



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:19 PM UTC

PDB ID : 4QY2 / pdb_00004qy2
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

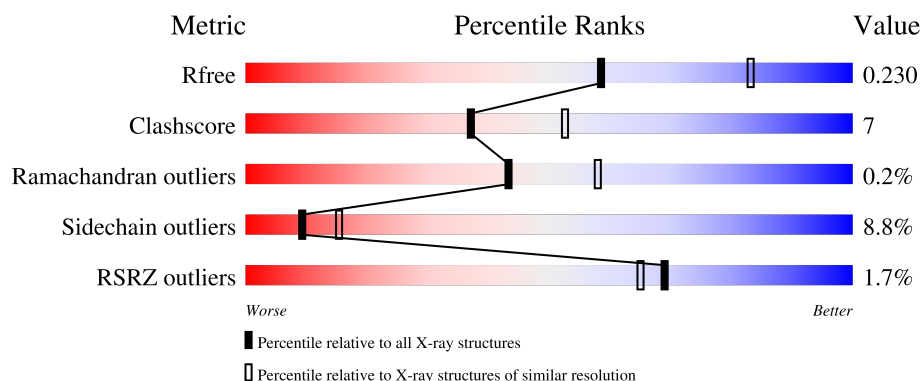
1 Overall quality at a glance

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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	% 80% 18%
1	K	318	% 80% 18%
2	B	174	2% 84% 13%
2	D	174	4% 79% 18%
2	F	174	2% 85% 11%
2	H	174	5% 74% 23%
2	J	174	5% 71% 25%
2	L	174	4% 80% 18%

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.

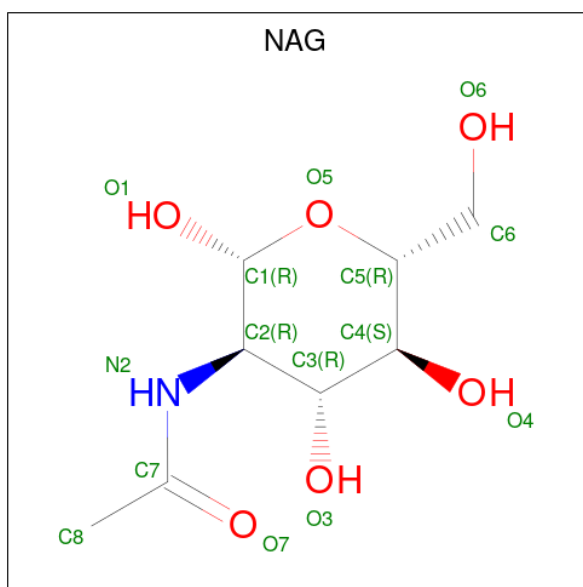
- Molecule 1 is a protein called hemagglutinin.

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.

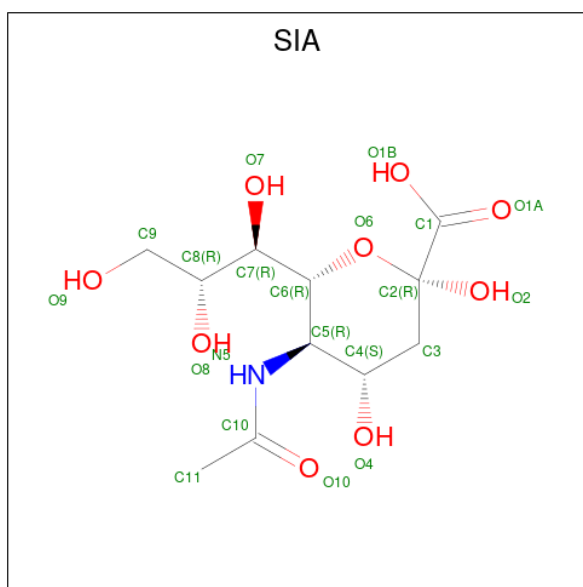
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	D	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	F	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	H	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	J	174	Total	C	N	O	S	0	0	0
			1402	866	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 (CCD ID: 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 (CCD ID: 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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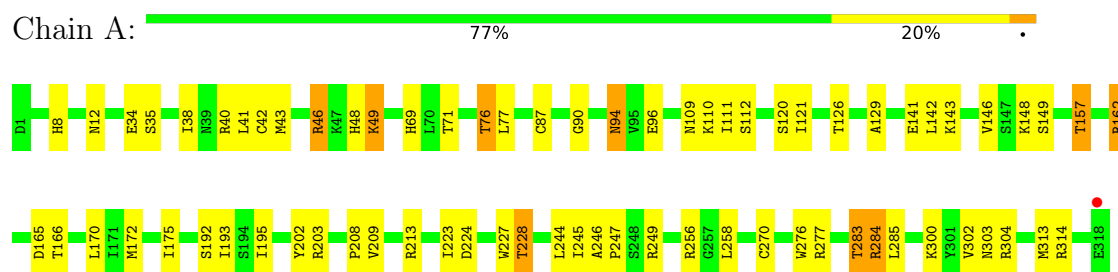
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	56	Total	O	0	0
			56	56		

