



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:06 PM GMT

PDB ID : 4GXU
Title : Crystal structure of antibody 1F1 bound to the 1918 influenza hemagglutinin
Authors : Ekiert, D.C.; Wilson, I.A.
Deposited on : 2012-09-04
Resolution : 3.29 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

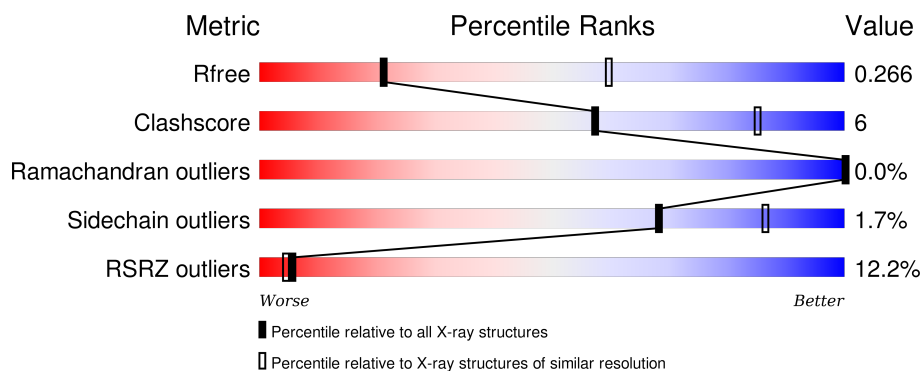
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	331	<div> <div>6%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	C	331	<div> <div>6%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	E	331	<div> <div>4%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	G	331	<div> <div>6%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	I	331	<div> <div>13%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	331	
2	B	176	
2	D	176	
2	F	176	
2	H	176	
2	J	176	
2	L	176	
3	M	231	
3	O	231	
3	Q	231	
3	S	231	
3	U	231	
3	W	231	
4	N	217	
4	P	217	
4	R	217	
4	T	217	
4	V	217	
4	X	217	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 38412 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	A	325	Total	C	N	O	S	0	7	0
			2568	1619	440	498	11			
1	C	325	Total	C	N	O	S	0	8	0
			2576	1623	442	500	11			
1	E	325	Total	C	N	O	S	0	8	0
			2576	1623	442	500	11			
1	G	325	Total	C	N	O	S	0	8	0
			2576	1623	442	500	11			
1	I	325	Total	C	N	O	S	0	8	0
			2576	1623	442	500	11			
1	K	325	Total	C	N	O	S	0	8	0
			2576	1623	442	500	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	EXPRESSION TAG	UNP Q9WFX3
A	8	ASP	-	EXPRESSION TAG	UNP Q9WFX3
A	9	PRO	-	EXPRESSION TAG	UNP Q9WFX3
A	10	GLY	-	EXPRESSION TAG	UNP Q9WFX3
C	7	ALA	-	EXPRESSION TAG	UNP Q9WFX3
C	8	ASP	-	EXPRESSION TAG	UNP Q9WFX3
C	9	PRO	-	EXPRESSION TAG	UNP Q9WFX3
C	10	GLY	-	EXPRESSION TAG	UNP Q9WFX3
E	7	ALA	-	EXPRESSION TAG	UNP Q9WFX3
E	8	ASP	-	EXPRESSION TAG	UNP Q9WFX3
E	9	PRO	-	EXPRESSION TAG	UNP Q9WFX3
E	10	GLY	-	EXPRESSION TAG	UNP Q9WFX3
G	7	ALA	-	EXPRESSION TAG	UNP Q9WFX3
G	8	ASP	-	EXPRESSION TAG	UNP Q9WFX3
G	9	PRO	-	EXPRESSION TAG	UNP Q9WFX3
G	10	GLY	-	EXPRESSION TAG	UNP Q9WFX3
I	7	ALA	-	EXPRESSION TAG	UNP Q9WFX3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	8	ASP	-	EXPRESSION TAG	UNP Q9WFX3
I	9	PRO	-	EXPRESSION TAG	UNP Q9WFX3
I	10	GLY	-	EXPRESSION TAG	UNP Q9WFX3
K	7	ALA	-	EXPRESSION TAG	UNP Q9WFX3
K	8	ASP	-	EXPRESSION TAG	UNP Q9WFX3
K	9	PRO	-	EXPRESSION TAG	UNP Q9WFX3
K	10	GLY	-	EXPRESSION TAG	UNP Q9WFX3

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	3	0
			1399	873	241	279	6			
2	D	171	Total	C	N	O	S	0	3	0
			1399	873	241	279	6			
2	F	171	Total	C	N	O	S	0	3	0
			1399	873	241	279	6			
2	H	171	Total	C	N	O	S	0	3	0
			1399	873	241	279	6			
2	J	171	Total	C	N	O	S	0	3	0
			1399	873	241	279	6			
2	L	171	Total	C	N	O	S	0	3	0
			1399	873	241	279	6			

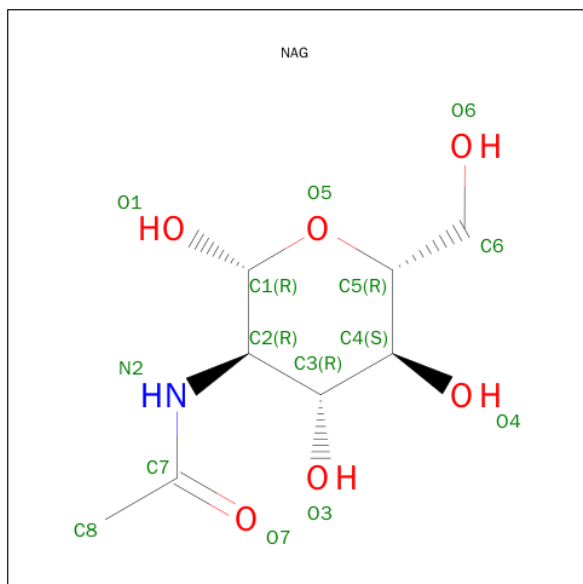
- Molecule 3 is a protein called Antibody 1F1, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	228	Total	C	N	O	S	0	4	0
			1758	1106	304	339	9			
3	O	125	Total	C	N	O	S	0	2	0
			1003	632	178	187	6			
3	Q	228	Total	C	N	O	S	0	5	0
			1766	1111	305	340	10			
3	S	125	Total	C	N	O	S	0	2	0
			1003	632	178	187	6			
3	U	125	Total	C	N	O	S	0	2	0
			1003	632	178	187	6			
3	W	125	Total	C	N	O	S	0	2	0
			1003	632	178	187	6			

- Molecule 4 is a protein called Antibody 1F1, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	214	Total	C	N	O	S	0	7	0
			1620	1019	268	329	4			
4	P	111	Total	C	N	O	S	0	7	0
			848	534	140	172	2			
4	R	214	Total	C	N	O	S	0	7	0
			1620	1019	268	329	4			
4	T	111	Total	C	N	O	S	0	7	0
			848	534	140	172	2			
4	V	111	Total	C	N	O	S	0	7	0
			848	534	140	172	2			
4	X	111	Total	C	N	O	S	0	7	0
			848	534	140	172	2			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		

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

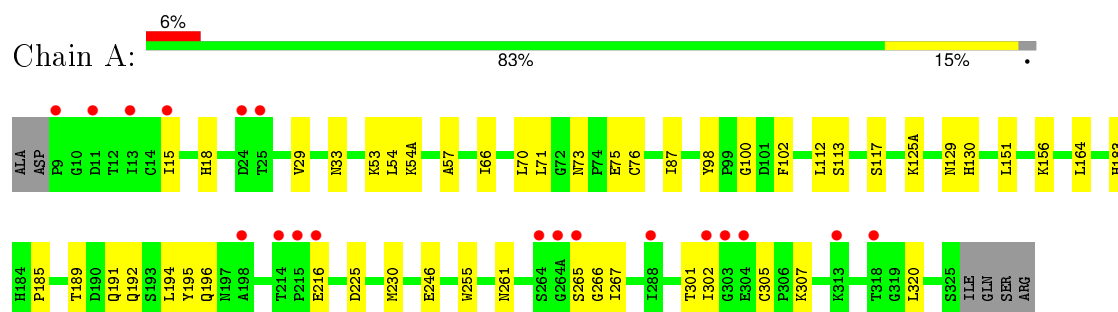
- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			39	22	2	15		
6	C	3	Total	C	N	O	0	0
			39	22	2	15		
6	E	3	Total	C	N	O	0	0
			39	22	2	15		
6	G	3	Total	C	N	O	0	0
			39	22	2	15		
6	I	3	Total	C	N	O	0	0
			39	22	2	15		
6	K	3	Total	C	N	O	0	0
			39	22	2	15		

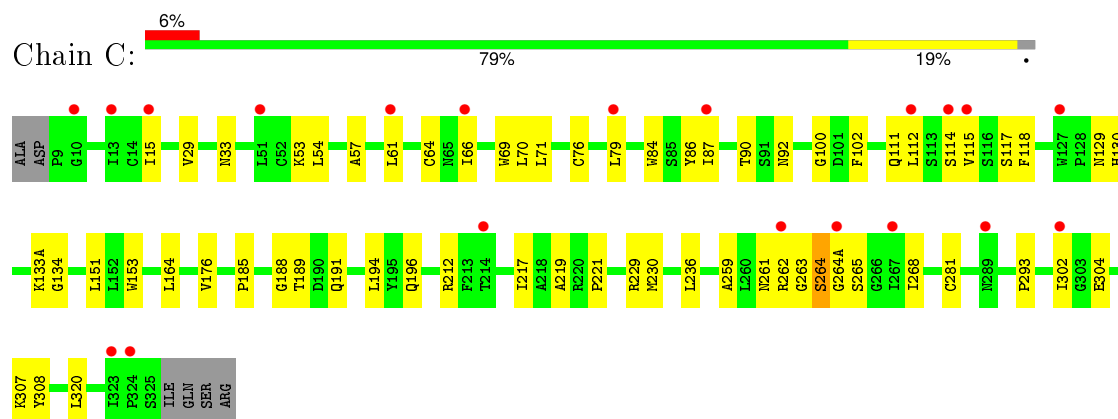
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

