



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2024 – 10:52 am BST

PDB ID : 2WRH  
Title : structure of H1 duck albert hemagglutinin with human receptor  
Authors : Liu, J.; Stevens, D.J.; Haire, L.F.; Walker, P.A.; Coombs, P.J.; Russell, R.J.;  
Gamblin, S.J.; Skehel, J.J.  
Deposited on : 2009-09-01  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

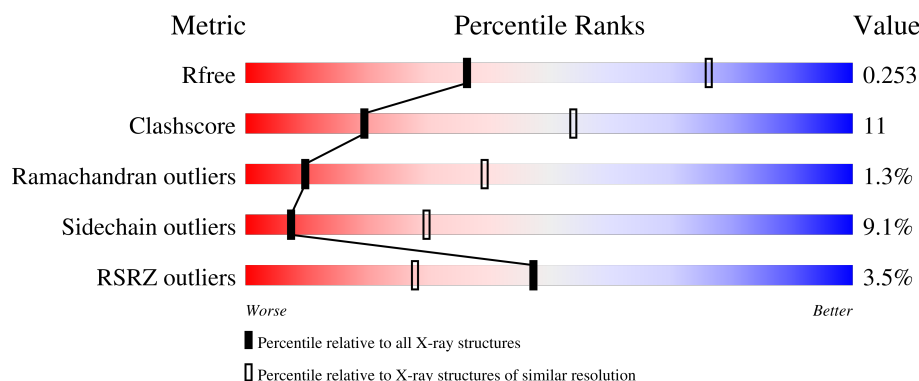
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	H	324	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>5%</div> </div> </div>
1	J	324	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>5%</div> </div> </div>
1	L	324	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>.</div> </div> </div>
2	I	222	<div> <div>3%</div> <div> <div></div> <div>56%</div> <div>14%</div> <div>.</div> <div>28%</div> </div> </div>
2	K	222	<div> <div>3%</div> <div> <div></div> <div>55%</div> <div>14%</div> <div>.</div> <div>28%</div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	M	222	 <p>2% 57% 13% 28%</p>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11332 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 HA1 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	322	Total	C	N	O	S	0	0	0
			2483	1558	430	484	11			
1	J	322	Total	C	N	O	S	0	0	0
			2483	1558	430	484	11			
1	L	322	Total	C	N	O	S	0	0	0
			2483	1558	430	484	11			

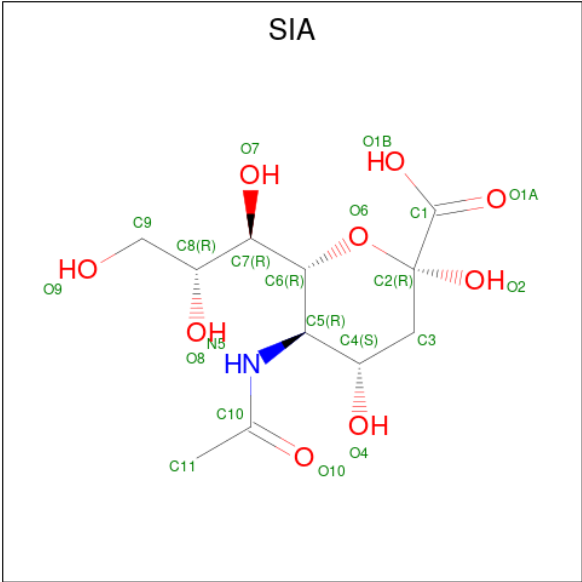
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	ASN	deletion	UNP Q9WCE0
H	?	-	THR	deletion	UNP Q9WCE0
H	327	ARG	ILE	conflict	UNP Q9WCE0
J	?	-	ASN	deletion	UNP Q9WCE0
J	?	-	THR	deletion	UNP Q9WCE0
J	327	ARG	ILE	conflict	UNP Q9WCE0
L	?	-	ASN	deletion	UNP Q9WCE0
L	?	-	THR	deletion	UNP Q9WCE0
L	327	ARG	ILE	conflict	UNP Q9WCE0

- Molecule 2 is a protein called HEMAGGLUTININ HA2 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	160	Total	C	N	O	S	0	0	0
			1274	794	219	255	6			
2	K	160	Total	C	N	O	S	0	0	0
			1274	794	219	255	6			
2	M	160	Total	C	N	O	S	0	0	0
			1274	794	219	255	6			

- Molecule 3 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: C<sub>11</sub>H<sub>19</sub>NO<sub>9</sub>).

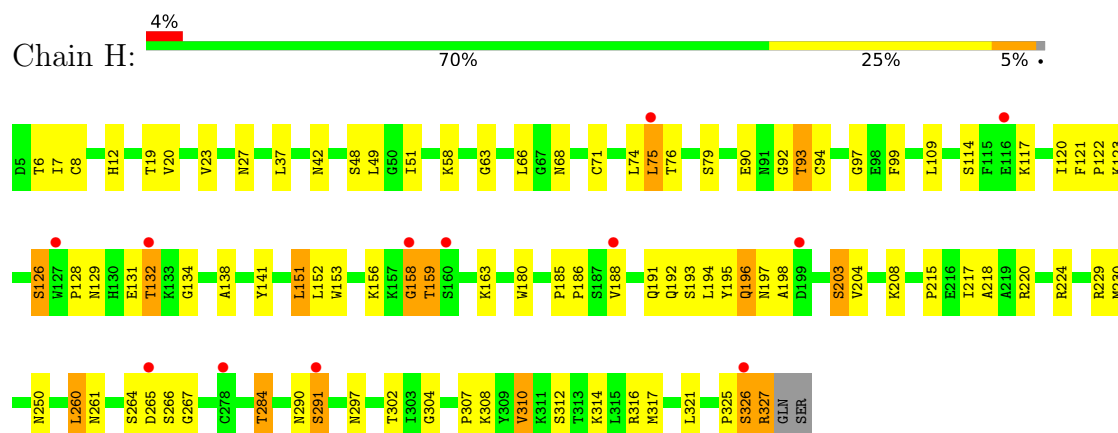


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			21	11	1	9		
3	J	1	Total	C	N	O	0	0
			20	11	1	8		
3	L	1	Total	C	N	O	0	0
			20	11	1	8		

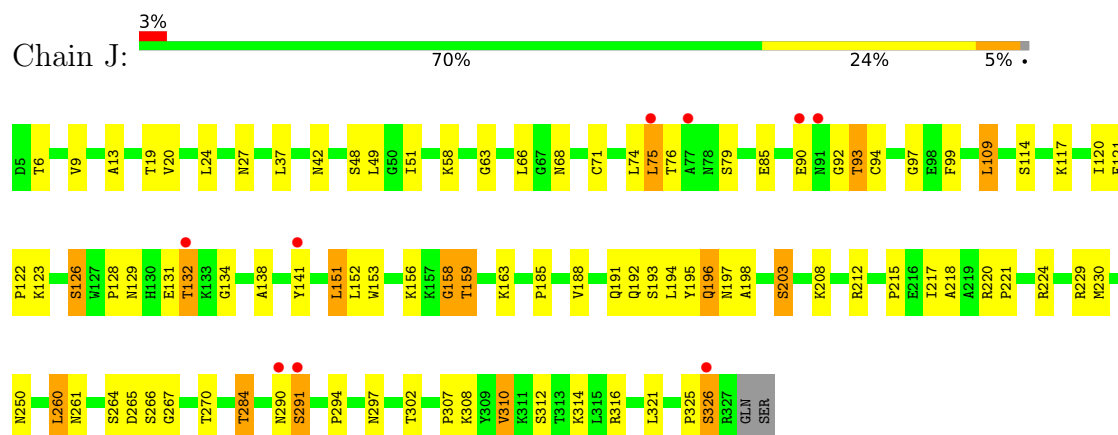
### 3 Residue-property plots [i](#)

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.