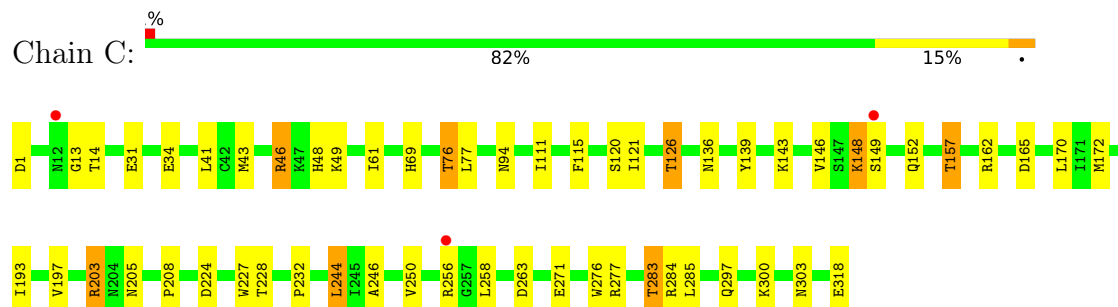
3 Residue-property plots

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.

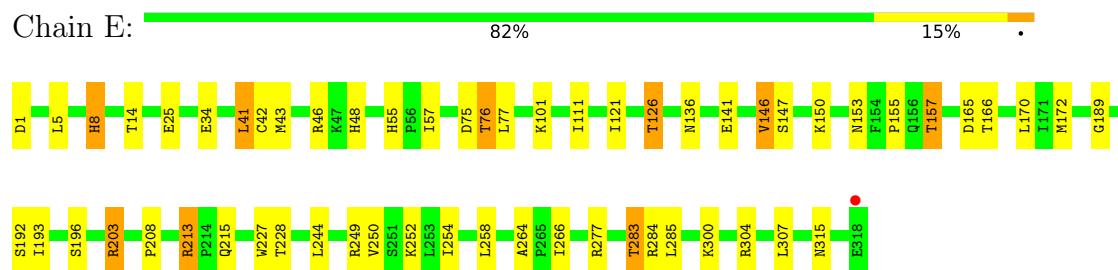
• Molecule 1: hemagglutinin



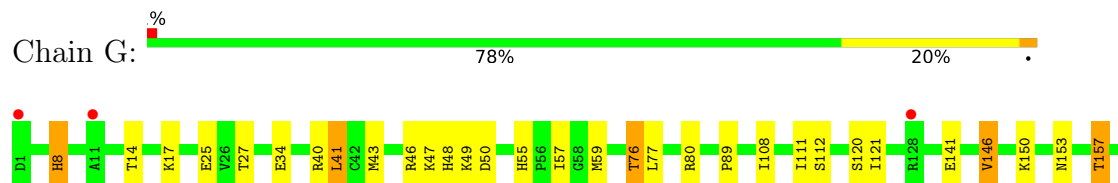
• Molecule 1: hemagglutinin

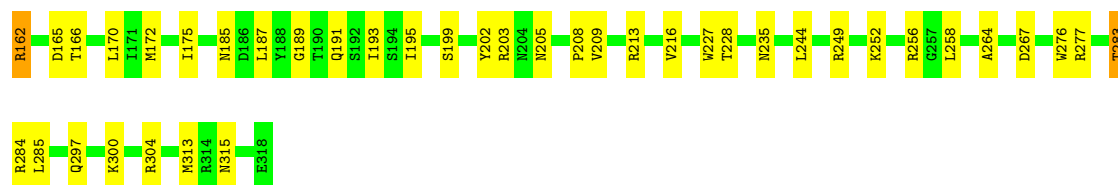


• Molecule 1: hemagglutinin

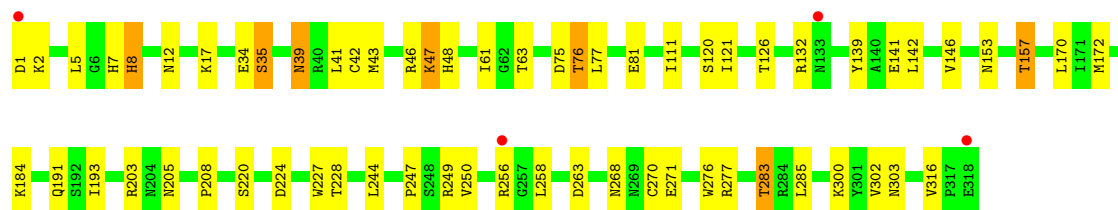
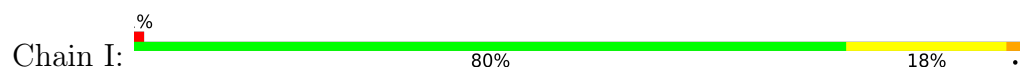


