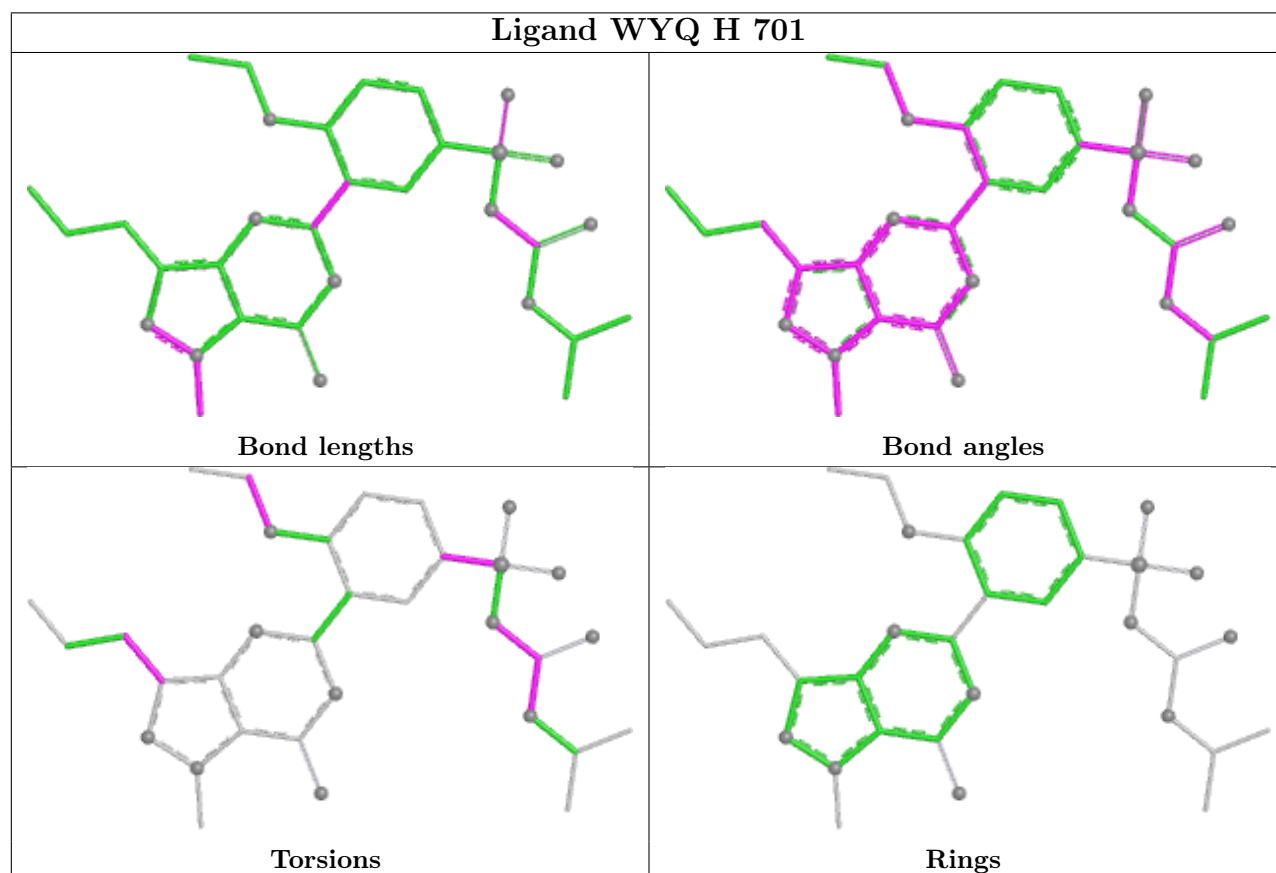
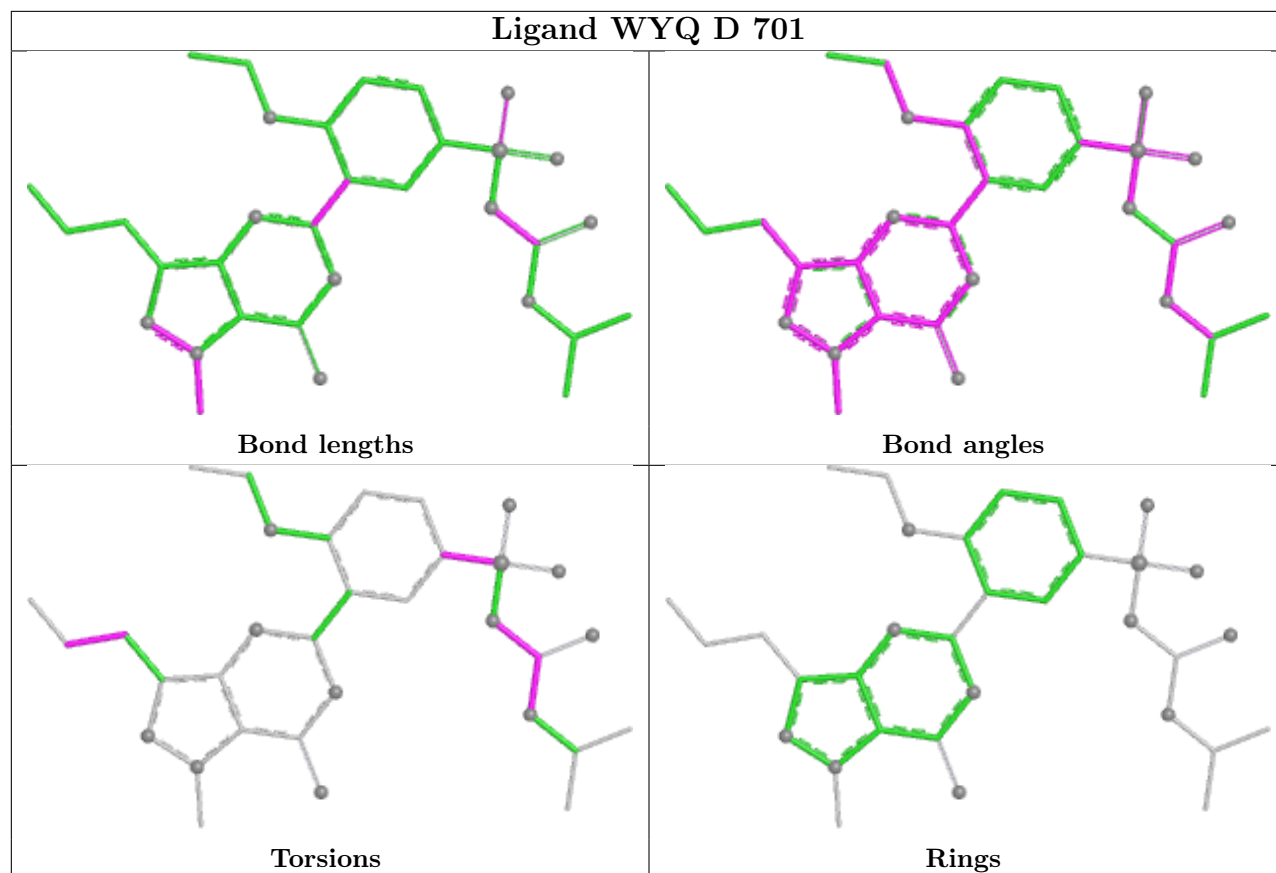
8 monomers are involved in 41 short contacts:

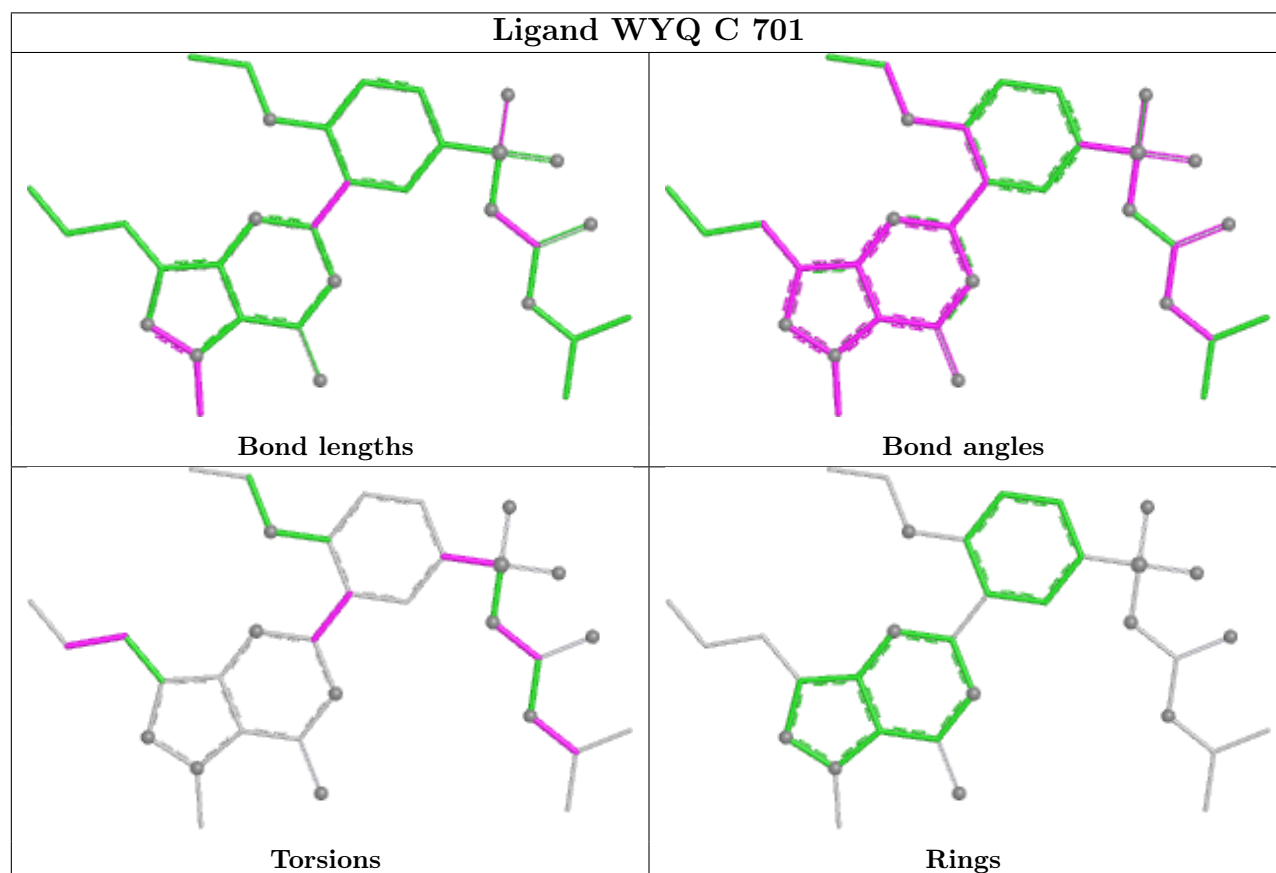
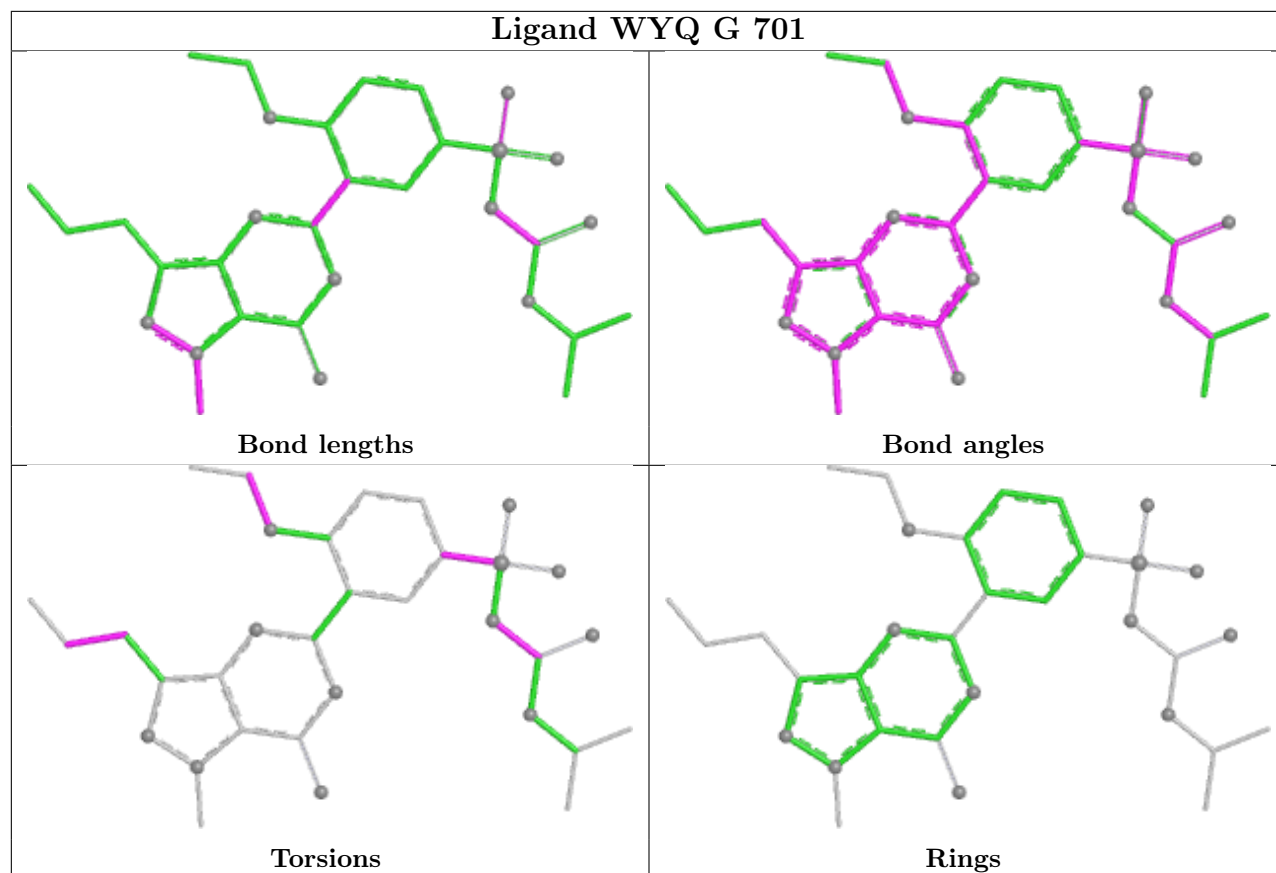
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	701	WYQ	4	0
2	D	701	WYQ	4	0
2	H	701	WYQ	3	0
2	G	701	WYQ	5	0
2	C	701	WYQ	4	0
2	B	701	WYQ	15	0
2	A	701	WYQ	3	0
2	F	701	WYQ	3	0