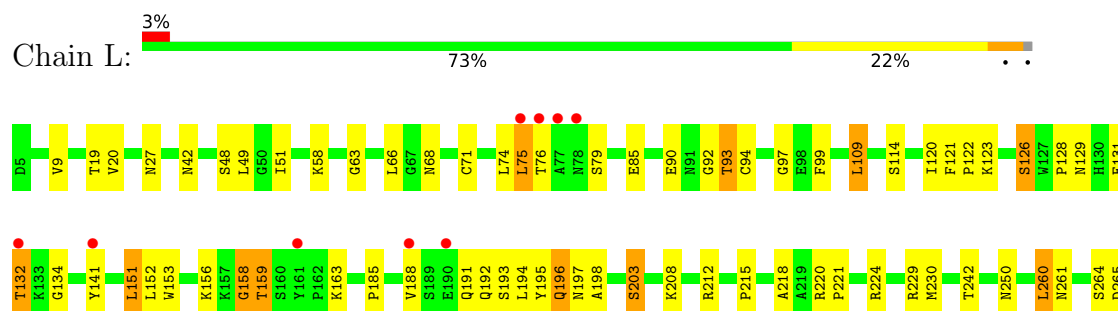
#### • Molecule 1: HEMAGGLUTININ HA1 CHAIN



#### • Molecule 1: HEMAGGLUTININ HA1 CHAIN

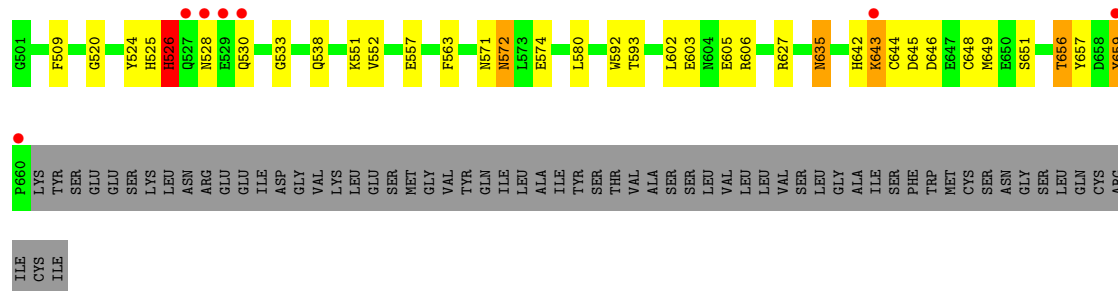


#### • Molecule 1: HEMAGGLUTININ HA1 CHAIN

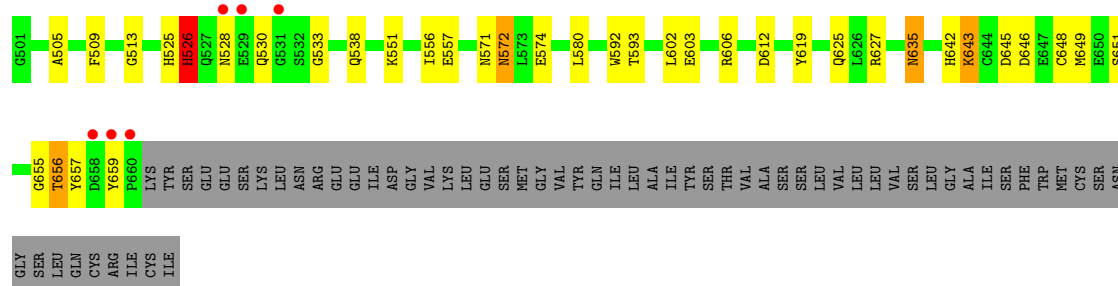




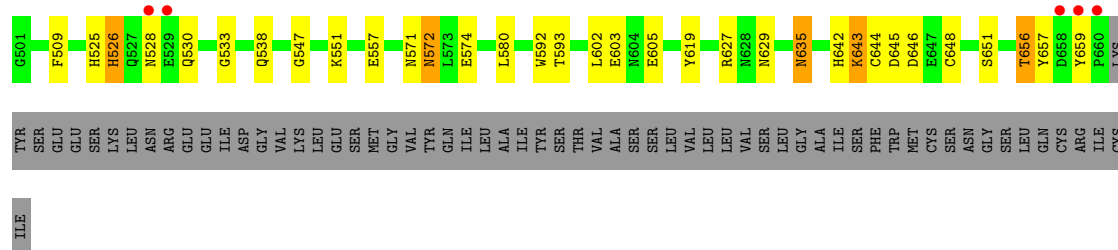
• Molecule 2: HEMAGGLUTININ HA2 CHAIN



• Molecule 2: HEMAGGLUTININ HA2 CHAIN



• Molecule 2: HEMAGGLUTININ HA2 CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.42Å 155.54Å 157.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.00 19.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.2 (19.98-3.00) 97.6 (19.98-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.98Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.229 , 0.252 0.228 , 0.253	Depositor DCC
$R_{free}$ test set	2576 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.1	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11332	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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: SIA

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	H	0.33	0/2546	0.52	0/3473
1	J	0.37	0/2546	0.54	0/3473
1	L	0.39	0/2546	0.55	0/3473
2	I	0.41	0/1300	0.54	0/1755
2	K	0.46	0/1300	0.55	0/1755
2	M	0.45	0/1300	0.54	0/1755
All	All	0.39	0/11538	0.54	0/15684

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2483	0	2339	71	0
1	J	2483	0	2339	66	0
1	L	2483	0	2339	58	0
2	I	1274	0	1158	34	0
2	K	1274	0	1156	27	0
2	M	1274	0	1158	23	0
3	H	21	0	17	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	20	0	16	1	0
3	L	20	0	16	1	0
All	All	11332	0	10538	249	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 11.