• Molecule 1: hemagglutinin

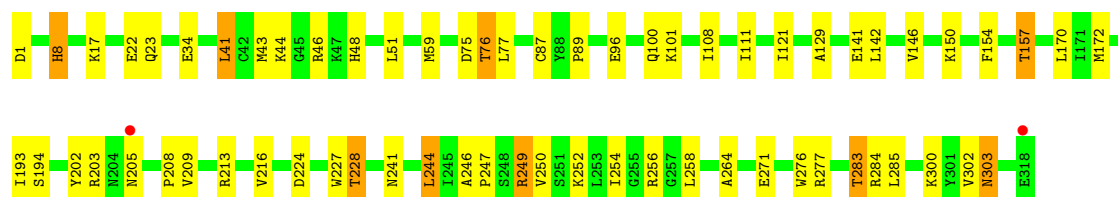
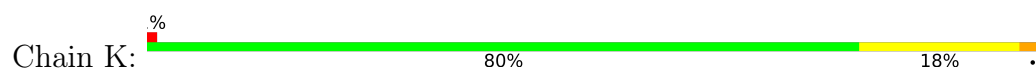




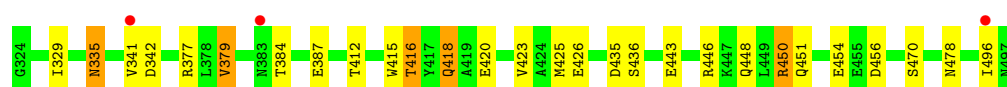
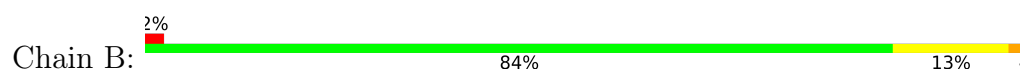
- Molecule 1: hemagglutinin



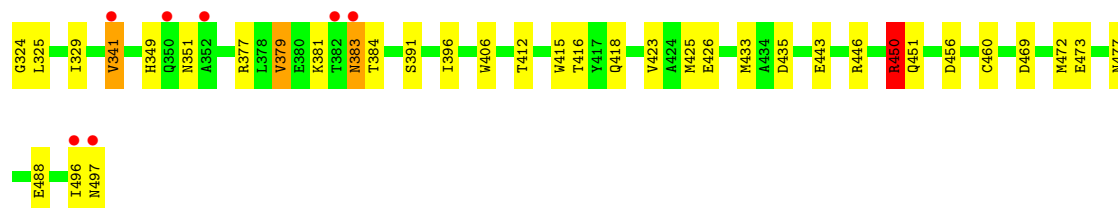
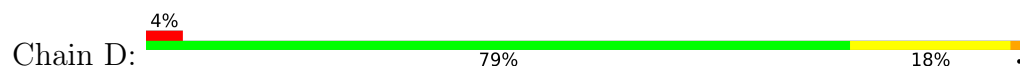
- Molecule 1: hemagglutinin



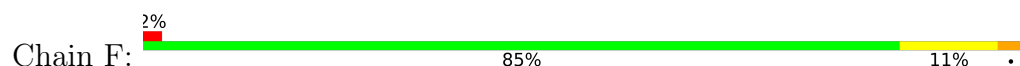
- Molecule 2: hemagglutinin

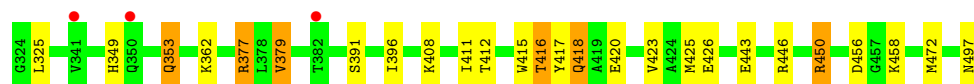


- Molecule 2: hemagglutinin

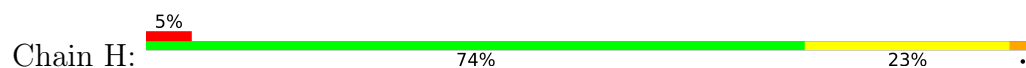


- Molecule 2: hemagglutinin

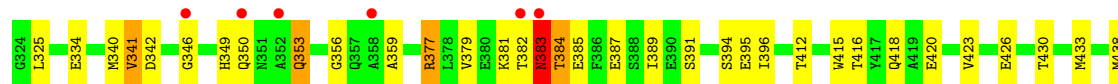




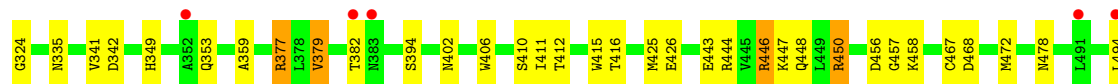
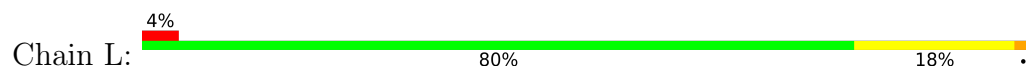
- Molecule 2: hemagglutinin