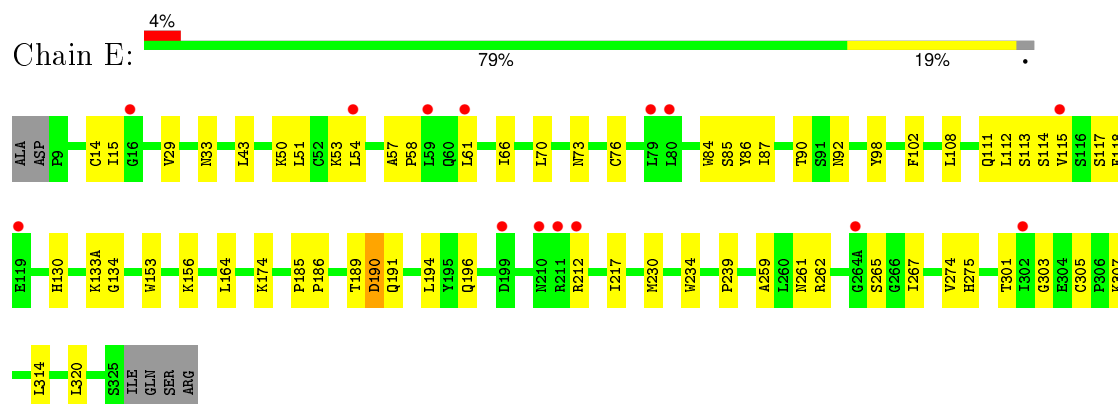
- Molecule 1: Hemagglutinin HA1 chain



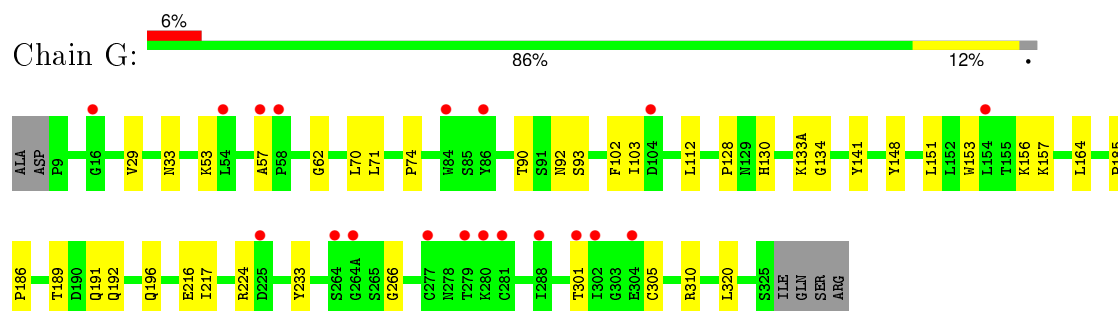
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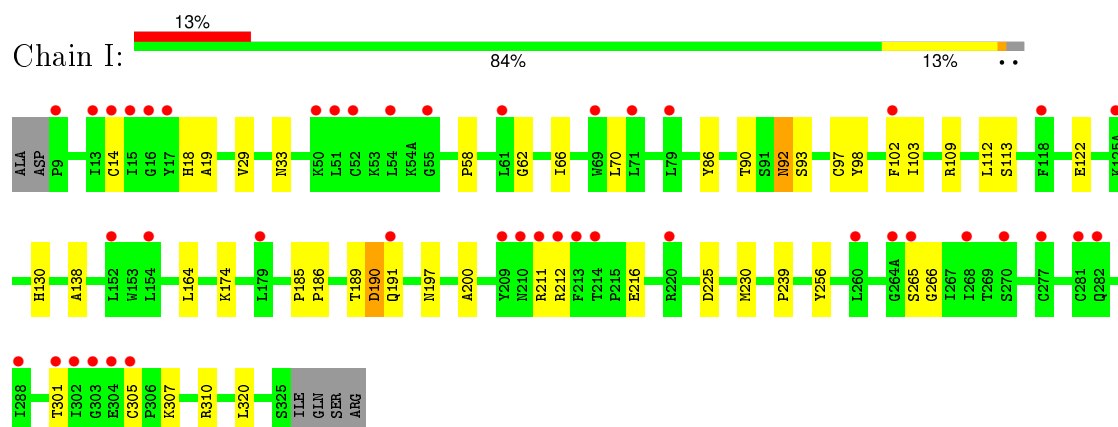
- Molecule 1: Hemagglutinin HA1 chain



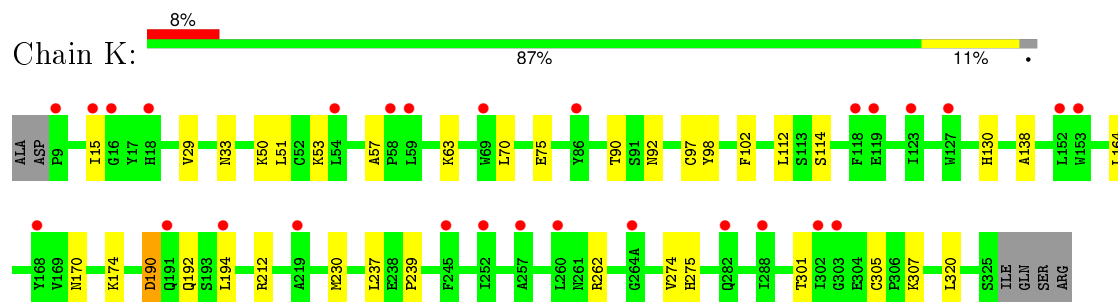
- Molecule 1: Hemagglutinin HA1 chain



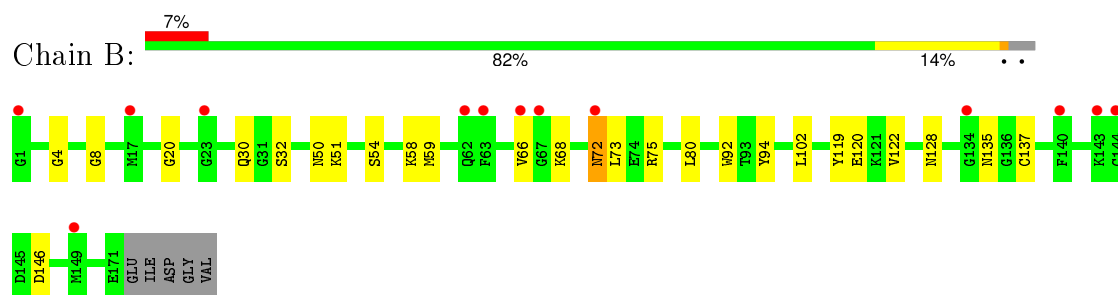
- Molecule 1: Hemagglutinin HA1 chain



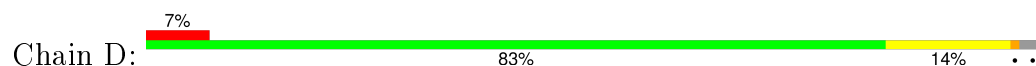
- Molecule 1: Hemagglutinin HA1 chain

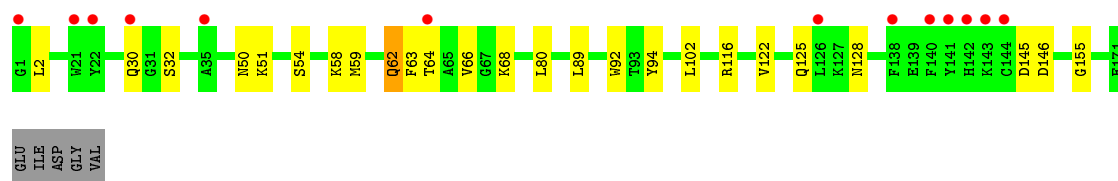


- Molecule 2: Hemagglutinin HA2 chain

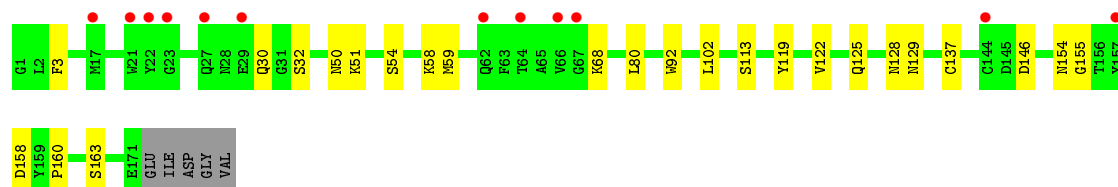
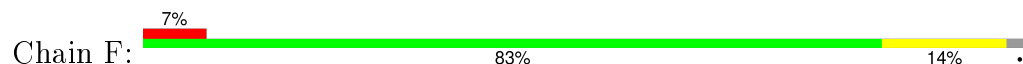


- Molecule 2: Hemagglutinin HA2 chain

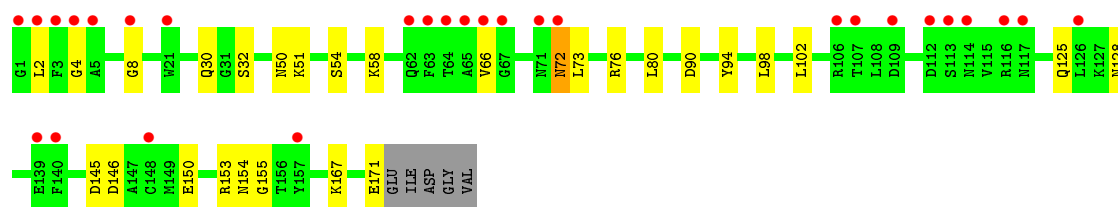
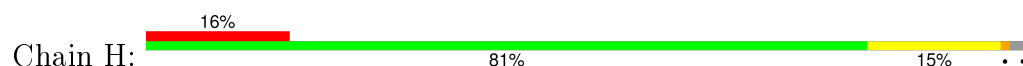




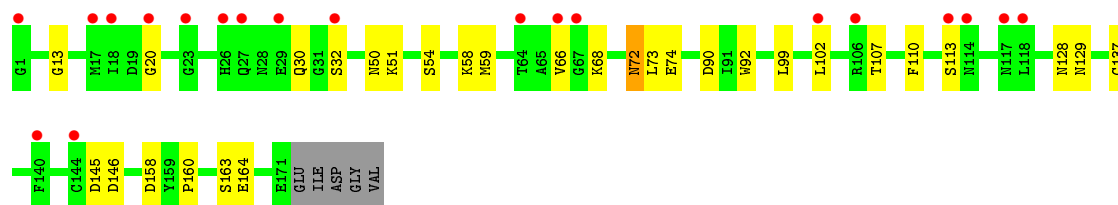
• Molecule 2: Hemagglutinin HA2 chain



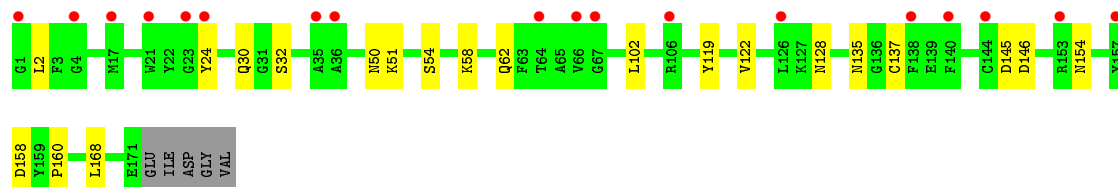
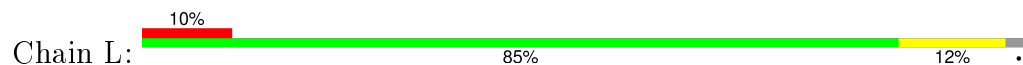
• Molecule 2: Hemagglutinin HA2 chain



