



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:28 PM UTC

PDB ID : 5HEX / pdb\_00005hex  
Title : Crystal Structure of Human Hexokinase 2 with cmpd 30, a 2-amino-6-benzenesulfonamide glucosamine  
Authors : Campobasso, N.; Zhao, B.; Smallwood, A.  
Deposited on : 2016-01-06  
Resolution : 2.73 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](mailto: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>.

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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)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

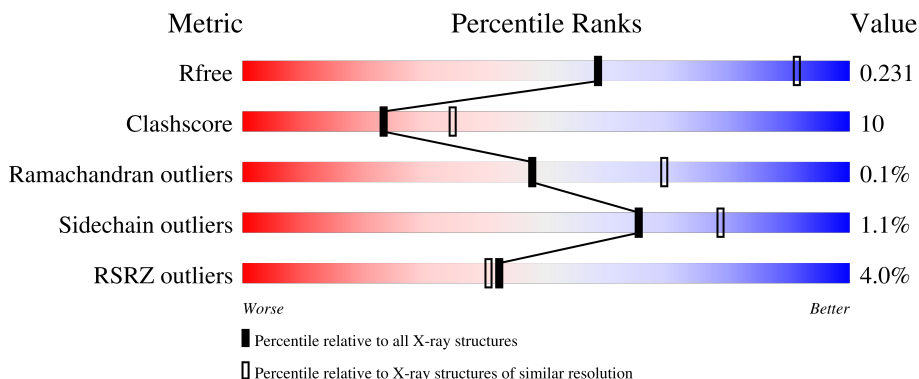
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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  $\geq 3$ , 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	923	 6% 72% 23% • 5%
1	B	923	 2% 80% 16% •

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13830 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 Hexokinase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	880	6771	4245	1191	1274	61	0	1	0
1	B	891	6847	4293	1195	1297	62	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

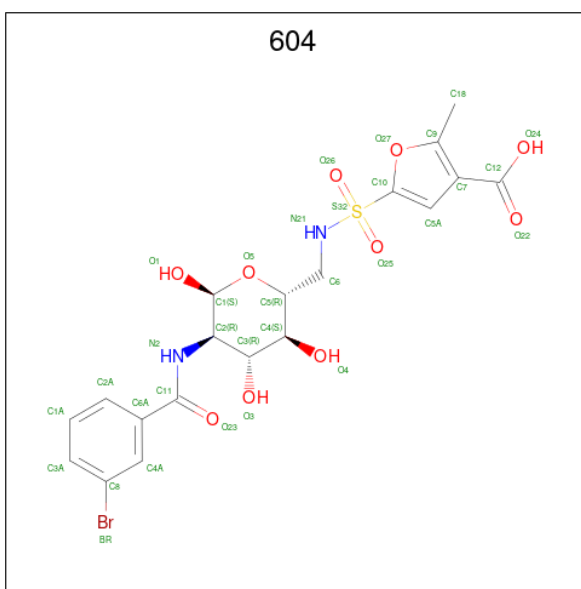
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP P52789
A	-4	GLY	-	expression tag	UNP P52789
A	-3	SER	-	expression tag	UNP P52789
A	-2	SER	-	expression tag	UNP P52789
A	-1	HIS	-	expression tag	UNP P52789
A	0	HIS	-	expression tag	UNP P52789
A	1	HIS	-	expression tag	UNP P52789
A	2	HIS	-	expression tag	UNP P52789
A	3	HIS	-	expression tag	UNP P52789
A	4	HIS	-	expression tag	UNP P52789
A	5	SER	-	expression tag	UNP P52789
A	6	SER	-	expression tag	UNP P52789
A	7	GLY	-	expression tag	UNP P52789
A	8	LEU	-	expression tag	UNP P52789
A	9	GLU	-	expression tag	UNP P52789
A	10	ASN	-	expression tag	UNP P52789
A	11	LEU	-	expression tag	UNP P52789
A	12	TYR	-	expression tag	UNP P52789
A	13	PHE	-	expression tag	UNP P52789
A	14	GLN	-	expression tag	UNP P52789
A	15	GLY	-	expression tag	UNP P52789
A	16	SER	-	expression tag	UNP P52789
B	-5	MET	-	initiating methionine	UNP P52789
B	-4	GLY	-	expression tag	UNP P52789
B	-3	SER	-	expression tag	UNP P52789

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP P52789
B	-1	HIS	-	expression tag	UNP P52789
B	0	HIS	-	expression tag	UNP P52789
B	1	HIS	-	expression tag	UNP P52789
B	2	HIS	-	expression tag	UNP P52789
B	3	HIS	-	expression tag	UNP P52789
B	4	HIS	-	expression tag	UNP P52789
B	5	SER	-	expression tag	UNP P52789
B	6	SER	-	expression tag	UNP P52789
B	7	GLY	-	expression tag	UNP P52789
B	8	LEU	-	expression tag	UNP P52789
B	9	GLU	-	expression tag	UNP P52789
B	10	ASN	-	expression tag	UNP P52789
B	11	LEU	-	expression tag	UNP P52789
B	12	TYR	-	expression tag	UNP P52789
B	13	PHE	-	expression tag	UNP P52789
B	14	GLN	-	expression tag	UNP P52789
B	15	GLY	-	expression tag	UNP P52789
B	16	SER	-	expression tag	UNP P52789

- Molecule 2 is 2-[(3-bromobenzene-1-carbonyl)amino]-6-[[[(4-carboxy-5-methylfuran-2-yl)sulfonyl]amino]-2,6-dideoxy- $\alpha$ -D-glucopyranos e (CCD ID: 604) (formula:  $C_{19}H_{21}BrN_2O_{10}S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	Br	C	N	O			S
2	A	1	33	1	19	2	10	1	0	0

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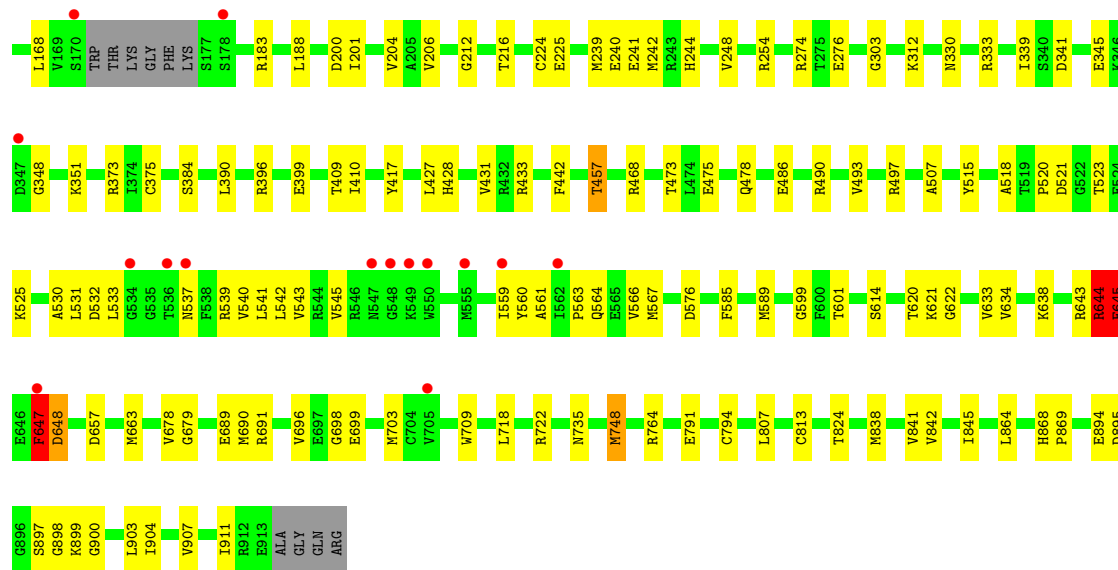
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	S	0	0
			33	1	19	2	10	1		
2	B	1	Total	Br	C	N	O	S	0	0
			30	1	16	2	10	1		
2	B	1	Total	Br	C	N	O	S	0	0
			33	1	19	2	10	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total	O	0	0
			31	31		
3	B	52	Total	O	0	0
			52	52		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.03Å 154.89Å 114.83Å 90.00° 96.34° 90.00°	Depositor
Resolution (Å)	114.12 – 2.73 114.12 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.8 (114.12-2.73) 93.7 (114.12-2.73)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.73Å)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.190 , 0.252 (Not available) , 0.231	Depositor DCC
$R_{free}$ test set	2919 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.4	Xtrriage
Anisotropy	0.502	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13830	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
604