- 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 0.190 , 0.230	Depositor DCC
R_{free} test set	7913 reflections (4.81%)	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)	0.30 , 31.5	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 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	A	0.41	0/2486	0.80	1/3368 (0.0%)
1	C	0.42	0/2486	0.81	1/3368 (0.0%)
1	E	0.42	0/2486	0.80	1/3368 (0.0%)
1	G	0.41	0/2486	0.78	0/3368
1	I	0.43	0/2486	0.81	1/3368 (0.0%)
1	K	0.40	0/2486	0.78	0/3368
2	B	0.41	0/1427	0.77	0/1926
2	D	0.41	0/1427	0.81	1/1926 (0.1%)
2	F	0.42	0/1427	0.79	0/1926
2	H	0.38	0/1427	0.79	2/1926 (0.1%)
2	J	0.38	0/1427	0.80	3/1926 (0.2%)
2	L	0.38	0/1427	0.78	1/1926 (0.1%)
All	All	0.41	0/23478	0.79	11/31764 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	341	VAL	N-CA-C	-6.39	106.28	112.29
2	H	457	GLY	N-CA-C	-6.07	106.25	115.00
2	H	341	VAL	N-CA-C	-5.95	106.70	112.29
2	D	341	VAL	N-CA-C	-5.92	106.73	112.29
1	I	2	LYS	N-CA-C	5.54	116.68	108.60
2	L	457	GLY	N-CA-C	-5.47	107.12	115.00
1	E	213	ARG	N-CA-C	5.43	113.10	108.22
2	J	383	ASN	CA-C-N	5.08	130.84	121.70
2	J	383	ASN	C-N-CA	5.08	130.84	121.70
1	C	148	LYS	N-CA-C	-5.04	105.79	111.28
1	A	284	ARG	N-CA-C	-5.03	107.19	113.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2437	0	2389	41	0
1	C	2437	0	2389	36	1
1	E	2437	0	2389	34	0
1	G	2437	0	2389	38	0
1	I	2437	0	2389	32	0
1	K	2437	0	2389	36	0
2	B	1402	0	1298	19	0
2	D	1402	0	1298	28	0
2	F	1402	0	1298	17	0
2	H	1402	0	1298	27	1
2	J	1402	0	1298	30	0
2	L	1402	0	1298	28	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	7	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	142	0	0	6	0
5	J	58	0	0	9	0
5	K	90	0	0	2	0
5	L	56	0	0	9	0
All	All	24413	0	22296	325	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 (325) 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
1:G:43:MET:HE3	1:G:46:ARG:HG3	1.62	0.82
2:L:377:ARG:NH2	2:L:426:GLU:OE2	2.11	0.82
1:C:43:MET:HE2	1:C:48:HIS:HB3	1.62	0.81
1:C:43:MET:HE3	1:C:46:ARG:HG3	1.62	0.81
1:A:43:MET:HE3	1:A:46:ARG:HG3	1.62	0.81
1:I:43:MET:HE2	1:I:48:HIS:HB3	1.63	0.80
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:G:43:MET:HE2	1:G:48:HIS:HB3	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:K:43:MET:HE3	1:K:46:ARG:HG3	1.76	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
1:A:304:ARG:NH1	2:B:420:GLU:OE1	2.28	0.67
1:A:43:MET:HE2	1:A:48:HIS:HB3	1.77	0.66
1:E:43:MET:HE3	1:E:46:ARG:HG3	1.77	0.66
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:D:349:HIS:HB2	2:D:472:MET:HE3	1.80	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:C:143:LYS:NZ	5:C:806:HOH:O	2.30	0.62
1:A:162:ARG:NH2	5:A:808:HOH:O	2.31	0.62
1:I:17:LYS:NZ	2:J:420:GLU:OE2	2.26	0.62
1:K:284:ARG:HB3	2:L:379:VAL:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:349:HIS:HB2	2:L:472:MET:HE3	1.82	0.60
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: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
1:I:43:MET:HE2	1:I:48:HIS:CB	2.34	0.57
2:L:468:ASP:OD1	5:L:739:HOH:O	2.17	0.57
1:A:43:MET:HE2	1:A:48:HIS:CB	2.35	0.56
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
2:J:446:ARG:HH12	2:J:447:LYS:HE3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:349:HIS:HB2	2:H:472:MET:HE3	1.90	0.53
1:G:43:MET:HE2	1:G:48:HIS:CB	2.37	0.53
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:C:43:MET:HE2	1:C:48:HIS:CB	2.37	0.53
1:G:284:ARG:HB3	2:H:379:VAL:HG22	1.90	0.53
2:J:349:HIS:HB2	2:J:472:MET:HE3	1.91	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: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
2:F:349:HIS:HB2	2:F:472:MET:HE3	1.92	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
1:E:75:ASP:OD2	1:E:76:THR:HG22	2.11	0.50
1:G:59:MET:HE2	1:G:108:ILE:HD12	1.93	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:G:43:MET:CE	1:G:48:HIS:HB3	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LYS:HG3	2:B:415:TRP:CE2	2.47	0.49
1:K:59:MET:HE2	1:K:108:ILE:HD12	1.93	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: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:G:50:ASP:CG	1:G:80:ARG:HH21	2.22	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: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
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
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
2:L:468:ASP:CG	5:L:739:HOH:O	2.58	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
2:H:462:GLU:CD	2:J:450:ARG:HH22	2.23	0.47
1:I:142:LEU:HD23	1:I:247:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:165:ASP:OD2	1:E:252:LYS:NZ	2.43	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
1:I:43:MET:HE1	1:I:76:THR:HG21	1.99	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:451:GLN:HB2	5:D:768:HOH:O	2.18	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:K:43:MET:HE2	1:K:48:HIS:CB	2.48	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: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
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:A:42:CYS:HB3	1:A:270:CYS:C	2.44	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:8:HIS:CE1	1:G:313:MET:HE3	2.54	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
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:G:205:ASN:CG	1:K:209:VAL:HG11	2.44	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
1:E:43:MET:HE2	1:E:48:HIS:HB3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:252:LYS:HE3	1:K:254:ILE:HD11	2.00	0.42
1:G:25:GLU:HG2	1:G:315:ASN: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
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:D:456:ASP:CG	2:D:460:CYS:HB2	2.45	0.42
1:G:199:SER:HG	1:G:202:TYR:H	1.68	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: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
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:I:43:MET:HE3	1:I:46:ARG:HB2	2.03	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:C:43:MET:CE	1:C:48:HIS:HB3	2.44	0.40
1:G:55:HIS:CE1	1:G:57:ILE:HD13	2.55	0.40
1:K:43:MET:HE2	1:K:48:HIS:HB3	2.04	0.40
1:C:300:LYS:HG3	2:D:415:TRP:CE2	2.57	0.40
2:J:477:ASN:ND2	5:J:737:HOH:O	2.30	0.40