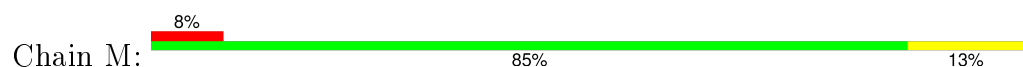
• Molecule 2: Hemagglutinin HA2 chain

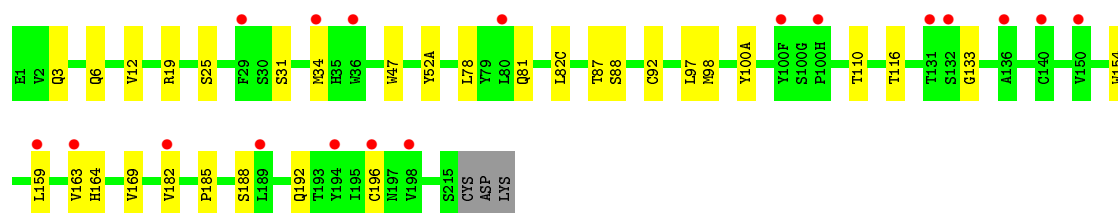


• Molecule 2: Hemagglutinin HA2 chain

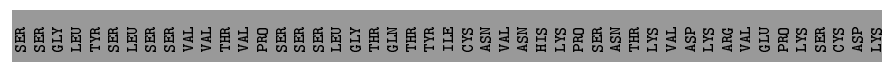
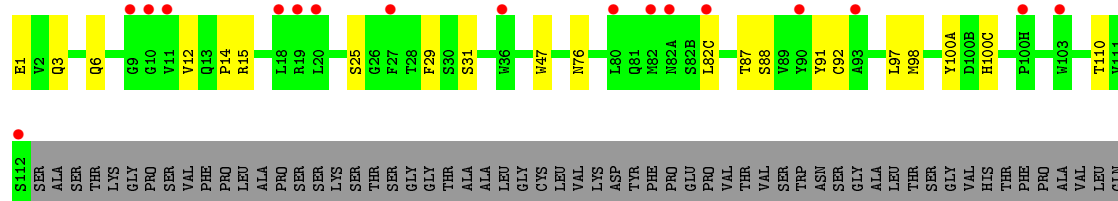


• Molecule 3: Antibody 1F1, heavy chain

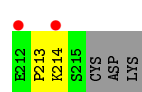
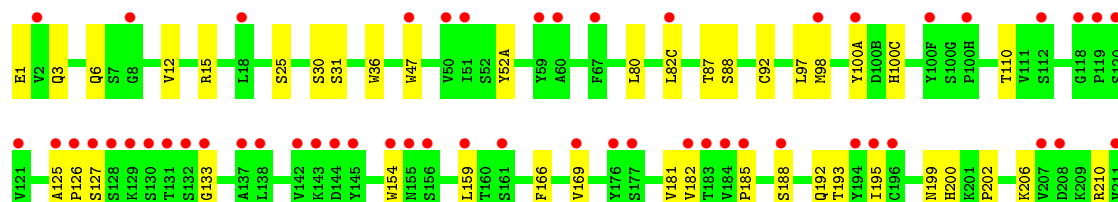
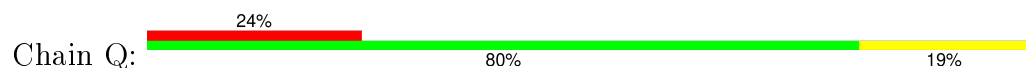




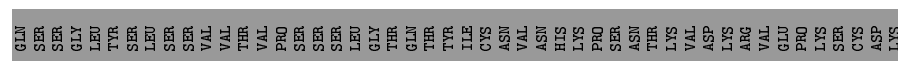
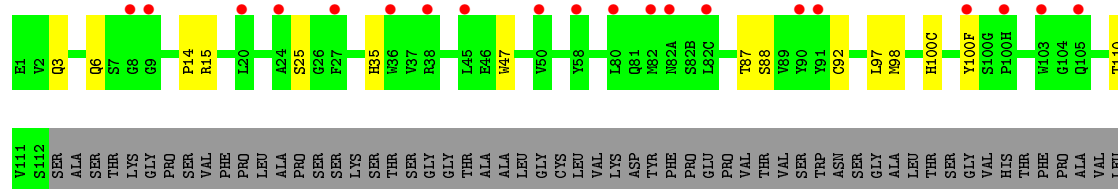
• Molecule 3: Antibody 1F1, heavy chain



• Molecule 3: Antibody 1F1, heavy chain

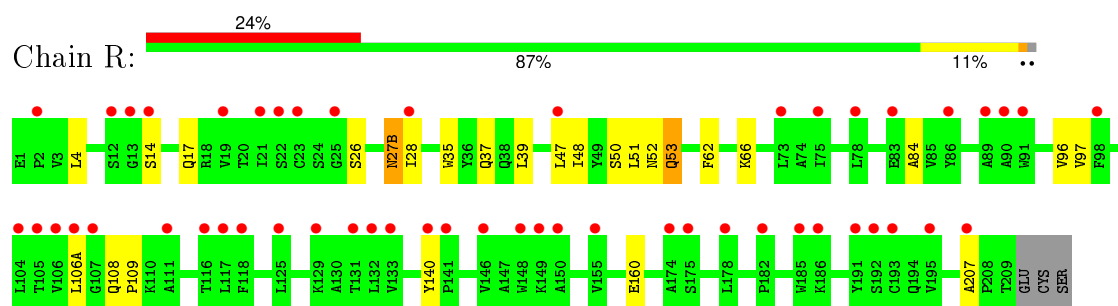


• Molecule 3: Antibody 1F1, heavy chain

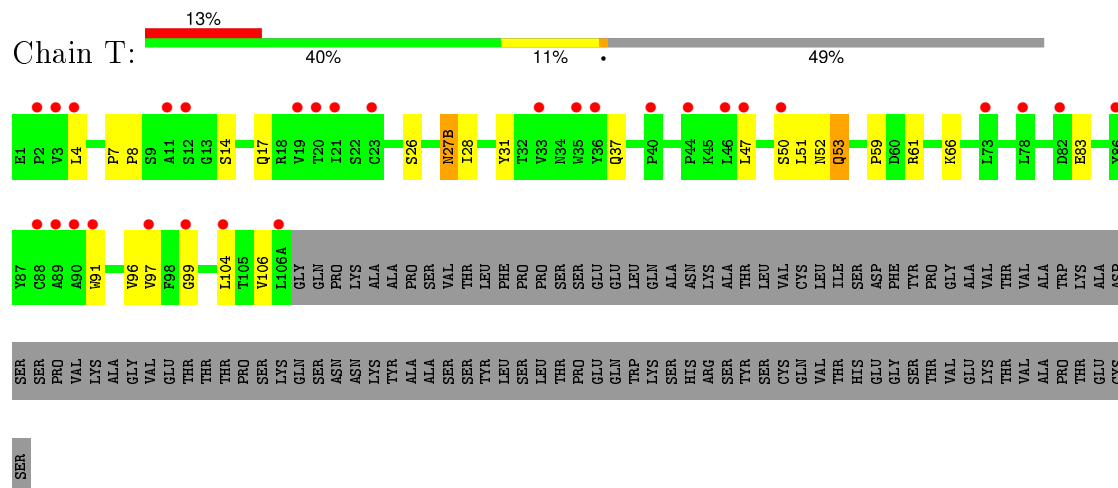


• Molecule 3: Antibody 1F1, heavy chain

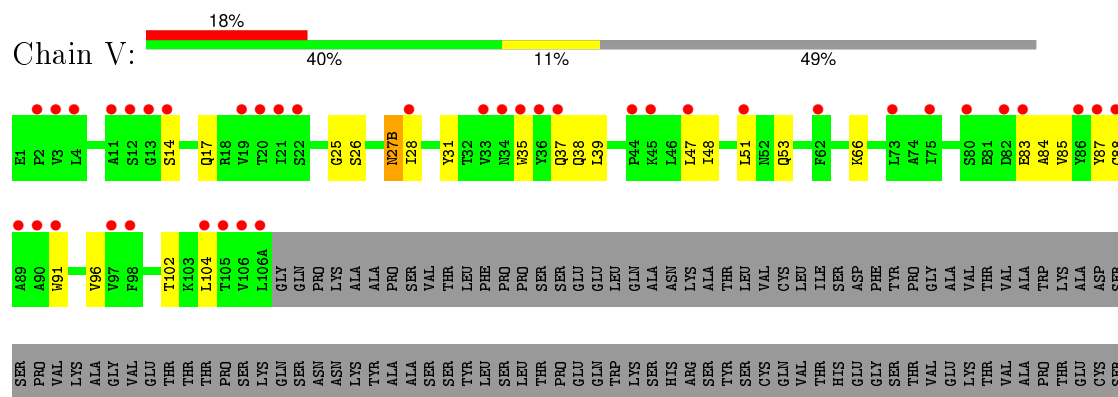




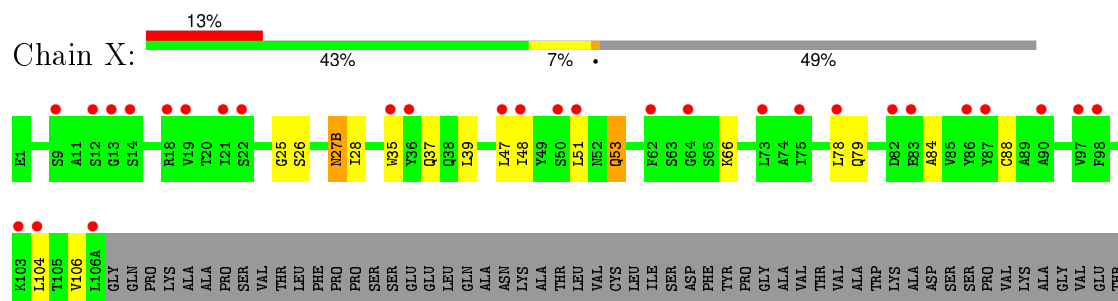
- Molecule 4: Antibody 1F1, light chain



- Molecule 4: Antibody 1F1, light chain



- Molecule 4: Antibody 1F1, light chain



THR	THR	PRO	SER	LYS	GLN	SER	ASN	LYS	TYR	ALA	ALA	SER	SER	TYR	LEU	SER	LEU	THR	PRO	GLU	GLN	TRP	LYS	SER	HIS	ARG	SER	SER	TYR	SER	CYS	GLN	VAL	THR	HIS	GLU	GLY	SER	THR	VAL	GLU	LYS	THR	VAL	ALA	PRO	THR	GLU	CYS	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	153.71Å 176.27Å 168.12Å 90.00° 92.14° 90.00°	Depositor
Resolution (Å)	35.04 – 3.29 45.23 – 3.29	Depositor EDS
% Data completeness (in resolution range)	80.1 (35.04-3.29) 80.3 (45.23-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.219 , 0.255 0.232 , 0.266	Depositor DCC
R_{free} test set	5441 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	104.3	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 57.4	EDS
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 108628 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	38412	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PCA, NAG, BMA

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	0.29	0/2633	0.62	0/3588
1	C	0.33	0/2641	0.71	1/3599 (0.0%)
1	E	0.31	0/2641	0.65	0/3599
1	G	0.28	0/2641	0.60	0/3599
1	I	0.26	0/2641	0.57	0/3599
1	K	0.28	0/2641	0.60	0/3599
2	B	0.32	0/1426	0.59	0/1920
2	D	0.34	0/1426	0.64	1/1920 (0.1%)
2	F	0.34	0/1426	0.62	0/1920
2	H	0.31	0/1426	0.52	0/1920
2	J	0.32	0/1426	0.56	0/1920
2	L	0.35	0/1426	0.60	2/1920 (0.1%)
3	M	0.28	0/1794	0.59	0/2444
3	O	0.24	0/1020	0.55	0/1383
3	Q	0.26	0/1802	0.58	0/2454
3	S	0.24	0/1020	0.58	0/1383
3	U	0.27	0/1020	0.59	0/1383
3	W	0.26	0/1020	0.55	0/1383
4	N	0.27	0/1662	0.58	0/2276
4	P	0.24	0/869	0.57	0/1189
4	R	0.25	0/1662	0.60	1/2276 (0.0%)
4	T	0.24	0/869	0.57	0/1189
4	V	0.24	0/869	0.59	0/1189
4	X	0.23	0/869	0.53	0/1189
All	All	0.29	0/38870	0.60	5/52841 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	207	ALA	C-N-CD	6.38	141.80	128.40
1	C	264	SER	N-CA-C	5.96	127.09	111.00
2	D	62	GLN	N-CA-C	-5.55	96.03	111.00
2	L	168	LEU	CB-CG-CD1	-5.25	102.07	111.00
2	L	168	LEU	CA-CB-CG	5.04	126.90	115.30