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	0.42	1/6878 (0.0%)	0.72	6/9262 (0.1%)
1	B	0.40	0/6952	0.67	6/9365 (0.1%)
All	All	0.41	1/13830 (0.0%)	0.69	12/18627 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	691	ARG	NE-CZ	-6.04	1.26	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	645	GLU	N-CA-C	11.35	127.97	107.99
1	B	647	PHE	CA-C-N	6.26	133.49	121.54
1	B	647	PHE	C-N-CA	6.26	133.49	121.54
1	A	644	ARG	CA-C-N	6.07	133.13	121.54
1	A	644	ARG	C-N-CA	6.07	133.13	121.54
1	A	142	GLN	CA-CB-CG	6.04	126.17	114.10
1	A	107	MET	CB-CG-SD	-5.91	94.98	112.70
1	B	644	ARG	CA-C-N	-5.49	114.34	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	644	ARG	C-N-CA	-5.49	114.34	122.41
1	B	648	ASP	N-CA-C	5.36	122.21	110.80
1	A	846	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	846	ARG	NE-CZ-NH1	-5.01	116.49	121.50

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	523	THR	Peptide
1	A	646	GLU	Peptide
1	B	622	GLY	Peptide
1	B	644	ARG	Peptide
1	B	645	GLU	Peptide
1	B	647	PHE	Peptide

## 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	6771	0	6696	174	0
1	B	6847	0	6763	108	0
2	A	66	0	0	2	0
2	B	63	0	0	2	0
3	A	31	0	0	4	0
3	B	52	0	0	1	0
All	All	13830	0	13459	280	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 10.