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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	316/318 (99%)	307 (97%)	9 (3%)	0	100	100
1	C	316/318 (99%)	310 (98%)	6 (2%)	0	100	100
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%)	21	32
2	D	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	21	32
2	F	172/174 (99%)	168 (98%)	3 (2%)	1 (1%)	21	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	172/174 (99%)	165 (96%)	6 (4%)	1 (1%)	21	32
2	J	172/174 (99%)	164 (95%)	7 (4%)	1 (1%)	21	32
2	L	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	21	32
All	All	2928/2952 (99%)	2835 (97%)	87 (3%)	6 (0%)	43	58

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%)	243 (90%)	26 (10%)	8	12
1	C	269/269 (100%)	247 (92%)	22 (8%)	10	18
1	E	269/269 (100%)	247 (92%)	22 (8%)	10	18
1	G	269/269 (100%)	246 (91%)	23 (9%)	10	16
1	I	269/269 (100%)	238 (88%)	31 (12%)	5	8
1	K	269/269 (100%)	245 (91%)	24 (9%)	9	15
2	B	148/148 (100%)	136 (92%)	12 (8%)	11	18
2	D	148/148 (100%)	139 (94%)	9 (6%)	17	30
2	F	148/148 (100%)	138 (93%)	10 (7%)	14	25
2	H	148/148 (100%)	138 (93%)	10 (7%)	14	25
2	J	148/148 (100%)	129 (87%)	19 (13%)	4	6
2	L	148/148 (100%)	137 (93%)	11 (7%)	13	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2502/2502 (100%)	2283 (91%)	219 (9%)	9 15

All (219) 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	146	VAL
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	341	VAL
2	B	342	ASP
2	B	379	VAL
2	B	384	THR
2	B	416	THR
2	B	418	GLN
2	B	423	VAL
2	B	425	MET
2	B	436	SER
2	B	470	SER

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Mol	Chain	Res	Type
2	B	496	ILE
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	146	VAL
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	277	ARG
1	C	283	THR
1	C	318	GLU
2	D	325	LEU
2	D	341	VAL
2	D	379	VAL
2	D	383	ASN
2	D	384	THR
2	D	423	VAL
2	D	425	MET
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	101	LYS
1	E	111	ILE
1	E	126	THR
1	E	146	VAL
1	E	150	LYS

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Mol	Chain	Res	Type
1	E	157	THR
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	277	ARG
1	E	283	THR
2	F	325	LEU
2	F	353	GLN
2	F	362	LYS
2	F	377	ARG
2	F	379	VAL
2	F	411	ILE
2	F	416	THR
2	F	418	GLN
2	F	425	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	146	VAL
1	G	150	LYS
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

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Mol	Chain	Res	Type
1	G	276	TRP
1	G	277	ARG
1	G	283	THR
2	H	379	VAL
2	H	385	GLU
2	H	416	THR
2	H	423	VAL
2	H	425	MET
2	H	438	MET
2	H	477	ASN
2	H	479	THR
2	H	496	ILE
2	H	497	ASN
1	I	1	ASP
1	I	5	LEU
1	I	8	HIS
1	I	35	SER
1	I	39	ASN
1	I	41	LEU
1	I	47	LYS
1	I	63	THR
1	I	76	THR
1	I	77	LEU
1	I	111	ILE
1	I	120	SER
1	I	126	THR
1	I	132	ARG
1	I	146	VAL
1	I	157	THR
1	I	170	LEU
1	I	184	LYS
1	I	203	ARG
1	I	220	SER
1	I	228	THR
1	I	244	LEU
1	I	250	VAL
1	I	256	ARG
1	I	258	LEU
1	I	263	ASP
1	I	271	GLU
1	I	276	TRP
1	I	277	ARG