All (249) 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:L:131:GLU:HG3	1:L:132:THR:H	1.24	1.01
1:H:131:GLU:HG3	1:H:132:THR:H	1.24	1.00
1:J:131:GLU:HG3	1:J:132:THR:H	1.21	0.99
2:K:528:ASN:HB3	2:K:530:GLN:H	1.37	0.89
2:M:528:ASN:HB3	2:M:530:GLN:H	1.39	0.87
2:I:528:ASN:HB3	2:I:530:GLN:H	1.39	0.86
1:H:8:CYS:O	2:I:524:TYR:HA	1.78	0.84
1:J:131:GLU:CG	1:J:132:THR:H	1.93	0.82
1:H:131:GLU:CG	1:H:132:THR:H	1.94	0.80
1:J:185:PRO:HG2	1:J:191:GLN:HE21	1.47	0.79
1:H:6:THR:O	2:I:526:HIS:HA	1.82	0.79
1:L:20:VAL:HG12	1:L:316:ARG:HG2	1.65	0.78
1:J:158:GLY:O	1:J:159:THR:HG22	1.85	0.76
1:L:131:GLU:CG	1:L:132:THR:H	1.95	0.76
2:M:644:CYS:HG	2:M:648:CYS:HG	0.77	0.76
1:L:134:GLY:HA3	1:L:153:TRP:HB3	1.67	0.75
1:H:185:PRO:HG2	1:H:191:GLN:HE21	1.52	0.75
1:H:134:GLY:HA3	1:H:153:TRP:HB3	1.69	0.74
1:J:185:PRO:HG2	1:J:191:GLN:NE2	2.02	0.74
1:J:20:VAL:HG12	1:J:316:ARG:HG2	1.68	0.74
1:L:185:PRO:HG2	1:L:191:GLN:HE21	1.53	0.74
1:H:158:GLY:O	1:H:159:THR:HG22	1.88	0.73
1:L:158:GLY:O	1:L:159:THR:HG22	1.88	0.73
1:J:74:LEU:O	1:J:76:THR:HG23	1.88	0.72
1:H:20:VAL:HG12	1:H:316:ARG:HG2	1.70	0.72
1:H:185:PRO:HG2	1:H:191:GLN:NE2	2.05	0.72
1:L:185:PRO:HG2	1:L:191:GLN:NE2	2.05	0.72
1:L:74:LEU:O	1:L:76:THR:HG23	1.91	0.70
2:M:551:LYS:HE3	2:M:603:GLU:OE2	1.91	0.70
1:J:156:LYS:NZ	1:J:196:GLN:HE21	1.90	0.70
1:H:156:LYS:NZ	1:H:196:GLN:HE21	1.91	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:134:GLY:HA3	1:J:153:TRP:HB3	1.73	0.69
1:H:7:ILE:HA	2:I:526:HIS:HA	1.74	0.69
1:H:74:LEU:O	1:H:76:THR:HG23	1.93	0.69
1:H:308:LYS:HG2	2:I:592:TRP:CE2	2.29	0.67
1:L:156:LYS:NZ	1:L:196:GLN:HE21	1.92	0.67
2:K:551:LYS:HE3	2:K:603:GLU:OE2	1.94	0.67
2:I:551:LYS:HE3	2:I:603:GLU:OE2	1.94	0.66
1:J:132:THR:HG23	1:J:132:THR:O	1.94	0.66
1:L:132:THR:HG23	1:L:132:THR:O	1.96	0.66
1:H:132:THR:HG23	1:H:132:THR:O	1.94	0.66
1:J:6:THR:O	2:K:526:HIS:HA	1.96	0.66
1:J:310:VAL:HG22	2:K:593:THR:HA	1.77	0.66
1:L:123:LYS:HE2	1:L:132:THR:OG1	1.96	0.65
1:L:308:LYS:HG2	2:M:592:TRP:CE2	2.32	0.65
1:H:123:LYS:HE2	1:H:132:THR:OG1	1.96	0.65
1:L:310:VAL:HG13	1:L:312:SER:H	1.62	0.64
2:M:642:HIS:HE1	2:M:657:TYR:OH	1.81	0.63
2:K:642:HIS:HE1	2:K:657:TYR:OH	1.81	0.63
1:L:19:THR:HG23	1:L:314:LYS:NZ	2.14	0.63
1:H:310:VAL:HG13	1:H:312:SER:H	1.64	0.63
2:I:642:HIS:HE1	2:I:657:TYR:OH	1.81	0.62
1:L:156:LYS:HZ2	1:L:196:GLN:HE21	1.45	0.62
1:H:156:LYS:HZ2	1:H:196:GLN:HE21	1.45	0.62
1:J:123:LYS:HE2	1:J:132:THR:OG1	1.99	0.62
1:J:310:VAL:HG13	1:J:312:SER:H	1.65	0.62
1:L:19:THR:HG23	1:L:314:LYS:HZ1	1.65	0.62
1:H:19:THR:HG23	1:H:314:LYS:NZ	2.15	0.61
1:J:156:LYS:HZ2	1:J:196:GLN:HE21	1.47	0.61
1:J:218:ALA:HB1	1:L:203:SER:OG	2.00	0.61
1:J:19:THR:HG23	1:J:314:LYS:NZ	2.15	0.61
1:L:310:VAL:HG22	2:M:593:THR:HA	1.82	0.61
1:J:63:GLY:HA3	1:J:92:GLY:HA2	1.82	0.60
1:L:63:GLY:HA3	1:L:92:GLY:HA2	1.83	0.60
1:H:93:THR:HG22	1:H:93:THR:O	2.03	0.59
1:H:63:GLY:HA3	1:H:92:GLY:HA2	1.85	0.59
1:H:156:LYS:HD2	1:H:196:GLN:HG2	1.85	0.59
1:H:327:ARG:HB2	1:H:327:ARG:NH1	2.17	0.59
1:J:131:GLU:O	1:J:132:THR:HB	2.03	0.59
1:L:156:LYS:HD2	1:L:196:GLN:HG2	1.85	0.58
1:J:131:GLU:CG	1:J:132:THR:N	2.66	0.58
1:J:308:LYS:HG2	2:K:592:TRP:CE2	2.38	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:571:ASN:OD1	2:K:574:GLU:HG3	2.05	0.57
1:L:93:THR:HG22	1:L:93:THR:O	2.03	0.57
1:J:217:ILE:O	1:L:212:ARG:NH1	2.37	0.57
1:J:156:LYS:HD2	1:J:196:GLN:HG2	1.85	0.57
1:H:325:PRO:O	1:H:327:ARG:HG3	2.05	0.56
1:H:131:GLU:CG	1:H:132:THR:N	2.67	0.55
2:I:525:HIS:O	2:I:533:GLY:O	2.25	0.55
1:L:131:GLU:O	1:L:132:THR:HB	2.07	0.55
1:J:93:THR:HG22	1:J:93:THR:O	2.06	0.55
2:M:525:HIS:O	2:M:533:GLY:O	2.25	0.55
2:I:528:ASN:ND2	2:I:646:ASP:OD1	2.40	0.54
1:H:131:GLU:O	1:H:132:THR:HB	2.08	0.54
1:H:8:CYS:O	2:I:524:TYR:CA	2.53	0.54
1:J:290:ASN:OD1	1:J:290:ASN:O	2.26	0.54
2:I:656:THR:O	2:I:656:THR:CG2	2.56	0.53
1:L:290:ASN:OD1	1:L:290:ASN:O	2.25	0.53
1:H:194:LEU:HD21	3:H:1328:SIA:H113	1.89	0.53
1:H:8:CYS:HB2	2:I:525:HIS:HB3	1.91	0.53
1:H:290:ASN:OD1	1:H:290:ASN:O	2.27	0.53
2:K:538:GLN:HA	2:K:538:GLN:NE2	2.22	0.53
1:L:131:GLU:CG	1:L:132:THR:N	2.68	0.53
2:M:530:GLN:HE22	2:M:645:ASP:HB2	1.73	0.53
1:J:63:GLY:CA	1:J:92:GLY:HA2	2.39	0.53
1:H:7:ILE:HA	2:I:526:HIS:CA	2.39	0.53
1:L:194:LEU:HD21	3:L:1328:SIA:H113	1.91	0.53
1:J:156:LYS:HE2	1:J:193:SER:O	2.09	0.52
1:H:156:LYS:HE2	1:H:193:SER:O	2.08	0.52
1:L:131:GLU:HG3	1:L:132:THR:N	2.08	0.52
1:J:131:GLU:HG3	1:J:132:THR:N	2.06	0.52
1:J:194:LEU:HD21	3:J:1328:SIA:H113	1.92	0.52
1:H:19:THR:HG23	1:H:314:LYS:HZ1	1.73	0.52
2:I:605:GLU:HG3	2:K:606:ARG:HH22	1.74	0.52
2:I:644:CYS:HG	2:I:648:CYS:HG	0.60	0.52
1:H:114:SER:HB3	1:H:261:ASN:HB2	1.91	0.52
1:J:294:PRO:HG3	2:K:556:ILE:HA	1.93	0.51
1:L:156:LYS:HE2	1:L:193:SER:O	2.10	0.51
2:K:525:HIS:O	2:K:533:GLY:O	2.29	0.51
1:H:310:VAL:HG22	2:I:593:THR:HA	1.92	0.51
1:J:310:VAL:CG1	1:J:312:SER:H	2.24	0.50
2:M:538:GLN:HA	2:M:538:GLN:NE2	2.25	0.50
1:J:74:LEU:O	1:J:75:LEU:C	2.49	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:114:SER:HB3	1:J:261:ASN:HB2	1.93	0.50
1:L:310:VAL:CG1	1:L:312:SER:H	2.23	0.50
2:K:651:SER:HB2	2:K:656:THR:HG22	1.94	0.50
1:H:195:TYR:O	1:H:197:ASN:N	2.44	0.50
1:J:122:PRO:O	1:J:126:SER:OG	2.29	0.50
2:K:530:GLN:HE22	2:K:645:ASP:HB2	1.76	0.50
2:M:509:PHE:O	2:M:635:ASN:HA	2.11	0.50
2:K:656:THR:O	2:K:656:THR:CG2	2.60	0.49
1:H:74:LEU:O	1:H:75:LEU:C	2.50	0.49
1:H:310:VAL:CG1	1:H:312:SER:H	2.23	0.49
1:L:195:TYR:O	1:L:197:ASN:N	2.45	0.49
1:J:24:LEU:O	2:M:547:GLY:HA2	2.11	0.49
1:H:291:SER:HB3	1:H:307:PRO:CG	2.43	0.49
1:L:291:SER:HB3	1:L:307:PRO:CG	2.42	0.49
1:L:63:GLY:CA	1:L:92:GLY:HA2	2.42	0.49
1:L:114:SER:HB3	1:L:261:ASN:HB2	1.94	0.49