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	2568	0	2488	40	0
1	C	2576	0	2493	54	1
1	E	2576	0	2493	51	0
1	G	2576	0	2493	31	0
1	I	2576	0	2493	32	0
1	K	2576	0	2493	23	0
2	B	1399	0	1312	22	0
2	D	1399	0	1312	24	0
2	F	1399	0	1312	19	0
2	H	1399	0	1312	22	0
2	J	1399	0	1312	25	0
2	L	1399	0	1312	13	0
3	M	1758	0	1718	20	0
3	O	1003	0	968	13	0
3	Q	1766	0	1726	26	0
3	S	1003	0	968	12	0
3	U	1003	0	968	18	0
3	W	1003	0	968	11	0
4	N	1620	0	1589	21	1
4	P	848	0	834	15	0
4	R	1620	0	1589	21	0
4	T	848	0	834	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	V	848	0	834	21	0
4	X	848	0	834	15	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
5	E	14	0	13	0	0
5	F	14	0	13	1	0
5	G	14	0	13	0	0
5	H	14	0	13	1	0
5	I	14	0	13	0	0
5	J	14	0	13	0	0
5	K	14	0	13	0	0
5	L	14	0	13	1	0
6	A	39	0	34	1	0
6	C	39	0	34	0	0
6	E	39	0	34	0	0
6	G	39	0	34	1	0
6	I	39	0	34	0	0
6	K	39	0	34	1	0
All	All	38412	0	37015	455	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 6.