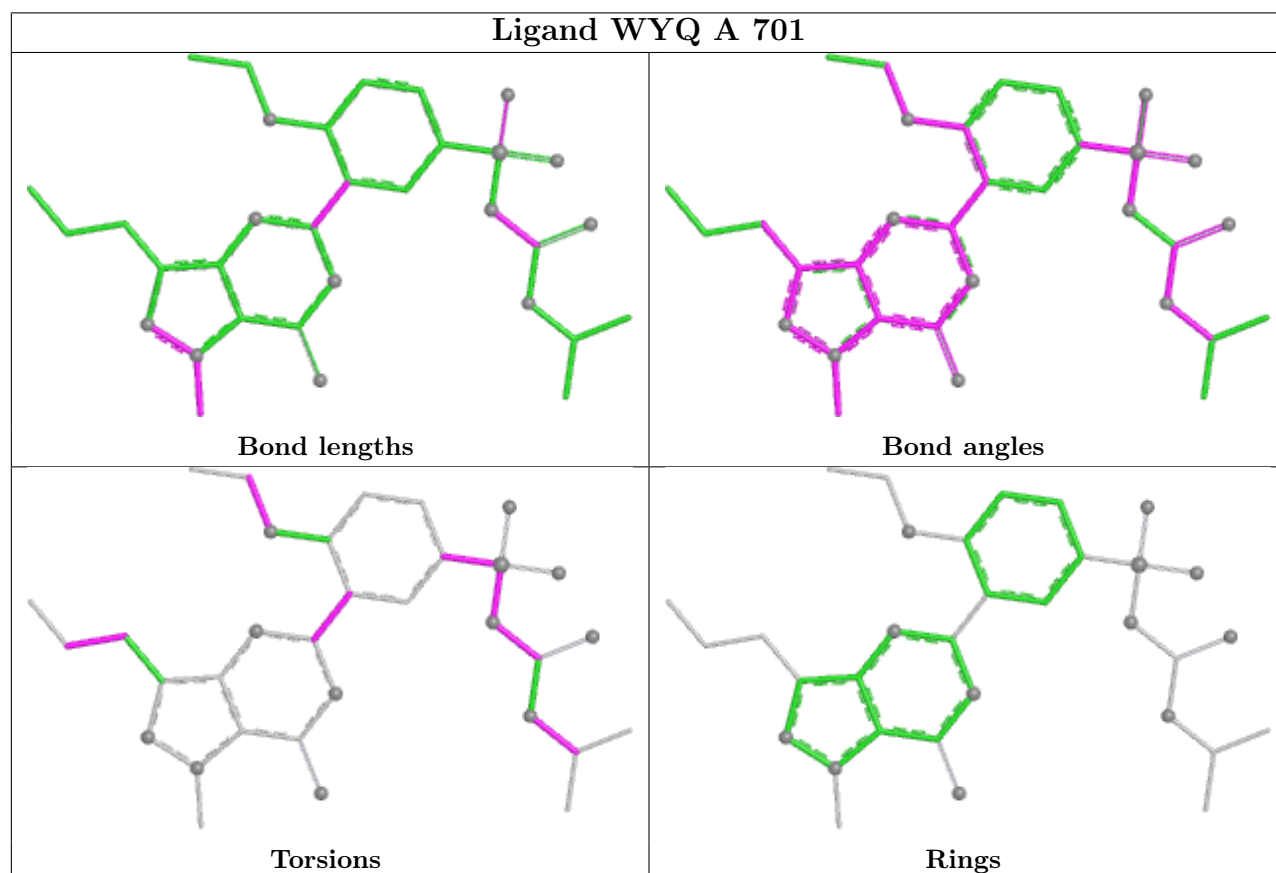
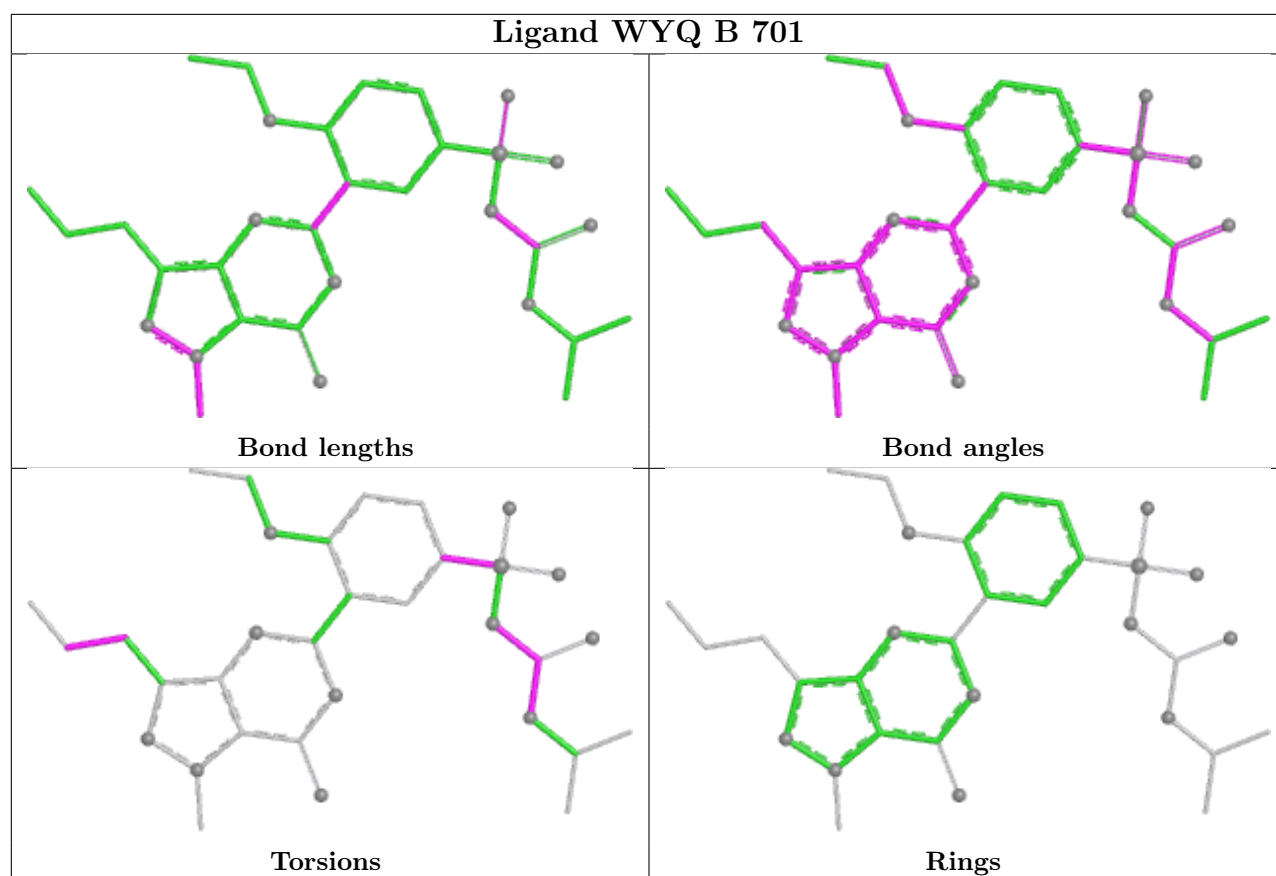
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