1:H:68:ASN:HB3	1:H:71:CYS:SG	2.52	0.49
2:I:538:GLN:HA	2:I:538:GLN:NE2	2.26	0.49
1:J:195:TYR:O	1:J:197:ASN:N	2.45	0.49
1:H:284:THR:HG22	1:H:302:THR:HG22	1.94	0.49
1:J:220:ARG:HD2	1:J:229:ARG:HG2	1.95	0.48
1:J:284:THR:HG22	1:J:302:THR:HG22	1.95	0.48
2:M:571:ASN:OD1	2:M:574:GLU:HG3	2.14	0.48
2:K:509:PHE:O	2:K:635:ASN:HA	2.13	0.48
1:L:74:LEU:O	1:L:75:LEU:C	2.52	0.48
2:M:656:THR:O	2:M:656:THR:CG2	2.62	0.48
2:M:528:ASN:ND2	2:M:646:ASP:OD1	2.46	0.48
1:H:75:LEU:HD21	1:H:117:LYS:HZ3	1.78	0.48
2:M:530:GLN:HE22	2:M:646:ASP:H	1.61	0.48
1:H:220:ARG:HD2	1:H:229:ARG:HG2	1.95	0.48
1:J:138:ALA:O	1:J:224:ARG:NH1	2.47	0.48
1:J:68:ASN:HB3	1:J:71:CYS:SG	2.54	0.48
1:J:9:VAL:HG21	2:K:619:TYR:HA	1.95	0.47
1:L:220:ARG:HD2	1:L:229:ARG:HG2	1.95	0.47
2:K:528:ASN:ND2	2:K:646:ASP:OD1	2.47	0.47
1:H:63:GLY:CA	1:H:92:GLY:HA2	2.44	0.47
1:H:215:PRO:HG3	1:H:250:ASN:ND2	2.29	0.47
2:I:643:LYS:HE3	2:I:643:LYS:HA	1.96	0.47
1:J:37:LEU:HD21	1:J:297:ASN:ND2	2.30	0.47
1:H:131:GLU:HG3	1:H:132:THR:N	2.08	0.47
2:I:509:PHE:O	2:I:635:ASN:HA	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:75:LEU:HD21	1:J:117:LYS:HZ3	1.81	0.46
1:J:19:THR:HG23	1:J:314:LYS:HZ1	1.79	0.46
1:J:97:GLY:HA3	1:J:230:MET:O	2.15	0.46
1:H:97:GLY:HA3	1:H:230:MET:O	2.15	0.46
2:K:643:LYS:HE3	2:K:643:LYS:HA	1.98	0.46
1:J:221:PRO:HG3	1:L:242:THR:O	2.16	0.46
2:K:505:ALA:HB3	2:K:612:ASP:OD2	2.15	0.46
2:K:530:GLN:HE22	2:K:646:ASP:H	1.64	0.46
1:J:291:SER:HB3	1:J:307:PRO:CG	2.46	0.46
2:I:530:GLN:HE22	2:I:646:ASP:H	1.62	0.46
2:K:625:GLN:NE2	2:K:655:GLY:HA2	2.30	0.46
1:L:120:ILE:HG23	1:L:121:PHE:N	2.30	0.46
1:H:37:LEU:HD21	1:H:297:ASN:ND2	2.30	0.45
2:I:530:GLN:HE22	2:I:645:ASP:HB2	1.80	0.45
1:J:48:SER:HB3	1:J:51:ILE:O	2.17	0.45
1:L:68:ASN:HB3	1:L:71:CYS:SG	2.56	0.45
1:H:138:ALA:O	1:H:224:ARG:NH1	2.49	0.45
2:K:625:GLN:HE22	2:K:655:GLY:HA2	1.81	0.45
1:L:260:LEU:HD23	1:L:260:LEU:C	2.36	0.45
1:H:48:SER:HB3	1:H:51:ILE:O	2.16	0.45
2:M:651:SER:HB2	2:M:656:THR:HG22	1.98	0.45
1:H:120:ILE:HG23	1:H:121:PHE:N	2.31	0.45
2:I:526:HIS:HB2	2:I:649:MET:SD	2.56	0.45
1:J:120:ILE:HG23	1:J:121:PHE:N	2.32	0.45
1:H:192:GLN:NE2	1:H:198:ALA:HB2	2.32	0.45
1:J:128:PRO:O	1:J:129:ASN:HB2	2.16	0.45
1:H:156:LYS:CD	1:H:196:GLN:HG2	2.46	0.45
1:H:304:GLY:HA2	2:I:563:PHE:CE1	2.51	0.45
2:M:642:HIS:CE1	2:M:657:TYR:OH	2.66	0.45
2:I:642:HIS:CE1	2:I:657:TYR:OH	2.66	0.45
1:H:12:HIS:HB2	2:I:520:GLY:O	2.17	0.44
1:H:260:LEU:HD23	1:H:260:LEU:O	2.17	0.44
1:H:266:SER:OG	1:H:267:GLY:N	2.50	0.44
1:H:217:ILE:O	1:J:212:ARG:NH1	2.50	0.44
1:H:203:SER:OG	1:L:218:ALA:HB1	2.17	0.44
1:H:325:PRO:O	1:H:326:SER:C	2.56	0.44
1:L:192:GLN:NE2	1:L:198:ALA:HB2	2.33	0.44
2:M:643:LYS:HE3	2:M:643:LYS:HA	2.00	0.44
1:H:291:SER:HB3	1:H:307:PRO:HG3	1.99	0.44
2:M:572:ASN:C	2:M:572:ASN:HD22	2.21	0.44
1:H:66:LEU:HD22	1:H:151:LEU:HD22	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:218:ALA:HB1	1:J:203:SER:OG	2.17	0.44
1:H:23:VAL:HG12	2:I:605:GLU:HB2	2.00	0.44
2:K:572:ASN:C	2:K:572:ASN:HD22	2.21	0.44
1:J:156:LYS:CD	1:J:196:GLN:HG2	2.47	0.43
1:L:215:PRO:HG3	1:L:250:ASN:ND2	2.33	0.43
1:L:260:LEU:HD23	1:L:260:LEU:O	2.16	0.43
1:H:260:LEU:HD23	1:H:260:LEU:C	2.39	0.43
1:J:109:LEU:HD12	1:J:109:LEU:HA	1.82	0.43
1:L:94:CYS:O	1:L:224:ARG:HD3	2.19	0.43
2:I:571:ASN:OD1	2:I:574:GLU:HG3	2.17	0.43
1:J:13:ALA:HB2	2:K:513:GLY:HA3	2.00	0.43
1:L:85:GLU:O	1:L:270:THR:HA	2.18	0.43
2:I:659:TYR:HD2	2:I:659:TYR:HA	1.70	0.43
1:H:122:PRO:O	1:H:126:SER:OG	2.36	0.43
1:L:66:LEU:HD22	1:L:151:LEU:HD22	2.01	0.43
1:L:128:PRO:O	1:L:129:ASN:HB2	2.18	0.43
1:H:128:PRO:O	1:H:129:ASN:HB2	2.18	0.43
1:J:66:LEU:HD22	1:J:151:LEU:HD22	2.01	0.43
1:L:284:THR:HG22	1:L:302:THR:HG22	1.99	0.43
1:L:97:GLY:HA3	1:L:230:MET:O	2.18	0.43
1:L:156:LYS:CD	1:L:196:GLN:HG2	2.47	0.43
1:J:19:THR:HG23	1:J:314:LYS:HZ2	1.84	0.43
1:L:291:SER:HB3	1:L:307:PRO:HG3	2.00	0.43
1:L:9:VAL:HG21	2:M:619:TYR:HA	2.01	0.42
2:I:606:ARG:HH22	2:M:605:GLU:HG3	1.84	0.42
1:J:85:GLU:O	1:J:270:THR:HA	2.20	0.42
1:J:192:GLN:NE2	1:J:198:ALA:HB2	2.34	0.42
2:I:551:LYS:CE	2:I:603:GLU:OE2	2.65	0.42
1:J:132:THR:O	1:J:132:THR:CG2	2.66	0.42
2:K:551:LYS:CE	2:K:603:GLU:OE2	2.66	0.42
1:H:94:CYS:O	1:H:224:ARG:HD3	2.20	0.42
1:J:266:SER:OG	1:J:267:GLY:N	2.52	0.42
1:J:325:PRO:O	1:J:326:SER:C	2.58	0.42
1:L:109:LEU:HD12	1:L:109:LEU:HA	1.83	0.42
1:L:48:SER:HB3	1:L:51:ILE:O	2.20	0.42
2:I:651:SER:HB2	2:I:656:THR:HG22	2.02	0.41
1:L:122:PRO:O	1:L:126:SER:OG	2.38	0.41
1:L:220:ARG:HB2	1:L:221:PRO:CD	2.51	0.41
2:M:629:ASN:HD22	2:M:629:ASN:HA	1.63	0.41
2:K:526:HIS:HB2	2:K:649:MET:SD	2.61	0.41
1:J:94:CYS:O	1:J:224:ARG:HD3	2.19	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:215:PRO:HG3	1:J:250:ASN:ND2	2.35	0.41
2:K:642:HIS:CE1	2:K:657:TYR:OH	2.67	0.41
1:H:317:MET:HE1	2:I:552:VAL:HA	2.03	0.41
1:H:327:ARG:HB2	1:H:327:ARG:CZ	2.50	0.41
1:L:266:SER:OG	1:L:267:GLY:N	2.50	0.41
1:J:260:LEU:HD23	1:J:260:LEU:C	2.41	0.41
2:I:528:ASN:OD1	2:I:644:CYS:O	2.39	0.40
2:I:572:ASN:C	2:I:572:ASN:HD22	2.24	0.40
1:J:291:SER:HB3	1:J:307:PRO:HG3	2.02	0.40
1:H:180:TRP:CZ2	1:H:204:VAL:HG21	2.56	0.40
1:H:185:PRO:HA	1:H:186:PRO:HD3	1.91	0.40
1:L:93:THR:O	1:L:93:THR:CG2	2.69	0.40
2:M:551:LYS:CE	2:M:603:GLU:OE2	2.65	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	H	320/324 (99%)	295 (92%)	20 (6%)	5 (2%)	8	34
1	J	320/324 (99%)	296 (92%)	19 (6%)	5 (2%)	8	34
1	L	320/324 (99%)	293 (92%)	22 (7%)	5 (2%)	8	34
2	I	158/222 (71%)	148 (94%)	9 (6%)	1 (1%)	22	57
2	K	158/222 (71%)	147 (93%)	10 (6%)	1 (1%)	22	57
2	M	158/222 (71%)	148 (94%)	9 (6%)	1 (1%)	22	57
All	All	1434/1638 (88%)	1327 (92%)	89 (6%)	18 (1%)	10	39

