



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 10:42 AM EDT

PDB ID : 4QY2
Title : Structure of H10 from human-infecting H10N8 virus in complex with human receptor analog
Authors : Wang, M.; Zhang, W.; Qi, J.; Wang, F.; Zhou, J.; Bi, Y.; Wu, Y.; Sun, H.; Liu, J.; Huang, C.; Li, X.; Yan, J.; Shu, Y.; Shi, Y.; Gao, G.F.
Deposited on : 2014-07-23
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

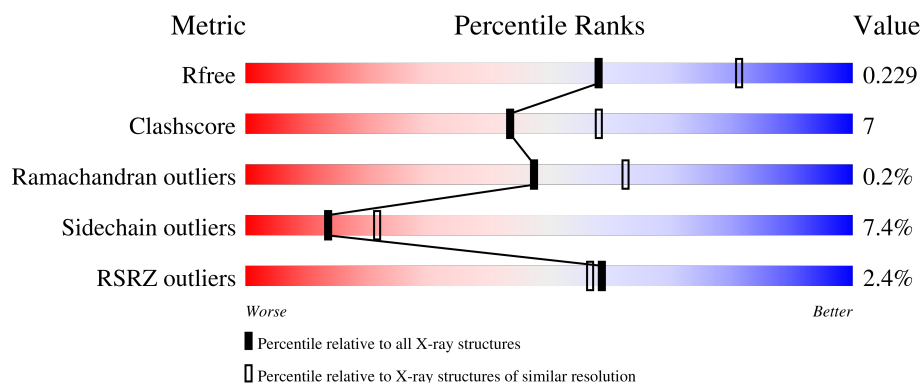
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	318	
1	C	318	
1	E	318	
1	G	318	

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Mol	Chain	Length	Quality of chain
1	I	318	<div> <div>2%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	K	318	<div> <div>%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
2	B	174	<div> <div>3%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
2	D	174	<div> <div>2%</div> <div>81%</div> <div>18%</div> <div>..</div> </div>
2	F	174	<div> <div>3%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
2	H	174	<div> <div>6%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
2	J	174	<div> <div>9%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
2	L	174	<div> <div>6%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24413 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 hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	C	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	E	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	G	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	I	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	K	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			

- Molecule 2 is a protein called hemagglutinin.

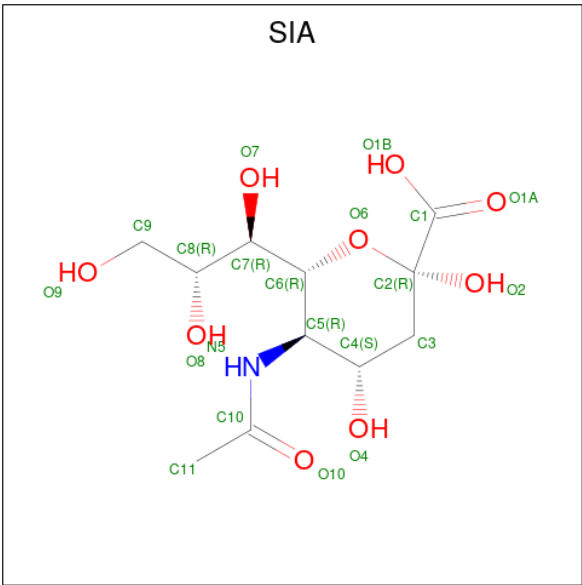
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	D	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	F	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	H	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	J	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	L	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: C₁₁H₁₉NO₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	128	Total	O	0	0
			128	128		
5	B	81	Total	O	0	0
			81	81		
5	C	124	Total	O	0	0
			124	124		
5	D	93	Total	O	0	0
			93	93		
5	E	161	Total	O	0	0
			161	161		
5	F	90	Total	O	0	0
			90	90		
5	G	126	Total	O	0	0
			126	126		
5	H	41	Total	O	0	0
			41	41		
5	I	142	Total	O	0	0
			142	142		
5	J	58	Total	O	0	0
			58	58		
5	K	90	Total	O	0	0
			90	90		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	56	Total	O	0	0
			56	56		

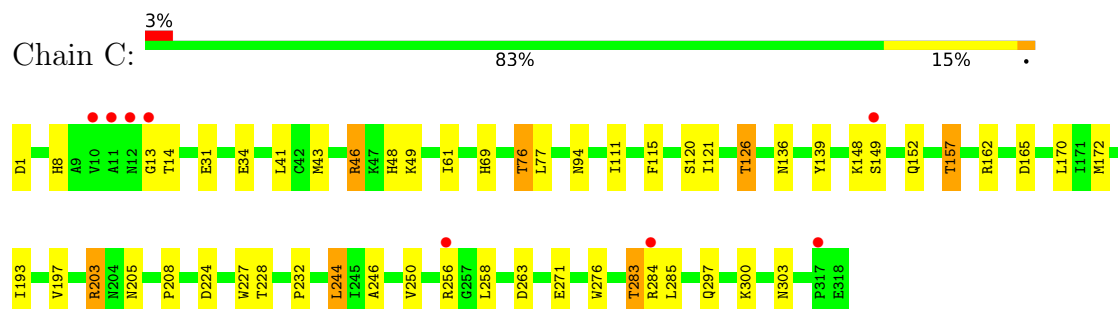
3 Residue-property plots [i](#)

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.

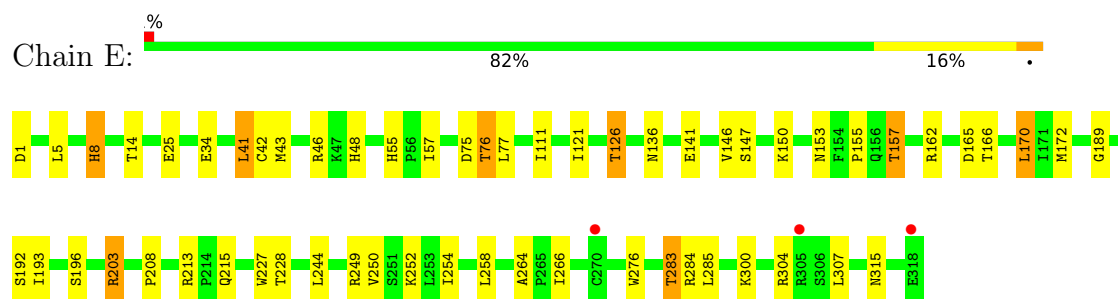
• Molecule 1: hemagglutinin



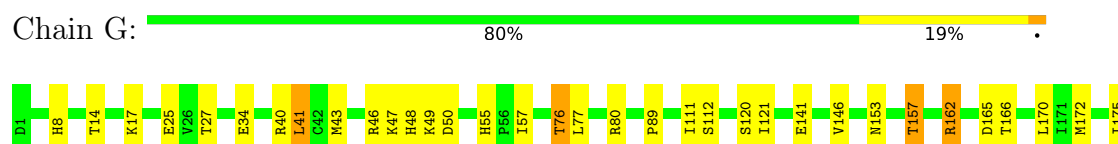
• Molecule 1: hemagglutinin



• Molecule 1: hemagglutinin

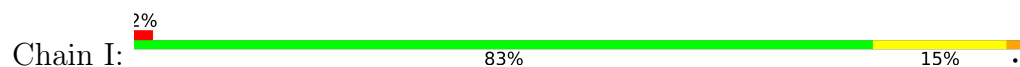


• Molecule 1: hemagglutinin

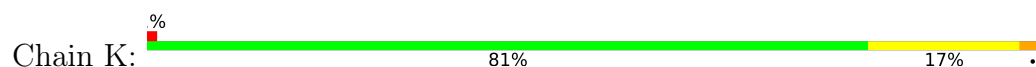




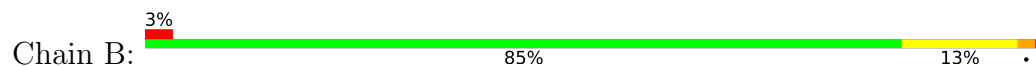
• Molecule 1: hemagglutinin



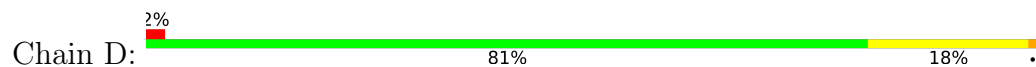
• Molecule 1: hemagglutinin



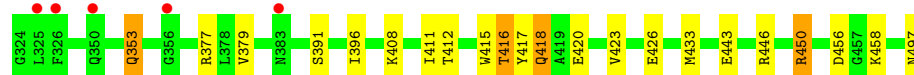
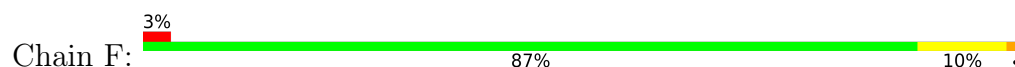
• Molecule 2: hemagglutinin



