Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 10:06 PM EST

PDB ID	:	3V94
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 (i) 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 (i)) were used in the production of this report:

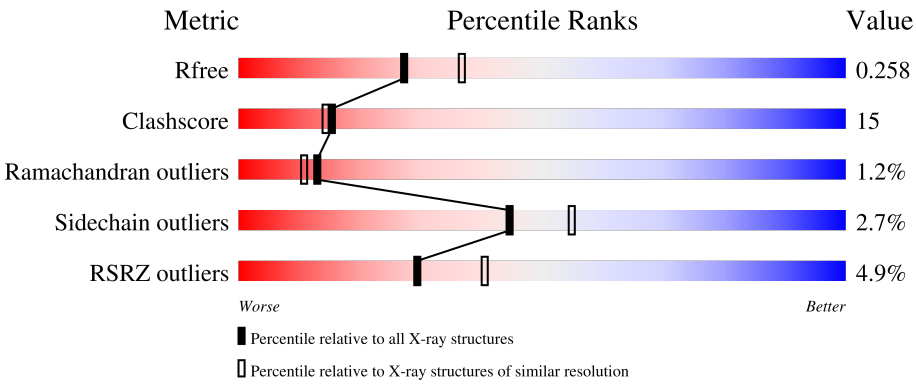
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (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 <=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	2%, 79%, 16%
1	B	345	3%, 73%, 21%
1	C	345	4%, 72%, 22%
1	D	345	6%, 66%, 27%
1	E	345	14%, 61%, 33%

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Mol	Chain	Length	Quality of chain
1	F	345	3% 76% 19%
1	G	345	4% 71% 24%
1	H	345	2% 71% 23%

2 Entry composition (i)

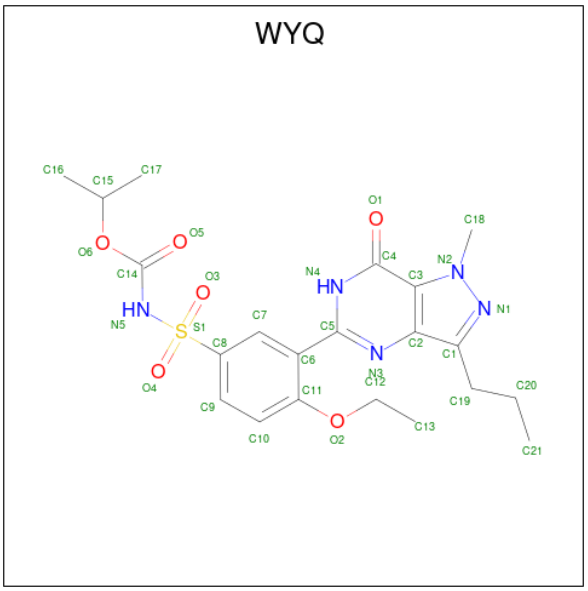
There are 5 unique types of molecules in this entry. The entry contains 21762 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- 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 (three-letter code: WYQ) (formula: $C_{21}H_{27}N_5O_6S$).



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 (three-letter code: 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 Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0
3	G	1	Total Zn 1 1	0	0
3	H	1	Total Zn 1 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

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

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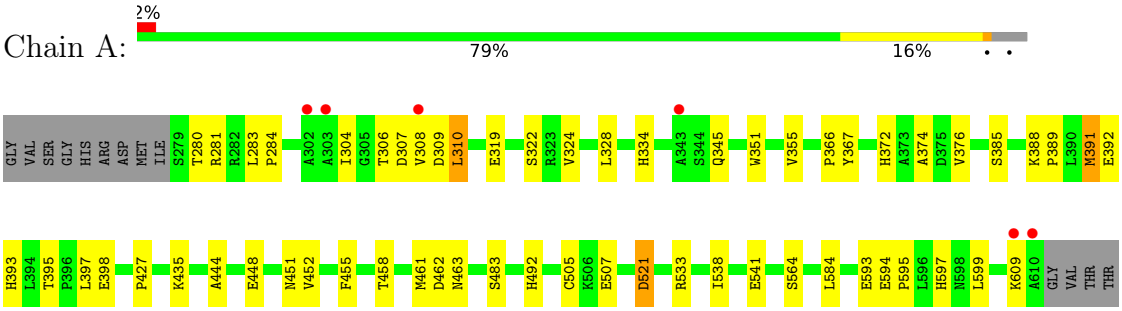
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	F	129	129	129	0	0
			Total	O		
5	G	132	132	132	0	0
			Total	O		
5	H	74	74	74	0	0

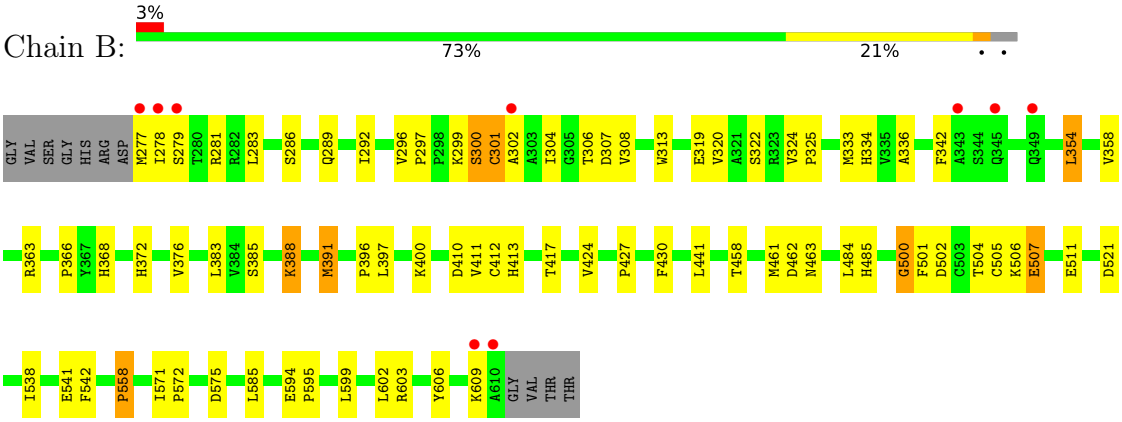
3 Residue-property plots (i)

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.

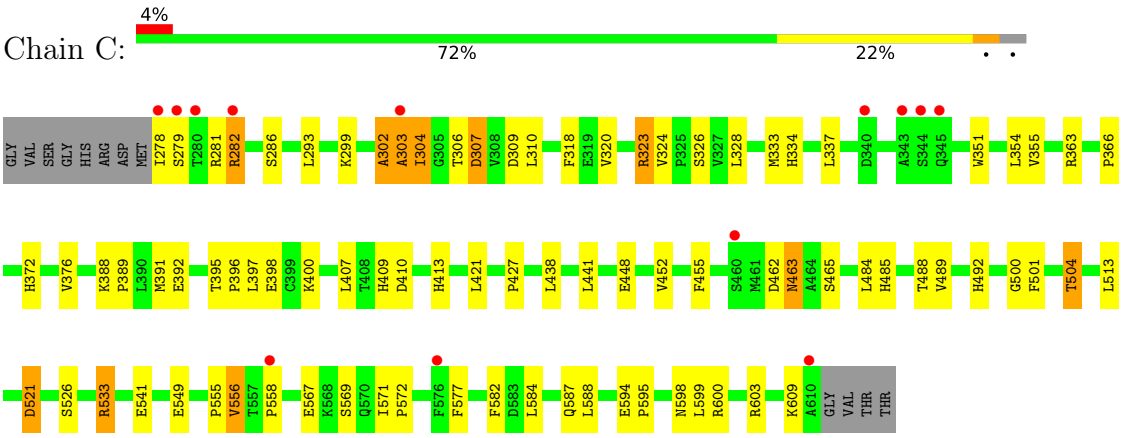
• Molecule 1: Cyclic nucleotide specific phosphodiesterase



• Molecule 1: Cyclic nucleotide specific phosphodiesterase

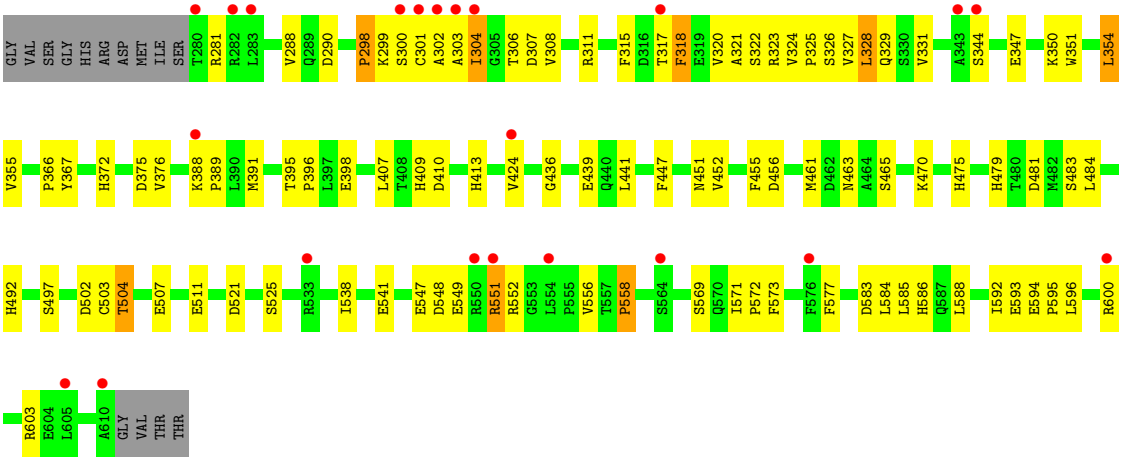


• Molecule 1: Cyclic nucleotide specific phosphodiesterase



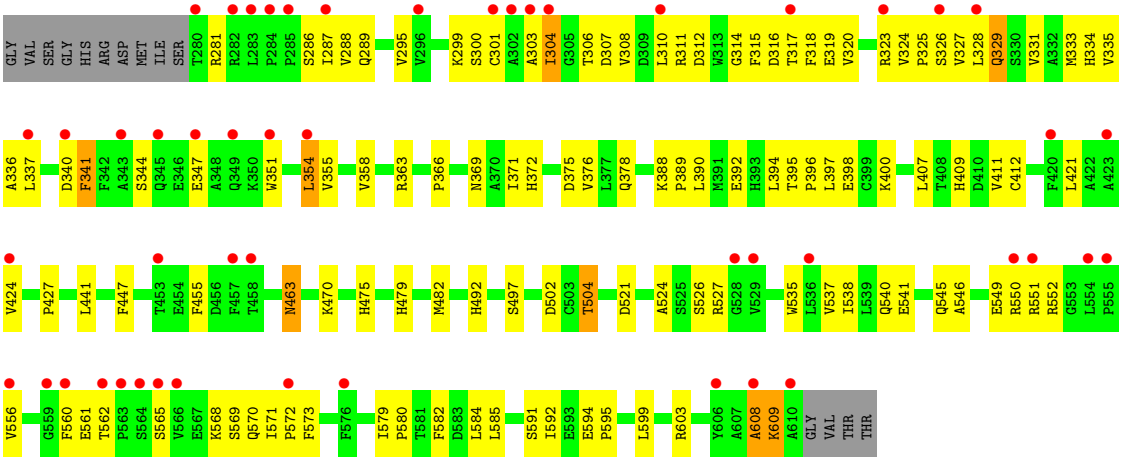
• Molecule 1: Cyclic nucleotide specific phosphodiesterase

Chain D:



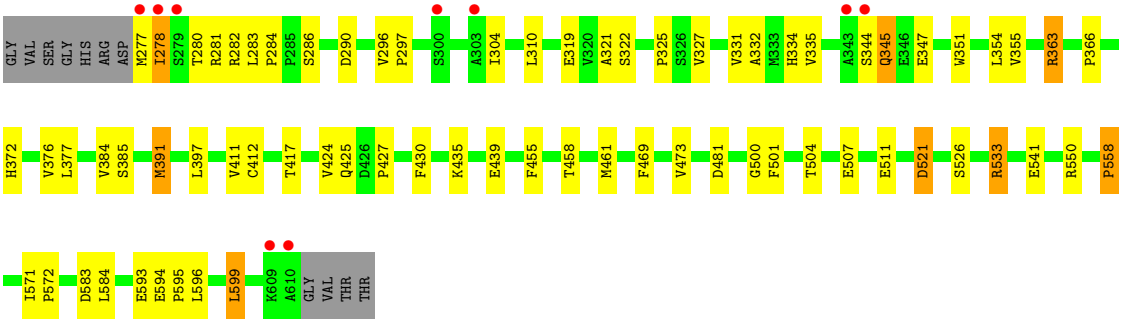
• Molecule 1: Cyclic nucleotide specific phosphodiesterase

Chain E:



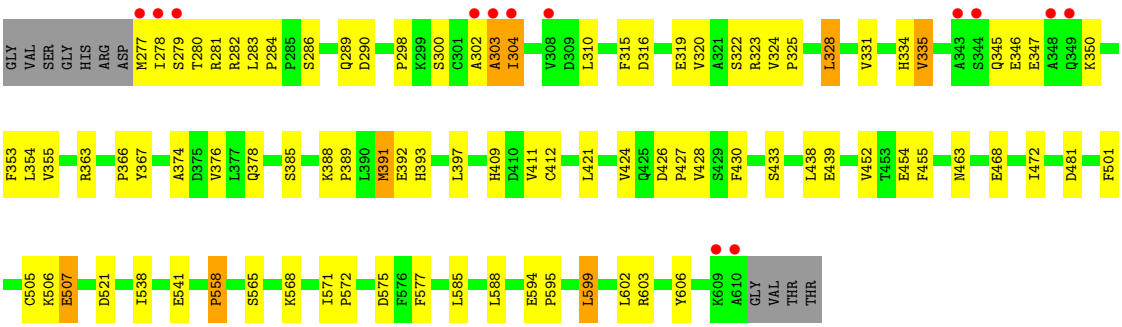
• Molecule 1: Cyclic nucleotide specific phosphodiesterase

Chain F:



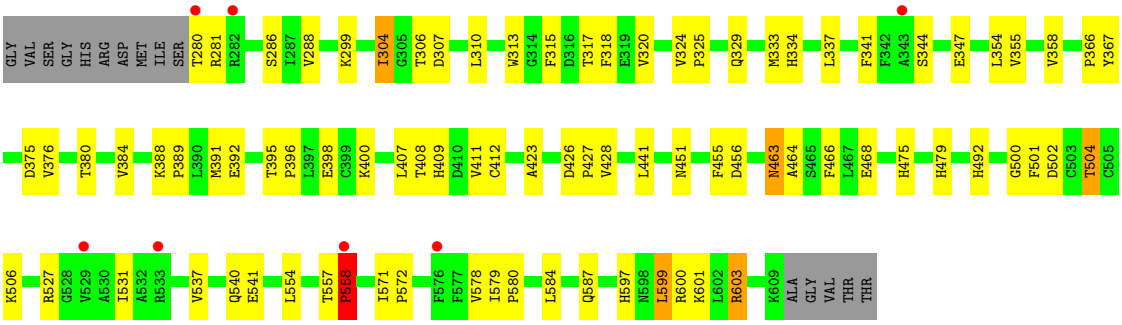
• Molecule 1: Cyclic nucleotide specific phosphodiesterase

Chain G:



• Molecule 1: Cyclic nucleotide specific phosphodiesterase

Chain H:



4 Data and refinement statistics (i)

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 47.09 – 2.33	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.33) 95.1 (47.09-2.33)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.69 (at 2.34Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.268 0.215 , 0.258	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 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, WYQ, MG

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	0.40	0/2639	0.61	1/3592 (0.0%)
1	B	0.39	0/2655	0.61	1/3613 (0.0%)
1	C	0.35	0/2647	0.57	1/3603 (0.0%)
1	D	0.33	0/2633	0.54	0/3584
1	E	0.33	0/2633	0.52	0/3584
1	F	0.37	0/2655	0.59	1/3613 (0.0%)
1	G	0.39	0/2655	0.59	0/3613
1	H	0.33	0/2628	0.55	0/3577
All	All	0.36	0/21145	0.57	4/28779 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	521	ASP	CB-CG-OD1	6.13	123.82	118.30
1	C	521	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	521	ASP	CB-CG-OD1	5.96	123.66	118.30
1	B	500	GLY	N-CA-C	5.25	126.24	113.10

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	2574	0	2531	52	0
1	B	2590	0	2551	97	0
1	C	2582	0	2542	72	0
1	D	2568	0	2526	95	0
1	E	2568	0	2526	102	0
1	F	2590	0	2551	62	0
1	G	2590	0	2551	85	0
1	H	2563	0	2521	79	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
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	618	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 15.

All (618) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:500:GLY:O	1:F:501:PHE:HB2	1.96	0.65
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:278:ILE:HD11	1:D:470:LYS:HZ3	1.62	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:B:278:ILE:HD11	1:D:470:LYS:HZ2	1.63	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:F:281:ARG:HH11	1:H:463:ASN:ND2	1.98	0.61
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:H:500:GLY:O	1:H:501:PHE:HB2	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:278:ILE:CD1	1:D:470:LYS:HZ2	2.15	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:D:424:VAL:HG12	1:D:424:VAL:O	2.03	0.58
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
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: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:E:550:ARG:C	1:E:552:ARG:H	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:306:THR:HG22	1:B:307:ASP:N	2.21	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
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:F:296:VAL:HG13	1:F:297:PRO:HD2	1.88	0.55
1:B:502:ASP:CG	1:B:504:THR:HG22	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:328:LEU:HD23	1:E:328:LEU:O	2.08	0.53
1:E:608:ALA:O	1:E:609:LYS:C	2.46	0.53
1:F:584:LEU:C	1:F:584:LEU:HD13	2.29	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:C:376:VAL:HG21	1:C:409:HIS:CE1	2.44	0.53
1:D:441:LEU:HD23	1:D:441:LEU:C	2.29	0.53
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: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: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: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: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:E:312:ASP:CG	1:E:314:GLY:H	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H:358:VAL:HG11	1:H:407:LEU:HD21	1.95	0.48
1:D:585:LEU:C	1:D:585:LEU:HD23	2.34	0.48
1:B:417:THR:HG22	2:B:701:WYQ:N5	2.23	0.48
1:B:585:LEU:HD23	1:B:585:LEU:C	2.33	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:E:585:LEU:HD23	1:E:585:LEU:C	2.34	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: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:B:397:LEU:HD23	1:B:397:LEU:C	2.35	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:G:397:LEU:HD23	1:G:397:LEU:C	2.34	0.47
1:D:308:VAL:HA	1:D:311:ARG:HH21	1.78	0.47
1:B:441:LEU:C	1:B:441:LEU:HD13	2.35	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:H:407:LEU:HD23	1:H:407:LEU:C	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:G:354:LEU:HD13	1:G:354:LEU:C	2.36	0.46
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: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:D:584:LEU:HD13	1:D:584:LEU:C	2.36	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:397:LEU:C	1:A:397:LEU:HD23	2.37	0.45
1:B:278:ILE:HG23	1:B:281:ARG:CB	2.44	0.45
1:B:278:ILE:CD1	1:D:470:LYS:HZ3	2.27	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:397:LEU:HD23	1:F:397:LEU:C	2.37	0.45
1:F:439:GLU:HG2	1:F:481:ASP:HB2	1.98	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: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: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: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: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:C:323:ARG:HB2	1:C:324:VAL:H	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:LEU:HD13	1:C:455:PHE:HB3	1.99	0.44
2:C:701:WYQ:H11	2:C:701:WYQ:H12	1.70	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:F:411:VAL:O	1:F:412:CYS:HB2	2.18	0.44
1:G:501:PHE:CE1	1:G:588:LEU:HD13	2.52	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:F:278:ILE:C	1:F:280:THR:H	2.21	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:326:SER:OG	1:E:329:GLN:HB2	2.17	0.43
1:G:310:LEU:HG	1:G:334:HIS:CD2	2.53	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: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:B:500:GLY:O	1:B:501:PHE:CB	2.63	0.43
1:A:507:GLU:CD	1:A:507:GLU:H	2.22	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:C:306:THR:O	1:C:309:ASP:HB2	2.19	0.42
1:C:397:LEU:C	1:C:397:LEU:HD23	2.39	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:550:ARG:C	1:E:552:ARG:N	2.73	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: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: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:G:585:LEU:HD23	1:G:585:LEU:C	2.41	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:G:281:ARG:O	1:G:282:ARG:HB2	2.20	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:320:VAL:C	1:D:322:SER:H	2.24	0.41
1:E:524:ALA:HB1	1:E:535:TRP:CD1	2.56	0.41
1:H:388:LYS:HE3	1:H:392:GLU:CD	2.39	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: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:G:316:ASP:CG	1:G:319:GLU:HB2	2.41	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
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:481:ASP:CG	1:D:483:SER:HB3	2.42	0.40
1:A:306:THR:O	1:A:309:ASP:HB2	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:561:GLU:O	1:E:562:THR:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/345 (96%)	325 (98%)	4 (1%)	1 (0%)	41	47
1	B	332/345 (96%)	319 (96%)	9 (3%)	4 (1%)	13	11
1	C	331/345 (96%)	308 (93%)	18 (5%)	5 (2%)	10	7
1	D	329/345 (95%)	309 (94%)	14 (4%)	6 (2%)	8	5
1	E	329/345 (95%)	302 (92%)	19 (6%)	8 (2%)	6	3
1	F	332/345 (96%)	319 (96%)	11 (3%)	2 (1%)	25	26
1	G	332/345 (96%)	315 (95%)	13 (4%)	4 (1%)	13	11
1	H	328/345 (95%)	308 (94%)	18 (6%)	2 (1%)	25	26
All	All	2643/2760 (96%)	2505 (95%)	106 (4%)	32 (1%)	13	11

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

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Mol	Chain	Res	Type
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 (i)

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%)	270 (98%)	6 (2%)	52	63
1	B	278/286 (97%)	271 (98%)	7 (2%)	47	58
1	C	277/286 (97%)	268 (97%)	9 (3%)	39	47
1	D	275/286 (96%)	267 (97%)	8 (3%)	42	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	275/286 (96%)	270 (98%)	5 (2%)	59	70
1	F	278/286 (97%)	269 (97%)	9 (3%)	39	47
1	G	278/286 (97%)	271 (98%)	7 (2%)	47	58
1	H	275/286 (96%)	267 (97%)	8 (3%)	42	52
All	All	2212/2288 (97%)	2153 (97%)	59 (3%)	44	55

All (59) 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	427	PRO
1	A	533	ARG
1	A	599	LEU
1	B	354	LEU
1	B	388	LYS
1	B	391	MET
1	B	484	LEU
1	B	507	GLU
1	B	558	PRO
1	B	599	LEU
1	C	282	ARG
1	C	307	ASP
1	C	318	PHE
1	C	328	LEU
1	C	391	MET
1	C	463	ASN
1	C	504	THR
1	C	533	ARG
1	C	558	PRO
1	D	290	ASP
1	D	318	PHE
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