All (18) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	H	132	THR
1	J	132	THR
1	J	326	SER
1	L	132	THR
1	H	75	LEU
1	H	158	GLY
1	H	196	GLN
1	H	326	SER
1	J	75	LEU
1	J	158	GLY
1	J	196	GLN
1	L	75	LEU
1	L	158	GLY
1	L	196	GLN
1	L	326	SER
2	I	526	HIS
2	K	526	HIS
2	M	526	HIS

### 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	H	263/280 (94%)	237 (90%)	26 (10%)	6	26
1	J	263/280 (94%)	238 (90%)	25 (10%)	7	28
1	L	263/280 (94%)	238 (90%)	25 (10%)	7	28
2	I	128/191 (67%)	118 (92%)	10 (8%)	10	36
2	K	128/191 (67%)	117 (91%)	11 (9%)	8	32
2	M	128/191 (67%)	118 (92%)	10 (8%)	10	36
All	All	1173/1413 (83%)	1066 (91%)	107 (9%)	7	30

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	27	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	42	ASN
1	H	49	LEU
1	H	58	LYS
1	H	79	SER
1	H	90	GLU
1	H	93	THR
1	H	99	PHE
1	H	109	LEU
1	H	126	SER
1	H	141	TYR
1	H	151	LEU
1	H	152	LEU
1	H	159	THR
1	H	163	LYS
1	H	188	VAL
1	H	203	SER
1	H	208	LYS
1	H	260	LEU
1	H	264	SER
1	H	265	ASP
1	H	284	THR
1	H	291	SER
1	H	310	VAL
1	H	321	LEU
1	H	327	ARG
2	I	526	HIS
2	I	557	GLU
2	I	572	ASN
2	I	580	LEU
2	I	602	LEU
2	I	627	ARG
2	I	635	ASN
2	I	643	LYS
2	I	656	THR
2	I	659	TYR
1	J	27	ASN
1	J	42	ASN
1	J	49	LEU
1	J	58	LYS
1	J	79	SER
1	J	90	GLU
1	J	93	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	99	PHE
1	J	109	LEU
1	J	126	SER
1	J	141	TYR
1	J	151	LEU
1	J	152	LEU
1	J	159	THR
1	J	163	LYS
1	J	188	VAL
1	J	203	SER
1	J	208	LYS
1	J	260	LEU
1	J	264	SER
1	J	265	ASP
1	J	284	THR
1	J	291	SER
1	J	310	VAL
1	J	321	LEU
2	K	526	HIS
2	K	557	GLU
2	K	572	ASN
2	K	580	LEU
2	K	602	LEU
2	K	627	ARG
2	K	635	ASN
2	K	643	LYS
2	K	648	CYS
2	K	656	THR
2	K	659	TYR
1	L	27	ASN
1	L	42	ASN
1	L	49	LEU
1	L	58	LYS
1	L	79	SER
1	L	90	GLU
1	L	93	THR
1	L	99	PHE
1	L	109	LEU
1	L	126	SER
1	L	141	TYR
1	L	151	LEU
1	L	152	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	159	THR
1	L	163	LYS
1	L	188	VAL
1	L	203	SER
1	L	208	LYS
1	L	260	LEU
1	L	264	SER
1	L	265	ASP
1	L	284	THR
1	L	291	SER
1	L	310	VAL
1	L	321	LEU
2	M	526	HIS
2	M	557	GLU
2	M	572	ASN
2	M	580	LEU
2	M	602	LEU
2	M	627	ARG
2	M	635	ASN
2	M	643	LYS
2	M	656	THR
2	M	659	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	27	ASN
1	H	42	ASN
1	H	130	HIS
1	H	191	GLN
1	H	196	GLN
1	H	250	ASN
1	H	290	ASN
2	I	530	GLN
2	I	538	GLN
2	I	572	ASN
2	I	625	GLN
2	I	629	ASN
2	I	642	HIS
1	J	27	ASN
1	J	42	ASN
1	J	130	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	191	GLN
1	J	196	GLN
1	J	250	ASN
1	J	290	ASN
2	K	530	GLN
2	K	538	GLN
2	K	572	ASN
2	K	625	GLN
2	K	629	ASN
2	K	642	HIS
1	L	27	ASN
1	L	42	ASN
1	L	130	HIS
1	L	191	GLN
1	L	196	GLN
1	L	250	ASN
1	L	290	ASN
2	M	530	GLN
2	M	538	GLN
2	M	572	ASN
2	M	625	GLN
2	M	629	ASN
2	M	642	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

3 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	SIA	H	1328	-	21,21,21	4.39	9 (42%)	25,31,31	3.76	8 (32%)
3	SIA	L	1328	-	20,20,21	4.29	6 (30%)	24,28,31	3.35	9 (37%)
3	SIA	J	1328	-	20,20,21	4.30	6 (30%)	24,28,31	3.35	9 (37%)

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	SIA	H	1328	-	-	6/20/38/38	0/1/1/1
3	SIA	L	1328	-	-	3/18/34/38	0/1/1/1
3	SIA	J	1328	-	-	3/18/34/38	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1328	SIA	C2-C1	13.48	1.64	1.52
3	L	1328	SIA	C2-C1	13.41	1.64	1.52
3	H	1328	SIA	O2-C2	12.56	1.55	1.39
3	L	1328	SIA	O4-C4	-7.41	1.27	1.43
3	J	1328	SIA	O4-C4	-7.39	1.27	1.43
3	H	1328	SIA	O4-C4	-7.34	1.27	1.43
3	H	1328	SIA	C2-C1	6.85	1.64	1.53
3	J	1328	SIA	C6-C5	6.51	1.63	1.53
3	L	1328	SIA	C6-C5	6.47	1.63	1.53
3	H	1328	SIA	C6-C5	6.46	1.63	1.53
3	H	1328	SIA	C3-C4	6.25	1.62	1.53
3	H	1328	SIA	C4-C5	5.92	1.58	1.53
3	L	1328	SIA	C4-C5	5.89	1.58	1.53
3	J	1328	SIA	C4-C5	5.88	1.58	1.53
3	L	1328	SIA	C3-C4	5.64	1.62	1.52
3	J	1328	SIA	C3-C4	5.64	1.62	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1328	SIA	O6-C6	-3.03	1.39	1.44
3	H	1328	SIA	O6-C6	-3.03	1.39	1.44
3	L	1328	SIA	O6-C6	-2.98	1.39	1.44
3	H	1328	SIA	O6-C2	2.88	1.46	1.43
3	H	1328	SIA	C3-C2	-2.19	1.49	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1328	SIA	O6-C6-C5	-13.68	96.43	109.78
3	J	1328	SIA	C6-O6-C2	12.29	137.63	111.34
3	L	1328	SIA	C6-O6-C2	12.26	137.56	111.34
3	H	1328	SIA	O6-C6-C7	8.30	120.09	107.29
3	H	1328	SIA	O1A-C1-C2	-5.86	114.72	123.59
3	J	1328	SIA	O6-C2-C3	-4.74	103.94	110.46
3	L	1328	SIA	O6-C2-C3	-4.72	103.96	110.46
3	J	1328	SIA	C11-C10-N5	4.58	123.85	116.10
3	H	1328	SIA	C11-C10-N5	4.57	123.84	116.10
3	L	1328	SIA	C11-C10-N5	4.55	123.80	116.10
3	J	1328	SIA	O1B-C1-C2	3.97	124.35	113.03
3	L	1328	SIA	O1B-C1-C2	3.96	124.32	113.03
3	H	1328	SIA	C5-N5-C10	3.76	132.32	123.18
3	J	1328	SIA	C5-N5-C10	3.75	132.30	123.18
3	L	1328	SIA	C5-N5-C10	3.75	132.29	123.18
3	J	1328	SIA	O1A-C1-C2	-3.31	114.76	122.57
3	L	1328	SIA	O1A-C1-C2	-3.30	114.78	122.57
3	L	1328	SIA	C6-C5-N5	-2.38	106.97	110.91
3	L	1328	SIA	C3-C4-C5	-2.37	108.60	111.46
3	J	1328	SIA	C6-C5-N5	-2.35	107.01	110.91
3	J	1328	SIA	C3-C4-C5	-2.32	108.65	111.46
3	H	1328	SIA	C6-C5-N5	-2.32	107.06	110.91
3	J	1328	SIA	O10-C10-N5	-2.29	117.73	121.95
3	L	1328	SIA	O10-C10-N5	-2.28	117.77	121.95
3	H	1328	SIA	O10-C10-N5	-2.26	117.79	121.95
3	H	1328	SIA	O4-C4-C3	-2.10	105.01	109.91