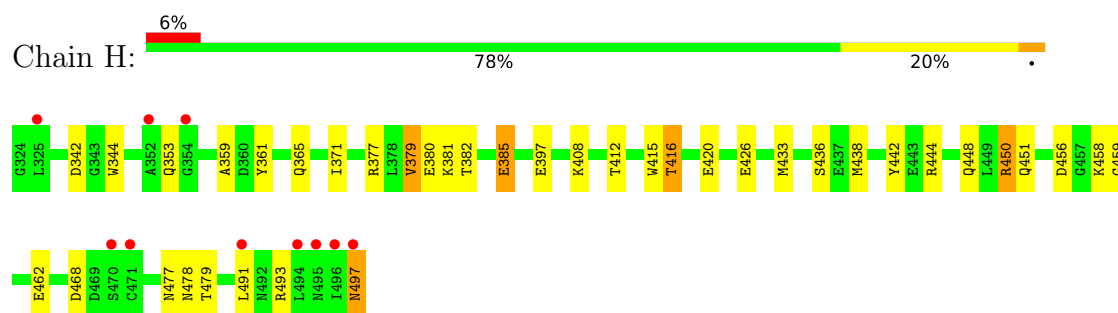
• Molecule 2: hemagglutinin



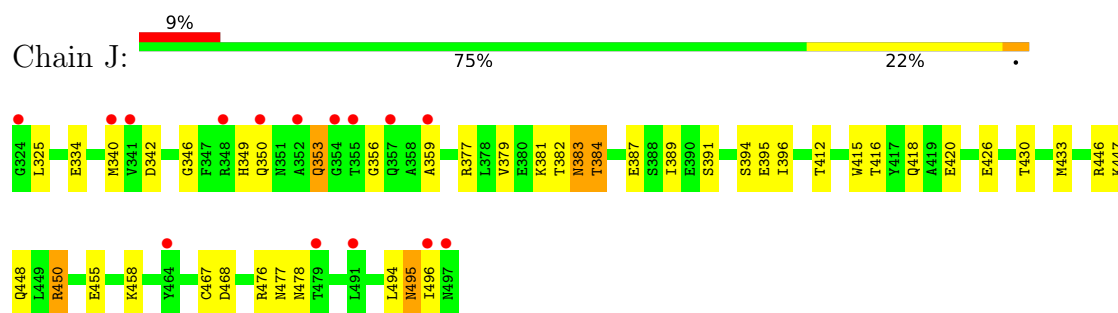
• Molecule 2: hemagglutinin



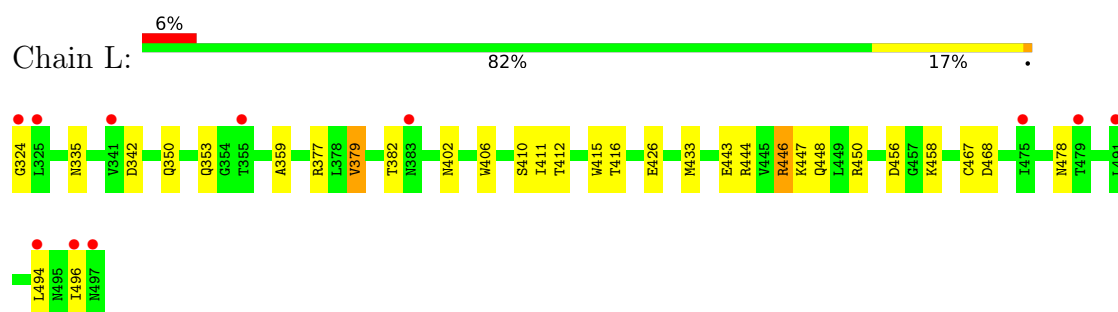
- Molecule 2: hemagglutinin



- Molecule 2: hemagglutinin



- Molecule 2: hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.00Å 118.51Å 124.51Å 98.69° 93.04° 96.51°	Depositor
Resolution (Å)	39.90 – 2.40 39.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (39.90-2.40) 92.5 (39.90-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.189 , 0.230 0.189 , 0.229	Depositor DCC
R_{free} test set	7913 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24413	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.34	0/2486	0.54	0/3368
1	C	0.34	0/2486	0.54	0/3368
1	E	0.35	0/2486	0.54	1/3368 (0.0%)
1	G	0.33	0/2486	0.52	0/3368
1	I	0.35	0/2486	0.55	0/3368
1	K	0.32	0/2486	0.52	0/3368
2	B	0.36	0/1427	0.50	0/1926
2	D	0.35	0/1427	0.53	0/1926
2	F	0.37	0/1427	0.51	0/1926
2	H	0.32	0/1427	0.48	0/1926
2	J	0.32	0/1427	0.49	0/1926
2	L	0.33	0/1427	0.47	0/1926
All	All	0.34	0/23478	0.52	1/31764 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	170	LEU	CA-CB-CG	5.21	127.28	115.30

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	2437	0	2389	40	0
1	C	2437	0	2389	34	1
1	E	2437	0	2389	31	0
1	G	2437	0	2389	34	0
1	I	2437	0	2389	31	0
1	K	2437	0	2389	32	0
2	B	1402	0	1298	19	0
2	D	1402	0	1298	27	0
2	F	1402	0	1298	16	0
2	H	1402	0	1298	26	1
2	J	1402	0	1298	29	0
2	L	1402	0	1298	27	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	1	0
3	D	14	0	13	1	0
3	E	14	0	13	1	0
3	F	14	0	13	0	0
3	G	14	0	13	1	0
3	H	14	0	13	0	0
3	I	14	0	13	0	0
3	J	14	0	13	0	0
3	K	14	0	13	0	0
3	L	14	0	13	0	0
4	E	21	0	18	1	0
5	A	128	0	0	8	0
5	B	81	0	0	4	0
5	C	124	0	0	6	0
5	D	93	0	0	7	0
5	E	161	0	0	7	0
5	F	90	0	0	3	0
5	G	126	0	0	4	0
5	H	41	0	0	4	0
5	I	142	0	0	6	0
5	J	58	0	0	9	0
5	K	90	0	0	3	0
5	L	56	0	0	9	0
All	All	24413	0	22296	306	1

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 7.