All (280) 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:A:865:TYR:HH	1:A:876:HIS:HE2	1.01	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:THR:HG21	1:A:449:SER:HB2	1.49	0.95
1:B:240:GLU:CD	1:B:396:ARG:HH12	1.77	0.91
1:B:663:MET:HG3	1:B:904:ILE:HG12	1.54	0.89
1:B:239:MET:HG3	1:B:254:ARG:HH21	1.37	0.86
1:A:793:ASP:O	1:A:820:LYS:NZ	2.09	0.85
1:B:634:VAL:HG12	1:B:638:LYS:HE2	1.56	0.84
1:B:239:MET:CB	1:B:254:ARG:NH2	2.39	0.84
1:B:274:ARG:NH1	3:B:1101:HOH:O	2.11	0.83
1:B:601:THR:HG21	1:B:897:SER:HA	1.62	0.81
1:B:239:MET:CG	1:B:254:ARG:HH21	1.94	0.80
1:A:138:MET:HE2	1:A:144:LYS:HA	1.63	0.80
1:A:538:PHE:CE1	1:A:560:TYR:HB2	2.18	0.79
1:B:239:MET:HG3	1:B:254:ARG:NH2	1.99	0.77
1:B:240:GLU:OE1	1:B:396:ARG:NH1	2.17	0.77
1:A:896:GLY:HA2	1:A:897:SER:HB2	1.67	0.77
1:B:134:LEU:HG	1:B:138:MET:HE3	1.68	0.76
1:A:44:ARG:HA	1:A:47:MET:HE3	1.68	0.75
1:B:542:LEU:HD23	1:B:589:MET:HE2	1.70	0.74
1:A:502:GLU:OE1	1:A:503:THR:HG23	1.88	0.73
1:B:645:GLU:OE1	1:B:647:PHE:HB3	1.87	0.73
1:B:239:MET:CB	1:B:254:ARG:HH21	2.01	0.73
1:A:405:ARG:NH1	1:A:436:PRO:O	2.20	0.73
1:A:405:ARG:NH2	1:A:439:ASP:OD1	2.22	0.72
1:A:141:LEU:O	1:A:142:GLN:HB3	1.88	0.71
1:A:490:ARG:NH1	1:A:717:CYS:O	2.23	0.71
1:A:538:PHE:HE2	1:A:578:ILE:HG12	1.54	0.71
1:A:580:GLN:HB2	1:A:644:ARG:HH21	1.54	0.71
1:A:580:GLN:HB2	1:A:644:ARG:NH2	2.06	0.70
1:A:523:THR:HG21	1:A:910:ARG:NH2	2.09	0.68
1:A:538:PHE:HE1	1:A:560:TYR:HB2	1.55	0.68
1:B:240:GLU:CD	1:B:396:ARG:NH1	2.52	0.67
1:A:497:ARG:HG2	1:A:507:ALA:HB2	1.75	0.67
1:A:523:THR:HG21	1:A:910:ARG:HH22	1.59	0.67
1:A:688:GLU:OE2	1:A:848:ASN:ND2	2.28	0.66
1:A:84:ASP:OD1	1:A:91:ARG:HB2	1.95	0.66
1:B:539:ARG:HG2	1:B:559:ILE:HG12	1.78	0.66
1:A:196:ARG:NH2	1:A:198:ASP:OD2	2.28	0.65
1:A:785:LYS:O	1:A:789:GLN:HG3	1.96	0.65
1:A:635:THR:O	1:A:639:GLU:HG3	1.97	0.65
1:A:844:ARG:NH1	1:A:848:ASN:OD1	2.30	0.65
1:B:497:ARG:HG2	1:B:507:ALA:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:ARG:HB3	1:B:699:GLU:HB3	1.80	0.64
1:A:523:THR:CG2	1:A:910:ARG:HH22	2.11	0.64
1:A:533:LEU:HD12	1:A:538:PHE:HD2	1.62	0.64
1:A:27:TYR:OH	1:B:399:GLU:OE2	2.08	0.63
1:B:339:ILE:HG23	1:B:375:CYS:HB3	1.81	0.63
1:A:673:GLU:OE1	1:A:702:ARG:NH1	2.32	0.63
1:B:239:MET:CG	1:B:254:ARG:NH2	2.58	0.63
1:A:515:TYR:HA	1:A:703:MET:HE2	1.81	0.62
1:A:673:GLU:OE2	1:A:849:ARG:NH2	2.33	0.62
1:B:239:MET:HB3	1:B:254:ARG:NH2	2.15	0.62
1:B:894:GLU:OE2	1:B:894:GLU:N	2.33	0.62
1:B:521:ASP:OD1	1:B:523:THR:HG22	1.99	0.62
1:A:495:MET:HA	1:A:511:MET:HE3	1.82	0.62
1:A:423:PHE:CD1	1:A:423:PHE:C	2.78	0.61
1:A:523:THR:CB	1:A:910:ARG:HH22	2.13	0.61
1:A:676:LEU:HD22	1:A:838:MET:HE3	1.82	0.61
1:A:722:ARG:HG2	1:A:744:MET:HE1	1.82	0.61
1:A:291:GLN:NE2	1:A:294:GLU:OE1	2.32	0.60
1:A:542:LEU:HD23	1:A:589:MET:HE2	1.83	0.60
1:A:207:VAL:HG11	1:A:456:VAL:HG21	1.83	0.60
1:A:538:PHE:CE2	1:A:578:ILE:HG12	2.35	0.60
1:B:341:ASP:HB3	1:B:351:LYS:HE2	1.84	0.60
1:B:690:MET:HE1	1:B:696:VAL:HG12	1.84	0.59
1:A:418:LYS:C	1:A:419:LYS:HD3	2.27	0.59
1:A:633:VAL:HA	1:A:636:LEU:HD12	1.84	0.59
1:A:862:GLY:HA2	2:A:1002:604:O22	2.02	0.59
1:B:239:MET:HB2	1:B:254:ARG:NH2	2.16	0.59
1:A:25:TYR:OH	1:A:312:LYS:NZ	2.33	0.59
1:A:83:LEU:HG	1:A:150:LEU:HD11	1.85	0.59
1:A:199:PHE:HD1	1:A:199:PHE:H	1.50	0.58
1:B:564:GLN:HA	1:B:567:MET:HB2	1.83	0.58
1:A:543:VAL:HG21	1:A:902:ALA:HB3	1.86	0.58
1:B:645:GLU:OE1	1:B:647:PHE:N	2.36	0.58
1:A:543:VAL:HG22	1:A:555:MET:SD	2.44	0.57
1:A:896:GLY:HA2	1:A:897:SER:CB	2.32	0.57
1:A:569:GLY:O	1:A:625:ALA:HA	2.04	0.57
1:B:240:GLU:OE2	1:B:396:ARG:NH1	2.31	0.57
1:A:90:PHE:CZ	1:A:112:TYR:HB2	2.40	0.56
1:A:533:LEU:HD12	1:A:538:PHE:CD2	2.41	0.56
1:A:528:PHE:HB2	1:A:902:ALA:HB1	1.88	0.56
1:A:202:ASP:OD2	1:A:461:TYR:OH	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:PHE:C	1:A:423:PHE:HD1	2.13	0.56
1:B:431:VAL:HG11	1:B:442:PHE:HZ	1.71	0.56
1:B:83:LEU:HG	1:B:150:LEU:HD11	1.87	0.55
1:B:486:GLU:O	1:B:490:ARG:HG3	2.07	0.55
1:A:470:ARG:HB2	1:A:761:PHE:CZ	2.41	0.55
1:B:225:GLU:HG2	1:B:254:ARG:HH22	1.72	0.55
1:A:910:ARG:CG	1:A:911:ILE:HD12	2.36	0.55
1:A:570:THR:HG23	1:A:573:GLU:H	1.71	0.54
1:B:212:GLY:O	1:B:216:THR:HG22	2.07	0.54
1:B:345:GLU:HB2	1:B:348:GLY:HA2	1.89	0.54
1:A:634:VAL:HG23	1:A:638:LYS:HE2	1.89	0.54
1:A:612:ASP:O	1:A:634:VAL:HG11	2.07	0.54
1:B:645:GLU:OE1	1:B:645:GLU:HA	2.08	0.54
1:B:791:GLU:OE1	1:B:824:THR:HA	2.09	0.53
1:B:417:TYR:OH	1:B:428:HIS:NE2	2.34	0.53
1:A:634:VAL:O	1:A:638:LYS:N	2.36	0.53
1:B:475:GLU:HA	1:B:478:GLN:OE1	2.08	0.53
1:A:29:MET:HE1	1:A:378:VAL:HG22	1.91	0.53
1:A:511:MET:HE1	1:A:707:MET:HE3	1.90	0.53
1:A:327:GLU:HG2	1:A:333:ARG:HH21	1.74	0.53
1:A:568:HIS:O	1:A:568:HIS:ND1	2.36	0.53
1:B:390:LEU:HD22	1:B:410:ILE:HD13	1.91	0.53
1:A:395:GLN:O	1:A:399:GLU:HG3	2.08	0.53
1:A:554:GLU:OE1	1:A:554:GLU:N	2.36	0.53
1:A:128:ASP:CG	1:A:195:ARG:HH21	2.16	0.52
1:A:488:LYS:NZ	1:A:882:LEU:O	2.36	0.52
1:A:428:HIS:HB3	1:A:432:ARG:NH1	2.24	0.52
1:B:242:MET:HE1	1:B:248:VAL:HG12	1.92	0.52
1:A:217:CYS:SG	1:A:445:SER:HB2	2.49	0.51
1:B:330:ASN:HB3	1:B:333:ARG:HD3	1.91	0.51
1:B:149:PRO:HB2	1:B:457:THR:HG21	1.92	0.51
1:B:530:ALA:HB3	1:B:541:LEU:HB2	1.93	0.51
1:A:33:ASP:OD1	1:A:433:ARG:NH1	2.43	0.51
1:B:20:GLN:O	1:B:24:GLN:HG3	2.11	0.51
1:A:503:THR:O	1:A:507:ALA:N	2.38	0.51
1:A:580:GLN:O	1:A:580:GLN:HG2	2.10	0.51
1:A:798:LEU:N	3:A:1105:HOH:O	2.44	0.51
1:B:149:PRO:HB2	1:B:457:THR:CG2	2.40	0.51
1:B:530:ALA:HA	1:B:599:GLY:O	2.11	0.51
1:A:447:ASP:CB	1:A:451:LYS:HD2	2.41	0.51
1:A:620:THR:HG22	1:A:621:LYS:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:VAL:HG22	1:B:560:TYR:HE1	1.76	0.51
1:A:107:MET:HE3	1:A:451:LYS:CG	2.41	0.50
1:A:403:GLU:OE1	1:A:405:ARG:N	2.30	0.50
1:A:44:ARG:HD3	3:A:1118:HOH:O	2.12	0.50
1:A:489:ARG:O	1:A:492:LYS:HB3	2.11	0.50
1:A:846:ARG:HG3	1:A:854:LEU:HD11	1.94	0.49
1:A:567:MET:HE3	1:A:623:PHE:CD2	2.47	0.49
1:B:718:LEU:O	1:B:722:ARG:HG3	2.12	0.49
1:A:199:PHE:N	1:A:199:PHE:CD1	2.81	0.49
1:A:408:SER:O	1:A:440:VAL:HA	2.13	0.49
1:B:33:ASP:OD1	1:B:433:ARG:NH1	2.46	0.49
1:A:303:GLY:HA2	1:A:339:ILE:HD11	1.95	0.49
1:B:532:ASP:HB3	1:B:897:SER:O	2.13	0.49
1:B:152:PHE:HB2	1:B:206:VAL:HG22	1.94	0.48
1:A:680:THR:HG23	2:A:1002:604:O24	2.13	0.48
1:A:851:LEU:HB3	1:A:854:LEU:HD21	1.95	0.48
1:B:303:GLY:HA2	1:B:339:ILE:HD11	1.95	0.48