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1328	SIA	O1A-C1-C2-O2
3	H	1328	SIA	O1A-C1-C2-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	H	1328	SIA	O1B-C1-C2-O2
3	H	1328	SIA	O1B-C1-C2-O6
3	H	1328	SIA	C11-C10-N5-C5
3	H	1328	SIA	O10-C10-N5-C5
3	J	1328	SIA	C11-C10-N5-C5
3	J	1328	SIA	O10-C10-N5-C5
3	L	1328	SIA	C11-C10-N5-C5
3	L	1328	SIA	O10-C10-N5-C5
3	J	1328	SIA	O1A-C1-C2-C3
3	L	1328	SIA	O1A-C1-C2-C3

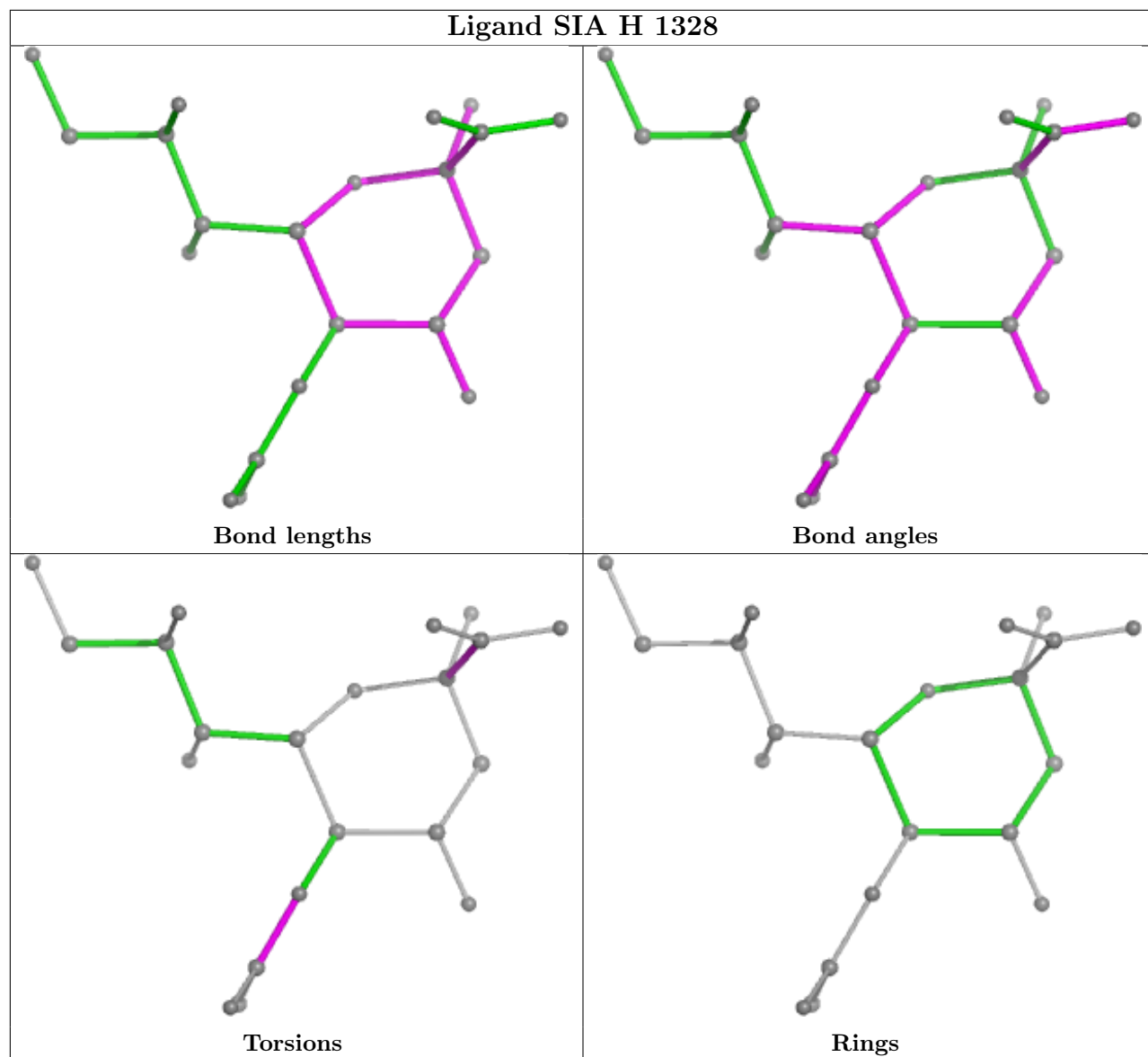
There are no ring outliers.

3 monomers are involved in 3 short contacts:

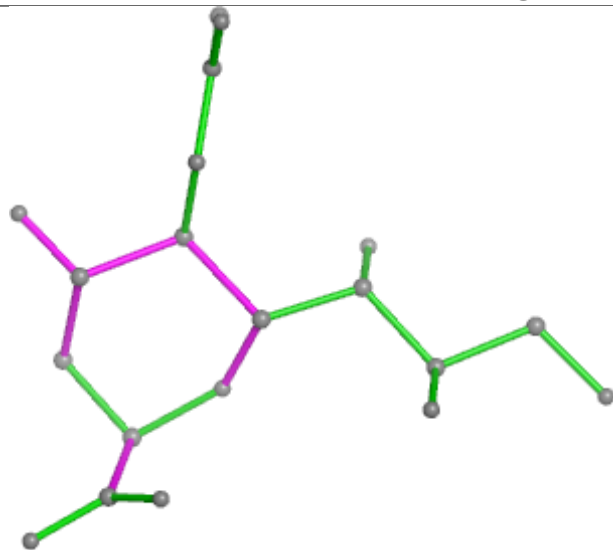
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1328	SIA	1	0
3	L	1328	SIA	1	0
3	J	1328	SIA	1	0