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Mol	Chain	Res	Type
1	I	283	THR
1	I	316	VAL
2	J	325	LEU
2	J	341	VAL
2	J	350	GLN
2	J	353	GLN
2	J	377	ARG
2	J	379	VAL
2	J	383	ASN
2	J	384	THR
2	J	385	GLU
2	J	395	GLU
2	J	418	GLN
2	J	423	VAL
2	J	433	MET
2	J	438	MET
2	J	448	GLN
2	J	450	ARG
2	J	452	ASN
2	J	491	LEU
2	J	495	ASN
1	K	1	ASP
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	170	LEU
1	K	203	ARG
1	K	213	ARG
1	K	228	THR
1	K	244	LEU
1	K	249	ARG
1	K	250	VAL
1	K	256	ARG
1	K	258	LEU
1	K	276	TRP

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Mol	Chain	Res	Type
1	K	277	ARG
1	K	283	THR
1	K	303	ASN
2	L	335	ASN
2	L	341	VAL
2	L	377	ARG
2	L	379	VAL
2	L	382	THR
2	L	394	SER
2	L	411	ILE
2	L	425	MET
2	L	446	ARG
2	L	450	ARG
2	L	467	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	185	ASN
1	A	205	ASN
1	C	82	ASN
2	D	428	GLN
1	E	8	HIS
1	E	136	ASN
1	E	205	ASN
1	E	231	GLN
2	F	353	GLN
2	F	428	GLN
2	F	484	GLN
1	G	8	HIS
1	G	182	GLN
2	H	350	GLN
2	H	365	GLN
2	H	428	GLN
2	H	484	GLN
1	I	7	HIS
1	I	8	HIS
1	I	39	ASN
1	I	205	ASN
1	I	231	GLN
1	I	268	ASN

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Mol	Chain	Res	Type
2	J	398	HIS
2	J	428	GLN
1	K	205	ASN
1	K	231	GLN
2	L	428	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	L	601	2	14,14,15	0.38	0	17,19,21	0.56	0
3	NAG	F	601	2	14,14,15	0.47	0	17,19,21	0.72	1 (5%)
3	NAG	J	601	2	14,14,15	0.47	0	17,19,21	0.57	0
3	NAG	H	601	2	14,14,15	0.33	0	17,19,21	0.46	0
3	NAG	I	601	1	14,14,15	0.38	0	17,19,21	0.52	0
4	SIA	E	602	-	21,21,21	0.96	1 (4%)	24,31,31	1.31	3 (12%)
3	NAG	D	601	2	14,14,15	0.65	0	17,19,21	0.59	0
3	NAG	C	601	1	14,14,15	0.45	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	K	601	1	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	A	601	1	14,14,15	0.31	0	17,19,21	0.55	0
3	NAG	E	601	1	14,14,15	0.38	0	17,19,21	0.55	0
3	NAG	B	601	2	14,14,15	0.55	0	17,19,21	0.50	0
3	NAG	G	601	1	14,14,15	0.19	0	17,19,21	0.50	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	L	601	2	-	2/6/23/26	0/1/1/1
3	NAG	F	601	2	-	0/6/23/26	0/1/1/1
3	NAG	J	601	2	-	0/6/23/26	0/1/1/1
3	NAG	H	601	2	-	2/6/23/26	0/1/1/1
3	NAG	I	601	1	-	2/6/23/26	0/1/1/1
4	SIA	E	602	-	-	7/20/38/38	0/1/1/1
3	NAG	D	601	2	-	0/6/23/26	0/1/1/1
3	NAG	C	601	1	-	2/6/23/26	0/1/1/1
3	NAG	K	601	1	-	2/6/23/26	0/1/1/1
3	NAG	A	601	1	-	2/6/23/26	0/1/1/1
3	NAG	E	601	1	-	1/6/23/26	0/1/1/1
3	NAG	B	601	2	-	0/6/23/26	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	3.30	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	3.95	113.46	109.84
4	E	602	SIA	C8-C7-C6	-2.63	108.11	113.05
3	F	601	NAG	C1-O5-C5	2.25	115.21	112.19
4	E	602	SIA	O1A-C1-C2	-2.22	120.15	123.85

There are no chirality outliers.

All (22) 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
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	O7-C7-C8-C9
4	E	602	SIA	C6-C7-C8-C9
4	E	602	SIA	C6-C7-C8-O8
3	E	601	NAG	O5-C5-C6-O6
4	E	602	SIA	O10-C10-N5-C5
4	E	602	SIA	O1A-C1-C2-O2
3	K	601	NAG	C4-C5-C6-O6
3	K	601	NAG	O5-C5-C6-O6
4	E	602	SIA	O7-C7-C8-O8
3	G	601	NAG	C4-C5-C6-O6