All (306) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ASN:ND2	5:C:792:HOH:O	1.81	0.99
1:G:46:ARG:HE	1:G:76:THR:HG21	1.33	0.93
2:J:381:LYS:O	5:J:734:HOH:O	1.90	0.90
1:I:7:HIS:NE2	5:I:746:HOH:O	2.07	0.87
1:I:224:ASP:OD1	5:I:748:HOH:O	1.92	0.85
2:F:497:ASN:O	5:F:754:HOH:O	1.94	0.85
2:D:488:GLU:OE1	5:D:761:HOH:O	1.94	0.84
1:A:46:ARG:HE	1:A:76:THR:HG21	1.41	0.83
3:E:601:NAG:O4	5:E:854:HOH:O	1.95	0.83
3:G:601:NAG:O4	5:G:767:HOH:O	1.96	0.83
2:L:377:ARG:NH2	2:L:426:GLU:OE2	2.11	0.82
2:D:377:ARG:NH2	2:D:426:GLU:OE2	2.15	0.80
1:A:71:THR:OG1	5:A:826:HOH:O	1.99	0.79
1:I:46:ARG:HE	1:I:76:THR:HG21	1.46	0.78
2:J:377:ARG:NH2	2:J:426:GLU:OE2	2.16	0.78
2:J:478:ASN:O	5:J:745:HOH:O	2.02	0.77
1:A:96:GLU:OE2	5:A:786:HOH:O	2.02	0.77
1:A:94:ASN:OD1	5:A:789:HOH:O	2.02	0.77
1:E:42:CYS:O	5:E:743:HOH:O	2.02	0.76
1:E:1:ASP:N	5:E:717:HOH:O	2.19	0.76
2:B:335:ASN:O	5:B:766:HOH:O	2.02	0.75
3:D:601:NAG:O7	5:D:702:HOH:O	2.04	0.75
2:F:377:ARG:NH2	2:F:426:GLU:OE2	2.18	0.75
2:L:478:ASN:OD1	5:L:715:HOH:O	2.04	0.75
1:G:27:THR:O	5:G:798:HOH:O	2.04	0.73
1:K:224:ASP:OD1	5:K:706:HOH:O	2.06	0.73
1:K:164:THR:OG1	5:K:741:HOH:O	2.06	0.73
2:B:377:ARG:NH2	2:B:426:GLU:OE2	2.21	0.73
1:E:215:GLN:O	5:E:806:HOH:O	2.06	0.72
1:G:304:ARG:NH1	2:H:420:GLU:OE1	2.24	0.71
2:J:334:GLU:HG3	5:J:724:HOH:O	1.90	0.70
2:J:389:ILE:O	5:J:749:HOH:O	2.08	0.70
1:G:17:LYS:NZ	2:H:420:GLU:OE2	2.25	0.70
1:K:41:LEU:HD13	1:K:264:ALA:HB3	1.75	0.69
2:L:443:GLU:OE2	2:L:446:ARG:NH1	2.25	0.69
2:L:448:GLN:NE2	5:L:715:HOH:O	2.26	0.69
1:C:31:GLU:O	5:C:721:HOH:O	2.10	0.68
2:J:387:GLU:OE1	5:J:708:HOH:O	2.11	0.68
1:A:12:ASN:O	5:A:765:HOH:O	2.10	0.68
1:C:46:ARG:HE	1:C:76:THR:HG21	1.58	0.67
1:K:17:LYS:HE3	1:K:22:GLU:HG3	1.76	0.67
1:E:304:ARG:NH1	2:F:420:GLU:OE1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ARG:NH1	2:B:420:GLU:OE1	2.28	0.67
1:I:8:HIS:O	5:I:771:HOH:O	2.12	0.66
2:L:377:ARG:HD2	5:L:736:HOH:O	1.96	0.66
2:F:456:ASP:HB3	2:F:458:LYS:H	1.62	0.65
2:B:412:THR:O	2:B:416:THR:HG23	1.96	0.65
2:B:456:ASP:OD2	5:B:781:HOH:O	2.13	0.65
2:F:353:GLN:H	2:F:353:GLN:HE21	1.44	0.65
1:A:224:ASP:OD1	5:A:734:HOH:O	2.14	0.65
1:C:13:GLY:O	5:C:807:HOH:O	2.15	0.64
2:L:412:THR:O	2:L:416:THR:HG23	1.98	0.64
2:D:412:THR:O	2:D:416:THR:HG23	1.98	0.63
1:E:283:THR:HG22	1:E:285:LEU:H	1.63	0.63
1:A:141:GLU:OE1	1:A:249:ARG:HD3	1.99	0.63
1:I:121:ILE:HD11	1:I:157:THR:HG21	1.80	0.63
1:I:141:GLU:OE1	1:I:249:ARG:HD3	1.99	0.62
1:A:162:ARG:NH2	5:A:808:HOH:O	2.31	0.62
1:K:284:ARG:HB3	2:L:379:VAL:HG22	1.83	0.61
2:F:391:SER:H	2:F:396:ILE:HD11	1.65	0.61
2:D:477:ASN:ND2	5:D:786:HOH:O	2.33	0.61
1:A:165:ASP:OD1	1:A:166:THR:N	2.32	0.61
1:I:48:HIS:HE1	1:I:268:ASN:HD21	1.49	0.60
1:I:81:GLU:OE1	5:I:758:HOH:O	2.16	0.60
1:E:41:LEU:HD13	1:E:264:ALA:HB3	1.84	0.60
1:E:147:SER:O	5:E:708:HOH:O	2.17	0.59
1:E:193:ILE:HG21	1:E:208:PRO:HG2	1.84	0.59
1:C:49:LYS:HD2	1:C:69:HIS:ND1	2.17	0.59
1:I:17:LYS:NZ	2:J:420:GLU:OE2	2.26	0.59
1:A:172:MET:HG2	1:A:227:TRP:HB3	1.83	0.59
1:A:110:LYS:NZ	1:A:141:GLU:OE2	2.32	0.59
2:F:443:GLU:OE2	2:F:446:ARG:NH1	2.36	0.59
2:J:391:SER:H	2:J:396:ILE:HD11	1.68	0.59
1:K:193:ILE:HG21	1:K:208:PRO:HG2	1.85	0.59
1:C:303:ASN:H	2:D:416:THR:CG2	2.16	0.59
2:H:456:ASP:HB3	2:H:458:LYS:H	1.68	0.58
2:D:391:SER:H	2:D:396:ILE:HD11	1.68	0.58
2:H:458:LYS:O	5:H:732:HOH:O	2.17	0.58
1:G:297:GLN:HG2	2:H:385:GLU:HG2	1.84	0.58
2:L:324:GLY:N	5:L:704:HOH:O	2.36	0.57
1:C:121:ILE:HD11	1:C:157:THR:HG21	1.86	0.57
2:B:443:GLU:OE2	2:B:446:ARG:NH1	2.37	0.57
1:C:303:ASN:H	2:D:416:THR:HG22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:468:ASP:OD1	5:L:739:HOH:O	2.17	0.57
2:D:469:ASP:OD1	5:D:748:HOH:O	2.17	0.56
2:B:454:GLU:OE1	2:D:450:ARG:NH1	2.35	0.56
1:C:126:THR:HG23	1:C:136:ASN:HB3	1.87	0.56
1:G:121:ILE:HD11	1:G:157:THR:HG21	1.88	0.56
2:J:455:GLU:OE1	2:L:446:ARG:NH2	2.38	0.56
2:L:410:SER:O	5:L:702:HOH:O	2.17	0.56
1:C:172:MET:HG2	1:C:227:TRP:HB3	1.87	0.56
2:D:443:GLU:OE1	2:D:446:ARG:NH1	2.39	0.55
1:K:172:MET:HG2	1:K:227:TRP:HB3	1.89	0.55
1:C:224:ASP:OD2	1:E:203:ARG:NH2	2.36	0.55
2:J:394:SER:OG	5:J:725:HOH:O	2.18	0.55
2:J:412:THR:O	2:J:416:THR:HG23	2.07	0.55
2:J:458:LYS:NZ	5:J:724:HOH:O	2.38	0.54
1:I:43:MET:HE3	1:I:46:ARG:HD3	1.89	0.54
2:J:446:ARG:HH12	2:J:447:LYS:HE3	1.72	0.54
1:A:34:GLU:HB2	1:A:283:THR:HG21	1.90	0.54
1:E:126:THR:HG23	1:E:136:ASN:HB3	1.90	0.54
1:K:46:ARG:HE	1:K:76:THR:HG21	1.73	0.54
1:C:284:ARG:HB3	2:D:379:VAL:HG22	1.90	0.54
1:G:141:GLU:OE1	1:G:249:ARG:HD3	2.08	0.53
2:H:444:ARG:O	5:H:719:HOH:O	2.19	0.53
2:H:397:GLU:OE2	5:H:727:HOH:O	2.19	0.53
2:H:353:GLN:HE22	2:H:468:ASP:HB2	1.72	0.53
1:G:284:ARG:HB3	2:H:379:VAL:HG22	1.90	0.53
1:K:121:ILE:HD11	1:K:157:THR:HG21	1.90	0.53
2:L:448:GLN:NE2	2:L:478:ASN:HA	2.23	0.52
1:A:256:ARG:NH2	2:B:387:GLU:OE1	2.43	0.52
1:E:34:GLU:HB2	1:E:283:THR:HG21	1.91	0.52
2:H:344:TRP:HH2	2:H:371:ILE:HD12	1.75	0.52
2:L:448:GLN:HE22	2:L:478:ASN:HA	1.75	0.52
1:G:252:LYS:NZ	5:G:802:HOH:O	2.43	0.51
1:E:8:HIS:HE1	5:E:724:HOH:O	1.92	0.51
1:C:224:ASP:OD1	5:C:714:HOH:O	2.19	0.51
1:G:43:MET:CE	1:G:48:HIS:HB3	2.40	0.51
1:K:34:GLU:HB2	1:K:283:THR:HG21	1.92	0.51
1:K:283:THR:HG22	1:K:285:LEU:H	1.75	0.51
1:I:34:GLU:HB2	1:I:283:THR:HG21	1.92	0.51
2:D:473:GLU:O	2:D:477:ASN:HB2	2.11	0.51
1:E:155:PRO:O	1:E:157:THR:HG22	2.11	0.51
1:G:172:MET:HG2	1:G:227:TRP:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ASP:OD2	1:E:76:THR:HG22	2.11	0.50
2:J:494:LEU:HB3	2:J:496:ILE:HG13	1.94	0.50
1:C:34:GLU:HB2	1:C:283:THR:HG21	1.93	0.50
1:G:89:PRO:HB3	1:G:216:VAL:HB	1.94	0.50
1:I:39:ASN:O	5:I:765:HOH:O	2.19	0.50
1:K:303:ASN:H	2:L:416:THR:CG2	2.25	0.50
1:I:302:VAL:HB	2:J:416:THR:HG22	1.93	0.50
1:G:209:VAL:HG11	1:I:205:ASN:HB2	1.94	0.50
2:D:456:ASP:OD1	2:D:460:CYS:HB2	2.12	0.49
1:G:193:ILE:HG21	1:G:208:PRO:HG2	1.94	0.49
1:A:300:LYS:HG3	2:B:415:TRP:CE2	2.47	0.49
1:G:41:LEU:HD13	1:G:264:ALA:HB3	1.94	0.49
2:H:381:LYS:NZ	2:H:382:THR:O	2.38	0.49
1:A:175:ILE:HD12	1:A:195:ILE:HD13	1.93	0.49
1:C:244:LEU:HD13	1:C:246:ALA:HB2	1.94	0.49
2:L:377:ARG:NH1	5:L:736:HOH:O	2.20	0.49
2:D:324:GLY:N	5:D:703:HOH:O	2.45	0.49
1:K:89:PRO:HB3	1:K:216:VAL:HB	1.95	0.48
2:H:342:ASP:HB3	2:H:359:ALA:HB2	1.95	0.48
2:H:377:ARG:NH2	2:H:426:GLU:OE2	2.46	0.48
2:D:374:LYS:NZ	2:D:426:GLU:OE1	2.43	0.48
2:L:444:ARG:O	2:L:448:GLN:HG3	2.13	0.48
1:A:193:ILE:HG21	1:A:208:PRO:HG2	1.94	0.48
2:H:448:GLN:NE2	2:H:478:ASN:HA	2.28	0.48
2:J:353:GLN:HE22	2:J:468:ASP:HA	1.78	0.48
2:H:436:SER:OG	5:H:733:HOH:O	2.20	0.48
1:I:300:LYS:HG3	2:J:415:TRP:CE2	2.48	0.48
1:K:141:GLU:OE1	1:K:249:ARG:HD3	2.14	0.48
2:B:448:GLN:NE2	2:B:478:ASN:HA	2.28	0.48
1:K:303:ASN:H	2:L:416:THR:HG22	1.77	0.48