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

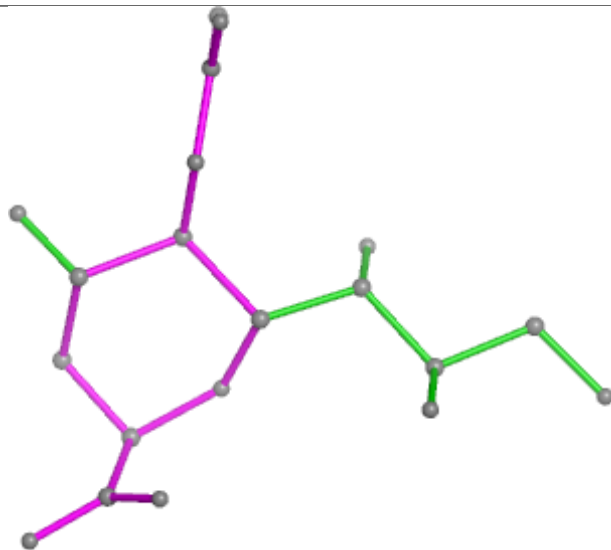




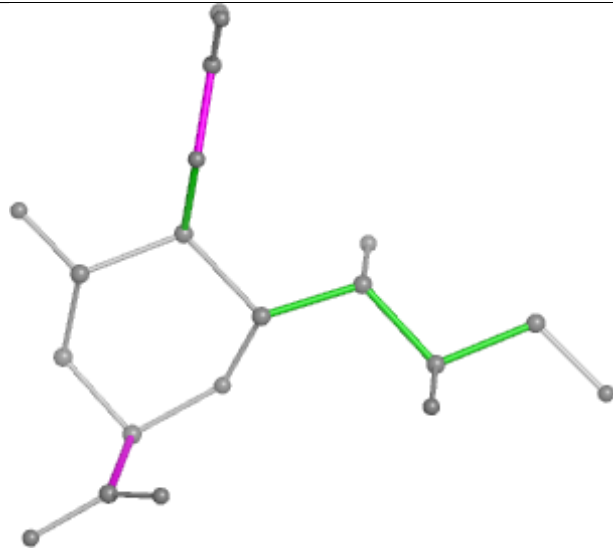
## Ligand SIA L 1328



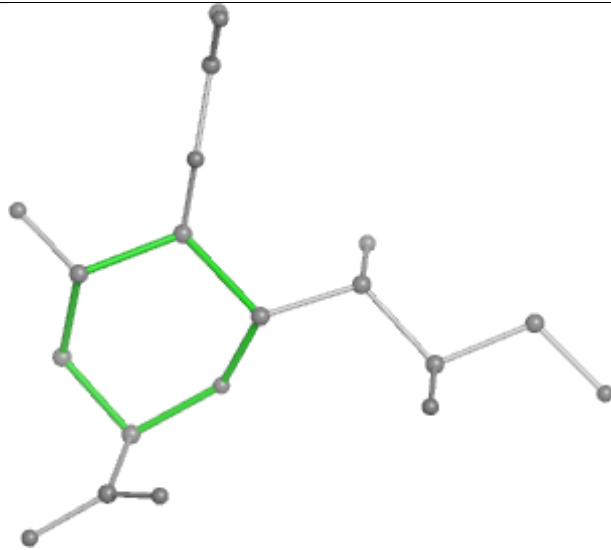
Bond lengths



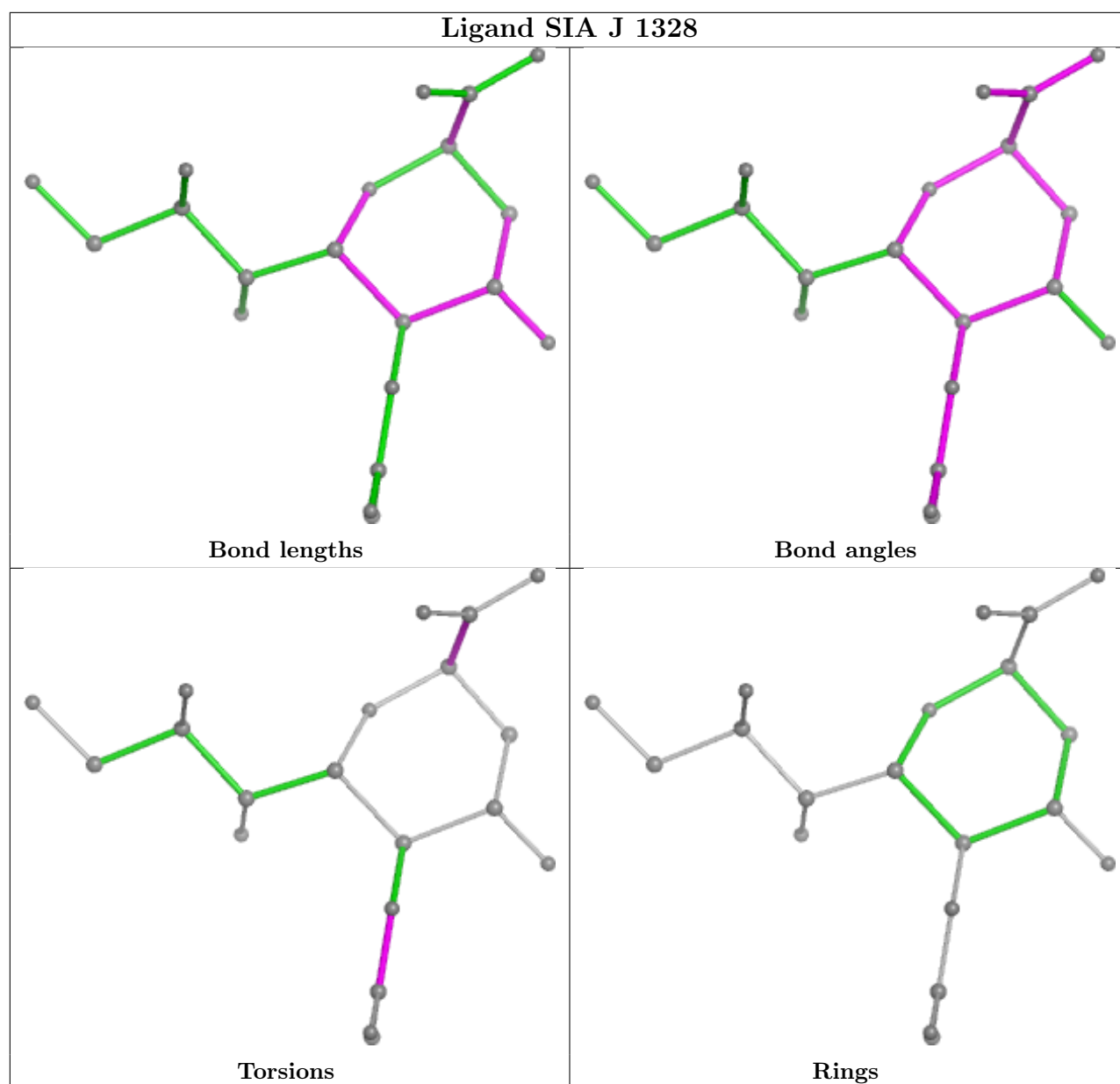
Bond angles



Torsions



Rings



## 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	H	322/324 (99%)	0.22	12 (3%) 45 27	44, 92, 145, 181	0
1	J	322/324 (99%)	-0.15	9 (2%) 55 33	40, 65, 105, 146	0
1	L	322/324 (99%)	-0.07	11 (3%) 48 28	43, 64, 133, 190	0
2	I	160/222 (72%)	-0.19	7 (4%) 39 23	43, 58, 96, 149	0
2	K	160/222 (72%)	-0.30	6 (3%) 44 26	37, 51, 81, 175	0
2	M	160/222 (72%)	-0.32	5 (3%) 51 30	41, 59, 99, 147	0
All	All	1446/1638 (88%)	-0.09	50 (3%) 47 28	37, 66, 129, 190	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	660	PRO	9.2
1	L	75	LEU	6.1
2	M	660	PRO	6.0
1	J	141	TYR	5.2
2	K	658	ASP	4.9
1	L	77	ALA	4.9
2	K	531	GLY	4.3
1	H	75	LEU	4.2
1	L	326	SER	4.1
1	H	278	CYS	3.9
2	K	659	TYR	3.9
1	L	291	SER	3.7
2	M	658	ASP	3.7
2	M	659	TYR	3.6
1	L	141	TYR	3.6
2	K	529	GLU	3.5
2	I	659	TYR	3.4
2	I	660	PRO	3.3
1	H	127	TRP	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	J	290	ASN	3.1
1	H	291	SER	3.0
2	I	528	ASN	3.0
1	J	75	LEU	2.9
1	L	78	ASN	2.9
1	H	188	VAL	2.8
1	H	158	GLY	2.8
2	I	529	GLU	2.7
2	I	530	GLN	2.7
1	L	190	GLU	2.6
1	H	132	THR	2.6
2	M	529	GLU	2.6
1	H	265	ASP	2.6
1	J	91	ASN	2.6
1	J	291	SER	2.6
1	L	76	THR	2.5
1	H	326	SER	2.5
1	H	116	GLU	2.4
1	J	90	GLU	2.4
1	H	199	ASP	2.4
1	J	77	ALA	2.3
1	H	160	SER	2.3
2	K	528	ASN	2.2
1	L	161	TYR	2.2
2	M	528	ASN	2.2
1	J	132	THR	2.2
1	J	326	SER	2.1
1	L	132	THR	2.1
2	I	643	LYS	2.1
2	I	527	GLN	2.1
1	L	188	VAL	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](#)