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Mol	Chain	Res	Type
1	E	354	LEU
1	E	463	ASN
1	E	504	THR
1	F	290	ASP
1	F	345	GLN
1	F	363	ARG
1	F	391	MET
1	F	424	VAL
1	F	504	THR
1	F	533	ARG
1	F	558	PRO
1	F	599	LEU
1	G	290	ASP
1	G	328	LEU
1	G	335	VAL
1	G	345	GLN
1	G	391	MET
1	G	507	GLU
1	G	599	LEU
1	H	304	ILE
1	H	318	PHE
1	H	391	MET
1	H	463	ASN
1	H	504	THR
1	H	558	PRO
1	H	599	LEU
1	H	603	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	HIS
1	A	345	GLN
1	A	360	ASN
1	A	393	HIS
1	A	451	ASN
1	A	463	ASN
1	B	289	GLN
1	B	334	HIS
1	B	345	GLN
1	B	463	ASN
1	B	479	HIS

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Mol	Chain	Res	Type
1	B	587	GLN
1	B	597	HIS
1	C	463	ASN
1	C	479	HIS
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	E	329	GLN
1	E	334	HIS
1	E	360	ASN
1	E	451	ASN
1	E	463	ASN
1	E	479	HIS
1	F	289	GLN
1	F	345	GLN
1	F	425	GLN
1	F	463	ASN
1	F	485	HIS
1	F	597	HIS
1	G	289	GLN
1	G	345	GLN
1	G	349	GLN
1	G	360	ASN
1	G	393	HIS
1	G	463	ASN
1	G	475	HIS
1	G	479	HIS
1	H	345	GLN
1	H	360	ASN
1	H	463	ASN
1	H	479	HIS
1	H	540	GLN
1	H	587	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B	701	-	31,35,35	2.54	6 (19%)	36,51,51	2.93	11 (30%)
2	WYQ	F	701	-	31,35,35	2.48	6 (19%)	36,51,51	2.90	10 (27%)
2	WYQ	A	701	-	31,35,35	2.49	6 (19%)	36,51,51	2.86	11 (30%)
2	WYQ	G	701	-	31,35,35	2.50	5 (16%)	36,51,51	2.79	11 (30%)
2	WYQ	D	701	-	31,35,35	2.48	6 (19%)	36,51,51	3.06	11 (30%)
2	WYQ	C	701	-	31,35,35	2.47	6 (19%)	36,51,51	2.79	11 (30%)
2	WYQ	E	701	-	31,35,35	2.50	6 (19%)	36,51,51	2.86	10 (27%)
2	WYQ	H	701	-	31,35,35	2.50	6 (19%)	36,51,51	3.01	11 (30%)

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	B	701	-	-	7/25/25/25	0/3/3/3
2	WYQ	F	701	-	-	10/25/25/25	0/3/3/3
2	WYQ	A	701	-	-	14/25/25/25	0/3/3/3
2	WYQ	G	701	-	-	9/25/25/25	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	WYQ	D	701	-	-	9/25/25/25	0/3/3/3
2	WYQ	C	701	-	-	12/25/25/25	0/3/3/3
2	WYQ	E	701	-	-	15/25/25/25	0/3/3/3
2	WYQ	H	701	-	-	9/25/25/25	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	WYQ	C14-N5	-8.22	1.33	1.38
2	E	701	WYQ	C14-N5	-8.06	1.33	1.38
2	H	701	WYQ	C14-N5	-8.04	1.33	1.38
2	G	701	WYQ	C14-N5	-8.04	1.33	1.38
2	A	701	WYQ	C14-N5	-8.01	1.33	1.38
2	D	701	WYQ	C14-N5	-7.94	1.33	1.38
2	C	701	WYQ	C14-N5	-7.84	1.33	1.38
2	F	701	WYQ	C14-N5	-7.84	1.33	1.38
2	B	701	WYQ	C18-N2	-6.99	1.33	1.47
2	G	701	WYQ	C18-N2	-6.98	1.33	1.47
2	D	701	WYQ	C18-N2	-6.96	1.33	1.47
2	F	701	WYQ	C18-N2	-6.94	1.33	1.47
2	C	701	WYQ	C18-N2	-6.94	1.33	1.47
2	H	701	WYQ	C18-N2	-6.93	1.33	1.47
2	E	701	WYQ	C18-N2	-6.92	1.33	1.47
2	A	701	WYQ	C18-N2	-6.91	1.33	1.47
2	B	701	WYQ	O3-S1	6.19	1.50	1.43
2	F	701	WYQ	O3-S1	6.15	1.50	1.43
2	H	701	WYQ	O3-S1	6.13	1.50	1.43
2	E	701	WYQ	O3-S1	6.09	1.50	1.43
2	C	701	WYQ	O3-S1	6.08	1.50	1.43
2	A	701	WYQ	O3-S1	6.08	1.50	1.43
2	D	701	WYQ	O3-S1	6.04	1.50	1.43
2	G	701	WYQ	O3-S1	6.02	1.50	1.43
2	B	701	WYQ	C6-C5	-4.54	1.39	1.47
2	E	701	WYQ	C6-C5	-4.45	1.39	1.47
2	F	701	WYQ	C6-C5	-4.45	1.39	1.47
2	D	701	WYQ	C6-C5	-4.44	1.39	1.47
2	G	701	WYQ	C6-C5	-4.44	1.39	1.47
2	A	701	WYQ	C6-C5	-4.43	1.39	1.47
2	C	701	WYQ	C6-C5	-4.40	1.39	1.47
2	H	701	WYQ	C6-C5	-4.38	1.39	1.47
2	G	701	WYQ	C3-C4	-2.42	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	WYQ	C3-C4	-2.41	1.39	1.45
2	A	701	WYQ	C3-C4	-2.40	1.39	1.45
2	C	701	WYQ	C3-C4	-2.39	1.39	1.45
2	E	701	WYQ	C3-C4	-2.38	1.39	1.45
2	H	701	WYQ	C3-C4	-2.35	1.39	1.45
2	F	701	WYQ	C3-C4	-2.35	1.39	1.45
2	D	701	WYQ	C3-C4	-2.35	1.39	1.45
2	B	701	WYQ	C2-N3	-2.10	1.34	1.38
2	A	701	WYQ	C2-N3	-2.09	1.34	1.38
2	F	701	WYQ	C2-N3	-2.06	1.34	1.38
2	H	701	WYQ	C2-N3	-2.04	1.34	1.38
2	C	701	WYQ	C2-N3	-2.02	1.34	1.38
2	E	701	WYQ	C2-N3	-2.01	1.34	1.38
2	D	701	WYQ	C2-N3	-2.01	1.34	1.38

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	701	WYQ	O6-C14-N5	10.97	119.81	108.56
2	H	701	WYQ	O6-C14-N5	10.62	119.45	108.56
2	F	701	WYQ	O6-C14-N5	10.57	119.40	108.56
2	E	701	WYQ	O6-C14-N5	9.84	118.64	108.56
2	B	701	WYQ	O6-C14-N5	9.59	118.39	108.56
2	A	701	WYQ	O6-C14-N5	9.09	117.88	108.56
2	C	701	WYQ	O6-C14-N5	8.72	117.50	108.56
2	A	701	WYQ	O3-S1-O4	-8.63	108.94	119.55
2	C	701	WYQ	O3-S1-O4	-8.59	108.99	119.55
2	D	701	WYQ	O3-S1-O4	-8.56	109.02	119.55
2	B	701	WYQ	O3-S1-O4	-8.56	109.03	119.55
2	H	701	WYQ	O3-S1-O4	-8.56	109.03	119.55
2	G	701	WYQ	O3-S1-O4	-8.53	109.06	119.55
2	G	701	WYQ	O6-C14-N5	8.51	117.29	108.56
2	E	701	WYQ	O3-S1-O4	-7.95	109.77	119.55
2	F	701	WYQ	O3-S1-O4	-7.56	110.26	119.55
2	H	701	WYQ	C1-N1-N2	6.62	110.19	104.48
2	A	701	WYQ	C1-N1-N2	6.61	110.18	104.48
2	E	701	WYQ	C1-N1-N2	6.59	110.17	104.48
2	D	701	WYQ	C1-N1-N2	6.56	110.14	104.48
2	B	701	WYQ	C1-N1-N2	6.48	110.07	104.48
2	C	701	WYQ	C1-N1-N2	6.46	110.05	104.48
2	F	701	WYQ	C1-N1-N2	6.45	110.04	104.48
2	G	701	WYQ	C1-N1-N2	6.43	110.02	104.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	701	WYQ	O6-C14-O5	-4.67	117.49	124.53
2	H	701	WYQ	O6-C14-O5	-4.37	117.94	124.53
2	G	701	WYQ	C3-C2-C1	-4.20	104.38	107.46
2	F	701	WYQ	O6-C14-O5	-4.13	118.30	124.53
2	E	701	WYQ	C3-C2-C1	-4.09	104.46	107.46
2	A	701	WYQ	C3-C2-C1	-4.05	104.49	107.46
2	D	701	WYQ	C3-C2-C1	-3.97	104.54	107.46
2	H	701	WYQ	C3-C2-C1	-3.90	104.60	107.46
2	C	701	WYQ	C3-C2-C1	-3.85	104.63	107.46
2	F	701	WYQ	C3-C2-C1	-3.78	104.69	107.46
2	B	701	WYQ	O6-C14-O5	-3.76	118.87	124.53
2	B	701	WYQ	C3-C2-C1	-3.76	104.70	107.46
2	E	701	WYQ	O6-C14-O5	-3.74	118.89	124.53
2	A	701	WYQ	O6-C14-O5	-3.59	119.12	124.53
2	B	701	WYQ	C15-O6-C14	-3.51	109.61	116.61
2	E	701	WYQ	C12-O2-C11	-3.35	110.75	118.05
2	C	701	WYQ	O6-C14-O5	-3.35	119.48	124.53
2	G	701	WYQ	O6-C14-O5	-3.33	119.51	124.53
2	D	701	WYQ	C12-O2-C11	-3.29	110.88	118.05
2	F	701	WYQ	C15-O6-C14	-3.28	110.08	116.61
2	D	701	WYQ	C8-S1-N5	3.26	110.91	105.97
2	C	701	WYQ	C8-S1-N5	3.20	110.81	105.97
2	B	701	WYQ	C8-S1-N5	3.18	110.78	105.97
2	G	701	WYQ	C8-S1-N5	3.14	110.72	105.97
2	A	701	WYQ	C11-C6-C5	-3.11	119.27	124.47
2	G	701	WYQ	C12-O2-C11	-3.06	111.38	118.05
2	H	701	WYQ	C12-O2-C11	-3.05	111.39	118.05
2	A	701	WYQ	C12-O2-C11	-3.05	111.39	118.05
2	C	701	WYQ	C12-O2-C11	-3.01	111.49	118.05
2	B	701	WYQ	C12-O2-C11	-2.95	111.63	118.05
2	C	701	WYQ	N4-C5-N3	-2.93	120.15	123.10
2	F	701	WYQ	C12-O2-C11	-2.92	111.69	118.05
2	H	701	WYQ	C8-S1-N5	2.90	110.36	105.97
2	B	701	WYQ	N4-C5-N3	-2.90	120.19	123.10
2	E	701	WYQ	C15-O6-C14	-2.88	110.87	116.61
2	G	701	WYQ	C11-C6-C5	-2.83	119.75	124.47
2	D	701	WYQ	N4-C5-N3	-2.80	120.28	123.10
2	A	701	WYQ	C8-S1-N5	2.78	110.19	105.97
2	F	701	WYQ	N4-C5-N3	-2.74	120.34	123.10
2	G	701	WYQ	N4-C5-N3	-2.73	120.35	123.10
2	E	701	WYQ	N4-C5-N3	-2.61	120.47	123.10
2	H	701	WYQ	N4-C5-N3	-2.56	120.52	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	701	WYQ	C11-C6-C5	-2.55	120.22	124.47
2	A	701	WYQ	N4-C5-N3	-2.54	120.55	123.10
2	H	701	WYQ	C15-O6-C14	-2.50	111.62	116.61
2	B	701	WYQ	C19-C1-C2	-2.43	126.19	130.34
2	C	701	WYQ	C19-C1-C2	-2.37	126.29	130.34
2	G	701	WYQ	C19-C1-C2	-2.35	126.32	130.34
2	C	701	WYQ	C11-C6-C5	-2.35	120.55	124.47
2	G	701	WYQ	C15-O6-C14	-2.34	111.95	116.61
2	H	701	WYQ	C19-C1-C2	-2.33	126.36	130.34
2	A	701	WYQ	C15-O6-C14	-2.32	111.98	116.61
2	C	701	WYQ	C15-O6-C14	-2.25	112.13	116.61
2	F	701	WYQ	C19-C1-C2	-2.24	126.52	130.34
2	D	701	WYQ	C11-C6-C5	-2.21	120.78	124.47
2	D	701	WYQ	C19-C1-C2	-2.18	126.62	130.34
2	A	701	WYQ	C19-C1-C2	-2.14	126.68	130.34
2	D	701	WYQ	C15-O6-C14	-2.14	112.35	116.61
2	E	701	WYQ	C19-C1-C2	-2.09	126.78	130.34
2	B	701	WYQ	C6-C5-N4	2.08	121.15	118.19
2	F	701	WYQ	C11-C6-C5	-2.06	121.03	124.47
2	E	701	WYQ	C11-C6-C5	-2.03	121.07	124.47