1:A:43:MET:CE	1:A:46:ARG:HG3	2.44	0.47
1:I:193:ILE:HG22	1:I:208:PRO:HD2	1.96	0.47
1:E:172:MET:HG2	1:E:227:TRP:HB3	1.95	0.47
1:G:283:THR:HG22	1:G:285:LEU:H	1.79	0.47
2:H:412:THR:O	2:H:416:THR:HG23	2.15	0.47
1:C:43:MET:CE	1:C:48:HIS:HB3	2.44	0.47
1:C:162:ARG:NH2	3:C:601:NAG:O6	2.47	0.47
2:L:402:ASN:OD1	5:L:701:HOH:O	2.20	0.47
1:A:202:TYR:CD2	1:A:228:THR:HG21	2.49	0.47
2:D:496:ILE:HD12	2:D:497:ASN:HB2	1.95	0.47
1:G:34:GLU:HB2	1:G:283:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:495:ASN:O	2:J:495:ASN:ND2	2.46	0.47
2:B:329:ILE:HD12	2:B:435:ASP:HA	1.97	0.47
1:C:43:MET:HE1	1:C:48:HIS:HB3	1.97	0.47
2:L:342:ASP:HB3	2:L:359:ALA:HB2	1.97	0.47
2:J:349:HIS:HD2	2:J:476:ARG:HH12	1.62	0.47
1:A:302:VAL:HA	2:B:416:THR:HG22	1.97	0.47
1:I:193:ILE:HG21	1:I:208:PRO:HG2	1.96	0.47
1:I:285:LEU:O	2:J:381:LYS:NZ	2.48	0.47
1:I:75:ASP:OD2	1:I:76:THR:HG22	2.14	0.47
1:I:142:LEU:HD23	1:I:247:PRO:HA	1.97	0.46
1:A:284:ARG:HB3	2:B:379:VAL:HG22	1.97	0.46
2:B:377:ARG:NH1	5:B:774:HOH:O	2.39	0.46
1:G:165:ASP:OD1	1:G:166:THR:N	2.44	0.46
1:C:263:ASP:HB2	5:C:748:HOH:O	2.15	0.46
2:H:442:TYR:CE1	2:H:459:GLY:HA2	2.50	0.46
1:K:8:HIS:O	5:K:722:HOH:O	2.20	0.46
1:G:55:HIS:HE1	1:G:57:ILE:HD13	1.80	0.46
1:E:284:ARG:HB3	2:F:379:VAL:HG22	1.98	0.46
2:H:377:ARG:O	2:H:380:GLU:HG2	2.16	0.46
1:I:303:ASN:H	2:J:416:THR:CG2	2.27	0.46
2:L:353:GLN:HE22	2:L:468:ASP:HB2	1.80	0.46
1:I:43:MET:CE	1:I:48:HIS:HB3	2.46	0.46
1:A:223:ILE:HD13	1:A:245:ILE:HG13	1.97	0.46
2:B:418:GLN:OE1	2:D:418:GLN:NE2	2.49	0.46
1:K:244:LEU:HD13	1:K:246:ALA:HB2	1.97	0.46
1:E:55:HIS:CE1	1:E:57:ILE:HG12	2.52	0.45
2:F:377:ARG:HD2	5:F:722:HOH:O	2.16	0.45
2:B:450:ARG:HG3	2:B:451:GLN:H	1.81	0.45
1:C:61:ILE:O	1:C:139:TYR:HB3	2.16	0.45
2:D:329:ILE:HD12	2:D:435:ASP:HA	1.97	0.45
1:A:109:ASN:ND2	5:A:813:HOH:O	2.49	0.45
2:B:387:GLU:HB2	5:B:705:HOH:O	2.16	0.45
2:J:382:THR:O	2:J:382:THR:OG1	2.33	0.45
1:E:146:VAL:HG21	4:E:602:SIA:H111	1.97	0.45
2:F:353:GLN:HE21	2:F:353:GLN:N	2.10	0.45
1:E:252:LYS:HE3	1:E:254:ILE:HD11	1.98	0.45
1:I:34:GLU:OE2	1:I:35:SER:N	2.49	0.45
1:E:284:ARG:NH2	5:E:853:HOH:O	2.49	0.45
1:A:209:VAL:HG11	1:C:205:ASN:HB2	1.99	0.45
1:I:42:CYS:HB3	1:I:270:CYS:O	2.17	0.45
1:I:172:MET:HG2	1:I:227:TRP:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:456:ASP:HB3	2:L:458:LYS:H	1.82	0.45
1:A:49:LYS:HD2	1:A:69:HIS:ND1	2.32	0.44
2:H:450:ARG:HG3	2:H:451:GLN:H	1.82	0.44
1:K:194:SER:HG	1:K:205:ASN:HD21	1.64	0.44
1:A:303:ASN:H	2:B:416:THR:HG21	1.83	0.44
1:K:302:VAL:HA	2:L:416:THR:HG22	2.00	0.44
1:A:46:ARG:HD3	5:A:708:HOH:O	2.17	0.44
2:B:418:GLN:HG2	2:F:417:TYR:CE1	2.53	0.44
2:J:349:HIS:NE2	2:J:356:GLY:HA3	2.32	0.44
2:D:451:GLN:HB2	5:D:768:HOH:O	2.18	0.44
1:G:43:MET:CE	1:G:46:ARG:HG3	2.48	0.44
1:G:162:ARG:HG3	1:G:235:ASN:OD1	2.16	0.44
1:G:185:ASN:HA	1:G:189:GLY:O	2.16	0.44
2:H:408:LYS:HG2	2:L:406:TRP:CH2	2.52	0.44
2:J:430:THR:OG1	5:J:706:HOH:O	2.21	0.44
1:A:142:LEU:HD23	1:A:247:PRO:HA	2.00	0.44
1:I:48:HIS:CE1	1:I:268:ASN:HD21	2.33	0.44
1:A:283:THR:HG22	1:A:285:LEU:H	1.83	0.44
2:D:406:TRP:CH2	2:F:408:LYS:HG2	2.53	0.43
2:J:342:ASP:HB3	2:J:359:ALA:HB2	2.00	0.43
1:A:121:ILE:HD11	1:A:157:THR:HG21	2.00	0.43
1:E:141:GLU:OE1	1:E:249:ARG:HD3	2.17	0.43
1:I:153:ASN:ND2	1:I:191:GLN:HB3	2.34	0.43
1:E:307:LEU:HB3	2:F:423:VAL:HG21	2.00	0.43
1:G:50:ASP:CG	1:G:80:ARG:HH21	2.22	0.43
1:K:193:ILE:HG22	1:K:208:PRO:HD2	2.00	0.43
1:K:300:LYS:HG3	2:L:415:TRP:CE2	2.53	0.43
1:G:256:ARG:NE	5:G:733:HOH:O	2.51	0.43
2:H:451:GLN:O	2:H:493:ARG:NH1	2.49	0.43
1:I:43:MET:HE2	1:I:48:HIS:HB3	2.00	0.43
2:H:497:ASN:OD1	2:H:497:ASN:N	2.52	0.43
1:E:25:GLU:HG2	1:E:315:ASN:HB3	2.01	0.43
1:G:40:ARG:NE	1:G:267:ASP:OD2	2.48	0.43
1:G:41:LEU:HD22	1:G:264:ALA:O	2.18	0.43
1:C:148:LYS:HB2	1:C:148:LYS:HE3	1.86	0.43
1:G:300:LYS:HG3	2:H:415:TRP:CE2	2.54	0.43
1:K:202:TYR:CD2	1:K:228:THR:HG21	2.54	0.43
1:E:43:MET:O	1:E:46:ARG:HG2	2.19	0.43
1:G:43:MET:HE3	1:G:48:HIS:HB3	2.01	0.43
1:K:142:LEU:HD23	1:K:247:PRO:HA	2.01	0.43
1:C:193:ILE:HG22	1:C:208:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:146:VAL:HG21	1:G:187:LEU:HD22	2.01	0.42
2:L:494:LEU:HB2	2:L:496:ILE:HG12	2.02	0.42
1:A:38:ILE:HG22	1:A:40:ARG:H	1.84	0.42
1:A:87:CYS:HB2	1:A:129:ALA:O	2.20	0.42
2:F:418:GLN:NE2	5:F:705:HOH:O	2.40	0.42
1:K:154:PHE:HB3	1:K:241:ASN:O	2.18	0.42
1:G:175:ILE:HD12	1:G:195:ILE:HD13	2.01	0.42
1:K:96:GLU:O	1:K:100:GLN:HG3	2.19	0.42
1:K:252:LYS:HE3	1:K:254:ILE:HD11	2.00	0.42
1:A:43:MET:HE1	1:A:46:ARG:HG3	2.01	0.42
1:G:25:GLU:HG2	1:G:315:ASN:HB3	2.02	0.42
2:L:468:ASP:CG	5:L:739:HOH:O	2.58	0.42
1:A:43:MET:HE2	1:A:48:HIS:HB3	2.02	0.42
1:A:148:LYS:HB2	1:A:148:LYS:HE3	1.87	0.42
1:C:149:SER:O	1:C:152:GLN:HB2	2.20	0.42
2:H:462:GLU:CD	2:J:450:ARG:HH22	2.23	0.42
1:K:75:ASP:OD2	1:K:76:THR:HG22	2.20	0.42
1:A:143:LYS:N	1:A:246:ALA:O	2.49	0.42
1:K:87:CYS:HB2	1:K:129:ALA:O	2.20	0.42
2:J:340:MET:SD	2:J:346:GLY:HA3	2.60	0.41
1:A:110:LYS:HB2	1:A:249:ARG:NH2	2.35	0.41
1:C:43:MET:CE	1:C:46:ARG:HG3	2.50	0.41
1:C:165:ASP:O	1:C:232:PRO:HB3	2.20	0.41
2:D:381:LYS:HG3	2:D:383:ASN:OD1	2.19	0.41
1:E:300:LYS:HG3	2:F:415:TRP:CE2	2.55	0.41
1:A:49:LYS:HB2	1:A:49:LYS:HE2	1.84	0.41
2:D:450:ARG:HG3	2:D:451:GLN:H	1.86	0.41
1:E:48:HIS:CD2	1:E:266:ILE:HD13	2.55	0.41
2:F:412:THR:O	2:F:416:THR:HG23	2.20	0.41
1:E:121:ILE:HD11	1:E:157:THR:HG21	2.02	0.41
1:I:61:ILE:O	1:I:139:TYR:HB3	2.20	0.41
1:A:90:GLY:HA3	1:A:223:ILE:O	2.20	0.41
1:C:1:ASP:N	5:D:701:HOH:O	2.52	0.41
1:C:1:ASP:OD2	2:D:351:ASN:HA	2.21	0.41
1:E:165:ASP:OD1	1:E:166:THR:N	2.42	0.41
1:I:47:LYS:HE2	1:I:47:LYS:HB3	1.53	0.41
1:C:285:LEU:O	2:D:381:LYS:NZ	2.54	0.41
1:C:303:ASN:HB2	2:D:416:THR:HG21	2.03	0.41
1:G:153:ASN:OD1	1:G:191:GLN:HG2	2.21	0.41
2:H:491:LEU:HD13	2:H:497:ASN:HA	2.02	0.41
1:I:12:ASN:HA	5:I:774:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:383:ASN:HA	2:J:384:THR:CB	2.50	0.41
1:K:34:GLU:HG2	1:K:283:THR:OG1	2.21	0.41
1:C:115:PHE:HA	5:C:752:HOH:O	2.20	0.41
1:E:46:ARG:HE	1:E:76:THR:HG21	1.85	0.41
2:L:446:ARG:HH12	2:L:447:LYS:HE3	1.85	0.41
1:G:55:HIS:CE1	1:G:57:ILE:HD13	2.55	0.40
1:C:300:LYS:HG3	2:D:415:TRP:CE2	2.57	0.40
1:G:43:MET:HE2	1:G:48:HIS:HB3	2.02	0.40
2:J:477:ASN:ND2	5:J:737:HOH:O	2.30	0.40
1:K:44:LYS:O	1:K:271:GLU:HG3	2.22	0.40
1:K:51:LEU:HD23	1:K:51:LEU:HA	1.91	0.40
1:C:297:GLN:HB3	2:D:383:ASN:HB2	2.04	0.40
1:E:153:ASN:HA	1:E:189:GLY:HA3	2.02	0.40
1:C:197:VAL:O	1:C:203:ARG:HA	2.22	0.40
1:E:5:LEU:HD13	1:E:5:LEU:HA	1.97	0.40
2:H:361:TYR:CZ	2:H:365:GLN:HG3	2.56	0.40
1:A:313:MET:HG3	1:A:314:ARG:O	2.21	0.40
1:K:193:ILE:HG21	1:K:193:ILE:HD13	1.83	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:SER:OG	2:H:497:ASN:OD1[1_456]	2.18	0.02