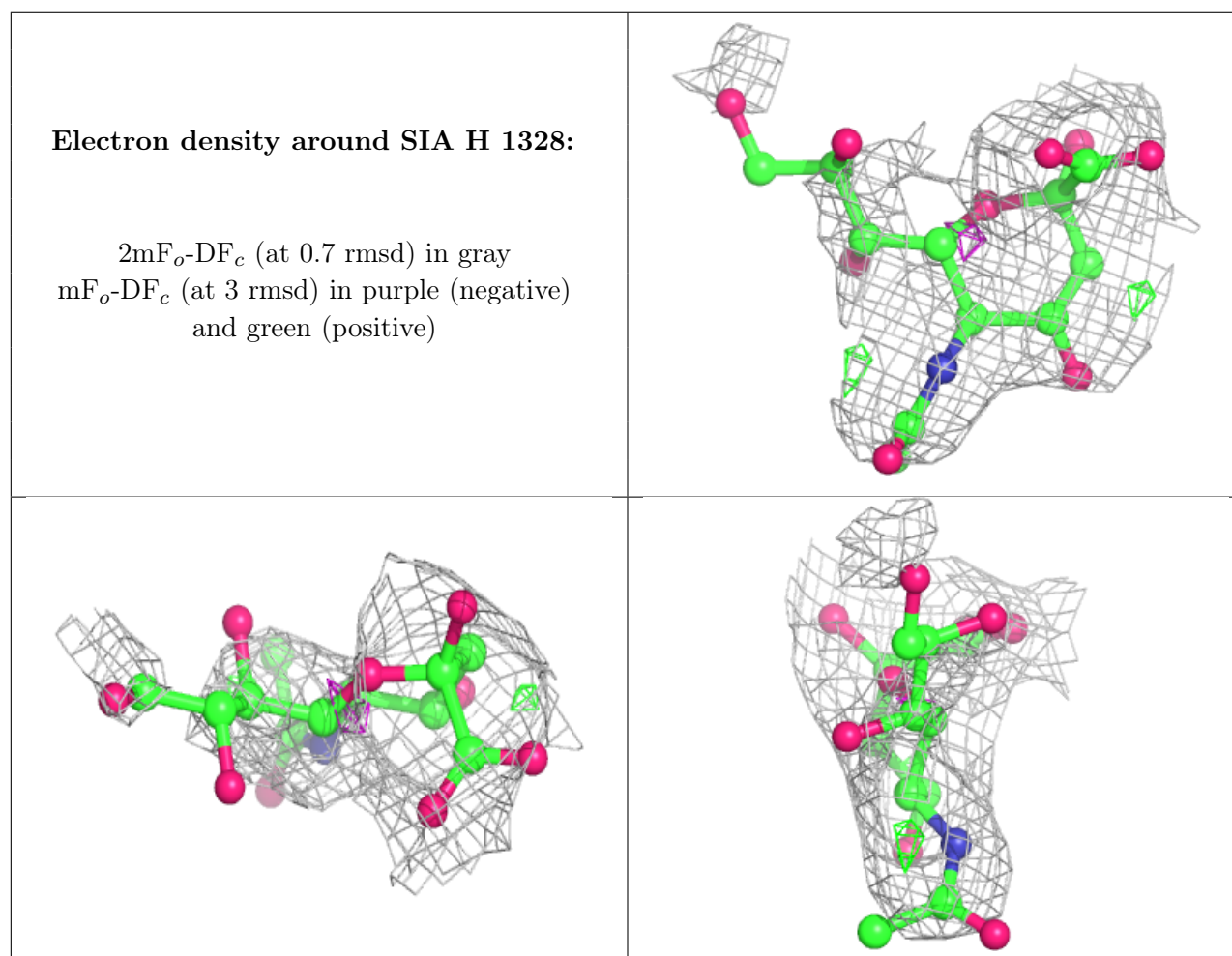
There are no monosaccharides in this entry.

## 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, 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.

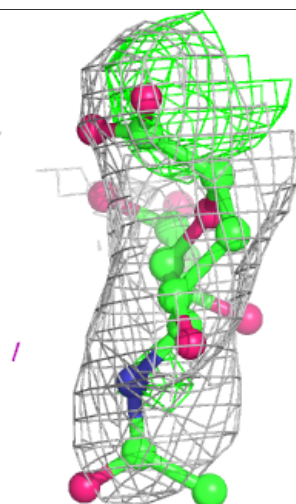
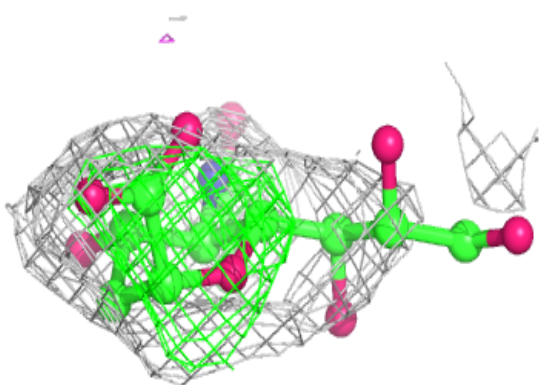
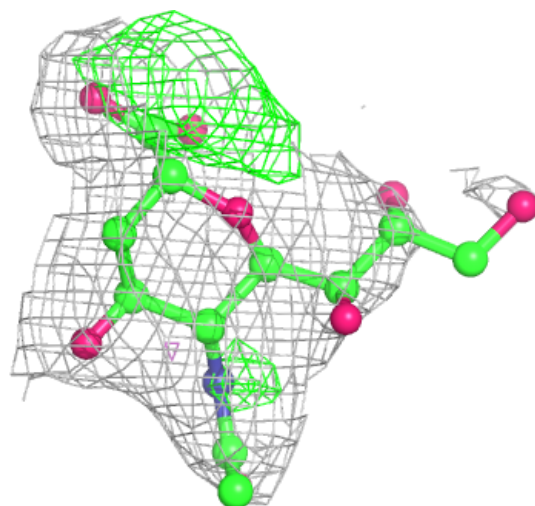
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SIA	H	1328	21/21	0.78	0.18	131,137,143,145	0
3	SIA	J	1328	20/21	0.82	0.24	117,123,129,131	0
3	SIA	L	1328	20/21	0.87	0.17	125,131,137,139	0

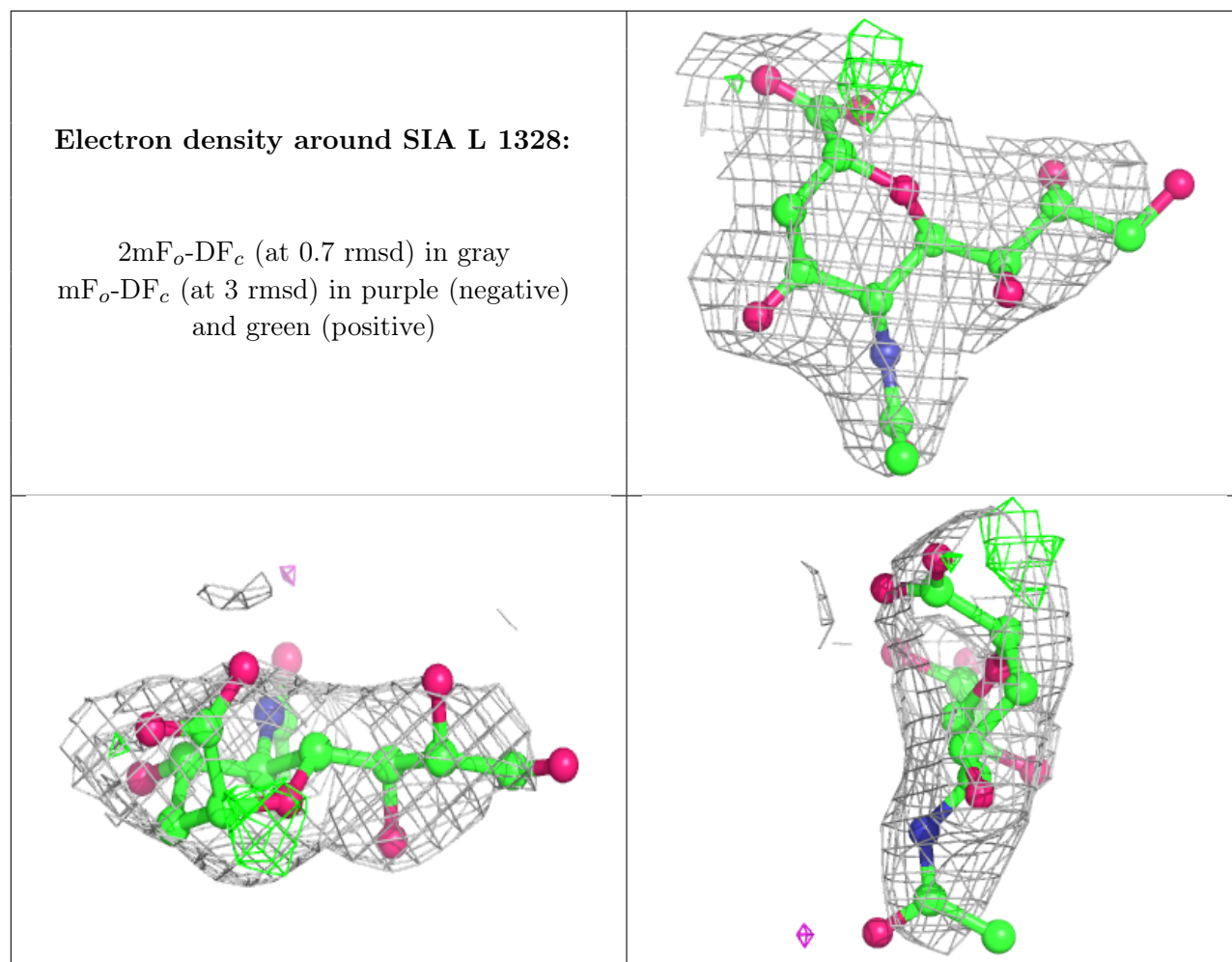
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



**Electron density around SIA J 1328:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.