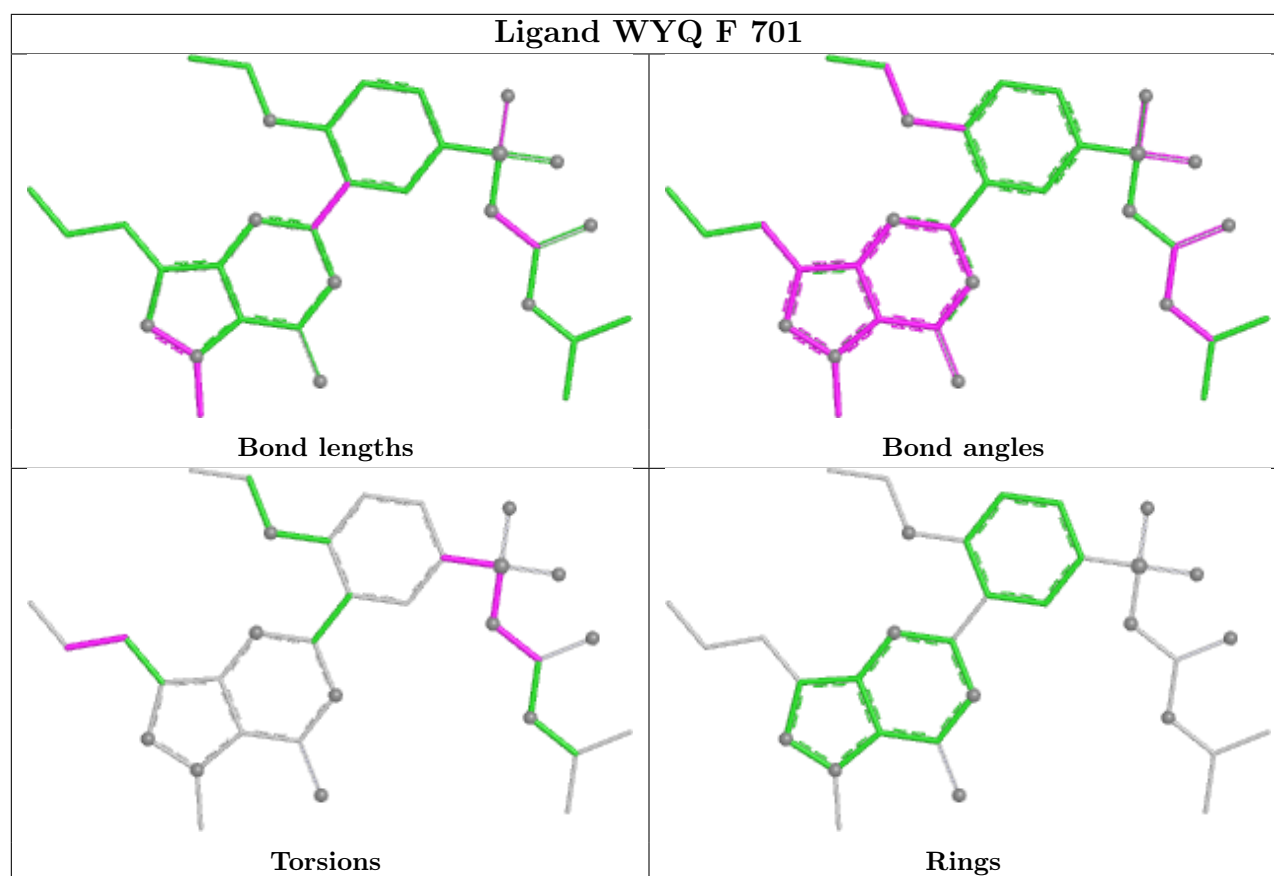
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	332/345 (96%)	-0.19	9 (2%) 56 62	11, 19, 44, 66	0
1	B	334/345 (96%)	-0.08	10 (2%) 52 59	10, 21, 45, 67	0
1	C	333/345 (96%)	0.28	20 (6%) 27 32	15, 29, 55, 79	0
1	D	331/345 (95%)	0.64	25 (7%) 20 24	18, 37, 65, 83	0
1	E	331/345 (95%)	1.32	71 (21%) 2 2	24, 45, 72, 86	0
1	F	334/345 (96%)	0.01	12 (3%) 46 52	13, 24, 46, 73	0
1	G	334/345 (96%)	0.53	18 (5%) 31 37	11, 28, 55, 86	0
1	H	330/345 (95%)	0.49	20 (6%) 27 32	17, 35, 60, 74	0
All	All	2659/2760 (96%)	0.37	185 (6%) 22 26	10, 29, 61, 86	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	278	ILE	9.0
1	B	278	ILE	8.8
1	F	278	ILE	7.9
1	G	277	MET	7.7
1	B	610	ALA	6.6
1	F	610	ALA	6.2
1	G	610	ALA	6.2
1	C	278	ILE	6.2
1	E	610	ALA	6.1
1	D	303	ALA	6.0
1	E	317	THR	4.7
1	A	308	VAL	4.7
1	F	277	MET	4.7
1	C	279	SER	4.7
1	G	279	SER	4.6
1	A	610	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	301	CYS	4.5
1	C	610	ALA	4.3
1	E	303	ALA	4.3
1	D	280	THR	4.3
1	D	610	ALA	4.3
1	H	280	THR	4.3
1	E	302	ALA	4.2
1	D	576	PHE	4.0
1	D	302	ALA	3.9
1	D	305	GLY	3.8
1	E	280	THR	3.8
1	E	607	ALA	3.7
1	B	277	MET	3.7
1	E	337	LEU	3.7
1	E	295	VAL	3.7
1	D	304	ILE	3.7
1	H	343	ALA	3.6
1	G	343	ALA	3.6
1	E	343	ALA	3.5
1	E	310	LEU	3.5
1	E	308	VAL	3.5
1	H	302	ALA	3.4
1	G	462	ASP	3.4
1	E	323	ARG	3.4
1	H	609	LYS	3.4
1	B	609	LYS	3.3
1	E	301	CYS	3.3
1	F	609	LYS	3.3
1	E	351	TRP	3.3
1	E	342	PHE	3.2
1	A	609	LYS	3.2
1	E	554	LEU	3.2
1	D	317	THR	3.1
1	E	318	PHE	3.1
1	E	576	PHE	3.1
1	E	324	VAL	3.1
1	E	354	LEU	3.1
1	F	279	SER	3.1
1	E	550	ARG	3.0
1	E	305	GLY	3.0
1	E	529	VAL	3.0
1	E	322	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	307	ASP	3.0
1	A	303	ALA	3.0
1	E	528	GLY	3.0
1	G	303	ALA	2.9
1	G	608	ALA	2.9
1	E	387	ALA	2.9
1	E	335	VAL	2.9
1	F	500	GLY	2.9
1	C	303	ALA	2.8
1	D	299	LYS	2.8
1	D	308	VAL	2.8
1	E	306	THR	2.8
1	B	462	ASP	2.8
1	D	300	SER	2.8
1	H	500	GLY	2.8
1	E	328	LEU	2.8
1	E	453	THR	2.8
1	C	500	GLY	2.8
1	H	558	PRO	2.8
1	C	343	ALA	2.8
1	C	576	PHE	2.8
1	A	462	ASP	2.7
1	F	462	ASP	2.7
1	B	500	GLY	2.7
1	E	486	SER	2.7
1	B	345	GLN	2.7
1	B	279	SER	2.7
1	C	280	THR	2.7
1	G	302	ALA	2.6
1	E	577	PHE	2.6
1	G	308	VAL	2.6
1	E	298	PRO	2.6
1	H	597	HIS	2.6
1	E	345	GLN	2.6
1	D	550	ARG	2.6
1	E	551	ARG	2.6
1	D	296	VAL	2.6
1	E	320	VAL	2.6
1	E	556	VAL	2.6
1	C	326	SER	2.6
1	G	300	SER	2.6
1	A	387	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	562	THR	2.6
1	F	282	ARG	2.5
1	H	310	LEU	2.5
1	E	555	PRO	2.5
1	H	301	CYS	2.5
1	G	280	THR	2.5
1	C	460	SER	2.5
1	E	420	PHE	2.5
1	E	542	PHE	2.5
1	C	307	ASP	2.5
1	A	302	ALA	2.5
1	H	604	GLU	2.4
1	G	304	ILE	2.4
1	G	609	LYS	2.4
1	H	601	LYS	2.4
1	B	346	GLU	2.4
1	E	297	PRO	2.4
1	H	387	ALA	2.4
1	H	305	GLY	2.4
1	C	486	SER	2.4
1	E	307	ASP	2.4
1	E	561	GLU	2.4
1	E	325	PRO	2.4
1	C	305	GLY	2.4
1	H	607	ALA	2.4
1	E	559	GLY	2.3
1	B	343	ALA	2.3
1	E	457	PHE	2.3
1	F	558	PRO	2.3
1	E	597	HIS	2.3
1	E	340	ASP	2.3
1	A	282	ARG	2.3
1	E	566	VAL	2.3
1	H	605	LEU	2.3
1	E	336	ALA	2.3
1	D	486	SER	2.3
1	E	287	ILE	2.3
1	E	560	PHE	2.2
1	C	298	PRO	2.2
1	E	321	ALA	2.2
1	D	306	THR	2.2
1	D	345	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	346	GLU	2.2
1	G	347	GLU	2.2
1	F	280	THR	2.2
1	F	343	ALA	2.2
1	C	304	ILE	2.2
1	E	605	LEU	2.2
1	E	327	VAL	2.2
1	C	282	ARG	2.2
1	F	296	VAL	2.2
1	D	298	PRO	2.2
1	E	364	PRO	2.2
1	D	559	GLY	2.2
1	E	485	HIS	2.2
1	E	412	CYS	2.2
1	H	317	THR	2.2
1	H	453	THR	2.2
1	E	296	VAL	2.1
1	D	560	PHE	2.1
1	D	344	SER	2.1
1	D	348	ALA	2.1
1	D	533	ARG	2.1
1	C	558	PRO	2.1
1	G	301	CYS	2.1
1	E	348	ALA	2.1
1	E	608	ALA	2.1
1	E	285	PRO	2.1
1	E	558	PRO	2.1
1	C	600	ARG	2.1
1	E	281	ARG	2.1
1	H	321	ALA	2.1
1	D	307	ASP	2.1
1	E	531	ILE	2.1
1	G	396	PRO	2.1
1	E	341	PHE	2.1
1	D	281	ARG	2.1
1	C	330	SER	2.0
1	C	607	ALA	2.0
1	E	338	ALA	2.0
1	E	304	ILE	2.0
1	H	323	ARG	2.0
1	H	600	ARG	2.0
1	E	349	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	609	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	WYQ	E	701	33/33	0.75	0.20	50,58,71,72	0
4	MG	E	703	1/1	0.79	0.13	39,39,39,39	0
2	WYQ	D	701	33/33	0.85	0.15	43,46,62,64	0
4	MG	D	703	1/1	0.88	0.14	33,33,33,33	0
2	WYQ	H	701	33/33	0.89	0.12	37,39,57,58	0
2	WYQ	A	701	33/33	0.89	0.13	14,21,52,53	0
2	WYQ	G	701	33/33	0.89	0.13	11,23,48,49	0
2	WYQ	C	701	33/33	0.91	0.12	25,34,54,55	0
4	MG	B	703	1/1	0.91	0.06	15,15,15,15	0
2	WYQ	F	701	33/33	0.91	0.13	11,19,59,61	0
2	WYQ	B	701	33/33	0.91	0.11	12,18,44,49	0
4	MG	C	703	1/1	0.94	0.09	17,17,17,17	0
4	MG	H	703	1/1	0.95	0.09	24,24,24,24	0
4	MG	G	703	1/1	0.96	0.12	27,27,27,27	0
4	MG	A	703	1/1	0.96	0.08	15,15,15,15	0
3	ZN	E	702	1/1	0.97	0.04	43,43,43,43	0
3	ZN	A	702	1/1	0.97	0.03	20,20,20,20	0
3	ZN	G	702	1/1	0.98	0.03	30,30,30,30	0
3	ZN	D	702	1/1	0.98	0.03	30,30,30,30	0
3	ZN	C	702	1/1	0.98	0.03	23,23,23,23	0
3	ZN	F	702	1/1	0.98	0.02	20,20,20,20	0
4	MG	F	703	1/1	0.99	0.10	15,15,15,15	0