All (455) 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)
4:X:27(B):ASN:HD22	4:X:28:ILE:H	1.15	0.95
4:R:27(B):ASN:HD22	4:R:28:ILE:H	1.14	0.95
4:T:27(B):ASN:HD22	4:T:28:ILE:H	1.15	0.94
4:V:27(B):ASN:HD22	4:V:28:ILE:H	1.15	0.94
4:P:27(B):ASN:HD22	4:P:28:ILE:H	1.13	0.91
4:N:27(B):ASN:HD22	4:N:28:ILE:H	1.13	0.90
1:C:129:ASN:ND2	3:Q:1:PCA:OE	2.05	0.89
1:C:111:GLN:O	1:C:114:SER:OG	1.94	0.85
1:G:156:LYS:NZ	4:T:50[A]:SER:OG	2.16	0.79
3:U:6:GLN:HE21	3:U:92:CYS:H	1.31	0.78
1:G:90:THR:OG1	1:G:92[A]:ASN:OD1	2.03	0.77
1:C:117:SER:OG	1:C:261:ASN:ND2	2.17	0.77
1:E:90:THR:OG1	1:E:92[A]:ASN:OD1	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:70:LEU:HD11	1:K:112:LEU:HD11	1.66	0.76
1:C:90:THR:OG1	1:C:92[A]:ASN:OD1	2.02	0.76
1:K:90:THR:OG1	1:K:92[A]:ASN:OD1	2.02	0.76
3:Q:6:GLN:HE21	3:Q:92:CYS:H	1.31	0.75
1:C:307:LYS:HE3	2:D:92:TRP:NE1	2.03	0.73
4:P:37:GLN:HB2	4:P:47[B]:LEU:HD11	1.71	0.73
1:E:196:GLN:NE2	4:R:52:ASN:OD1	2.22	0.71
2:J:30:GLN:HE22	2:J:146:ASP:H	1.38	0.71
3:M:169[A]:VAL:HG21	4:N:160:GLU:HB3	1.71	0.71
1:I:70:LEU:HD11	1:I:112:LEU:HD11	1.73	0.71
2:H:50:ASN:ND2	1:K:29:VAL:O	2.21	0.71
4:N:37:GLN:HB2	4:N:47[B]:LEU:HD11	1.72	0.70
4:T:37:GLN:HB2	4:T:47[B]:LEU:HD11	1.73	0.70
1:C:264(A):GLY:O	2:D:64:THR:HG22	1.92	0.69
4:X:37:GLN:HB2	4:X:47[B]:LEU:HD11	1.73	0.69
1:G:224:ARG:NH1	6:G:403:NAG:O6	2.25	0.69
1:I:197:ASN:HB2	1:I:200:ALA:HB2	1.74	0.68
4:V:37:GLN:HB2	4:V:47[B]:LEU:HD11	1.73	0.68
4:R:37:GLN:HB2	4:R:47[B]:LEU:HD11	1.75	0.68
3:W:6:GLN:HE21	3:W:92:CYS:H	1.40	0.68
2:B:50:ASN:ND2	1:C:29:VAL:O	2.25	0.68
2:B:30:GLN:HE22	2:B:146:ASP:H	1.39	0.68
1:K:50:LYS:HD2	1:K:275:HIS:HB2	1.77	0.68
3:S:87:THR:HG23	3:S:110:THR:HA	1.76	0.67
4:N:27(B):ASN:ND2	4:N:28:ILE:H	1.92	0.67
2:D:30:GLN:HE22	2:D:146:ASP:H	1.42	0.67
2:D:50:ASN:ND2	1:E:29:VAL:O	2.27	0.67
4:X:27(B):ASN:ND2	4:X:28:ILE:H	1.92	0.66
6:K:402:NAG:H61	6:K:403:NAG:H82	1.75	0.66
3:M:6:GLN:HE21	3:M:92:CYS:H	1.42	0.66
1:E:117:SER:OG	1:E:261:ASN:ND2	2.29	0.66
4:X:26:SER:H	4:X:27(B):ASN:HD21	1.43	0.66
1:A:216:GLU:OE1	1:E:212:ARG:HB3	1.96	0.66
1:I:266:GLY:HA3	2:J:66:VAL:HG11	1.78	0.66
1:K:51:LEU:HB2	1:K:274:VAL:HG22	1.77	0.66
2:H:30:GLN:HE22	2:H:146:ASP:H	1.44	0.65
4:T:51:LEU:HD21	4:T:66:LYS:HG2	1.78	0.65
1:G:216:GLU:OE1	1:I:212:ARG:HB3	1.96	0.65
1:E:111:GLN:O	1:E:114:SER:OG	2.13	0.65
1:G:192:GLN:HE21	4:T:53:GLN:HB3	1.60	0.65
4:X:39:LEU:HD23	4:X:84:ALA:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:6:GLN:HE21	3:S:92:CYS:H	1.45	0.64
4:N:51:LEU:HD21	4:N:66:LYS:HG2	1.80	0.63
3:O:6:GLN:HE21	3:O:92:CYS:H	1.46	0.63
3:Q:126:PRO:HG2	3:Q:213:PRO:HA	1.80	0.63
3:Q:159:LEU:HD21	3:Q:182:VAL:HG11	1.80	0.63
4:P:26:SER:H	4:P:27(B):ASN:HD21	1.46	0.63
4:X:51:LEU:HD21	4:X:66:LYS:HG2	1.79	0.63
4:T:27(B):ASN:ND2	4:T:28:ILE:H	1.93	0.63
3:O:87:THR:HG23	3:O:110:THR:HA	1.81	0.63
1:G:29:VAL:O	2:J:50:ASN:ND2	2.29	0.62
4:R:27(B):ASN:ND2	4:R:28:ILE:H	1.91	0.62
1:C:114:SER:OG	1:C:262:ARG:NH1	2.30	0.62
1:A:70:LEU:HD11	1:A:112:LEU:HD11	1.82	0.62
4:P:27(B):ASN:ND2	4:P:28:ILE:H	1.92	0.62
2:L:30:GLN:HE22	2:L:146:ASP:H	1.48	0.62
1:A:156:LYS:NZ	4:N:50[A]:SER:OG	2.25	0.61
4:R:26:SER:H	4:R:27(B):ASN:HD21	1.47	0.61
4:V:27(B):ASN:ND2	4:V:28:ILE:H	1.93	0.61
1:A:66[A]:ILE:HD11	1:A:87:ILE:HG21	1.82	0.61
4:V:26:SER:H	4:V:27(B):ASN:HD21	1.46	0.61
3:S:35:HIS:HE1	3:S:100(F):TYR:HB3	1.66	0.61
4:X:78[B]:LEU:HD11	4:X:104:LEU:HD21	1.83	0.61
1:E:84:TRP:HH2	1:E:118:PHE:CE2	2.18	0.60
3:M:163:VAL:HG22	3:M:182:VAL:HG22	1.82	0.60
4:R:51:LEU:HD21	4:R:66:LYS:HG2	1.82	0.60
1:A:113:SER:O	1:A:265:SER:HB3	2.01	0.60
1:G:217:ILE:O	1:I:212:ARG:NH2	2.35	0.59
4:T:26:SER:H	4:T:27(B):ASN:HD21	1.50	0.59
2:J:30:GLN:NE2	2:J:146:ASP:H	2.00	0.58
1:A:29:VAL:O	2:F:50:ASN:ND2	2.35	0.58
3:M:87:THR:HG23	3:M:110:THR:HA	1.85	0.58
1:E:114:SER:OG	1:E:262:ARG:NH1	2.35	0.58
2:F:125:GLN:HE22	2:F:155:GLY:HA2	1.68	0.58
4:N:26:SER:H	4:N:27(B):ASN:HD21	1.49	0.58
2:F:30:GLN:HE22	2:F:146:ASP:H	1.52	0.58
4:X:26:SER:H	4:X:27(B):ASN:ND2	2.01	0.57
2:D:30:GLN:NE2	2:D:146:ASP:H	2.02	0.57
4:P:39:LEU:HD23	4:P:84:ALA:HB2	1.85	0.57
2:F:54:SER:O	2:F:58:LYS:HG2	2.05	0.57
4:R:26:SER:H	4:R:27(B):ASN:ND2	2.02	0.57
1:E:84:TRP:HH2	1:E:118:PHE:HE2	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66[A]:ILE:HD11	1:C:87:ILE:HG21	1.85	0.57
1:C:302:ILE:HG12	2:D:66:VAL:HG12	1.86	0.57
1:I:216:GLU:OE1	1:K:212:ARG:HB3	2.04	0.56
2:B:54:SER:O	2:B:58:LYS:HG2	2.05	0.56
2:H:72[A]:ASN:HD22	2:H:73:LEU:N	2.03	0.56
3:U:87:THR:HG23	3:U:110:THR:HA	1.87	0.56
2:B:72[A]:ASN:HD22	2:B:73:LEU:N	2.04	0.56
1:A:15:ILE:HG12	2:B:119:TYR:HA	1.87	0.56
1:I:186:PRO:HB2	3:U:98[A]:MET:SD	2.46	0.56
3:U:19[A]:ARG:NH1	3:U:81:GLN:OE1	2.39	0.56
1:G:185:PRO:HG2	1:G:191:GLN:HE21	1.71	0.56
2:D:54:SER:O	2:D:58:LYS:HG2	2.06	0.56
2:D:68:LYS:HE3	2:F:80:LEU:N	2.20	0.55
1:A:192:GLN:HE21	4:N:53:GLN:HB3	1.71	0.55
1:C:53:LYS:HG2	1:C:57:ALA:HA	1.87	0.55
4:V:51:LEU:HD11	4:V:66:LYS:HB3	1.88	0.55
1:C:111:GLN:HB3	1:C:262:ARG:HH12	1.72	0.55
1:A:185:PRO:HG2	1:A:191:GLN:HE21	1.72	0.55
3:M:12:VAL:HG21	3:M:82(C):LEU:HD13	1.87	0.55
1:E:53:LYS:HG2	1:E:57:ALA:HA	1.88	0.55
1:G:266:GLY:HA3	2:H:66:VAL:HG11	1.88	0.55
1:E:54[A]:LEU:HD11	1:E:303:GLY:HA3	1.88	0.55
1:G:128:PRO:O	1:G:157:LYS:NZ	2.33	0.55
1:A:130:HIS:CE1	1:A:164:LEU:HB3	2.42	0.55
1:G:70:LEU:HD11	1:G:112:LEU:HD11	1.90	0.55
1:C:188:GLY:HA2	1:C:217:ILE:HD13	1.88	0.55
1:A:129:ASN:ND2	3:O:1:PCA:OE	2.40	0.54
4:T:26:SER:H	4:T:27(B):ASN:ND2	2.05	0.54
3:M:164:HIS:CE1	4:N:167:GLN:HG2	2.42	0.54
2:H:125:GLN:NE2	2:H:155:GLY:HA2	2.22	0.54
1:G:196:GLN:NE2	4:T:52:ASN:OD1	2.40	0.54
3:M:47:TRP:CG	4:N:96:VAL:HB	2.42	0.54
4:V:25:GLY:HA3	4:V:27(B):ASN:HD21	1.73	0.54
1:C:114:SER:O	1:C:262:ARG:HA	2.07	0.54
1:C:84:TRP:CZ3	1:C:118:PHE:HE2	2.25	0.54
1:A:194:LEU:HD11	3:M:100(A):TYR:CZ	2.42	0.54
2:J:72[A]:ASN:HD22	2:J:73:LEU:N	2.05	0.54
4:P:26:SER:H	4:P:27(B):ASN:ND2	2.06	0.54
3:U:6:GLN:HE21	3:U:92:CYS:N	2.05	0.54
2:J:54:SER:O	2:J:58:LYS:HG2	2.08	0.54
3:S:35:HIS:CE1	3:S:100(F):TYR:HB3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:39:LEU:HD23	4:V:84:ALA:HB2	1.90	0.54
3:Q:169[A]:VAL:HG21	4:R:160:GLU:HB3	1.90	0.54
2:J:129:ASN:HD21	2:J:163:SER:HA	1.73	0.54
1:C:221:PRO:O	1:C:229:ARG:NH2	2.31	0.53
1:C:133(A):LYS:HD3	3:O:100(C):HIS:CD2	2.43	0.53
1:C:70:LEU:HD11	1:C:112:LEU:HD11	1.89	0.53
4:X:25:GLY:HA3	4:X:27(B):ASN:HD21	1.74	0.53
2:L:54:SER:O	2:L:58:LYS:HG2	2.08	0.53
2:B:80:LEU:N	2:F:68:LYS:HE3	2.23	0.53
4:X:79:GLN:O	4:X:106:VAL:HG21	2.08	0.53
4:V:26:SER:H	4:V:27(B):ASN:ND2	2.06	0.53
1:I:310:ARG:NH1	2:J:90:ASP:OD1	2.39	0.53
4:N:150:ALA:HB1	4:N:188:HIS:CD2	2.44	0.52
1:A:189:THR:HG22	3:M:97:LEU:HD23	1.89	0.52
1:I:97:CYS:HB2	1:I:138:ALA:O	2.09	0.52
1:C:196:GLN:NE2	4:P:52:ASN:OD1	2.40	0.52
1:E:185:PRO:HG2	1:E:191:GLN:HE21	1.74	0.52
4:X:35:TRP:HB2	4:X:48:ILE:HB	1.92	0.52
1:C:114:SER:HB2	1:C:263:GLY:H	1.74	0.52
4:R:35:TRP:HB2	4:R:48:ILE:HB	1.92	0.52
2:H:2:LEU:O	2:J:113:SER:OG	2.28	0.52
4:X:27(B):ASN:HD22	4:X:28:ILE:N	1.96	0.52
1:E:130:HIS:CE1	1:E:164:LEU:HB3	2.44	0.52
3:Q:12:VAL:HG21	3:Q:82(C):LEU:HD13	1.92	0.52
1:G:74:PRO:HB2	1:G:141:TYR:HB2	1.91	0.52
4:P:35:TRP:HB2	4:P:48:ILE:HB	1.91	0.52
1:C:29:VAL:CG2	2:D:102:LEU:HD23	2.40	0.52
3:Q:154:TRP:HB3	3:Q:159:LEU:HD23	1.92	0.52
1:C:54[A]:LEU:HD13	1:C:86:TYR:CE2	2.44	0.52
1:E:54[A]:LEU:HB3	1:E:85:SER:HB2	1.93	0.51
2:B:68:LYS:HE3	2:D:80:LEU:N	2.25	0.51
1:I:29:VAL:O	2:L:50:ASN:ND2	2.39	0.51
1:E:51:LEU:HB2	1:E:274:VAL:HG22	1.92	0.51
3:Q:47:TRP:CG	4:R:96:VAL:HB	2.46	0.51
1:G:310:ARG:NH1	2:H:90:ASP:OD1	2.34	0.51
1:I:98:TYR:CD2	1:I:230:MET:HB2	2.46	0.51
1:E:66[A]:ILE:HD11	1:E:87:ILE:HG21	1.92	0.51
1:G:29:VAL:HG11	2:J:51:LYS:HE2	1.93	0.51
1:I:90:THR:OG1	1:I:92[A]:ASN:OD1	2.21	0.51
2:H:51:LYS:HE2	1:K:29:VAL:HG11	1.93	0.51
1:C:281:CYS:HB2	1:C:304:GLU:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:12:VAL:HG21	3:O:82(C):LEU:HD13	1.93	0.50
1:I:130:HIS:CE1	1:I:164:LEU:HB3	2.46	0.50
4:R:106(A):LEU:HA	4:R:140:TYR:OH	2.12	0.50
1:K:130:HIS:CE1	1:K:164:LEU:HB3	2.47	0.50
4:R:14:SER:H	4:R:17:GLN:NE2	2.09	0.50
3:Q:166:PHE:HE2	3:Q:181:VAL:HG12	1.76	0.50
1:C:304:GLU:HG3	2:D:62:GLN:O	2.12	0.50
1:I:185:PRO:HG2	1:I:191:GLN:HE21	1.75	0.50
2:L:154:ASN:HB2	5:L:201:NAG:H82	1.94	0.50
3:W:87:THR:HG23	3:W:110:THR:HA	1.94	0.50
1:E:50:LYS:HD2	1:E:275:HIS:HB2	1.94	0.50
1:G:186:PRO:HB2	3:S:98[A]:MET:SD	2.51	0.50
1:E:307:LYS:HE3	2:F:92:TRP:NE1	2.26	0.50
3:S:14:PRO:O	3:S:15:ARG:HB2	2.12	0.50
3:U:6:GLN:NE2	3:U:92:CYS:H	2.05	0.49
1:C:15:ILE:HD11	2:D:122:VAL:HG21	1.94	0.49
1:I:225:ASP:OD1	3:U:52(A):TYR:OH	2.30	0.49
1:E:133(A):LYS:HD3	3:Q:100(C):HIS:CD2	2.48	0.49
3:S:47:TRP:CG	4:T:96:VAL:HB	2.47	0.49
1:E:114:SER:O	1:E:262:ARG:HA	2.12	0.49
4:R:51:LEU:HD11	4:R:66:LYS:HB3	1.94	0.49
1:E:113:SER:O	1:E:265:SER:HB3	2.12	0.49
1:C:61:LEU:HA	1:C:79:LEU:HD21	1.94	0.49
1:K:15:ILE:HG12	2:L:119:TYR:HA	1.95	0.49
2:B:51:LYS:HE2	1:C:29:VAL:HG11	1.94	0.49
1:I:62:GLY:O	1:I:93:SER:OG	2.20	0.49
1:A:29:VAL:HG11	2:F:51:LYS:HE2	1.94	0.49
1:C:76:CYS:HB3	1:C:79:LEU:HD12	1.94	0.49
4:V:35:TRP:CZ3	4:V:88:CYS:HB3	2.47	0.49
4:P:80:SER:HA	4:P:106:VAL:HG11	1.95	0.49
3:M:159:LEU:HD21	3:M:182:VAL:HG11	1.94	0.49
2:H:54:SER:O	2:H:58:LYS:HG2	2.13	0.49
1:C:29:VAL:HG21	2:D:102:LEU:HD23	1.95	0.49
4:P:83:GLU:HG3	4:P:104:LEU:O	2.13	0.49
2:H:125:GLN:HE22	2:H:155:GLY:HA2	1.78	0.48
1:C:293:PRO:HB3	2:D:59:MET:HG3	1.94	0.48
4:V:51:LEU:HD21	4:V:66:LYS:HG2	1.94	0.48
1:K:97:CYS:HB2	1:K:138:ALA:O	2.13	0.48
1:E:98:TYR:CD2	1:E:230:MET:HB2	2.48	0.48
4:N:39:LEU:HD23	4:N:84:ALA:HB2	1.94	0.48
1:A:156:LYS:HZ1	4:N:50[A]:SER:HG	1.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LYS:HE3	2:B:92:TRP:CE2	2.48	0.48
4:N:27(B):ASN:HD22	4:N:28:ILE:N	1.96	0.48
3:O:31:SER:O	3:O:98[B]:MET:HG3	2.14	0.48
1:E:70:LEU:HD11	1:E:112:LEU:CD1	2.44	0.48
4:V:14:SER:H	4:V:17:GLN:NE2	2.11	0.48
4:R:39:LEU:HD23	4:R:84:ALA:HB2	1.96	0.48
1:I:189:THR:HG22	3:U:97:LEU:HD23	1.95	0.48
1:I:301:THR:HB	1:I:305:CYS:SG	2.53	0.48
1:I:113:SER:O	1:I:265:SER:HB3	2.14	0.48
4:N:51:LEU:HD11	4:N:66:LYS:HB3	1.96	0.48
1:K:192:GLN:HE21	4:X:53:GLN:NE2	2.12	0.47
4:R:27(B):ASN:HD22	4:R:28:ILE:N	1.97	0.47
1:E:307:LYS:HE3	2:F:92:TRP:CE2	2.49	0.47
1:A:307:LYS:HE3	2:B:92:TRP:NE1	2.29	0.47
3:Q:193:THR:HB	3:Q:210:ARG:HD3	1.95	0.47
1:C:236:LEU:HD11	1:C:262:ARG:NH2	2.30	0.47
1:E:115:VAL:HA	1:E:261:ASN:O	2.15	0.47
3:W:39:GLN:HB2	3:W:45:LEU:HD23	1.95	0.47
4:T:26:SER:N	4:T:27(B):ASN:HD21	2.13	0.47
3:Q:36:TRP:CE2	3:Q:80:LEU:HB2	2.50	0.47
4:T:51:LEU:HD11	4:T:66:LYS:HD3	1.97	0.47
1:A:29:VAL:HG21	2:B:102:LEU:HD23	1.97	0.47
1:E:73:ASN:HB3	1:E:76:CYS:SG	2.55	0.47
3:U:47:TRP:CG	4:V:96:VAL:HB	2.50	0.47
4:T:31:TYR:CZ	4:T:91:TRP:HD1	2.32	0.47
1:A:125(A):LYS:HD2	1:A:255:TRP:CH2	2.49	0.47
3:O:29:PHE:HB3	3:O:76:ASN:HD22	1.79	0.47
1:A:196:GLN:NE2	4:N:52:ASN:OD1	2.42	0.47
1:G:29:VAL:HG21	2:H:102:LEU:HD23	1.95	0.47
1:C:71:LEU:HD22	1:C:151:LEU:HD11	1.97	0.47
4:P:25:GLY:HA3	4:P:27(B):ASN:HD21	1.79	0.46
1:A:302:ILE:HG12	2:B:66:VAL:HG12	1.97	0.46
1:K:194:LEU:HD11	3:W:100(A):TYR:CZ	2.50	0.46
1:K:174:LYS:N	1:K:239:PRO:HG3	2.29	0.46
4:N:26:SER:H	4:N:27(B):ASN:ND2	2.13	0.46
3:U:100(F):TYR:HB2	4:V:91:TRP:CZ3	2.49	0.46
4:X:26:SER:N	4:X:27(B):ASN:HD21	2.11	0.46
1:C:130:HIS:CE1	1:C:164:LEU:HB3	2.49	0.46
2:H:154:ASN:HB2	5:H:201:NAG:H82	1.96	0.46
1:A:18:HIS:HB2	2:B:20:GLY:O	2.15	0.46
4:T:27(B):ASN:HD22	4:T:28:ILE:N	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:35:TRP:HB2	4:V:48:ILE:HB	1.97	0.46
2:F:3:PHE:CE1	2:F:113:SER:HB2	2.51	0.46
3:M:185:PRO:HG2	3:M:188:SER:OG	2.15	0.46
3:Q:127:SER:HB3	3:Q:214:LYS:HD2	1.96	0.46
1:C:115:VAL:HA	1:C:261:ASN:O	2.16	0.46
4:T:14:SER:H	4:T:17:GLN:NE2	2.14	0.46
2:D:51:LYS:HE2	1:E:29:VAL:HG11	1.98	0.46
1:C:70:LEU:HD11	1:C:112:LEU:CD1	2.45	0.46
4:V:27(B):ASN:HD22	4:V:28:ILE:N	1.98	0.46
1:C:265:SER:O	2:D:66:VAL:HG21	2.16	0.46
2:H:80:LEU:N	2:J:68:LYS:HE3	2.30	0.46
3:Q:87:THR:HG23	3:Q:110:THR:HA	1.97	0.45
1:A:183:HIS:ND1	1:A:195:TYR:OH	2.49	0.45
3:Q:30:SER:O	3:Q:52(A):TYR:HB2	2.16	0.45
1:E:84:TRP:CH2	1:E:118:PHE:CE2	3.03	0.45
3:O:47:TRP:CG	4:P:96:VAL:HB	2.51	0.45
4:T:4:LEU:HB2	4:T:99:GLY:HA2	1.98	0.45
1:C:212:ARG:NH2	1:E:217:ILE:O	2.44	0.45
1:I:18:HIS:HB2	2:J:20:GLY:O	2.15	0.45
1:K:114:SER:OG	1:K:262:ARG:NH1	2.49	0.45
4:T:83:GLU:OE2	4:T:106:VAL:N	2.42	0.45
3:U:31:SER:O	3:U:98[B]:MET:HG3	2.16	0.45
3:M:164:HIS:HE1	4:N:167:GLN:HG2	1.82	0.45
1:I:29:VAL:HG21	2:J:102:LEU:HD23	1.98	0.45
1:C:64:CYS:HB2	1:C:79:LEU:HD11	1.98	0.45
3:Q:199:ASN:ND2	3:Q:206:LYS:HE2	2.31	0.45
3:M:19[A]:ARG:NH1	3:M:81:GLN:OE1	2.44	0.45
1:C:194:LEU:HD11	3:O:100(A):TYR:CZ	2.52	0.45
4:R:26:SER:N	4:R:27(B):ASN:HD21	2.12	0.45
1:A:29:VAL:CG2	2:B:102:LEU:HD23	2.47	0.45
1:G:130:HIS:CE1	1:G:164:LEU:HB3	2.52	0.45
3:W:34:MET:HB3	3:W:78:LEU:HD22	1.98	0.45
1:A:15:ILE:HD11	2:B:122:VAL:HG21	1.99	0.45
3:U:6:GLN:NE2	3:U:91:TYR:HA	2.32	0.45
1:E:29:VAL:CG2	2:F:102:LEU:HD23	2.46	0.45
4:V:35:TRP:CH2	4:V:88:CYS:HB3	2.52	0.45
2:J:158:ASP:OD1	2:J:160:PRO:HD2	2.17	0.45
4:T:59:PRO:HB2	4:T:61:ARG:HG2	1.98	0.45
3:Q:195:ILE:HG12	3:Q:210:ARG:HB2	1.98	0.45
1:C:189:THR:HG22	3:O:97:LEU:HD23	1.99	0.45
1:E:174:LYS:CA	1:E:239:PRO:HG3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54[B]:LEU:HD12	1:E:86:TYR:CD2	2.52	0.45
1:I:29:VAL:HG11	2:L:51:LYS:HE2	1.99	0.45
1:G:71:LEU:HD22	1:G:151:LEU:HD11	1.98	0.45
1:A:185:PRO:HG2	1:A:191:GLN:NE2	2.32	0.44
1:K:53:LYS:HG2	1:K:57:ALA:HA	1.99	0.44
1:A:73:ASN:HB3	1:A:76:CYS:SG	2.57	0.44
3:O:6:GLN:HE21	3:O:91:TYR:HA	1.83	0.44
1:C:100:GLY:HA3	1:C:230:MET:O	2.16	0.44
1:C:84:TRP:CH2	1:C:118:PHE:HE2	2.35	0.44
1:G:53:LYS:HG2	1:G:57:ALA:HA	1.99	0.44
2:D:125:GLN:NE2	2:D:155:GLY:HA2	2.31	0.44
1:E:15:ILE:HD11	2:F:122:VAL:HG21	1.99	0.44
1:G:29:VAL:CG2	2:H:102:LEU:HD23	2.48	0.44
1:A:71:LEU:HD22	1:A:151:LEU:HD11	1.99	0.44
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.99	0.44
3:M:154:TRP:CH2	3:M:196[B]:CYS:HB2	2.53	0.44
1:A:266:GLY:HA3	2:B:66:VAL:HG11	1.98	0.44
1:I:29:VAL:CG2	2:J:102:LEU:HD23	2.48	0.44
2:H:150:GLU:OE2	2:H:153:ARG:NH1	2.51	0.44
1:I:19:ALA:HB2	2:J:13:GLY:HA3	1.99	0.44
1:A:98:TYR:CD2	1:A:230:MET:HB2	2.53	0.44
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.99	0.44
1:E:15:ILE:HG12	2:F:119:TYR:HA	1.99	0.44
2:B:4:GLY:O	2:B:8:GLY:HA3	2.18	0.44
3:U:12:VAL:O	3:U:111:VAL:HA	2.18	0.44
1:C:111:GLN:O	1:C:262:ARG:NH1	2.51	0.44
2:F:30:GLN:HE22	2:F:146:ASP:N	2.14	0.44
3:Q:31:SER:O	3:Q:98[B]:MET:HG3	2.17	0.44
1:A:54[A]:LEU:HG	1:A:54(A):LYS:HG2	2.00	0.44
4:N:108:GLN:HB2	4:N:109:PRO:HD2	2.00	0.44
1:G:134:GLY:HA3	1:G:153:TRP:HB3	2.00	0.44
2:F:129:ASN:HD21	2:F:163:SER:HA	1.83	0.44
2:H:30:GLN:NE2	2:H:146:ASP:H	2.13	0.43
2:L:2:LEU:HD12	2:L:2:LEU:HA	1.77	0.43
4:N:120:PRO:HD2	4:N:185:TRP:CE2	2.53	0.43
4:T:83:GLU:HG3	4:T:104:LEU:O	2.17	0.43
2:H:167:LYS:O	2:H:171:GLU:HG3	2.18	0.43
1:A:225:ASP:OD1	3:M:52(A):TYR:OH	2.31	0.43
4:V:83:GLU:HG3	4:V:104:LEU:O	2.18	0.43
2:L:30:GLN:NE2	2:L:145:ASP:HB2	2.33	0.43
1:E:194:LEU:HD11	3:Q:100(A):TYR:OH	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:CYS:HA	2:F:137:CYS:HA	2.01	0.43
3:M:34:MET:HB3	3:M:78:LEU:HD22	2.00	0.43
2:H:94:TYR:CE1	2:J:59:MET:SD	3.11	0.43
1:C:69:TRP:CD1	1:C:79:LEU:HD13	2.53	0.43
2:L:158:ASP:OD1	2:L:160:PRO:HD2	2.19	0.43
3:W:19[A]:ARG:NH1	3:W:81:GLN:HB2	2.33	0.43
2:J:30:GLN:NE2	2:J:145:ASP:HB2	2.34	0.43
2:D:63:PHE:O	2:D:64:THR:C	2.56	0.43
4:T:4:LEU:HG	4:T:97[A]:VAL:HG12	2.00	0.43
4:R:4:LEU:HG	4:R:97[A]:VAL:HG12	2.00	0.43
4:V:47[A]:LEU:HD12	4:V:47[A]:LEU:HA	1.91	0.43
2:H:30:GLN:NE2	2:H:145:ASP:HB2	2.34	0.43
1:E:43:LEU:HB2	1:E:314:LEU:HB2	2.00	0.43
2:D:2:LEU:HA	2:D:2:LEU:HD12	1.88	0.43
1:G:103[B]:ILE:HG13	1:G:233:TYR:CE2	2.54	0.43
1:E:189:THR:HG22	3:Q:97:LEU:HD23	2.01	0.43
2:J:164:GLU:OE2	3:M:116:THR:HG21	2.19	0.43
1:K:29:VAL:CG2	2:L:102:LEU:HD23	2.49	0.43
1:E:58:PRO:HB3	1:E:86:TYR:CZ	2.54	0.43
4:P:51:LEU:HD21	4:P:66:LYS:HG2	2.01	0.43
2:D:30:GLN:NE2	2:D:145:ASP:HB2	2.34	0.43
1:C:308:TYR:CD2	2:D:89:LEU:HD13	2.53	0.43
4:V:38:GLN:HE21	4:V:87:TYR:HE2	1.65	0.43
1:C:268:ILE:HG23	1:C:302:ILE:HD11	2.00	0.42
1:G:189:THR:HG22	3:S:97:LEU:HD23	2.00	0.42
1:K:190:ASP:OD1	1:K:190:ASP:N	2.52	0.42
1:A:113:SER:HB3	1:A:266:GLY:HA2	2.00	0.42
2:H:76:ARG:NH2	2:J:74:GLU:OE2	2.52	0.42
1:G:185:PRO:HG2	1:G:191:GLN:NE2	2.33	0.42
2:J:129:ASN:ND2	2:J:163:SER:HA	2.33	0.42
1:I:58:PRO:HB3	1:I:86:TYR:CZ	2.54	0.42
4:P:27(B):ASN:HD22	4:P:28:ILE:N	1.96	0.42
2:H:98:LEU:HD21	2:J:99:LEU:HD13	2.01	0.42
1:A:117:SER:OG	1:A:261:ASN:ND2	2.47	0.42
3:W:29:PHE:CD2	3:W:76:ASN:HA	2.55	0.42
4:R:48:ILE:HA	4:R:53:GLN:O	2.20	0.42
2:J:107:THR:O	2:J:110:PHE:HB3	2.19	0.42
1:A:75:GLU:HG3	6:A:402:NAG:HN2	1.83	0.42
1:E:185:PRO:HG2	1:E:191:GLN:NE2	2.34	0.42
1:K:63:LYS:HE3	1:K:75:GLU:HB3	2.01	0.42
2:B:135:ASN:OD1	2:B:137:CYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:15:ARG:N	3:Q:82(C):LEU:O	2.36	0.42
3:W:36:TRP:CE2	3:W:80:LEU:HB2	2.55	0.42
1:C:115:VAL:HG11	1:C:118:PHE:HD2	1.85	0.42
1:G:133(A):LYS:HD3	3:S:100(C):HIS:CD2	2.55	0.42
4:V:27(B):ASN:O	4:V:31:TYR:N	2.42	0.42
3:Q:195:ILE:HA	3:Q:210:ARG:HA	2.02	0.42
1:K:98:TYR:CD2	1:K:230:MET:HB2	2.54	0.42
3:U:12:VAL:HG21	3:U:82(C):LEU:HD13	2.02	0.41
1:A:246:GLU:OE2	1:C:219:ALA:HB3	2.20	0.41
1:I:174:LYS:HA	1:I:239:PRO:HG3	2.01	0.41
2:B:59:MET:SD	2:D:94:TYR:CD1	3.13	0.41
3:U:30:SER:O	3:U:52(A):TYR:HB2	2.20	0.41
1:A:100:GLY:HA3	1:A:230:MET:O	2.20	0.41
1:E:186:PRO:HB2	3:Q:98[A]:MET:SD	2.60	0.41
3:Q:185:PRO:HG2	3:Q:188:SER:OG	2.19	0.41
1:G:71:LEU:O	1:G:148:TYR:HB3	2.20	0.41
3:Q:200:HIS:CD2	3:Q:202:PRO:HD2	2.55	0.41
1:A:53:LYS:HG2	1:A:57:ALA:HA	2.01	0.41
3:U:36:TRP:CE2	3:U:80:LEU:HB2	2.54	0.41
1:C:84:TRP:CH2	1:C:118:PHE:CE2	3.09	0.41
1:G:133(A):LYS:HB3	3:S:100(C):HIS:CG	2.56	0.41
1:A:301:THR:HB	1:A:305:CYS:SG	2.61	0.41
1:E:190:ASP:OD1	1:E:190:ASP:N	2.53	0.41
1:I:66[B]:ILE:HD12	1:I:109:ARG:HG2	2.02	0.41
4:R:47[A]:LEU:HD21	4:R:62:PHE:CD1	2.55	0.41
1:E:61:LEU:HD11	1:E:66[A]:ILE:HD13	2.03	0.41
1:E:174:LYS:HD2	1:E:259:ALA:HB1	2.02	0.41
1:G:301:THR:HB	1:G:305:CYS:SG	2.61	0.41
4:P:26:SER:N	4:P:27(B):ASN:HD21	2.16	0.41
1:E:87:ILE:HB	1:E:267:ILE:HG12	2.03	0.41
3:O:29:PHE:CD2	3:O:76:ASN:HA	2.56	0.41
3:W:82:MET:HE2	3:W:82(C):LEU:HD21	2.03	0.41
3:O:14:PRO:O	3:O:15:ARG:HB2	2.21	0.41
1:C:176:VAL:HA	1:C:259:ALA:HA	2.03	0.41
3:U:2:VAL:HA	3:U:25:SER:O	2.19	0.41
3:M:31:SER:O	3:M:98:MET:HG3	2.20	0.41
1:E:108:LEU:HD22	1:E:234:TRP:CD1	2.56	0.41
2:B:94:TYR:CD1	2:F:59:MET:SD	3.13	0.41
1:G:62:GLY:O	1:G:93:SER:OG	2.27	0.41
4:R:108:GLN:HB2	4:R:109:PRO:HD2	2.02	0.41
1:K:301:THR:HB	1:K:305:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:24:TYR:HE2	2:L:122:VAL:HG21	1.85	0.41
1:I:190:ASP:OD1	1:I:190:ASP:N	2.54	0.41
2:F:158:ASP:OD1	2:F:160:PRO:HD2	2.21	0.41
3:W:40:ALA:HA	3:W:88:SER:HA	2.03	0.41
1:E:156:LYS:HZ1	4:R:50[B]:SER:HB3	1.85	0.41
4:T:7:PRO:HA	4:T:8:PRO:HD3	1.94	0.41
1:A:87:ILE:HB	1:A:267:ILE:HG12	2.01	0.41
4:X:35:TRP:CZ3	4:X:88:CYS:HB3	2.56	0.41
1:K:170:ASN:ND2	1:K:237:LEU:O	2.54	0.41
2:B:120:GLU:CD	2:D:116:ARG:HH22	2.24	0.40
1:C:185:PRO:HG2	1:C:191:GLN:HE21	1.85	0.40
1:C:307:LYS:HE3	2:D:92:TRP:CD1	2.56	0.40
2:B:75:ARG:CZ	1:E:111:GLN:HE22	2.34	0.40
1:C:54[A]:LEU:HD13	1:C:86:TYR:HE2	1.87	0.40
1:I:122:GLU:HG3	1:I:256:TYR:CZ	2.55	0.40
2:L:135:ASN:OD1	2:L:137:CYS:HB2	2.21	0.40
1:E:108:LEU:HB2	1:E:234:TRP:CE2	2.57	0.40
1:I:103[B]:ILE:HG21	1:I:211:ARG:HH22	1.85	0.40
4:V:85:VAL:HA	4:V:102:THR:O	2.22	0.40
1:I:307:LYS:HE3	2:J:92:TRP:NE1	2.36	0.40
1:K:307:LYS:HD3	2:L:62:GLN:OE1	2.22	0.40
3:U:53:ASP:CG	3:U:55:ARG:HG3	2.41	0.40
3:M:6:GLN:HE21	3:M:92:CYS:N	2.16	0.40
3:M:47:TRP:CD1	4:N:96:VAL:HB	2.56	0.40
3:Q:125:ALA:HB3	3:Q:214:LYS:HE3	2.03	0.40
2:F:154:ASN:HB2	5:F:201:NAG:H82	2.04	0.40
3:S:100(F):TYR:HB2	4:T:91:TRP:CZ3	2.56	0.40
1:K:194:LEU:HD11	3:W:100(A):TYR:OH	2.22	0.40
1:G:133(A):LYS:HB3	3:S:100(C):HIS:CD2	2.57	0.40
1:E:301:THR:HB	1:E:305:CYS:SG	2.61	0.40
1:I:14:CYS:HA	2:J:137:CYS:HA	2.04	0.40
2:H:4:GLY:O	2:H:8:GLY:HA3	2.21	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:264:SER:OG	4:N:189:ARG:N[2_444]	2.17	0.03