1:B:468:ARG:HD2	1:B:468:ARG:HA	1.63	0.48
1:B:899:LYS:O	1:B:903:LEU:HG	2.14	0.48
1:A:338:ASP:CG	1:A:358:ARG:HH12	2.22	0.48
1:A:353:ARG:O	1:A:357:MET:HG3	2.14	0.48
1:A:218:GLY:HA2	1:A:221:ASP:O	2.13	0.48
1:A:338:ASP:OD2	1:A:358:ARG:NH1	2.47	0.48
1:A:87:GLY:C	1:A:89:ASN:H	2.21	0.48
1:A:96:LYS:HB3	1:A:106:GLU:HB3	1.96	0.48
1:A:503:THR:O	1:A:506:SER:N	2.47	0.48
1:A:523:THR:HB	1:A:910:ARG:HH22	1.79	0.48
1:B:36:LEU:HD11	1:B:384:SER:HB3	1.95	0.48
1:A:419:LYS:HD3	1:A:419:LYS:N	2.28	0.47
1:B:19:VAL:HG13	1:B:373:ARG:NE	2.28	0.47
1:A:451:LYS:H	1:A:451:LYS:HG3	1.51	0.47
1:A:558:LYS:HD2	1:A:588:TYR:CD2	2.48	0.47
1:A:861:ASP:CG	1:A:894:GLU:HA	2.39	0.47
1:A:481:HIS:HD1	1:A:481:HIS:C	2.22	0.47
1:B:200:ASP:OD1	1:B:201:ILE:N	2.47	0.47
1:A:33:ASP:OD2	1:A:433:ARG:HD2	2.15	0.47
1:A:444:ARG:NH1	3:A:1103:HOH:O	2.36	0.47
1:A:865:TYR:CE2	1:A:872:ALA:HB2	2.50	0.47
1:A:164:ASP:OD1	1:A:164:ASP:N	2.45	0.47
1:B:531:LEU:HD13	1:B:533:LEU:HD11	1.96	0.47
1:A:447:ASP:HB3	1:A:451:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:SER:O	1:A:184:ASP:HA	2.15	0.46
1:B:663:MET:HE1	1:B:907:VAL:HG21	1.96	0.46
1:B:895:ASP:CG	1:B:898:GLY:HA3	2.40	0.46
1:A:722:ARG:HG2	1:A:744:MET:CE	2.45	0.46
1:A:846:ARG:HD2	1:A:852:ASP:O	2.15	0.46
1:A:327:GLU:CG	1:A:333:ARG:HH21	2.29	0.46
1:A:910:ARG:HG2	1:A:911:ILE:HD12	1.97	0.46
1:A:527:ASP:OD1	1:A:544:ARG:HD3	2.16	0.46
1:A:576:ASP:OD1	1:A:643:ARG:NH1	2.35	0.46
1:A:39:ILE:HD11	1:A:273:ILE:HG13	1.98	0.46
1:A:91:ARG:HD2	1:A:109:ASN:HD22	1.80	0.46
1:B:81:LEU:HD13	1:B:138:MET:HE2	1.97	0.46
1:B:690:MET:HE3	1:B:698:GLY:O	2.15	0.46
1:A:254:ARG:HD2	3:A:1115:HOH:O	2.15	0.46
1:A:686:TYR:HB2	1:A:845:ILE:HD11	1.97	0.46
1:B:107:MET:HE2	1:B:107:MET:HB3	1.66	0.46
1:B:239:MET:HB3	1:B:254:ARG:HH21	1.73	0.45
1:A:225:GLU:CD	1:A:254:ARG:HH22	2.25	0.45
1:A:620:THR:HG22	1:A:621:LYS:N	2.31	0.45
1:B:100:ASN:OD1	1:B:101:GLY:N	2.48	0.45
1:A:632:ASP:OD1	1:A:634:VAL:HG22	2.16	0.45
1:B:515:TYR:HA	1:B:703:MET:HE2	1.98	0.45
1:A:690:MET:HG3	1:A:701:GLY:C	2.42	0.45
1:A:865:TYR:HD2	1:A:865:TYR:O	1.99	0.45
1:B:164:ASP:HB3	1:B:204:VAL:O	2.17	0.45
1:A:418:LYS:NZ	1:A:445:SER:O	2.38	0.45
1:B:396:ARG:CG	1:B:396:ARG:HH11	2.29	0.45
1:B:678:VAL:HG12	1:B:864:LEU:HD23	1.99	0.45
1:A:94:TRP:CZ2	1:A:96:LYS:HB2	2.52	0.44
1:A:853:ALA:C	1:A:854:LEU:HD23	2.42	0.44
1:A:417:TYR:C	1:A:417:TYR:CD1	2.96	0.44
1:A:612:ASP:O	1:A:634:VAL:HG21	2.18	0.44
1:B:576:ASP:CG	1:B:643:ARG:HH21	2.25	0.44
1:A:846:ARG:NH1	1:A:885:LYS:HB2	2.33	0.44
1:A:497:ARG:HG2	1:A:507:ALA:CB	2.45	0.44
1:A:238:TYR:CD2	1:A:239:MET:O	2.71	0.44
1:A:137:PHE:O	1:A:141:LEU:HB2	2.17	0.43
1:A:347:ASP:OD2	1:A:350:ARG:HB2	2.18	0.43
1:A:734:LEU:C	1:A:736:PRO:HD3	2.43	0.43
1:A:110:GLN:NE2	1:A:111:ILE:H	2.17	0.43
1:B:244:HIS:HB3	1:B:396:ARG:HH22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:841:VAL:O	1:B:845:ILE:HG13	2.18	0.43
1:A:83:LEU:HD12	1:A:152:PHE:CE1	2.53	0.43
1:A:115:PRO:HB2	1:A:117:ASP:OD1	2.17	0.43
1:A:167:PHE:CE1	1:A:184:ASP:HB2	2.53	0.43
1:A:495:MET:HG2	1:A:511:MET:CE	2.47	0.43
1:A:762:THR:O	1:A:770:GLY:HA2	2.18	0.43
1:B:543:VAL:HG11	1:B:903:LEU:HD21	1.99	0.43
1:B:241:GLU:HG2	1:B:813:CYS:SG	2.59	0.43
1:A:502:GLU:CD	1:A:503:THR:N	2.77	0.43
1:A:607:GLN:HG3	1:A:609:ASN:HD21	1.83	0.43
1:A:851:LEU:HD23	1:A:854:LEU:HD22	2.00	0.43
1:A:45:LYS:HE2	1:B:794:CYS:SG	2.58	0.43
1:B:563:PRO:HB2	1:B:566:VAL:HG12	2.00	0.43
1:B:90:PHE:CD1	1:B:90:PHE:N	2.87	0.42
1:A:63:MET:SD	1:A:259:MET:HG2	2.59	0.42
1:A:658:THR:HG21	1:A:683:ASN:HB3	2.00	0.42
1:A:690:MET:HE2	1:A:690:MET:HB3	1.81	0.42
1:A:23:ASP:CG	1:A:373:ARG:HH21	2.28	0.42
1:B:614:SER:O	1:B:633:VAL:HG23	2.19	0.42
1:A:607:GLN:HE21	1:A:609:ASN:ND2	2.18	0.42
1:B:473:THR:OG1	1:B:764:ARG:NH2	2.52	0.42
1:B:518:ALA:HB3	1:B:911:ILE:HD11	2.00	0.42
1:B:33:ASP:OD2	1:B:433:ARG:HD2	2.19	0.42
1:B:657:ASP:OD2	2:B:1002:604:N21	2.52	0.42
1:B:679:GLY:HA3	2:B:1002:604:O24	2.19	0.42
1:A:184:ASP:O	1:A:188:LEU:HG	2.20	0.42
1:A:270:LEU:HD13	1:A:296:MET:HE1	2.01	0.42
1:B:183:ARG:HH11	1:B:188:LEU:HD21	1.85	0.42
1:A:19:VAL:HG13	1:A:373:ARG:NE	2.35	0.41
1:A:544:ARG:HB3	1:A:554:GLU:CD	2.45	0.41
1:B:497:ARG:HG2	1:B:507:ALA:CB	2.48	0.41
1:B:520:PRO:HG3	1:B:663:MET:HE1	2.00	0.41
1:B:537:ASN:HA	1:B:561:ALA:HA	2.02	0.41
1:B:838:MET:O	1:B:842:VAL:HG22	2.19	0.41
1:A:201:ILE:HD12	1:A:201:ILE:HA	1.93	0.41
1:B:163:LEU:HD12	1:B:163:LEU:HA	1.88	0.41
1:B:735:ASN:OD1	1:B:735:ASN:N	2.53	0.41
1:A:591:MET:O	1:A:594:VAL:HG23	2.20	0.41
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.87	0.41
1:A:677:ILE:O	1:A:682:SER:HA	2.20	0.41
1:B:644:ARG:O	1:B:644:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ASP:CG	1:A:634:VAL:HG22	2.45	0.41
1:B:620:THR:OG1	1:B:621:LYS:HG3	2.20	0.41
1:A:495:MET:HE2	1:A:844:ARG:HG2	2.01	0.41
1:A:91:ARG:CD	1:A:109:ASN:HD22	2.33	0.41
1:A:486:GLU:O	1:A:490:ARG:HG3	2.21	0.41
1:B:19:VAL:HG13	1:B:373:ARG:HE	1.86	0.41
1:B:427:LEU:O	1:B:431:VAL:HG12	2.20	0.41
1:A:412:VAL:HG11	1:A:417:TYR:CE2	2.55	0.41
1:A:544:ARG:HB3	1:A:554:GLU:OE2	2.21	0.41
1:A:639:GLU:O	1:A:643:ARG:HG3	2.21	0.41
1:B:900:GLY:O	1:B:904:ILE:HG13	2.21	0.41
1:A:431:VAL:O	1:A:435:VAL:HG22	2.20	0.41
1:A:585:PHE:HA	1:A:588:TYR:HB3	2.03	0.41
1:A:610:SER:HB3	1:A:613:GLU:HB3	2.02	0.41
1:B:276:GLU:CD	1:B:312:LYS:HE2	2.46	0.41
1:B:525:LYS:HA	1:B:545:VAL:HG12	2.03	0.41
1:B:663:MET:HE3	1:B:663:MET:HB3	1.75	0.41
1:A:412:VAL:HG11	1:A:417:TYR:CD2	2.56	0.40
1:B:645:GLU:OE1	1:B:645:GLU:CA	2.69	0.40
1:B:748:MET:HE2	1:B:748:MET:HB3	1.75	0.40
1:A:441:ARG:HH22	1:A:443:LEU:HD13	1.86	0.40
1:A:532:ASP:HA	1:A:601:THR:HB	2.03	0.40
1:B:17:ASP:N	1:B:17:ASP:OD1	2.54	0.40
1:B:540:VAL:HG21	1:B:585:PHE:HB2	2.02	0.40
1:A:403:GLU:CD	1:A:404:GLU:H	2.28	0.40
1:A:615:ILE:HD13	1:A:632:ASP:HA	2.02	0.40
1:B:543:VAL:HG12	1:B:545:VAL:HG23	2.03	0.40
1:B:22:VAL:HG11	1:B:373:ARG:HG3	2.03	0.40
1:A:199:PHE:HD1	1:A:199:PHE:N	2.15	0.40
1:A:274:ARG:HG2	1:A:296:MET:SD	2.61	0.40
1:A:860:VAL:HG11	1:A:865:TYR:CD1	2.56	0.40
1:B:224:CYS:HA	1:B:409:THR:O	2.22	0.40
1:B:868:HIS:CG	1:B:869:PRO:HD2	2.57	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	875/923 (95%)	850 (97%)	25 (3%)	0	100	100
1	B	887/923 (96%)	870 (98%)	16 (2%)	1 (0%)	48	69
All	All	1762/1846 (95%)	1720 (98%)	41 (2%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	648	ASP