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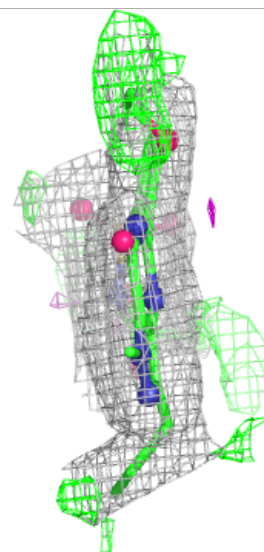
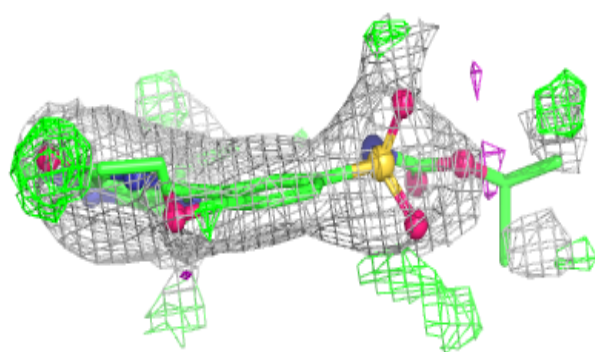
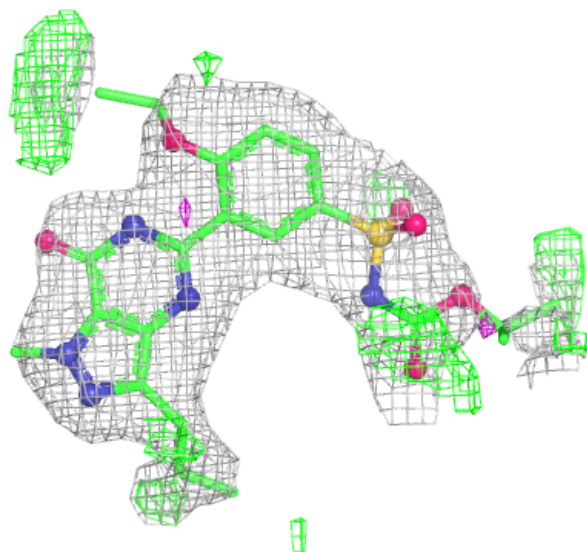
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	H	702	1/1	0.99	0.03	29,29,29,29	0
3	ZN	B	702	1/1	0.99	0.02	20,20,20,20	0