There are no chirality outliers.

All (85) 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	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
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

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Mol	Chain	Res	Type	Atoms
2	E	701	WYQ	C14-N5-S1-O4
2	E	701	WYQ	C14-N5-S1-C8
2	E	701	WYQ	C2-C1-C19-C20
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	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	A	701	WYQ	C1-C19-C20-C21
2	E	701	WYQ	C1-C19-C20-C21
2	F	701	WYQ	C1-C19-C20-C21
2	H	701	WYQ	C9-C8-S1-O4
2	A	701	WYQ	C17-C15-O6-C14
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	C	701	WYQ	C9-C8-S1-O4
2	F	701	WYQ	C7-C8-S1-O3
2	F	701	WYQ	C9-C8-S1-O3
2	H	701	WYQ	C7-C8-S1-O4
2	C	701	WYQ	C9-C8-S1-N5
2	A	701	WYQ	C16-C15-O6-C14
2	C	701	WYQ	C7-C8-S1-N5
2	F	701	WYQ	C7-C8-S1-N5
2	A	701	WYQ	C7-C8-S1-O4
2	D	701	WYQ	C7-C8-S1-N5
2	D	701	WYQ	C9-C8-S1-N5
2	A	701	WYQ	C13-C12-O2-C11
2	H	701	WYQ	C7-C8-S1-N5

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Mol	Chain	Res	Type	Atoms
2	B	701	WYQ	C9-C8-S1-O4
2	A	701	WYQ	C9-C8-S1-O4
2	E	701	WYQ	C10-C11-O2-C12
2	H	701	WYQ	C9-C8-S1-N5
2	G	701	WYQ	C7-C8-S1-O4
2	F	701	WYQ	C14-N5-S1-O3
2	A	701	WYQ	N4-C5-C6-C7
2	E	701	WYQ	N4-C5-C6-C7
2	G	701	WYQ	C9-C8-S1-O4
2	C	701	WYQ	C16-C15-O6-C14
2	H	701	WYQ	C13-C12-O2-C11
2	C	701	WYQ	N3-C5-C6-C7
2	E	701	WYQ	N3-C5-C6-C7
2	C	701	WYQ	N4-C5-C6-C11
2	C	701	WYQ	C17-C15-O6-C14
2	F	701	WYQ	C9-C8-S1-N5
2	A	701	WYQ	C14-N5-S1-C8
2	C	701	WYQ	N3-C5-C6-C11
2	B	701	WYQ	C7-C8-S1-O4
2	E	701	WYQ	C6-C11-O2-C12
2	G	701	WYQ	N4-C5-C6-C7
2	A	701	WYQ	N3-C5-C6-C7
2	E	701	WYQ	C9-C8-S1-O3
2	E	701	WYQ	N4-C5-C6-C11
2	E	701	WYQ	C7-C8-S1-O3
2	C	701	WYQ	C1-C19-C20-C21

There are no ring outliers.

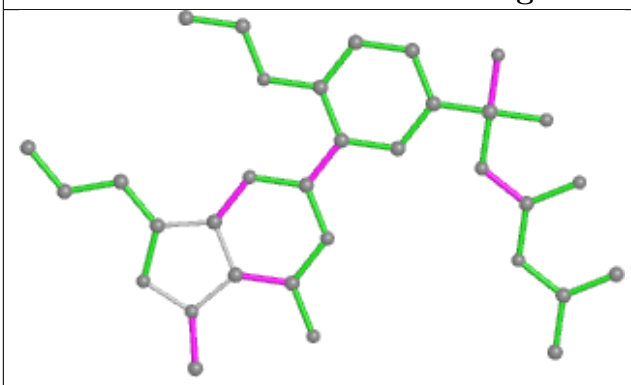
8 monomers are involved in 41 short contacts:

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

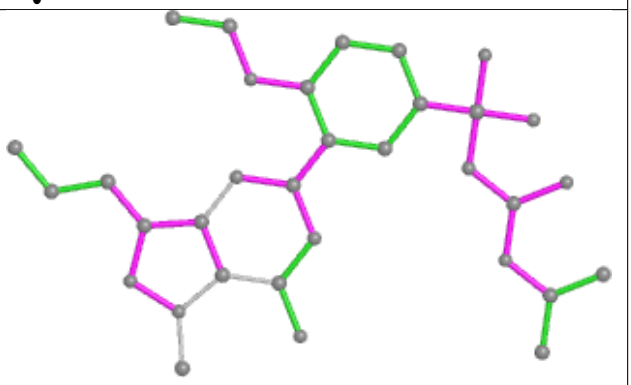
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