### 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	719/782 (92%)	712 (99%)	7 (1%)	68	80
1	B	729/782 (93%)	720 (99%)	9 (1%)	63	77
All	All	1448/1564 (93%)	1432 (99%)	16 (1%)	65	79

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	VAL
1	A	199	PHE
1	A	201	ILE
1	A	417	TYR
1	A	423	PHE

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Mol	Chain	Res	Type
1	A	481	HIS
1	A	709	TRP
1	B	90	PHE
1	B	124	THR
1	B	168	LEU
1	B	457	THR
1	B	493	VAL
1	B	689	GLU
1	B	709	TRP
1	B	748	MET
1	B	807	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	110	GLN
1	A	476	HIS
1	A	478	GLN
1	A	537	ASN
1	A	609	ASN
1	A	739	GLN
1	B	159	HIS
1	B	580	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	604	B	1002	-	32,35,35	1.61	2 (6%)	47,52,52	1.77	10 (21%)
2	604	A	1002	-	32,35,35	1.62	3 (9%)	47,52,52	1.68	10 (21%)
2	604	B	1001	-	28,31,35	2.13	6 (21%)	39,45,52	2.25	11 (28%)
2	604	A	1001	-	32,35,35	1.63	2 (6%)	47,52,52	1.87	9 (19%)

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	604	B	1002	-	-	7/23/44/44	0/3/3/3
2	604	A	1002	-	-	7/23/44/44	0/3/3/3
2	604	B	1001	-	-	7/22/42/44	0/2/2/3
2	604	A	1001	-	-	3/23/44/44	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	604	S32-N21	8.37	1.74	1.61
2	A	1001	604	S32-N21	7.50	1.72	1.61
2	A	1002	604	S32-N21	6.78	1.71	1.61
2	B	1002	604	S32-N21	6.66	1.71	1.61
2	B	1001	604	C8-C4A	-3.73	1.38	1.47
2	A	1002	604	C7-C12	3.48	1.54	1.48
2	B	1001	604	C7-C12	3.18	1.53	1.48
2	B	1002	604	C7-C12	2.99	1.53	1.48
2	B	1001	604	C6A-C4A	2.23	1.38	1.32
2	B	1001	604	BR-C8	-2.16	1.92	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	604	C11-N2	2.10	1.39	1.34
2	A	1002	604	O22-C12	2.04	1.27	1.22
2	A	1001	604	C7-C12	2.01	1.51	1.48

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	604	O25-S32-N21	7.11	114.05	107.41
2	B	1001	604	O26-S32-C10	-6.37	97.47	107.07
2	B	1002	604	O26-S32-N21	5.78	112.81	107.41
2	B	1001	604	O25-S32-N21	4.85	111.95	107.41
2	A	1002	604	O25-S32-N21	4.77	111.87	107.41
2	B	1001	604	C1-C2-C3	-4.48	104.43	110.54
2	B	1001	604	O26-S32-N21	4.40	111.53	107.41
2	A	1002	604	C1-O5-C5	-4.22	105.49	113.65
2	A	1001	604	O26-S32-C10	-4.03	101.00	107.07
2	B	1002	604	C6-N21-S32	-3.84	112.52	119.99
2	A	1002	604	O22-C12-C7	-3.78	114.84	122.67
2	A	1001	604	C5A-C7-C9	3.74	108.46	106.24
2	B	1002	604	O25-S32-N21	-3.60	104.05	107.41
2	B	1001	604	O25-S32-C10	-3.42	101.92	107.07
2	A	1002	604	O26-S32-C10	-3.37	101.99	107.07
2	B	1002	604	O22-C12-C7	-3.32	115.80	122.67
2	B	1001	604	O5-C5-C6	3.24	111.38	105.89
2	A	1001	604	O22-C12-C7	-3.24	115.97	122.67
2	B	1001	604	O22-C12-C7	-3.19	116.08	122.67
2	A	1001	604	O26-S32-N21	3.15	110.35	107.41
2	A	1001	604	O24-C12-O22	3.07	131.20	123.90
2	B	1001	604	O5-C1-C2	3.03	112.56	109.52
2	B	1001	604	C6A-C11-N2	2.93	119.62	114.61
2	B	1001	604	O23-C11-C6A	-2.88	116.30	122.95
2	A	1001	604	C18-C9-C7	-2.85	131.85	134.58
2	A	1001	604	O27-C9-C18	2.78	119.51	115.88
2	B	1002	604	C5A-C7-C9	2.62	107.80	106.24
2	A	1002	604	O5-C1-C2	-2.57	106.94	109.52
2	A	1002	604	O5-C5-C6	2.37	109.90	105.89
2	A	1002	604	O24-C12-O22	2.24	129.24	123.90
2	B	1002	604	O5-C5-C6	2.23	109.67	105.89
2	A	1001	604	O27-C9-C7	-2.19	108.64	109.75
2	B	1002	604	O26-S32-C10	-2.17	103.80	107.07
2	B	1002	604	O23-C11-N2	2.15	126.55	122.47
2	B	1001	604	O24-C12-O22	2.10	128.89	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1002	604	O25-S32-C10	-2.04	103.98	107.07
2	A	1002	604	C5A-C7-C9	2.04	107.45	106.24
2	A	1002	604	C3-C4-C5	-2.04	106.54	110.23
2	A	1002	604	BR-C8-C3A	2.02	122.05	119.30
2	B	1002	604	O24-C12-O22	2.01	128.69	123.90