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	316/318 (99%)	307 (97%)	9 (3%)	0	100	100
1	C	316/318 (99%)	310 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	316/318 (99%)	308 (98%)	8 (2%)	0	100	100
1	G	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
1	I	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
1	K	316/318 (99%)	303 (96%)	13 (4%)	0	100	100
2	B	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	25	36
2	D	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	25	36
2	F	172/174 (99%)	168 (98%)	3 (2%)	1 (1%)	25	36
2	H	172/174 (99%)	165 (96%)	6 (4%)	1 (1%)	25	36
2	J	172/174 (99%)	164 (95%)	7 (4%)	1 (1%)	25	36
2	L	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	25	36
All	All	2928/2952 (99%)	2835 (97%)	87 (3%)	6 (0%)	47	62

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	450	ARG
2	D	450	ARG
2	F	450	ARG
2	H	450	ARG
2	J	450	ARG
2	L	450	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/269 (100%)	244 (91%)	25 (9%)	9	13
1	C	269/269 (100%)	249 (93%)	20 (7%)	13	22
1	E	269/269 (100%)	248 (92%)	21 (8%)	12	19
1	G	269/269 (100%)	248 (92%)	21 (8%)	12	19
1	I	269/269 (100%)	245 (91%)	24 (9%)	9	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	269/269 (100%)	245 (91%)	24 (9%)	9	14
2	B	148/148 (100%)	138 (93%)	10 (7%)	16	25
2	D	148/148 (100%)	142 (96%)	6 (4%)	30	48
2	F	148/148 (100%)	142 (96%)	6 (4%)	30	48
2	H	148/148 (100%)	140 (95%)	8 (5%)	22	36
2	J	148/148 (100%)	136 (92%)	12 (8%)	11	18
2	L	148/148 (100%)	140 (95%)	8 (5%)	22	36
All	All	2502/2502 (100%)	2317 (93%)	185 (7%)	13	22