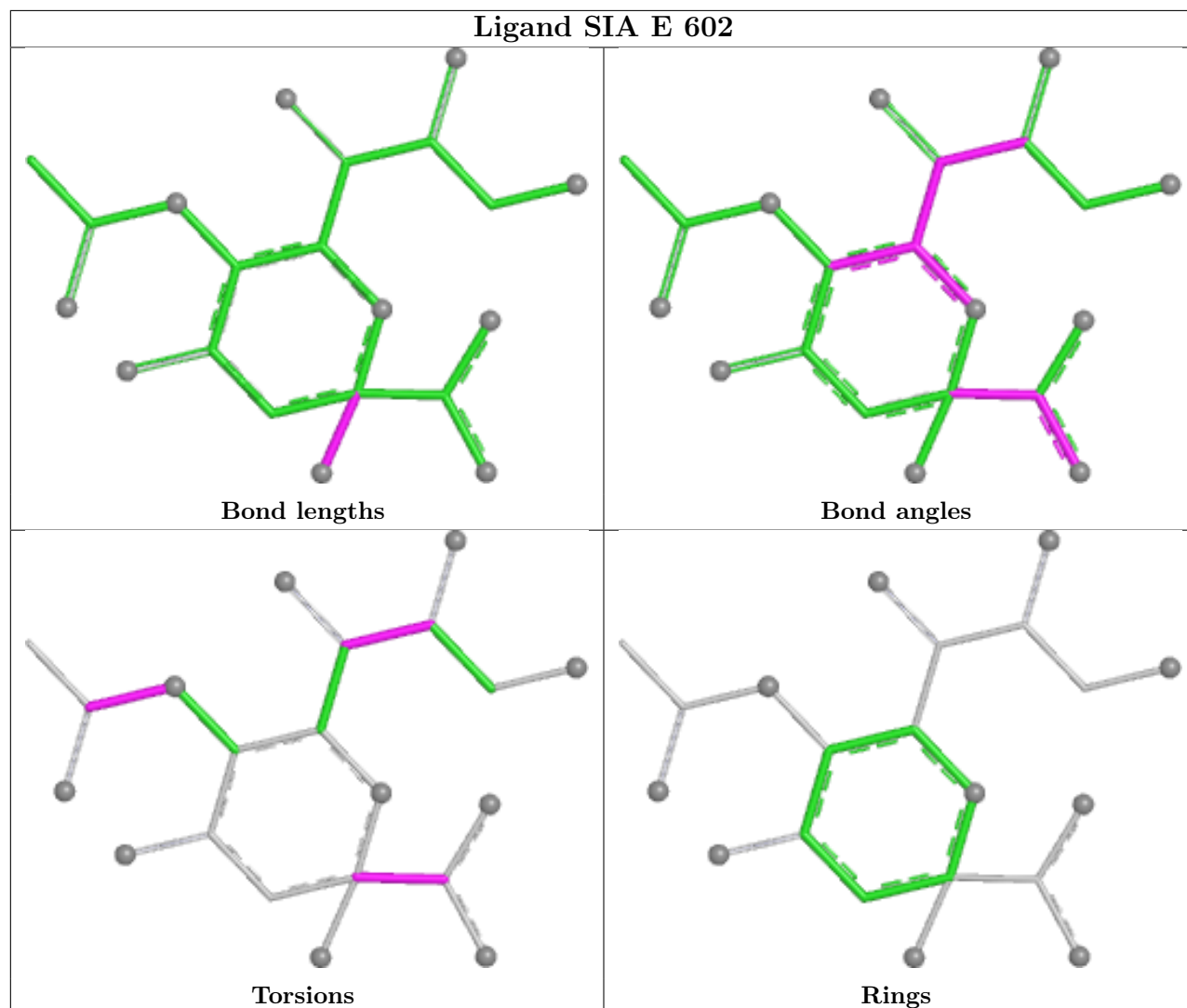
There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	602	SIA	1	0
3	D	601	NAG	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%)	-0.21	1 (0%) 90 88	21, 35, 57, 90	0
1	C	318/318 (100%)	-0.13	3 (0%) 81 78	19, 37, 55, 90	0
1	E	318/318 (100%)	-0.18	1 (0%) 90 88	20, 33, 52, 97	0
1	G	318/318 (100%)	-0.13	3 (0%) 81 78	24, 38, 60, 89	0
1	I	318/318 (100%)	-0.17	4 (1%) 75 71	17, 34, 58, 100	0
1	K	318/318 (100%)	-0.04	2 (0%) 85 83	26, 39, 62, 105	0
2	B	174/174 (100%)	-0.09	3 (1%) 69 65	22, 37, 61, 126	0
2	D	174/174 (100%)	-0.05	7 (4%) 42 38	21, 37, 74, 130	0
2	F	174/174 (100%)	-0.18	3 (1%) 69 65	18, 37, 61, 97	0
2	H	174/174 (100%)	0.36	8 (4%) 37 33	20, 53, 89, 177	0
2	J	174/174 (100%)	0.38	8 (4%) 37 33	22, 51, 88, 145	0
2	L	174/174 (100%)	0.27	7 (4%) 42 38	21, 49, 87, 146	0
All	All	2952/2952 (100%)	-0.05	50 (1%) 69 65	17, 38, 70, 177	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	496	ILE	8.0
2	J	496	ILE	6.9
2	H	497	ASN	5.1
1	I	133	ASN	4.9
2	D	382	THR	4.9
2	L	496	ILE	4.7
2	B	496	ILE	4.3
2	L	497	ASN	4.1
2	J	497	ASN	3.9
2	D	497	ASN	3.8
2	D	496	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	149	SER	3.3
2	J	382	THR	3.2
2	J	346	GLY	3.1
2	D	352	ALA	2.8
2	L	352	ALA	2.8
1	C	256	ARG	2.7
2	F	341	VAL	2.6
2	F	382	THR	2.6
2	L	491	LEU	2.6
2	D	350	GLN	2.6
2	D	383	ASN	2.6
1	E	318	GLU	2.5
2	H	491	LEU	2.5
1	I	318	GLU	2.5
2	J	358	ALA	2.5
1	K	205	ASN	2.4
2	H	356	GLY	2.4
2	L	382	THR	2.3
2	D	341	VAL	2.3
1	C	12	ASN	2.3
2	B	383	ASN	2.3
2	H	352	ALA	2.3
1	K	318	GLU	2.3
2	J	350	GLN	2.3
2	L	383	ASN	2.2
2	J	352	ALA	2.2
2	F	350	GLN	2.2
2	H	382	THR	2.2
2	B	341	VAL	2.2
1	I	1	ASP	2.2
1	G	11	ALA	2.2
2	H	464	TYR	2.1
2	H	381	LYS	2.1
1	A	318	GLU	2.1
2	L	494	LEU	2.1
1	G	1	ASP	2.1
2	J	383	ASN	2.1
1	G	128	ARG	2.0
1	I	256	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](#)