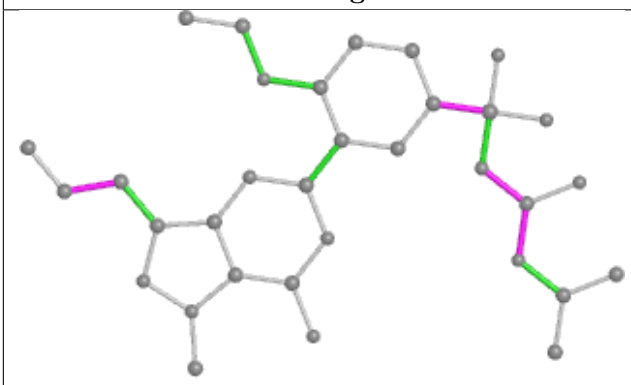
Ligand WYQ B 701



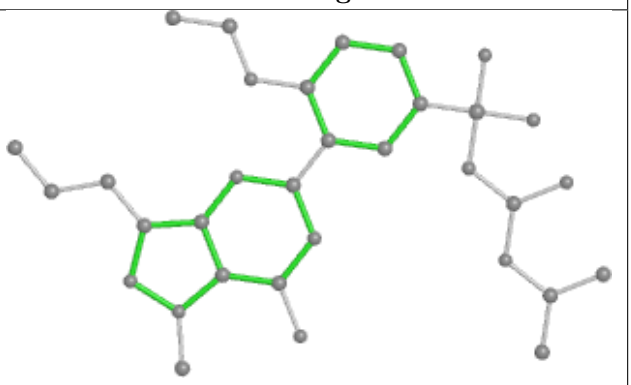
Bond lengths



Bond angles

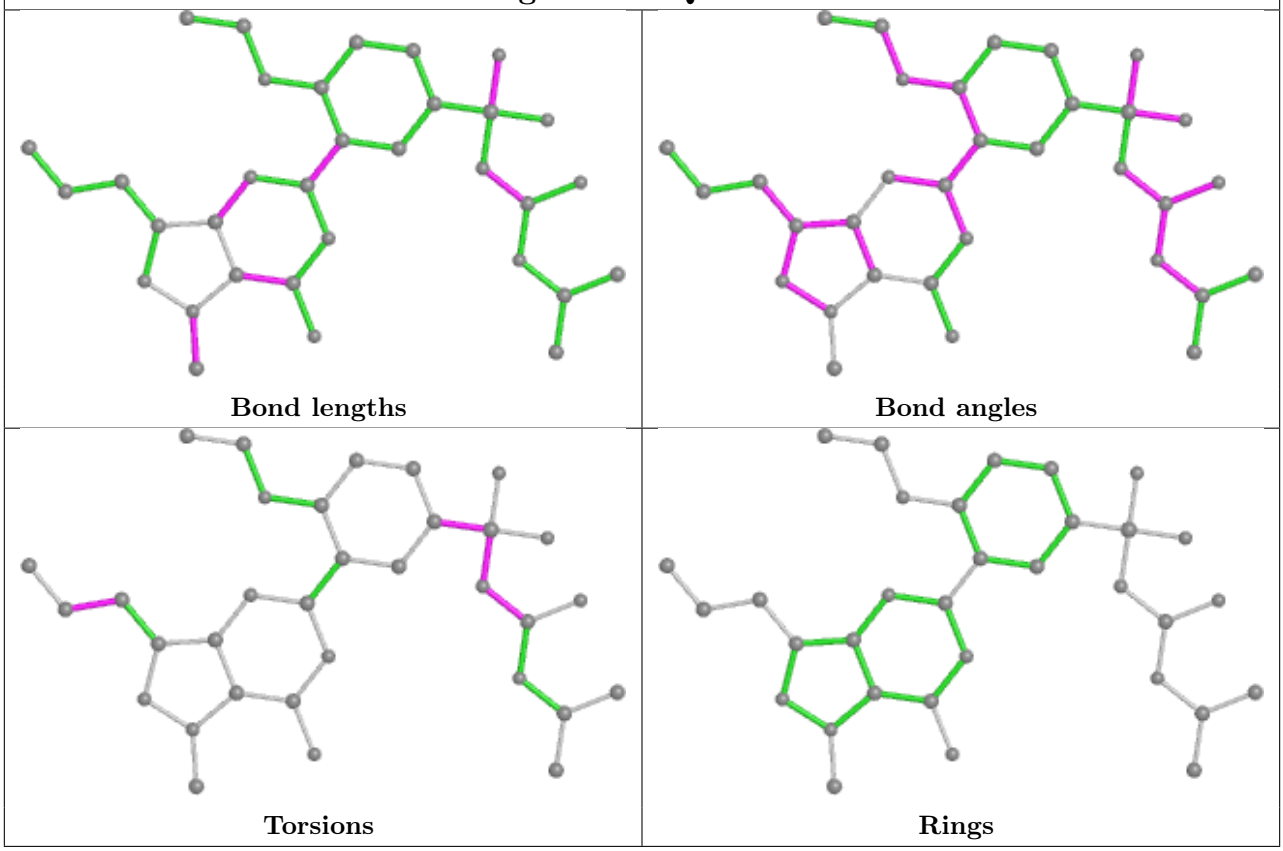


Torsions

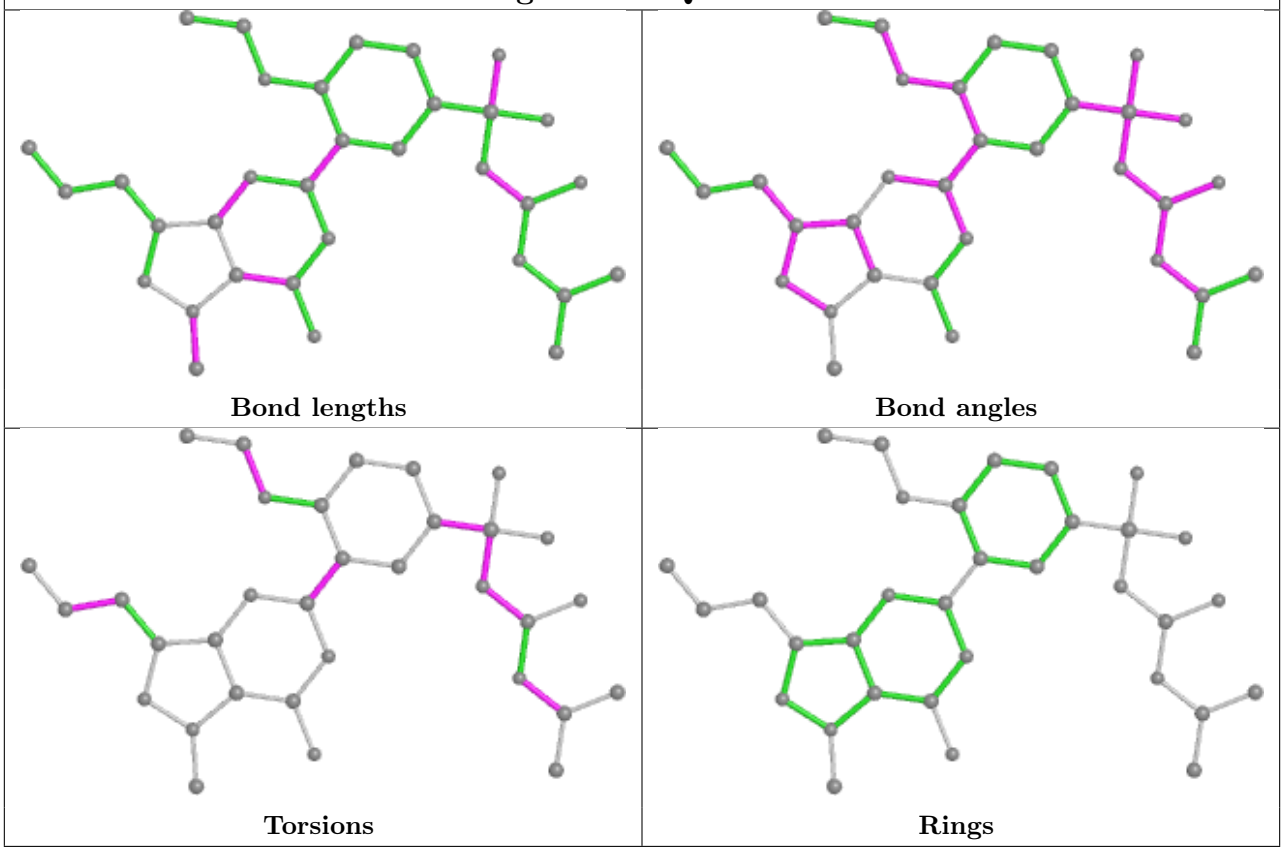


Rings

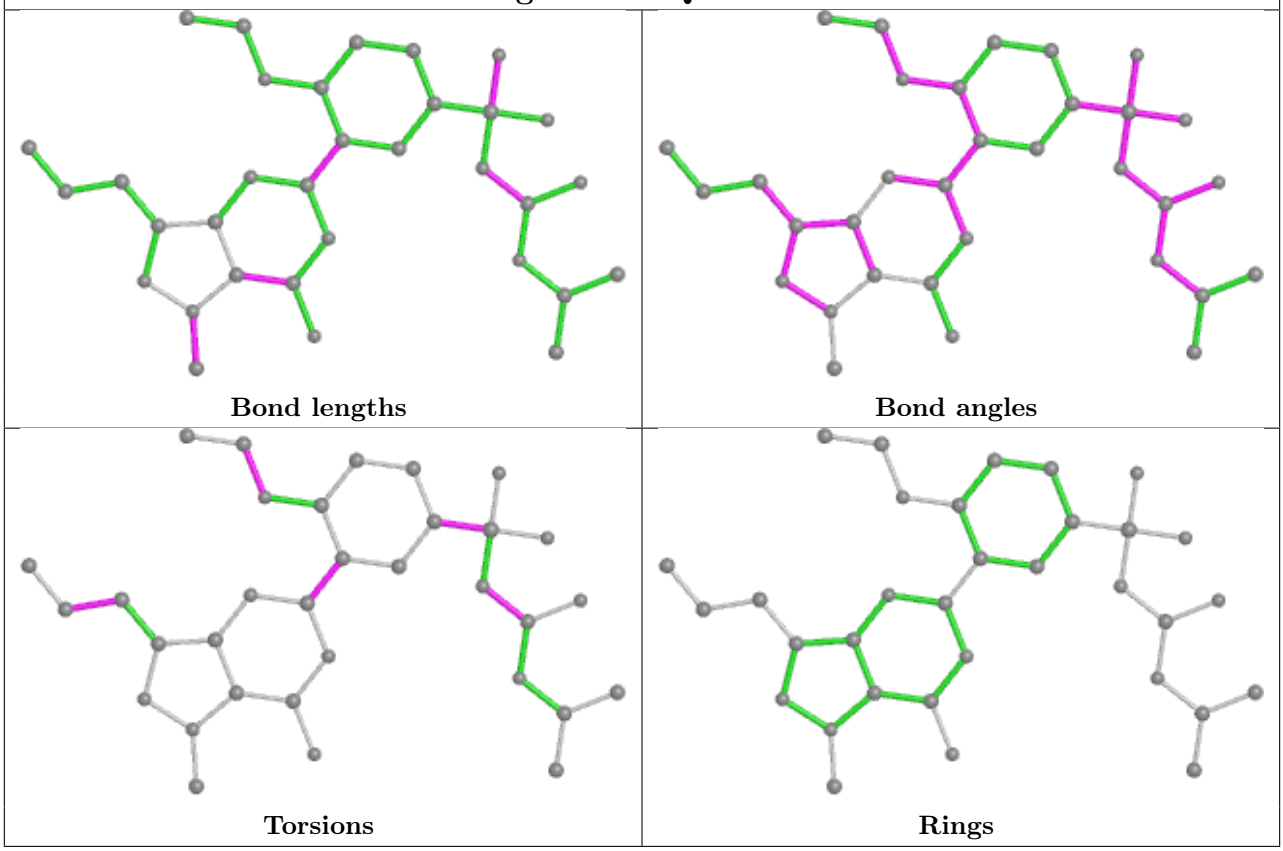
Ligand WYQ F 701