There are no chirality outliers.

All (24) torsion outliers are listed below:

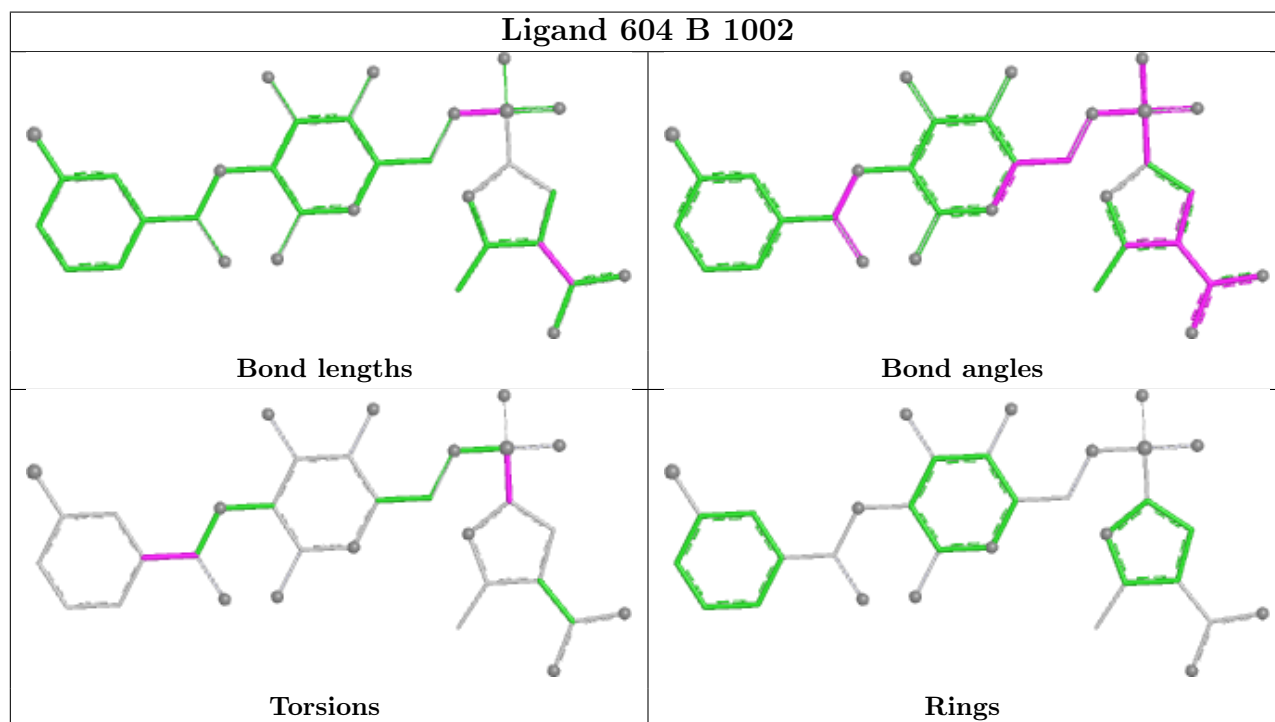
Mol	Chain	Res	Type	Atoms
2	A	1001	604	C5A-C10-S32-O26
2	B	1002	604	O23-C11-C6A-C2A
2	B	1002	604	O23-C11-C6A-C4A
2	B	1001	604	C5A-C10-S32-O26
2	B	1002	604	C5A-C10-S32-O26
2	B	1002	604	N2-C11-C6A-C2A
2	A	1002	604	C6-N21-S32-O25
2	B	1002	604	N2-C11-C6A-C4A
2	B	1001	604	O23-C11-C6A-C4A
2	B	1001	604	N2-C11-C6A-C4A
2	A	1002	604	O23-C11-C6A-C4A
2	A	1002	604	N2-C11-C6A-C4A
2	B	1001	604	C4-C5-C6-N21
2	A	1002	604	C6-N21-S32-O26
2	A	1002	604	C6-N21-S32-C10
2	A	1002	604	O23-C11-C6A-C2A
2	A	1002	604	N2-C11-C6A-C2A
2	B	1001	604	C6-N21-S32-O25
2	A	1001	604	C5A-C10-S32-N21
2	B	1001	604	C5A-C10-S32-N21
2	B	1002	604	C5A-C10-S32-N21
2	A	1001	604	O27-C10-S32-O26
2	B	1001	604	O27-C10-S32-O26
2	B	1002	604	O27-C10-S32-O26