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.

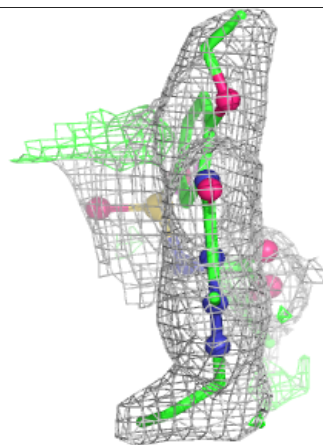
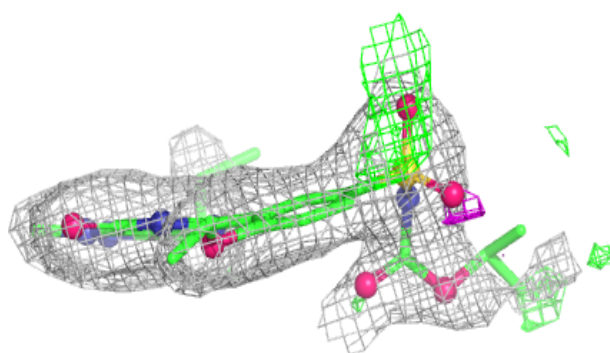
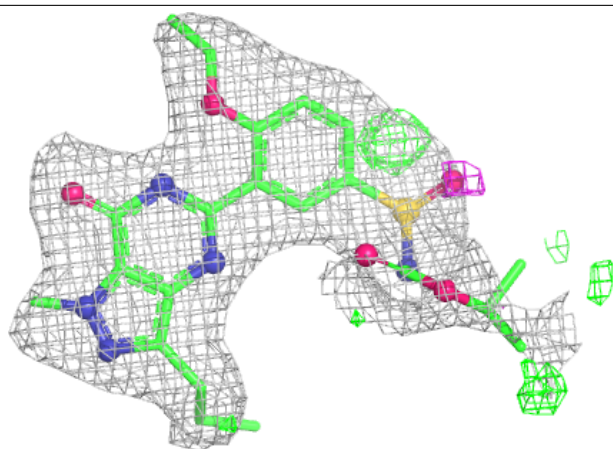
Electron density around WYQ E 701:

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



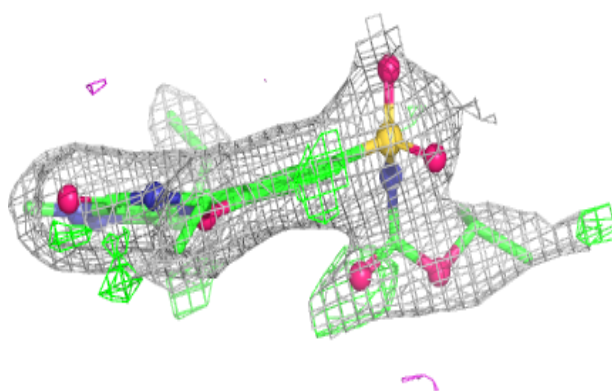
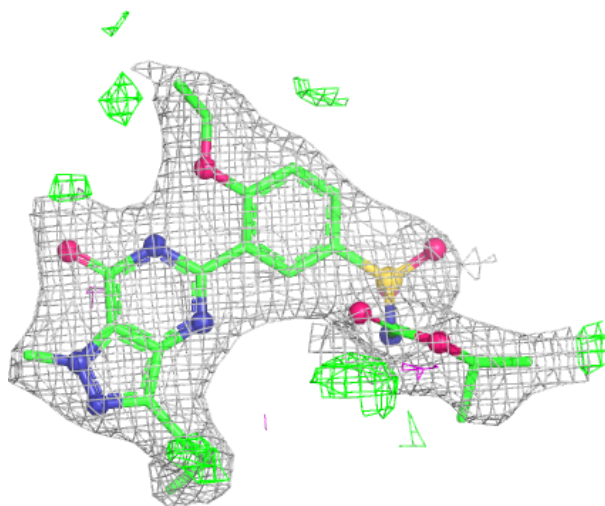
Electron density around WYQ D 701:

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



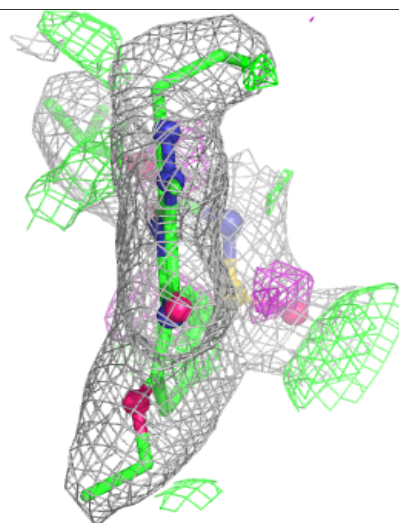
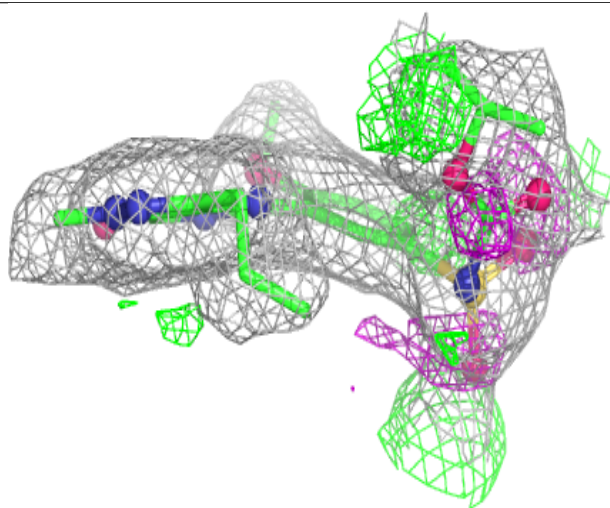
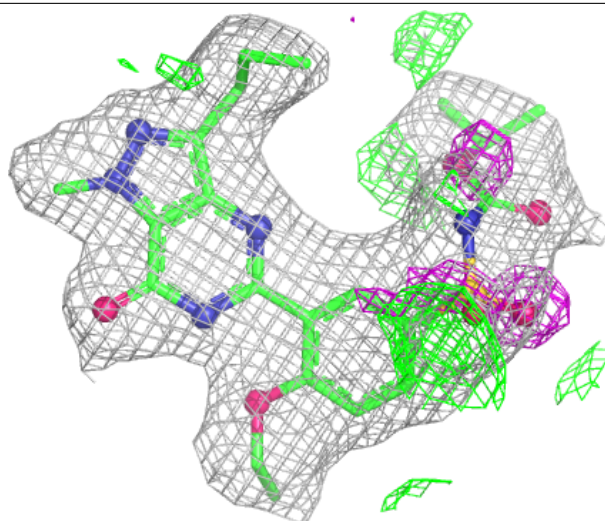
Electron density around WYQ H 701:

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



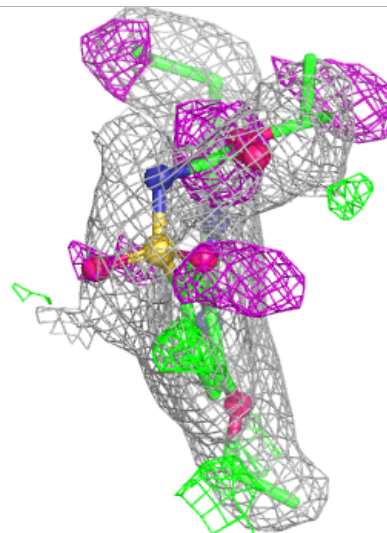
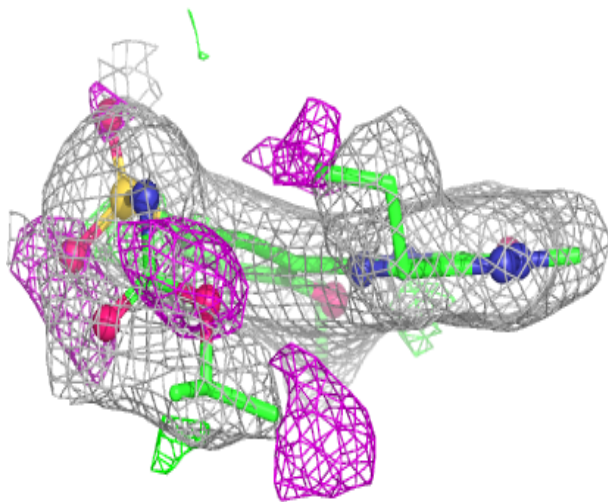
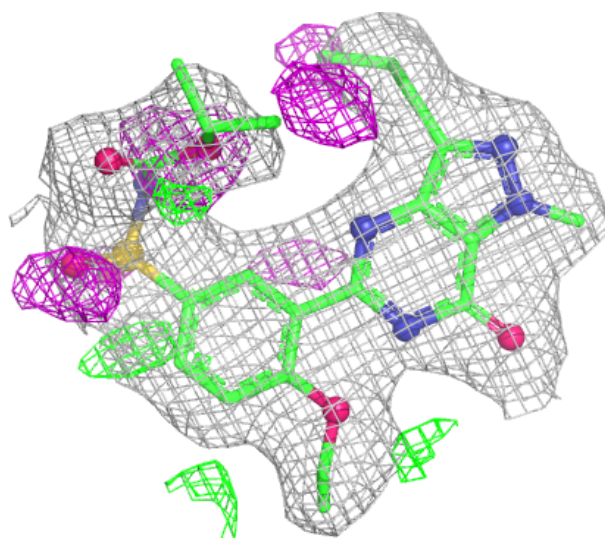
Electron density around WYQ A 701:

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



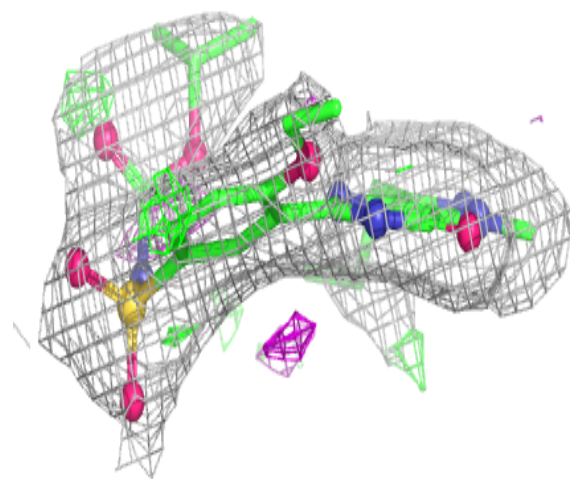
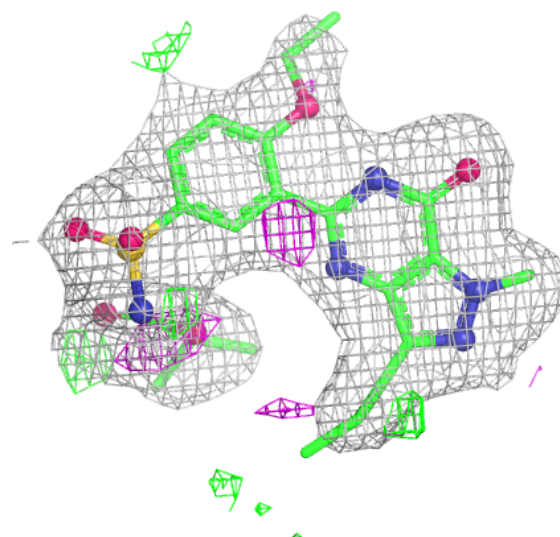
Electron density around WYQ G 701:

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



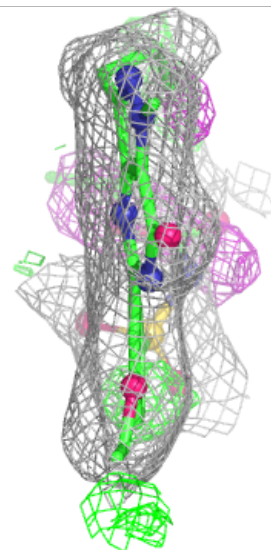
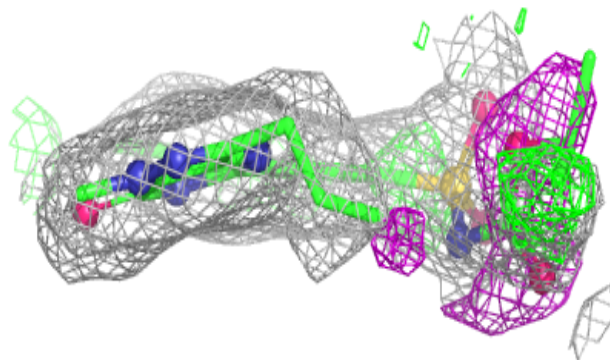
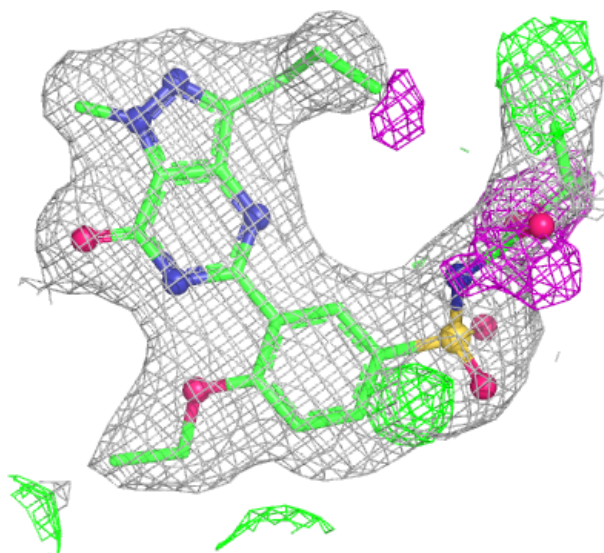
Electron density around WYQ C 701:

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



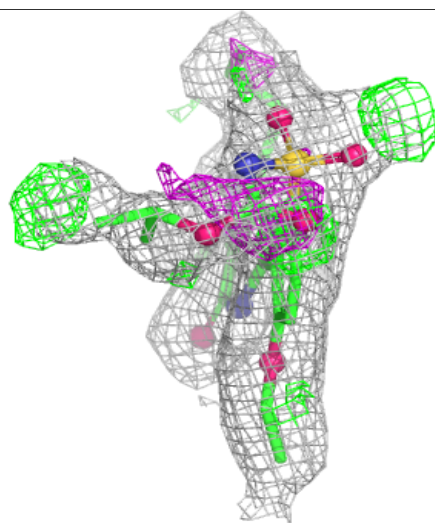
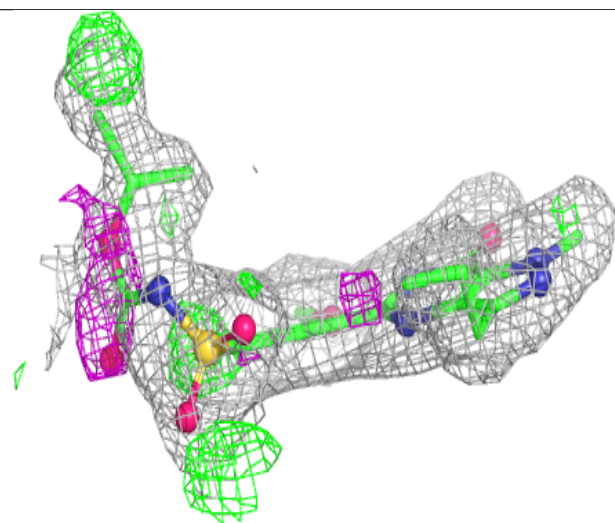
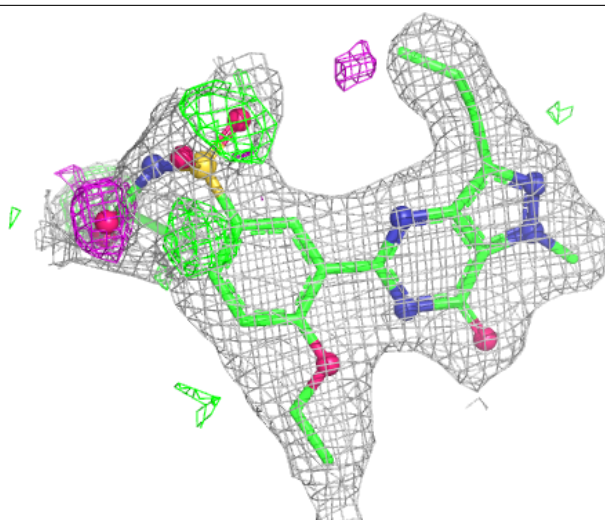
Electron density around WYQ F 701:

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



Electron density around WYQ B 701:

$2mF_o-DF_c$ (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.