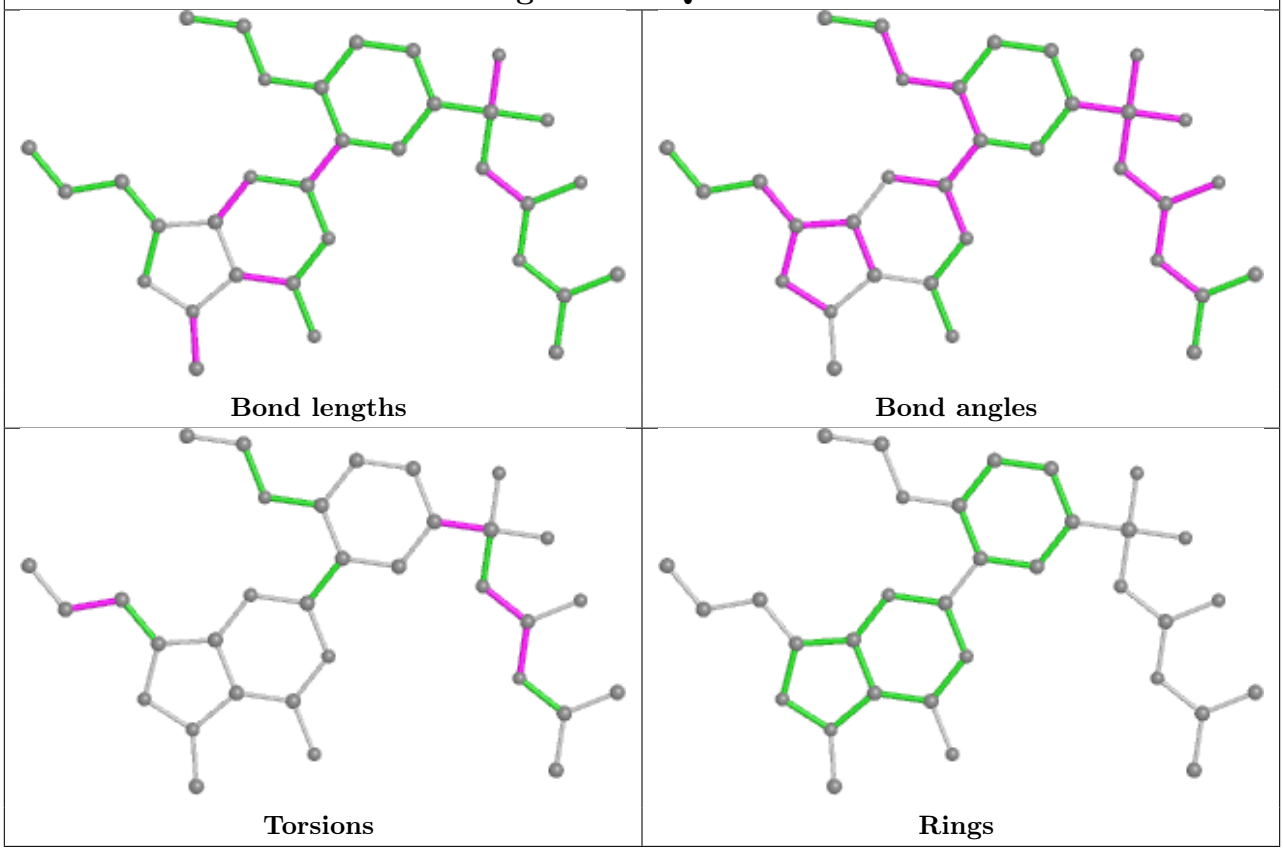
Ligand WYQ A 701



Ligand WYQ G 701



Ligand WYQ D 701



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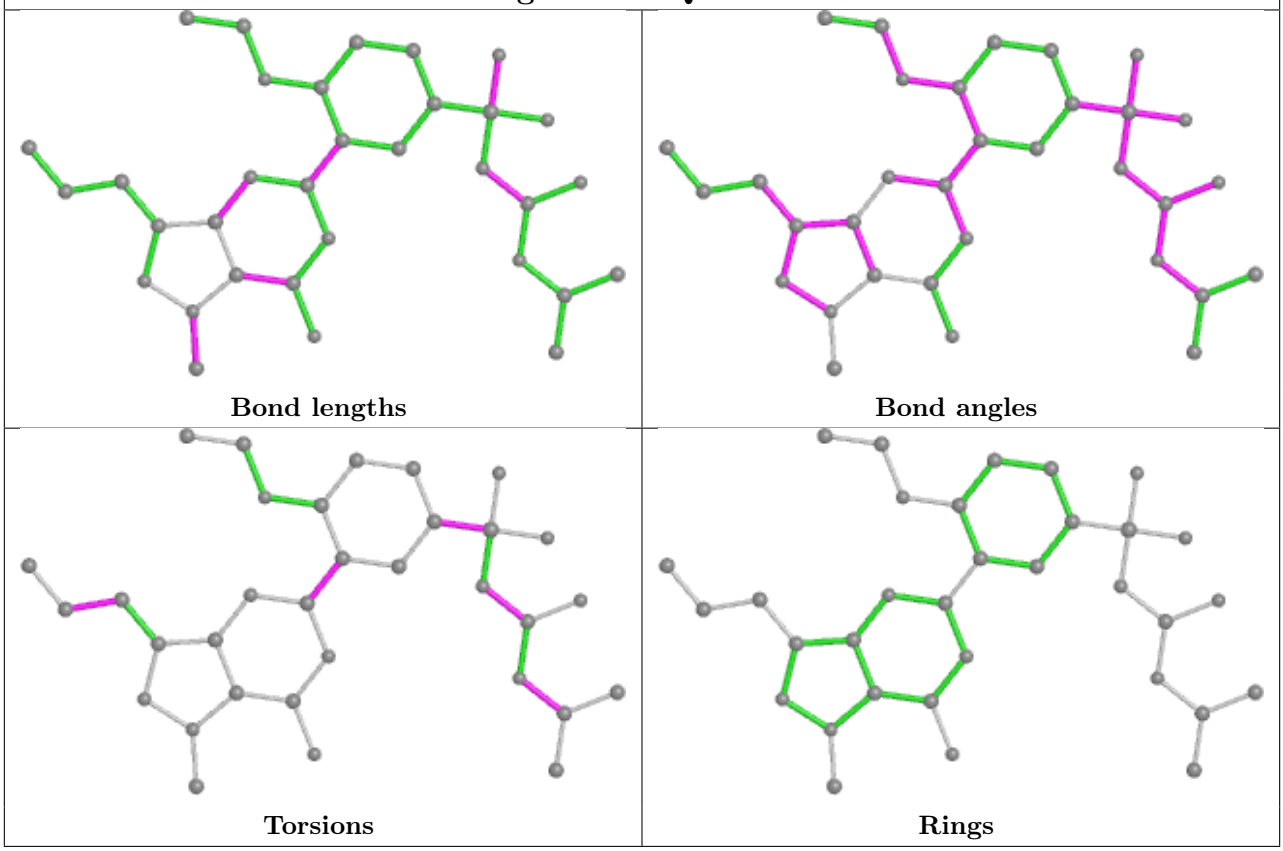

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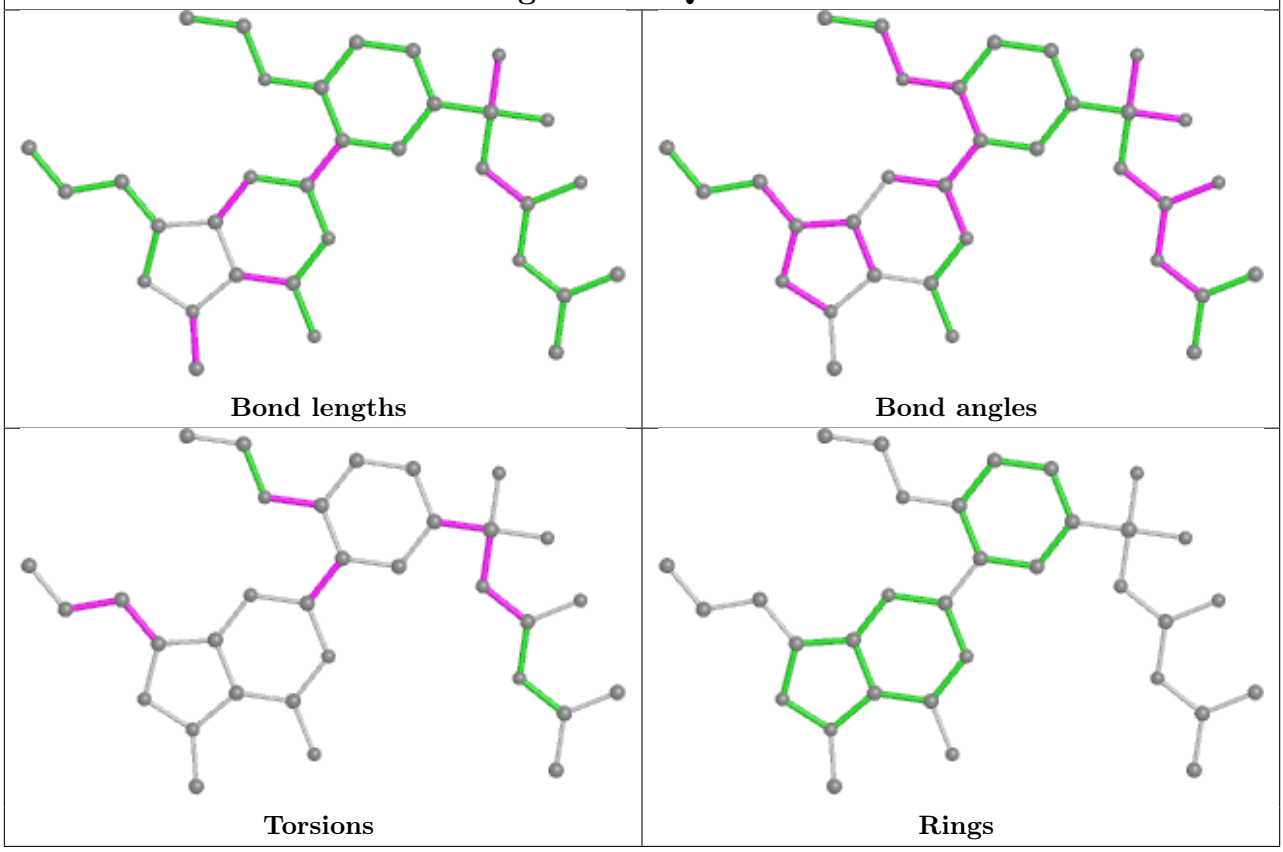