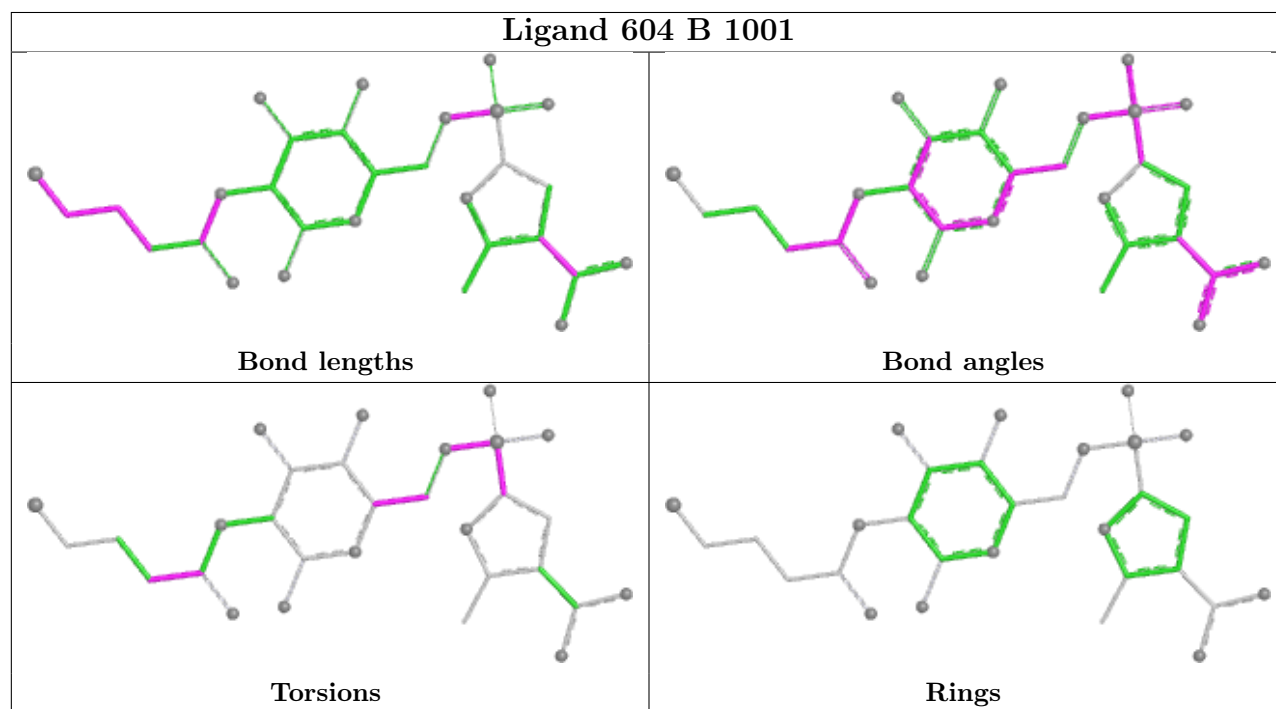
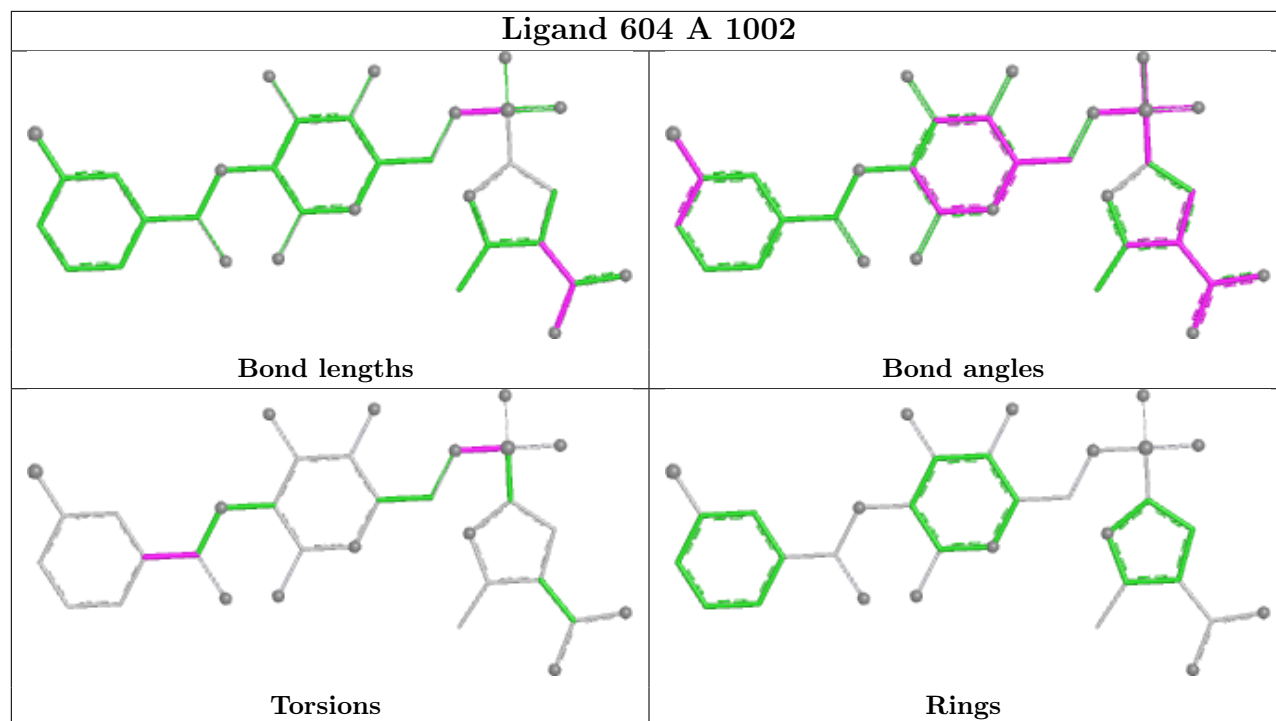
There are no ring outliers.

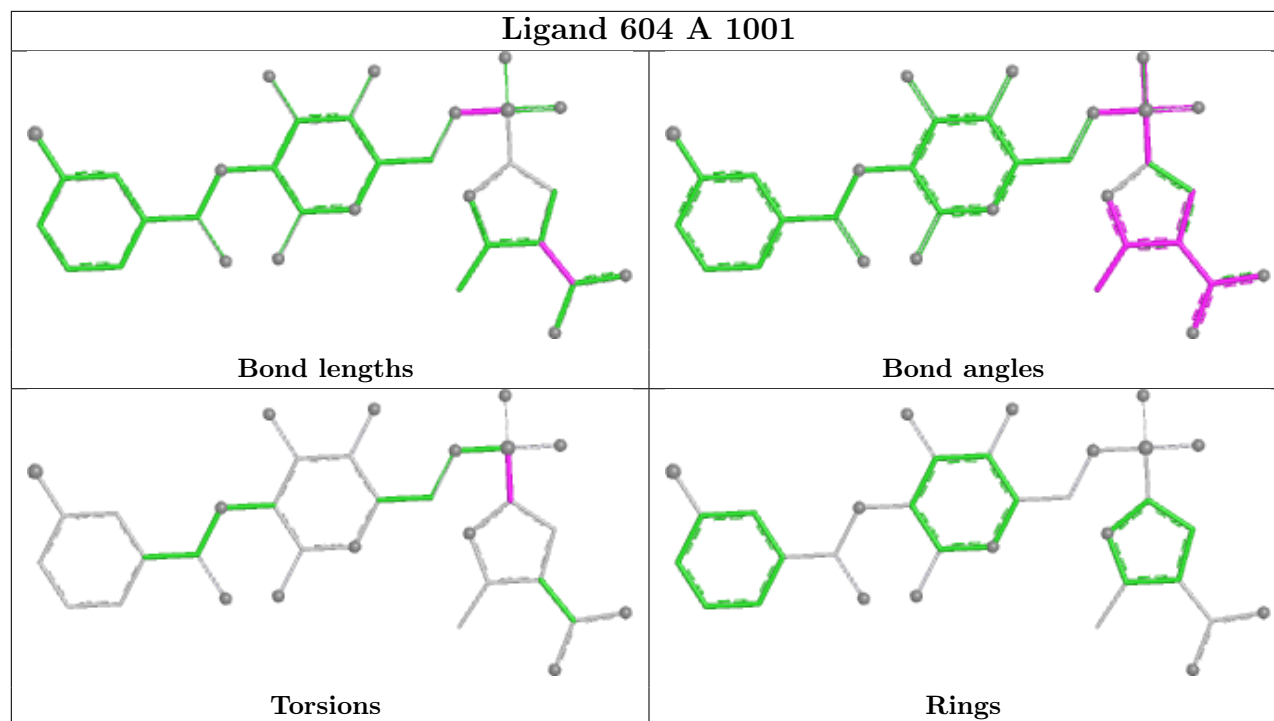
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	604	2	0
2	A	1002	604	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	880/923 (95%)	0.29	53 (6%) 27 27	21, 47, 80, 100	1 (0%)
1	B	891/923 (96%)	-0.09	17 (1%) 66 63	19, 36, 70, 94	0
All	All	1771/1846 (95%)	0.10	70 (3%) 42 40	19, 41, 77, 100	1 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	911	ILE	6.5
1	A	118	ILE	3.9
1	A	640	ALA	3.9
1	A	648	ASP	3.7
1	A	670	PRO	3.7
1	B	549	LYS	3.5
1	A	854	LEU	3.4
1	A	898	GLY	3.4
1	A	853	ALA	3.2
1	B	170	SER	3.1
1	B	102	LEU	3.0
1	A	447	ASP	3.0
1	A	499	LEU	3.0
1	B	178	SER	3.0
1	A	111	ILE	3.0
1	A	169	VAL	3.0
1	A	895	ASP	2.9
1	A	88	THR	2.9
1	A	555	MET	2.9
1	B	537	ASN	2.9
1	A	113	ALA	2.9
1	A	647	PHE	2.9
1	B	347	ASP	2.8
1	B	534	GLY	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	865	TYR	2.8
1	B	101	GLY	2.7
1	B	536	THR	2.7
1	A	641	ILE	2.7
1	A	602	PHE	2.7
1	A	556	HIS	2.7
1	A	697	GLU	2.6
1	A	850	GLY	2.6
1	B	550	TRP	2.6
1	B	647	PHE	2.6
1	A	542	LEU	2.6
1	A	855	LYS	2.6
1	A	570	THR	2.6
1	A	568	HIS	2.5
1	A	693	VAL	2.5
1	A	89	ASN	2.4
1	A	540	VAL	2.4
1	A	705	VAL	2.4
1	A	897	SER	2.4
1	A	891	LEU	2.4
1	A	910	ARG	2.3
1	A	115	PRO	2.3
1	B	705	VAL	2.3
1	A	523	THR	2.3
1	A	112	TYR	2.2
1	B	547	ASN	2.2
1	A	86	GLY	2.2
1	B	555	MET	2.2
1	A	883	ALA	2.2
1	A	586	LEU	2.2
1	A	588	TYR	2.2
1	A	695	LEU	2.2
1	A	701	GLY	2.1
1	A	896	GLY	2.1
1	A	85	LEU	2.1
1	A	594	VAL	2.1
1	A	538	PHE	2.1
1	A	894	GLU	2.1
1	A	552	GLY	2.1
1	B	548	GLY	2.1
1	B	559	ILE	2.1
1	B	562	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	590	GLY	2.0
1	A	505	ALA	2.0
1	A	87	GLY	2.0
1	A	539	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