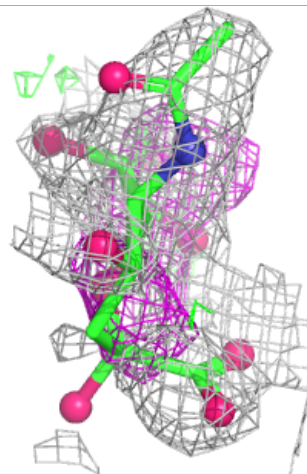
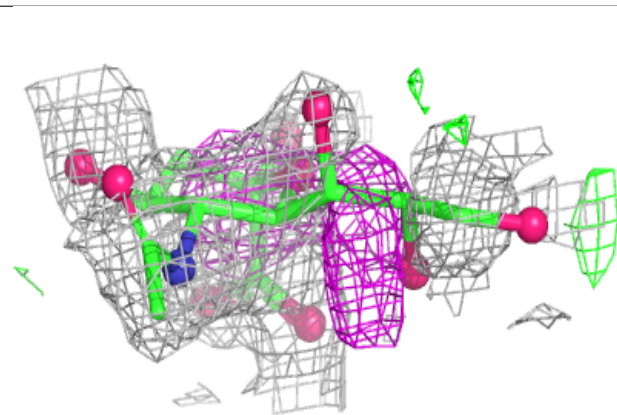
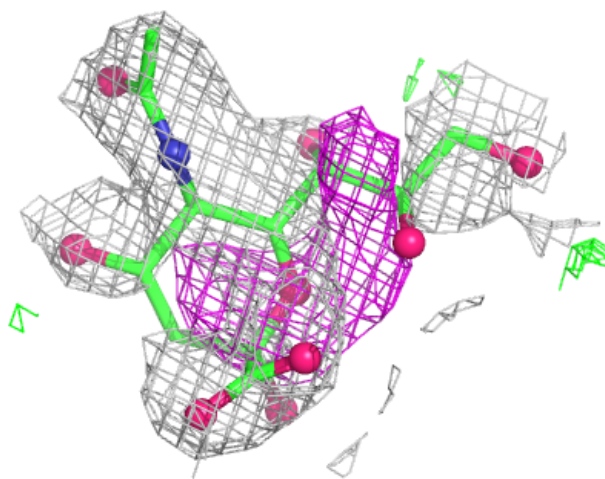
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SIA	E	602	21/21	0.74	0.20	73,92,103,105	0
3	NAG	C	601	14/15	0.76	0.11	50,56,64,71	0
3	NAG	I	601	14/15	0.80	0.11	39,58,63,69	0
3	NAG	B	601	14/15	0.83	0.09	36,43,51,51	0
3	NAG	L	601	14/15	0.83	0.10	32,47,54,57	0
3	NAG	G	601	14/15	0.83	0.12	69,82,86,88	0
3	NAG	E	601	14/15	0.84	0.11	50,61,72,73	0
3	NAG	F	601	14/15	0.84	0.09	33,41,50,52	0
3	NAG	J	601	14/15	0.86	0.08	30,38,42,42	0
3	NAG	K	601	14/15	0.86	0.13	51,60,67,68	0
3	NAG	A	601	14/15	0.87	0.09	52,68,74,74	0
3	NAG	H	601	14/15	0.90	0.08	32,50,53,54	0
3	NAG	D	601	14/15	0.90	0.08	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.