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	35	SER
1	A	41	LEU
1	A	46	ARG
1	A	49	LYS
1	A	76	THR
1	A	77	LEU
1	A	94	ASN
1	A	111	ILE
1	A	112	SER
1	A	120	SER
1	A	126	THR
1	A	149	SER
1	A	157	THR
1	A	162	ARG
1	A	170	LEU
1	A	192	SER
1	A	203	ARG
1	A	213	ARG
1	A	228	THR
1	A	244	LEU
1	A	258	LEU
1	A	276	TRP
1	A	277	ARG
1	A	283	THR
2	B	335	ASN
2	B	342	ASP
2	B	385	GLU

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Mol	Chain	Res	Type
2	B	416	THR
2	B	418	GLN
2	B	425	MET
2	B	433	MET
2	B	436	SER
2	B	450	ARG
2	B	470	SER
1	C	8	HIS
1	C	14	THR
1	C	41	LEU
1	C	46	ARG
1	C	76	THR
1	C	77	LEU
1	C	111	ILE
1	C	120	SER
1	C	126	THR
1	C	157	THR
1	C	170	LEU
1	C	203	ARG
1	C	228	THR
1	C	244	LEU
1	C	250	VAL
1	C	256	ARG
1	C	258	LEU
1	C	271	GLU
1	C	276	TRP
1	C	283	THR
2	D	325	LEU
2	D	341	VAL
2	D	383	ASN
2	D	384	THR
2	D	433	MET
2	D	450	ARG
1	E	8	HIS
1	E	14	THR
1	E	41	LEU
1	E	76	THR
1	E	77	LEU
1	E	111	ILE
1	E	126	THR
1	E	150	LYS
1	E	157	THR

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Mol	Chain	Res	Type
1	E	162	ARG
1	E	170	LEU
1	E	192	SER
1	E	196	SER
1	E	203	ARG
1	E	213	ARG
1	E	228	THR
1	E	244	LEU
1	E	250	VAL
1	E	258	LEU
1	E	276	TRP
1	E	283	THR
2	F	353	GLN
2	F	411	ILE
2	F	416	THR
2	F	418	GLN
2	F	433	MET
2	F	450	ARG
1	G	8	HIS
1	G	14	THR
1	G	41	LEU
1	G	47	LYS
1	G	49	LYS
1	G	76	THR
1	G	77	LEU
1	G	111	ILE
1	G	112	SER
1	G	120	SER
1	G	157	THR
1	G	162	ARG
1	G	170	LEU
1	G	203	ARG
1	G	213	ARG
1	G	228	THR
1	G	244	LEU
1	G	258	LEU
1	G	276	TRP
1	G	277	ARG
1	G	283	THR
2	H	379	VAL
2	H	385	GLU
2	H	416	THR

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Mol	Chain	Res	Type
2	H	433	MET
2	H	438	MET
2	H	477	ASN
2	H	479	THR
2	H	497	ASN
1	I	1	ASP
1	I	8	HIS
1	I	35	SER
1	I	39	ASN
1	I	41	LEU
1	I	47	LYS
1	I	76	THR
1	I	77	LEU
1	I	111	ILE
1	I	126	THR
1	I	132	ARG
1	I	149	SER
1	I	157	THR
1	I	170	LEU
1	I	184	LYS
1	I	203	ARG
1	I	228	THR
1	I	244	LEU
1	I	250	VAL
1	I	258	LEU
1	I	263	ASP
1	I	276	TRP
1	I	277	ARG
1	I	283	THR
2	J	325	LEU
2	J	350	GLN
2	J	353	GLN
2	J	379	VAL
2	J	383	ASN
2	J	384	THR
2	J	395	GLU
2	J	418	GLN
2	J	433	MET
2	J	448	GLN
2	J	467	CYS
2	J	495	ASN
1	K	1	ASP