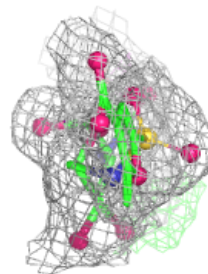
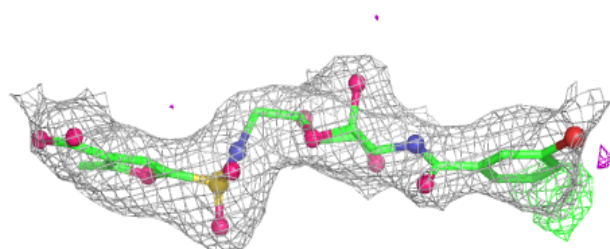
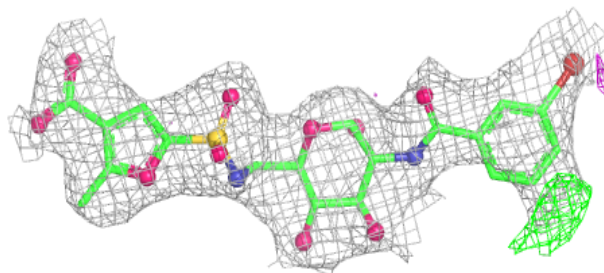
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q < 0.9
2	604	A	1002	33/33	0.92	0.10	36,45,72,147	0
2	604	B	1002	33/33	0.95	0.07	27,33,51,111	0
2	604	A	1001	33/33	0.96	0.08	24,35,42,73	0
2	604	B	1001	30/33	0.97	0.07	21,29,46,78	0

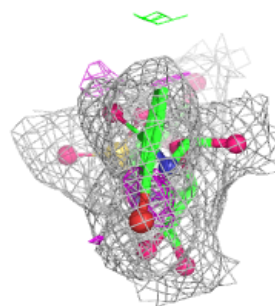
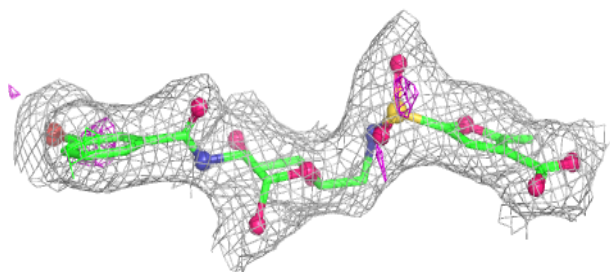
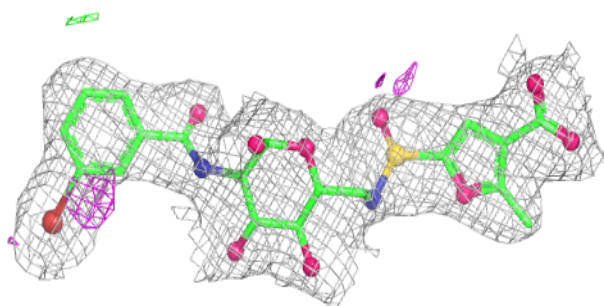
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 604 A 1002:**

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

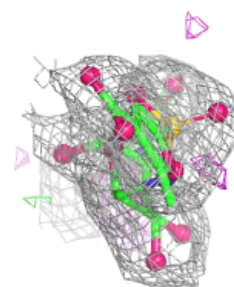
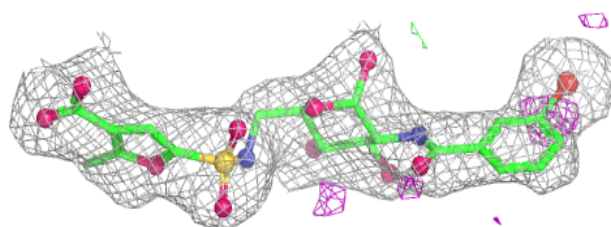
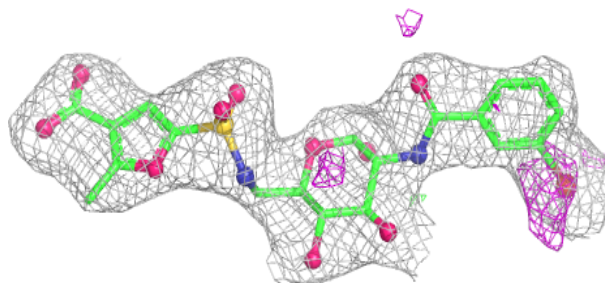
**Electron density around 604 B 1002:**

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

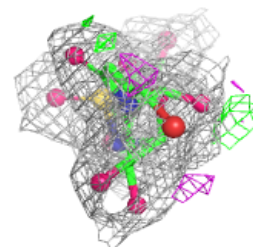
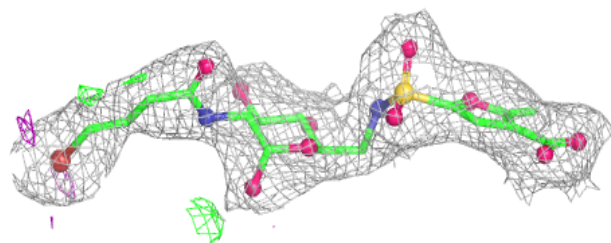
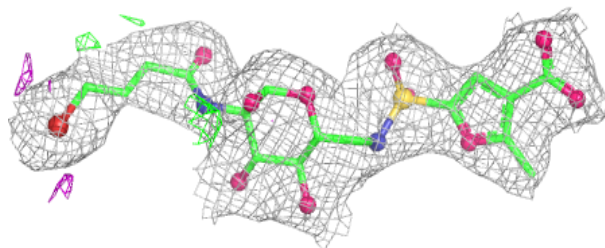


**Electron density around 604 A 1001:**

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

**Electron density around 604 B 1001:**

$2mF_o-DF_c$  (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.