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	330/331 (100%)	322 (98%)	8 (2%)	0	100	100
1	C	331/331 (100%)	324 (98%)	7 (2%)	0	100	100
1	E	331/331 (100%)	322 (97%)	9 (3%)	0	100	100
1	G	331/331 (100%)	324 (98%)	7 (2%)	0	100	100
1	I	331/331 (100%)	324 (98%)	7 (2%)	0	100	100
1	K	331/331 (100%)	322 (97%)	9 (3%)	0	100	100
2	B	172/176 (98%)	169 (98%)	3 (2%)	0	100	100
2	D	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
2	F	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
2	H	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
2	J	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
2	L	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
3	M	230/231 (100%)	224 (97%)	5 (2%)	1 (0%)	39	76
3	O	125/231 (54%)	123 (98%)	2 (2%)	0	100	100
3	Q	231/231 (100%)	225 (97%)	5 (2%)	1 (0%)	39	76
3	S	125/231 (54%)	123 (98%)	2 (2%)	0	100	100
3	U	125/231 (54%)	123 (98%)	2 (2%)	0	100	100
3	W	125/231 (54%)	123 (98%)	2 (2%)	0	100	100
4	N	219/217 (101%)	214 (98%)	5 (2%)	0	100	100
4	P	116/217 (54%)	113 (97%)	3 (3%)	0	100	100
4	R	219/217 (101%)	215 (98%)	4 (2%)	0	100	100
4	T	116/217 (54%)	113 (97%)	3 (3%)	0	100	100
4	V	116/217 (54%)	113 (97%)	3 (3%)	0	100	100
4	X	116/217 (54%)	113 (97%)	3 (3%)	0	100	100
All	All	4880/5730 (85%)	4779 (98%)	99 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	133	GLY
3	Q	133	GLY