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Mol	Chain	Res	Type
1	K	8	HIS
1	K	23	GLN
1	K	41	LEU
1	K	76	THR
1	K	77	LEU
1	K	101	LYS
1	K	111	ILE
1	K	146	VAL
1	K	150	LYS
1	K	157	THR
1	K	162	ARG
1	K	170	LEU
1	K	203	ARG
1	K	213	ARG
1	K	228	THR
1	K	244	LEU
1	K	250	VAL
1	K	258	LEU
1	K	263	ASP
1	K	276	TRP
1	K	277	ARG
1	K	283	THR
1	K	303	ASN
2	L	335	ASN
2	L	350	GLN
2	L	379	VAL
2	L	382	THR
2	L	411	ILE
2	L	433	MET
2	L	446	ARG
2	L	467	CYS

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

Mol	Chain	Res	Type
1	A	205	ASN
1	E	8	HIS
2	H	484	GLN
1	I	268	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	F	601	2	14,14,15	0.46	0	17,19,21	0.70	1 (5%)
3	NAG	D	601	2	14,14,15	0.62	0	17,19,21	0.58	0
3	NAG	I	601	1	14,14,15	0.36	0	17,19,21	0.50	0
3	NAG	L	601	2	14,14,15	0.37	0	17,19,21	0.54	0
4	SIA	E	602	-	21,21,21	1.01	1 (4%)	25,31,31	1.30	3 (12%)
3	NAG	K	601	1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	H	601	2	14,14,15	0.32	0	17,19,21	0.44	0
3	NAG	C	601	1	14,14,15	0.43	0	17,19,21	0.52	0
3	NAG	B	601	2	14,14,15	0.51	0	17,19,21	0.49	0
3	NAG	A	601	1	14,14,15	0.29	0	17,19,21	0.53	0
3	NAG	J	601	2	14,14,15	0.44	0	17,19,21	0.55	0
3	NAG	E	601	1	14,14,15	0.39	0	17,19,21	0.53	0
3	NAG	G	601	1	14,14,15	0.20	0	17,19,21	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	601	2	-	0/6/23/26	0/1/1/1
3	NAG	D	601	2	-	0/6/23/26	0/1/1/1
3	NAG	I	601	1	-	2/6/23/26	0/1/1/1
3	NAG	L	601	2	-	2/6/23/26	0/1/1/1
4	SIA	E	602	-	-	6/20/38/38	0/1/1/1
3	NAG	K	601	1	-	2/6/23/26	0/1/1/1
3	NAG	H	601	2	-	2/6/23/26	0/1/1/1
3	NAG	C	601	1	-	2/6/23/26	0/1/1/1
3	NAG	B	601	2	-	0/6/23/26	0/1/1/1
3	NAG	A	601	1	-	2/6/23/26	0/1/1/1
3	NAG	J	601	2	-	0/6/23/26	0/1/1/1
3	NAG	E	601	1	-	1/6/23/26	0/1/1/1
3	NAG	G	601	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	602	SIA	O2-C2	3.65	1.44	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	602	SIA	O6-C6-C5	3.78	113.46	109.78
4	E	602	SIA	C8-C7-C6	-2.60	108.11	113.03
4	E	602	SIA	O1A-C1-C2	-2.27	120.15	123.59
3	F	601	NAG	C1-O5-C5	2.22	115.21	112.19

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	601	NAG	O5-C5-C6-O6
3	C	601	NAG	O5-C5-C6-O6
3	L	601	NAG	C4-C5-C6-O6
3	C	601	NAG	C4-C5-C6-O6
3	I	601	NAG	C4-C5-C6-O6
3	L	601	NAG	O5-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6
3	A	601	NAG	C4-C5-C6-O6

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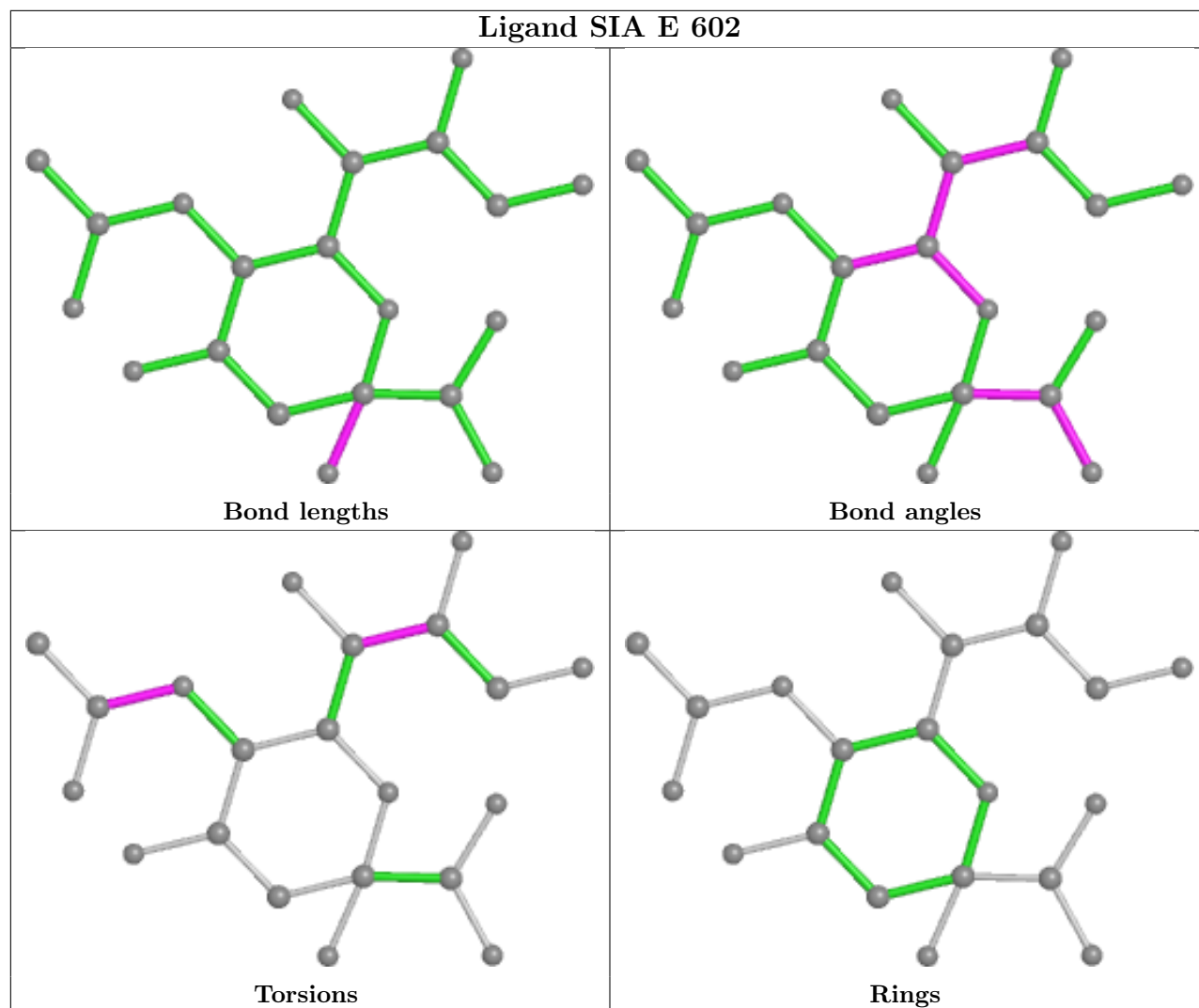
Mol	Chain	Res	Type	Atoms
3	G	601	NAG	O5-C5-C6-O6
3	H	601	NAG	C4-C5-C6-O6
3	H	601	NAG	O5-C5-C6-O6
4	E	602	SIA	C11-C10-N5-C5
4	E	602	SIA	C6-C7-C8-C9
4	E	602	SIA	O7-C7-C8-C9
3	E	601	NAG	O5-C5-C6-O6
4	E	602	SIA	O10-C10-N5-C5
4	E	602	SIA	C6-C7-C8-O8
3	K	601	NAG	C4-C5-C6-O6
3	K	601	NAG	O5-C5-C6-O6
3	G	601	NAG	C4-C5-C6-O6
4	E	602	SIA	O7-C7-C8-O8