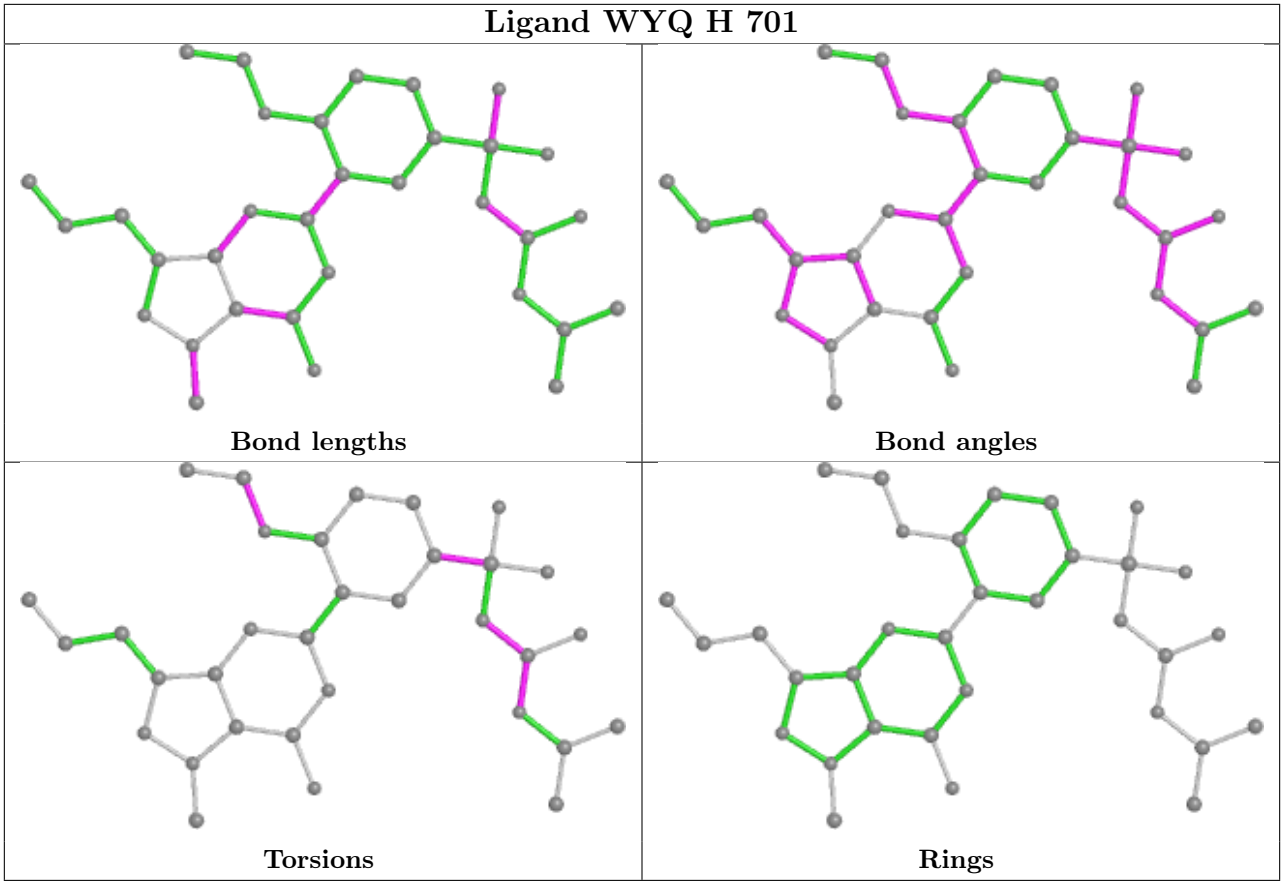

5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.20	6 (1%)	68	76	11, 19, 44, 66	0
1	B	334/345 (96%)	-0.10	9 (2%)	54	64	10, 21, 45, 67	0
1	C	333/345 (96%)	0.03	13 (3%)	39	50	15, 29, 55, 79	0
1	D	331/345 (95%)	0.27	22 (6%)	18	26	18, 37, 65, 83	0
1	E	331/345 (95%)	0.88	50 (15%)	2	3	24, 45, 72, 86	0
1	F	334/345 (96%)	-0.08	9 (2%)	54	64	13, 24, 46, 73	0
1	G	334/345 (96%)	0.23	13 (3%)	39	50	11, 28, 55, 86	0
1	H	330/345 (95%)	0.10	7 (2%)	63	73	17, 35, 60, 74	0
All	All	2659/2760 (96%)	0.14	129 (4%)	29	40	10, 29, 61, 86	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	278	ILE	15.5
1	G	277	MET	13.0
1	F	610	ALA	10.9
1	E	610	ALA	10.7
1	F	278	ILE	9.3
1	B	278	ILE	9.1
1	B	610	ALA	9.0
1	E	303	ALA	8.6
1	C	279	SER	7.8
1	C	278	ILE	7.8
1	A	610	ALA	7.4
1	G	610	ALA	5.7
1	H	343	ALA	5.1
1	F	277	MET	4.9
1	B	277	MET	4.7
1	G	304	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	303	ALA	4.6
1	E	287	ILE	4.4
1	G	279	SER	4.4
1	E	304	ILE	4.4
1	E	554	LEU	4.3
1	E	301	CYS	4.1
1	E	317	THR	4.1
1	E	354	LEU	4.0
1	E	550	ARG	4.0
1	F	609	LYS	3.8
1	E	280	THR	3.8
1	E	282	ARG	3.8
1	E	285	PRO	3.7
1	D	301	CYS	3.7
1	B	609	LYS	3.7
1	G	343	ALA	3.7
1	F	343	ALA	3.6
1	G	349	GLN	3.6
1	E	529	VAL	3.6
1	D	303	ALA	3.5
1	E	424	VAL	3.5
1	G	302	ALA	3.4
1	E	351	TRP	3.4
1	E	420	PHE	3.4
1	E	555	PRO	3.3
1	C	280	THR	3.3
1	D	343	ALA	3.3
1	E	343	ALA	3.3
1	H	280	THR	3.3
1	E	556	VAL	3.3
1	G	303	ALA	3.2
1	A	308	VAL	3.2
1	A	343	ALA	3.2
1	C	282	ARG	3.2
1	D	550	ARG	3.2
1	E	323	ARG	3.2
1	C	576	PHE	3.2
1	E	576	PHE	3.1
1	B	345	GLN	3.1
1	E	423	ALA	3.1
1	D	280	THR	3.0
1	E	283	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	343	ALA	3.0
1	D	300	SER	3.0
1	B	349	GLN	2.9
1	D	302	ALA	2.9
1	E	302	ALA	2.9
1	H	558	PRO	2.9
1	H	576	PHE	2.9
1	D	554	LEU	2.9
1	B	343	ALA	2.9
1	G	348	ALA	2.9
1	E	453	THR	2.9
1	C	344	SER	2.8
1	D	344	SER	2.8
1	E	310	LEU	2.8
1	D	610	ALA	2.7
1	E	559	GLY	2.7
1	E	560	PHE	2.7
1	E	345	GLN	2.7
1	F	303	ALA	2.7
1	E	562	THR	2.7
1	A	303	ALA	2.7
1	E	563	PRO	2.6
1	E	536	LEU	2.6
1	E	566	VAL	2.6
1	G	344	SER	2.6
1	B	302	ALA	2.6
1	A	302	ALA	2.6
1	D	282	ARG	2.5
1	E	347	GLU	2.5
1	C	460	SER	2.5
1	H	529	VAL	2.5
1	G	609	LYS	2.5
1	D	576	PHE	2.5
1	E	328	LEU	2.4
1	E	564	SER	2.4
1	E	337	LEU	2.4
1	A	609	LYS	2.4
1	D	605	LEU	2.4
1	C	345	GLN	2.4
1	F	300	SER	2.4
1	D	304	ILE	2.3
1	H	282	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	551	ARG	2.3
1	C	610	ALA	2.3
1	F	344	SER	2.3
1	G	308	VAL	2.3
1	E	284	PRO	2.3
1	B	279	SER	2.3
1	C	558	PRO	2.3
1	D	551	ARG	2.2
1	E	457	PHE	2.2
1	H	533	ARG	2.2
1	D	317	THR	2.2
1	E	608	ALA	2.2
1	E	606	TYR	2.2
1	E	528	GLY	2.2
1	D	388	LYS	2.2
1	E	296	VAL	2.1
1	D	564	SER	2.1
1	D	424	VAL	2.1
1	E	340	ASP	2.1
1	D	283	LEU	2.1
1	D	533	ARG	2.1
1	D	600	ARG	2.1
1	C	340	ASP	2.1
1	E	572	PRO	2.1
1	E	326	SER	2.1
1	F	279	SER	2.1
1	E	565	SER	2.0
1	E	349	GLN	2.0
1	E	458	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

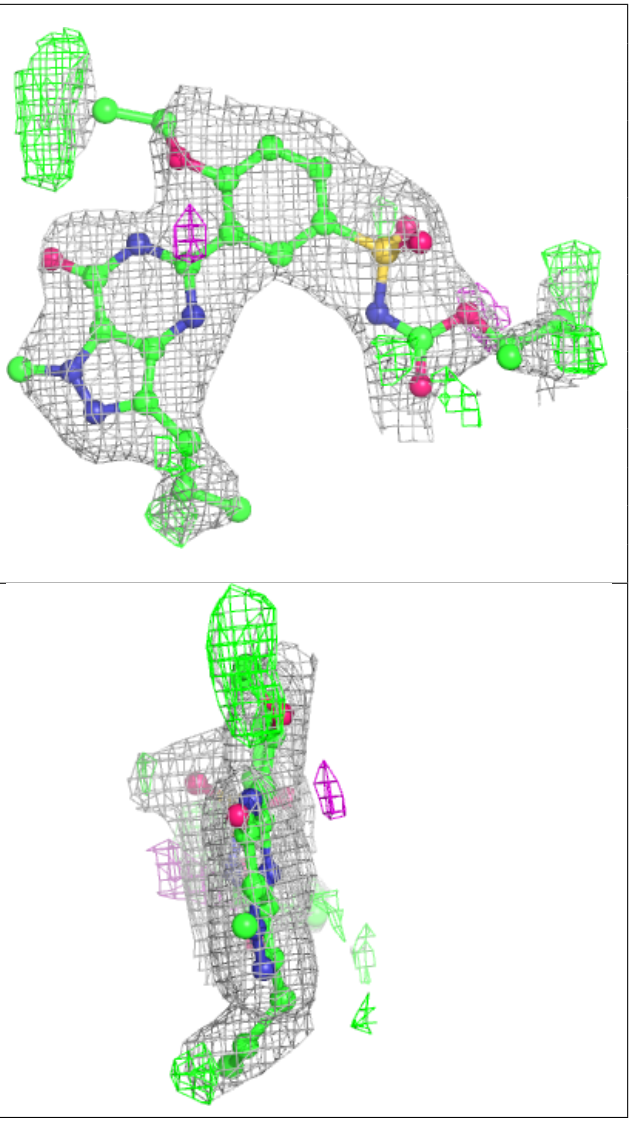
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	E	703	1/1	0.65	0.15	39,39,39,39	0
4	MG	G	703	1/1	0.83	0.22	27,27,27,27	0
2	WYQ	E	701	33/33	0.86	0.23	50,58,71,72	0
4	MG	D	703	1/1	0.86	0.22	33,33,33,33	0
2	WYQ	D	701	33/33	0.88	0.19	43,46,62,64	0
2	WYQ	G	701	33/33	0.91	0.17	11,23,48,49	0
2	WYQ	H	701	33/33	0.91	0.18	37,39,57,58	0
4	MG	A	703	1/1	0.91	0.16	15,15,15,15	0
2	WYQ	A	701	33/33	0.92	0.17	14,21,52,53	0
2	WYQ	B	701	33/33	0.92	0.15	12,18,44,49	0
2	WYQ	F	701	33/33	0.92	0.18	11,19,59,61	0
4	MG	C	703	1/1	0.93	0.21	17,17,17,17	0
2	WYQ	C	701	33/33	0.93	0.16	25,34,54,55	0
4	MG	H	703	1/1	0.95	0.22	24,24,24,24	0
4	MG	B	703	1/1	0.96	0.17	15,15,15,15	0
3	ZN	D	702	1/1	0.98	0.08	30,30,30,30	0
3	ZN	E	702	1/1	0.98	0.05	43,43,43,43	0
3	ZN	G	702	1/1	0.98	0.08	30,30,30,30	0
4	MG	F	703	1/1	0.98	0.17	15,15,15,15	0
3	ZN	A	702	1/1	0.98	0.08	20,20,20,20	0
3	ZN	C	702	1/1	0.98	0.07	23,23,23,23	0
3	ZN	H	702	1/1	0.99	0.10	29,29,29,29	0
3	ZN	F	702	1/1	0.99	0.07	20,20,20,20	0
3	ZN	B	702	1/1	0.99	0.08	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.

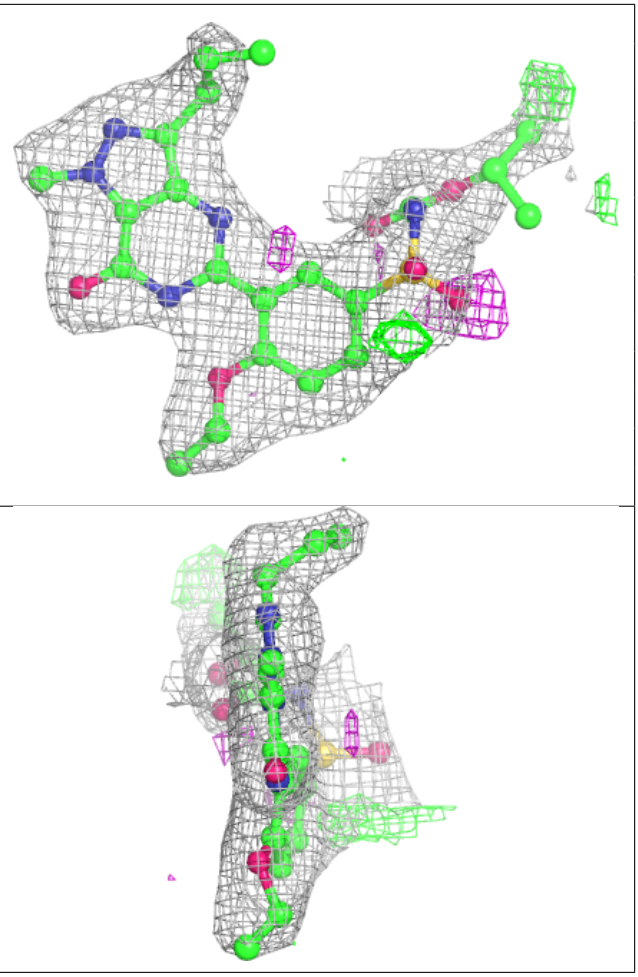
Electron density around WYQ E 701:

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



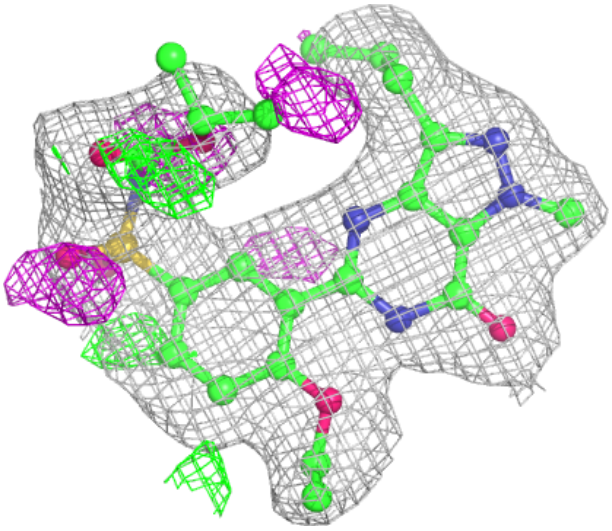
Electron density around WYQ D 701:

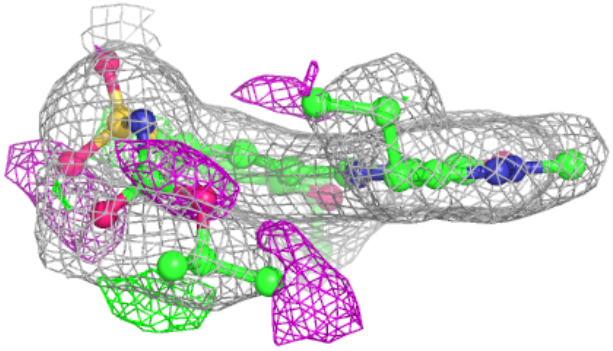
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

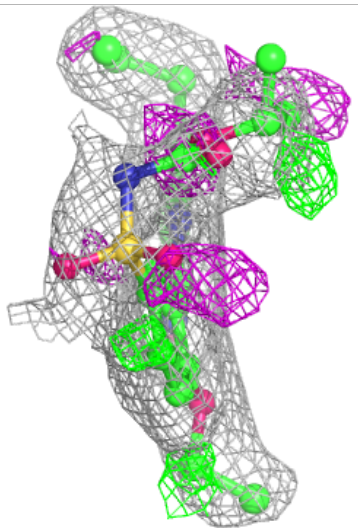


Electron density around WYQ G 701:

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

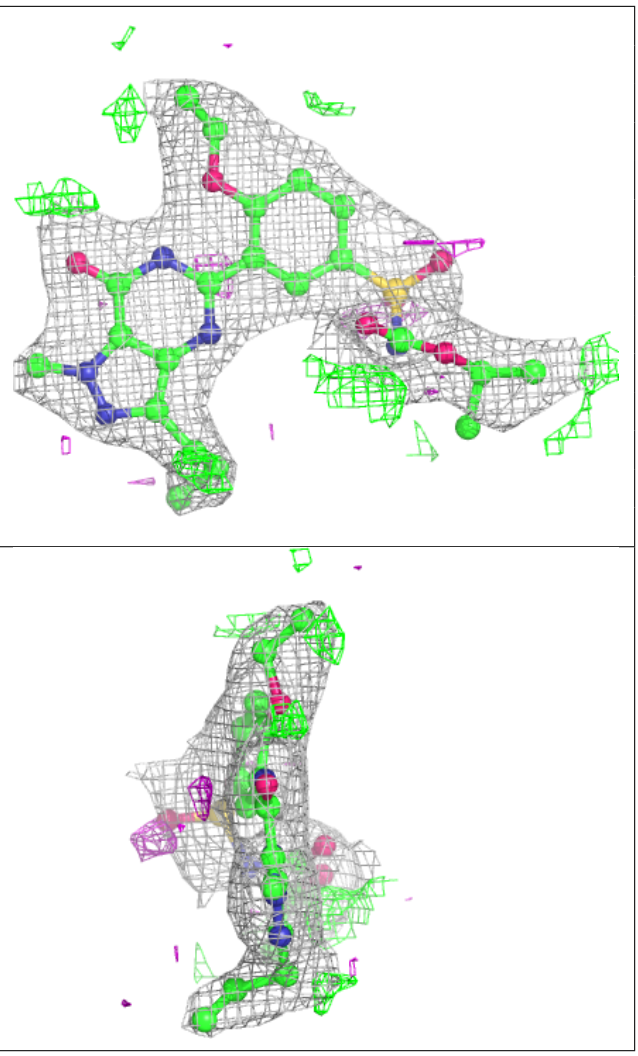






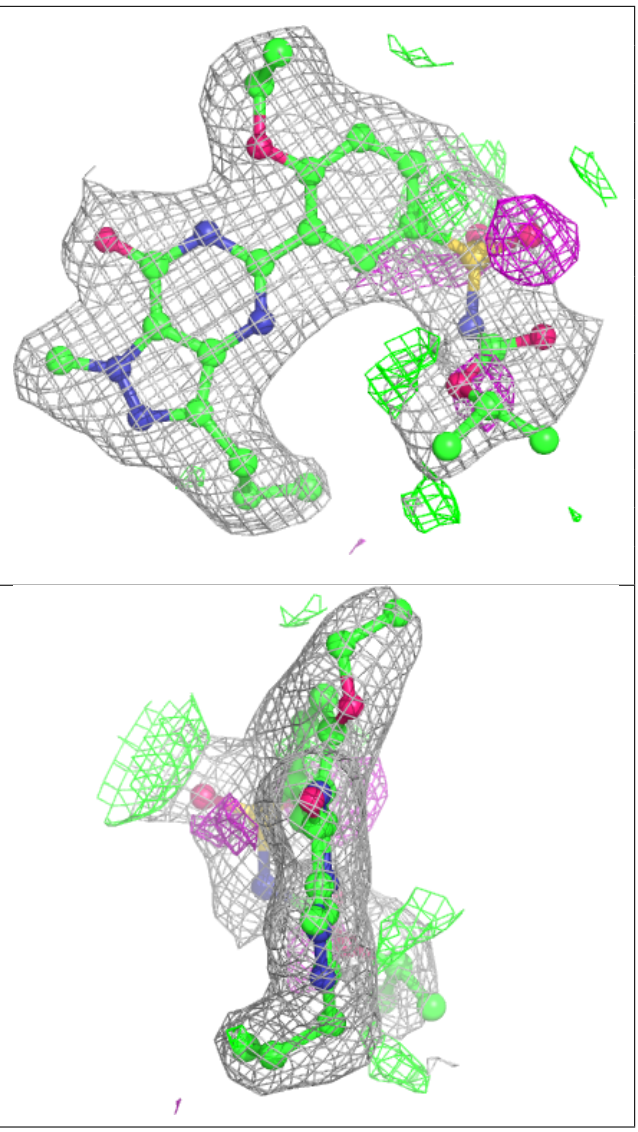
Electron density around WYQ H 701:

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



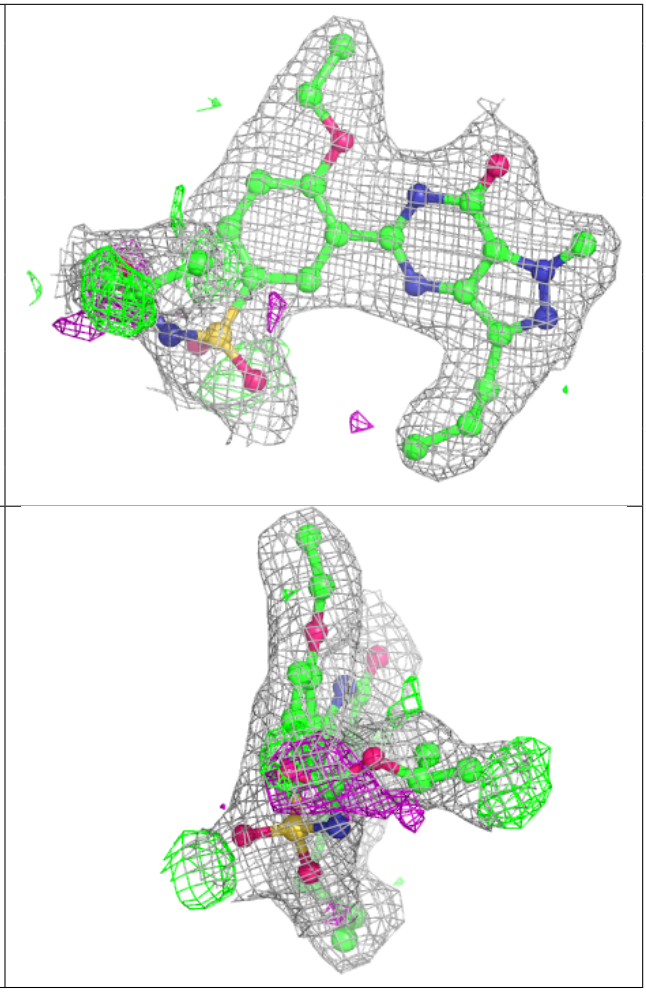
Electron density around WYQ A 701:

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



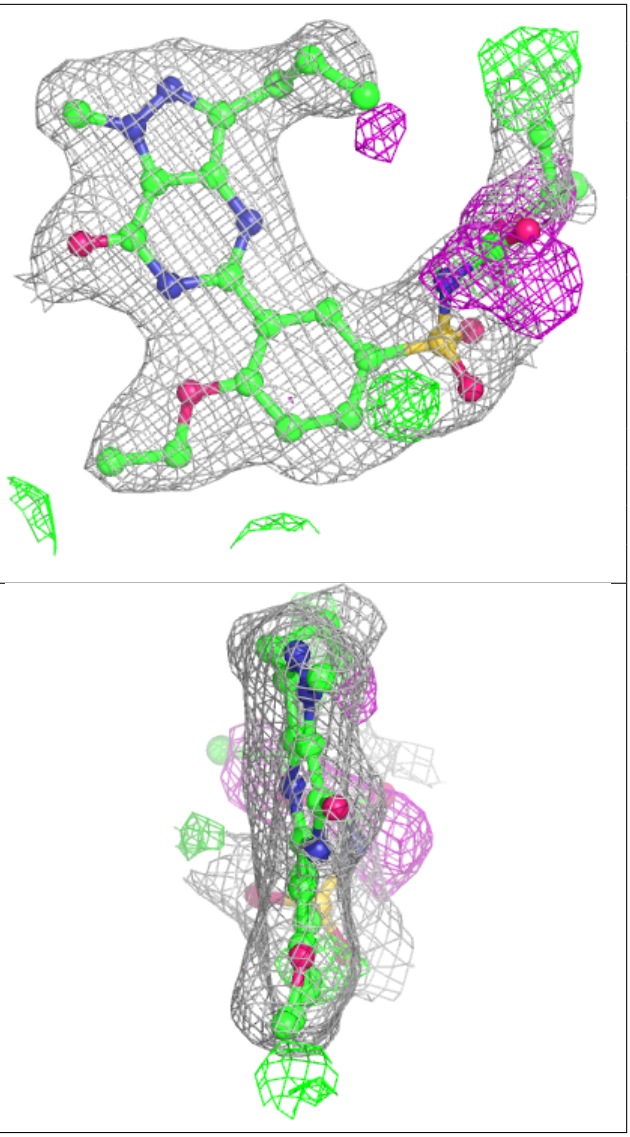
Electron density around WYQ B 701:

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



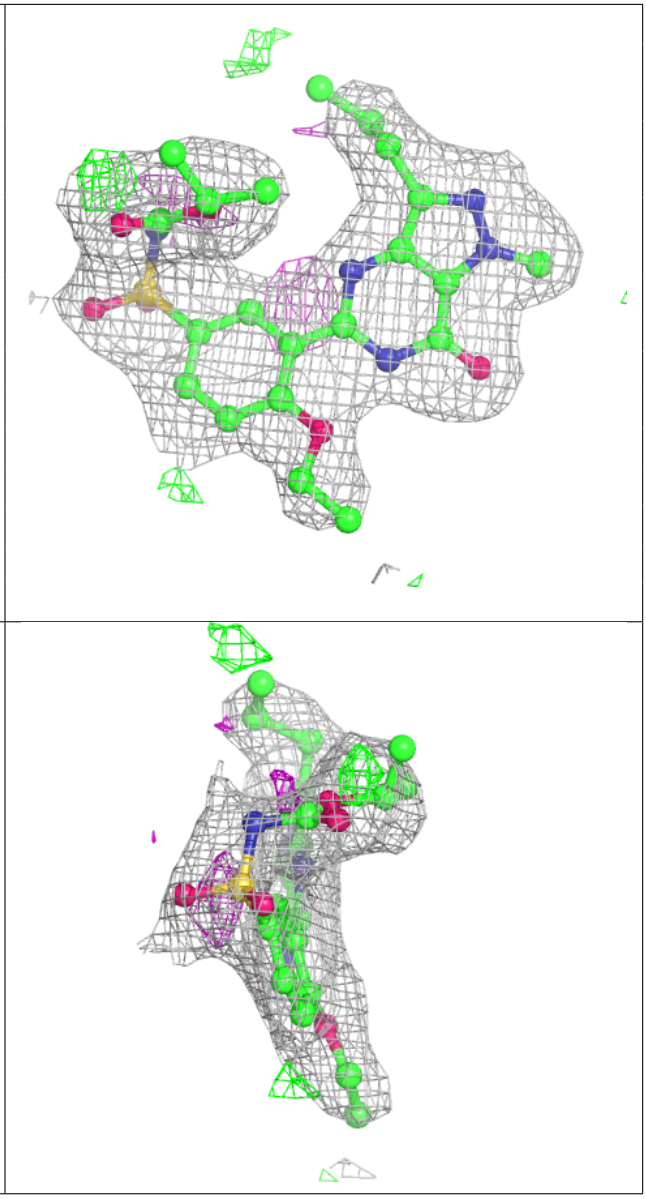
Electron density around WYQ F 701:

$2mF_o$-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 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)



6.5 Other polymers (i)

There are no such residues in this entry.