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	287/285 (101%)	284 (99%)	3 (1%)	82	91
1	C	288/285 (101%)	285 (99%)	3 (1%)	82	91
1	E	288/285 (101%)	284 (99%)	4 (1%)	74	88
1	G	288/285 (101%)	285 (99%)	3 (1%)	82	91
1	I	288/285 (101%)	282 (98%)	6 (2%)	61	84
1	K	288/285 (101%)	284 (99%)	4 (1%)	74	88
2	B	149/150 (99%)	145 (97%)	4 (3%)	52	81
2	D	149/150 (99%)	147 (99%)	2 (1%)	76	89
2	F	149/150 (99%)	147 (99%)	2 (1%)	76	89
2	H	149/150 (99%)	145 (97%)	4 (3%)	52	81
2	J	149/150 (99%)	145 (97%)	4 (3%)	52	81
2	L	149/150 (99%)	147 (99%)	2 (1%)	76	89
3	M	197/196 (100%)	193 (98%)	4 (2%)	63	84
3	O	106/196 (54%)	103 (97%)	3 (3%)	51	80
3	Q	198/196 (101%)	194 (98%)	4 (2%)	63	84
3	S	106/196 (54%)	103 (97%)	3 (3%)	51	80
3	U	106/196 (54%)	103 (97%)	3 (3%)	51	80
3	W	106/196 (54%)	103 (97%)	3 (3%)	51	80
4	N	185/181 (102%)	183 (99%)	2 (1%)	80	90
4	P	97/181 (54%)	95 (98%)	2 (2%)	61	84
4	R	185/181 (102%)	183 (99%)	2 (1%)	80	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	T	97/181 (54%)	95 (98%)	2 (2%)	61	84
4	V	97/181 (54%)	95 (98%)	2 (2%)	61	84
4	X	97/181 (54%)	95 (98%)	2 (2%)	61	84
All	All	4198/4872 (86%)	4125 (98%)	73 (2%)	68	86

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	102	PHE
1	A	320	LEU
2	B	32	SER
2	B	72[A]	ASN
2	B	72[B]	ASN
2	B	128	ASN
1	C	33	ASN
1	C	102	PHE
1	C	320	LEU
2	D	32	SER
2	D	128	ASN
1	E	33	ASN
1	E	102	PHE
1	E	190	ASP
1	E	320	LEU
2	F	32	SER
2	F	128	ASN
1	G	33	ASN
1	G	102	PHE
1	G	320	LEU
2	H	32	SER
2	H	72[A]	ASN
2	H	72[B]	ASN
2	H	128	ASN
1	I	33	ASN
1	I	92[A]	ASN
1	I	92[B]	ASN
1	I	102	PHE
1	I	190	ASP
1	I	320	LEU
2	J	32	SER
2	J	72[A]	ASN