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	601	NAG	1	0
4	E	602	SIA	1	0
3	C	601	NAG	1	0
3	E	601	NAG	1	0
3	G	601	NAG	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	318/318 (100%)	-0.13	1 (0%) 94 93	21, 35, 57, 90	0
1	C	318/318 (100%)	-0.04	8 (2%) 57 55	19, 37, 55, 90	0
1	E	318/318 (100%)	-0.08	3 (0%) 84 82	20, 33, 52, 97	0
1	G	318/318 (100%)	-0.13	0 100 100	23, 38, 60, 89	0
1	I	318/318 (100%)	-0.02	5 (1%) 72 70	17, 34, 58, 100	0
1	K	318/318 (100%)	-0.03	4 (1%) 77 75	26, 39, 62, 105	0
2	B	174/174 (100%)	0.35	6 (3%) 45 44	22, 37, 61, 126	0
2	D	174/174 (100%)	0.28	4 (2%) 60 58	21, 37, 74, 130	0
2	F	174/174 (100%)	0.23	5 (2%) 51 50	18, 37, 61, 97	0
2	H	174/174 (100%)	0.65	10 (5%) 23 22	20, 53, 89, 177	0
2	J	174/174 (100%)	0.70	15 (8%) 10 9	22, 51, 88, 145	0
2	L	174/174 (100%)	0.52	11 (6%) 20 18	21, 49, 87, 146	0
All	All	2952/2952 (100%)	0.11	72 (2%) 59 57	17, 38, 70, 177	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	497	ASN	21.9
2	J	496	ILE	14.7
2	H	496	ILE	13.8
2	J	497	ASN	11.6
2	L	497	ASN	10.1
2	B	497	ASN	8.8
2	D	497	ASN	8.6
2	L	496	ILE	5.9
2	D	496	ILE	5.4
2	H	494	LEU	4.7
2	B	496	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	I	133	ASN	4.4
2	J	341	VAL	4.4
2	H	491	LEU	3.8
2	L	494	LEU	3.8
1	K	317	PRO	3.7
2	L	383	ASN	3.6
2	D	382	THR	3.5
1	C	11	ALA	3.3
2	H	495	ASN	3.2
2	J	479	THR	3.2
2	H	352	ALA	3.2
1	C	12	ASN	3.0
2	J	464	TYR	3.0
2	H	470	SER	3.0
1	C	149	SER	2.9
2	B	383	ASN	2.8
2	H	354	GLY	2.7
2	J	355	THR	2.6
2	J	348	ARG	2.6
2	J	354	GLY	2.6
2	L	324	GLY	2.6
2	F	325	LEU	2.6
1	C	256	ARG	2.5
2	J	491	LEU	2.5
2	L	491	LEU	2.5
1	K	269	ASN	2.5
1	C	10	VAL	2.4
1	E	305	ARG	2.4
2	B	326	PHE	2.4
2	J	357	GLN	2.4
2	F	350	GLN	2.4
2	J	350	GLN	2.4
2	L	355	THR	2.4
1	I	149	SER	2.4
2	H	325	LEU	2.3
1	K	11	ALA	2.3
1	E	318	GLU	2.3
2	H	471	CYS	2.3
2	L	341	VAL	2.3
2	J	352	ALA	2.3
1	I	12	ASN	2.3
1	C	317	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	475	ILE	2.3
2	L	479	THR	2.2
2	F	356	GLY	2.2
2	F	383	ASN	2.2
2	J	340	MET	2.2
2	L	325	LEU	2.2
1	C	284	ARG	2.1
1	I	9	ALA	2.1
2	J	324	GLY	2.1
2	B	491	LEU	2.1
2	F	326	PHE	2.1
1	A	167	ALA	2.1
1	C	13	GLY	2.1
1	I	2	LYS	2.1
1	K	118	GLY	2.1
2	D	350	GLN	2.0
1	E	270	CYS	2.0
2	B	359	ALA	2.0
2	J	359	ALA	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(\AA^2)	Q<0.9
4	SIA	E	602	21/21	0.60	0.40	73,92,103,105	0
3	NAG	I	601	14/15	0.84	0.18	39,58,63,69	0
3	NAG	C	601	14/15	0.86	0.17	50,56,64,71	0
3	NAG	B	601	14/15	0.90	0.14	36,43,51,51	0

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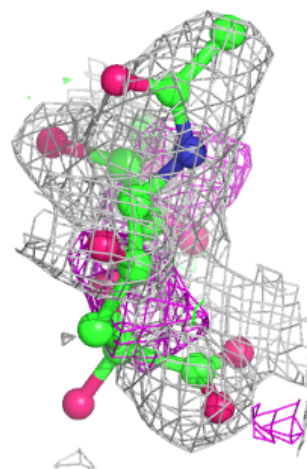
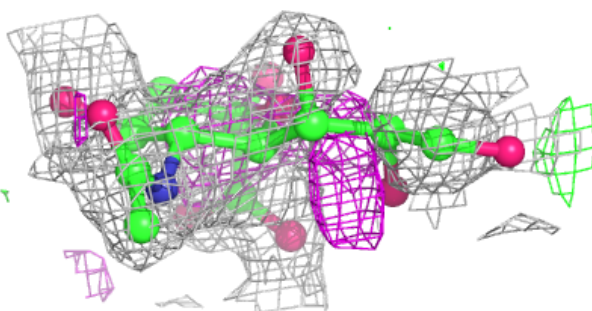
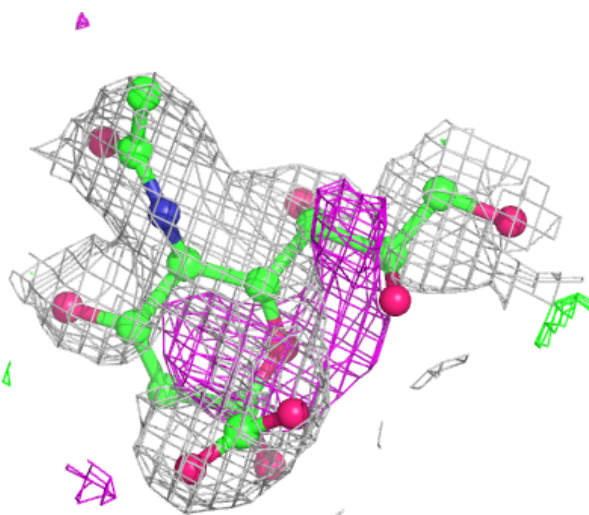
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	K	601	14/15	0.90	0.16	51,60,67,68	0
3	NAG	G	601	14/15	0.90	0.15	69,82,86,88	0
3	NAG	E	601	14/15	0.92	0.12	50,61,72,73	0
3	NAG	F	601	14/15	0.93	0.18	33,41,50,52	0
3	NAG	A	601	14/15	0.93	0.12	52,68,74,74	0
3	NAG	L	601	14/15	0.93	0.11	32,47,54,57	0
3	NAG	H	601	14/15	0.93	0.19	32,50,53,54	0
3	NAG	J	601	14/15	0.94	0.10	30,38,42,42	0
3	NAG	D	601	14/15	0.94	0.13	30,41,48,51	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 SIA E 602:

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.