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Mol	Chain	Res	Type
2	J	72 B	ASN
2	J	128	ASN
1	K	33	ASN
1	K	102	PHE
1	K	190	ASP
1	K	320	LEU
2	L	32	SER
2	L	128	ASN
3	M	3	GLN
3	M	25	SER
3	M	88	SER
3	M	192	GLN
4	N	27(B)	ASN
4	N	53	GLN
3	O	3	GLN
3	O	25	SER
3	O	88	SER
4	P	27(B)	ASN
4	P	53	GLN
3	Q	3	GLN
3	Q	25	SER
3	Q	88	SER
3	Q	192	GLN
4	R	27(B)	ASN
4	R	53	GLN
3	S	3	GLN
3	S	25	SER
3	S	88	SER
4	T	27(B)	ASN
4	T	53	GLN
3	U	3	GLN
3	U	25	SER
3	U	88	SER
4	V	27(B)	ASN
4	V	53	GLN
3	W	3	GLN
3	W	25	SER
3	W	88	SER
4	X	27(B)	ASN
4	X	53	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	192	GLN
1	A	196	GLN
1	A	197	ASN
1	A	250	ASN
2	B	30	GLN
2	B	43	ASN
2	B	125	GLN
2	B	128	ASN
2	B	129	ASN
1	C	129	ASN
1	C	191	GLN
1	C	197	ASN
1	C	250	ASN
1	C	261	ASN
2	D	30	GLN
2	D	43	ASN
2	D	125	GLN
2	D	128	ASN
2	D	129	ASN
1	E	129	ASN
1	E	191	GLN
1	E	197	ASN
1	E	250	ASN
1	E	261	ASN
2	F	30	GLN
2	F	43	ASN
2	F	125	GLN
2	F	128	ASN
2	F	129	ASN
1	G	191	GLN
1	G	192	GLN
1	G	197	ASN
1	G	250	ASN
2	H	30	GLN
2	H	43	ASN
2	H	125	GLN
2	H	128	ASN
2	H	129	ASN
1	I	191	GLN
1	I	197	ASN
1	I	250	ASN
2	J	30	GLN

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Mol	Chain	Res	Type
2	J	43	ASN
2	J	125	GLN
2	J	128	ASN
2	J	129	ASN
1	K	191	GLN
1	K	197	ASN
1	K	250	ASN
2	L	30	GLN
2	L	43	ASN
2	L	125	GLN
2	L	128	ASN
2	L	129	ASN
3	M	3	GLN
3	M	39	GLN
3	M	164	HIS
3	M	192	GLN
4	N	17	GLN
4	N	27(B)	ASN
4	N	38	GLN
4	N	52	ASN
3	O	3	GLN
3	O	39	GLN
3	O	76	ASN
3	O	100(C)	HIS
4	P	17	GLN
4	P	27(B)	ASN
4	P	34	ASN
4	P	38	GLN
4	P	53	GLN
3	Q	3	GLN
3	Q	39	GLN
3	Q	164	HIS
3	Q	171	GLN
3	Q	192	GLN
4	R	17	GLN
4	R	27(B)	ASN
4	R	38	GLN
4	R	53	GLN
3	S	3	GLN
3	S	39	GLN
3	S	100(C)	HIS
4	T	17	GLN

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Mol	Chain	Res	Type
4	T	27(B)	ASN
4	T	38	GLN
3	U	3	GLN
3	U	39	GLN
4	V	17	GLN
4	V	27(B)	ASN
4	V	38	GLN
4	V	53	GLN
3	W	3	GLN
3	W	76	ASN
4	X	17	GLN
4	X	27(B)	ASN
4	X	53	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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	PCA	M	1	3	7,8,9	1.57	1 (14%)	9,10,12	1.99	4 (44%)
4	PCA	N	1	4	7,8,9	1.60	1 (14%)	9,10,12	2.33	6 (66%)
3	PCA	O	1	3	7,8,9	1.48	1 (14%)	9,10,12	1.90	4 (44%)
4	PCA	P	1	4	7,8,9	1.62	1 (14%)	9,10,12	2.44	5 (55%)
3	PCA	Q	1	3	7,8,9	1.46	1 (14%)	9,10,12	1.89	3 (33%)
4	PCA	R	1	4	7,8,9	1.56	1 (14%)	9,10,12	2.21	5 (55%)
3	PCA	S	1	3	7,8,9	1.55	1 (14%)	9,10,12	1.92	4 (44%)
4	PCA	T	1	4	7,8,9	1.55	1 (14%)	9,10,12	2.13	5 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PCA	U	1	3	7,8,9	1.54	1 (14%)	9,10,12	1.81	3 (33%)
4	PCA	V	1	4	7,8,9	1.59	1 (14%)	9,10,12	2.32	6 (66%)
3	PCA	W	1	3	7,8,9	1.55	1 (14%)	9,10,12	1.92	3 (33%)
4	PCA	X	1	4	7,8,9	1.51	1 (14%)	9,10,12	2.08	5 (55%)

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	PCA	M	1	3	-	0/0/11/13	0/1/1/1
4	PCA	N	1	4	-	0/0/11/13	0/1/1/1
3	PCA	O	1	3	-	0/0/11/13	0/1/1/1
4	PCA	P	1	4	-	0/0/11/13	0/1/1/1
3	PCA	Q	1	3	-	0/0/11/13	0/1/1/1
4	PCA	R	1	4	-	0/0/11/13	0/1/1/1
3	PCA	S	1	3	-	0/0/11/13	0/1/1/1
4	PCA	T	1	4	-	0/0/11/13	0/1/1/1
3	PCA	U	1	3	-	0/0/11/13	0/1/1/1
4	PCA	V	1	4	-	0/0/11/13	0/1/1/1
3	PCA	W	1	3	-	0/0/11/13	0/1/1/1
4	PCA	X	1	4	-	0/0/11/13	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	1	PCA	CD-N	3.64	1.45	1.33
3	O	1	PCA	CD-N	3.78	1.46	1.33
4	X	1	PCA	CD-N	3.86	1.46	1.33
3	U	1	PCA	CD-N	3.96	1.46	1.33
4	T	1	PCA	CD-N	3.98	1.47	1.33
4	R	1	PCA	CD-N	3.99	1.47	1.33
3	W	1	PCA	CD-N	3.99	1.47	1.33
3	S	1	PCA	CD-N	3.99	1.47	1.33
4	N	1	PCA	CD-N	4.00	1.47	1.33
3	M	1	PCA	CD-N	4.02	1.47	1.33
4	V	1	PCA	CD-N	4.03	1.47	1.33
4	P	1	PCA	CD-N	4.15	1.47	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	1	PCA	CB-CA-C	-4.35	106.81	112.76
4	N	1	PCA	CA-N-CD	-3.67	101.53	113.81
4	V	1	PCA	CA-N-CD	-3.38	102.47	113.81
4	R	1	PCA	CB-CA-C	-3.37	108.16	112.76
3	O	1	PCA	CA-N-CD	-3.22	103.02	113.81
3	Q	1	PCA	CA-N-CD	-3.21	103.04	113.81
4	P	1	PCA	CA-N-CD	-3.18	103.16	113.81
4	R	1	PCA	CA-N-CD	-3.11	103.39	113.81
3	M	1	PCA	CA-N-CD	-3.10	103.42	113.81
4	T	1	PCA	CA-N-CD	-3.09	103.44	113.81
4	V	1	PCA	OE-CD-CG	-3.09	119.90	126.81
3	S	1	PCA	CA-N-CD	-3.07	103.51	113.81
4	X	1	PCA	CA-N-CD	-3.07	103.53	113.81
4	V	1	PCA	CB-CA-C	-3.05	108.59	112.76
3	W	1	PCA	CA-N-CD	-3.04	103.62	113.81
4	P	1	PCA	OE-CD-CG	-3.02	120.07	126.81
4	N	1	PCA	OE-CD-CG	-3.01	120.08	126.81
3	U	1	PCA	CA-N-CD	-2.99	103.81	113.81
4	T	1	PCA	CB-CA-C	-2.90	108.80	112.76
4	X	1	PCA	CB-CA-C	-2.80	108.93	112.76
4	R	1	PCA	OE-CD-CG	-2.68	120.83	126.81
3	M	1	PCA	OE-CD-CG	-2.63	120.93	126.81
3	W	1	PCA	OE-CD-CG	-2.57	121.07	126.81
4	T	1	PCA	OE-CD-CG	-2.51	121.21	126.81
3	S	1	PCA	OE-CD-CG	-2.45	121.34	126.81
4	N	1	PCA	O-C-CA	-2.35	119.24	125.44
3	U	1	PCA	OE-CD-CG	-2.34	121.58	126.81
4	T	1	PCA	O-C-CA	-2.28	119.42	125.44
4	X	1	PCA	OE-CD-CG	-2.28	121.72	126.81
3	O	1	PCA	OE-CD-CG	-2.28	121.73	126.81
4	X	1	PCA	O-C-CA	-2.23	119.54	125.44
4	N	1	PCA	CB-CA-C	-2.18	109.78	112.76
3	M	1	PCA	O-C-CA	-2.18	119.69	125.44
4	V	1	PCA	O-C-CA	-2.15	119.77	125.44
3	S	1	PCA	O-C-CA	-2.14	119.78	125.44
4	P	1	PCA	O-C-CA	-2.10	119.90	125.44
4	R	1	PCA	O-C-CA	-2.02	120.09	125.44
3	O	1	PCA	CG-CD-N	2.01	115.27	108.04
4	V	1	PCA	CG-CD-N	2.13	115.71	108.04
3	Q	1	PCA	CG-CD-N	2.17	115.85	108.04
4	N	1	PCA	CG-CD-N	2.22	116.03	108.04
4	R	1	PCA	CB-CA-N	2.38	110.16	103.20
4	P	1	PCA	CB-CA-N	2.44	110.34	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	1	PCA	CB-CA-N	2.45	110.35	103.20
4	X	1	PCA	CB-CA-N	2.48	110.44	103.20
3	W	1	PCA	CB-CA-N	2.53	110.60	103.20
3	U	1	PCA	CB-CA-N	2.55	110.64	103.20
3	M	1	PCA	CB-CA-N	2.59	110.75	103.20
4	V	1	PCA	CB-CA-N	2.64	110.89	103.20
3	S	1	PCA	CB-CA-N	2.65	110.93	103.20
3	Q	1	PCA	CB-CA-N	2.75	111.23	103.20
3	O	1	PCA	CB-CA-N	2.87	111.57	103.20
4	N	1	PCA	CB-CA-N	3.07	112.17	103.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	1	PCA	1	0
3	Q	1	PCA	1	0

5.5 Carbohydrates

18 carbohydrates 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	$\# Z > 2$
6	NAG	A	402	1,6	14,14,15	0.48	0	15,19,21	1.15	3 (20%)
6	NAG	A	403	6	14,14,15	0.57	0	15,19,21	1.04	1 (6%)
6	BMA	A	404	6	11,11,12	0.66	0	14,15,17	0.74	0
6	NAG	C	402	1,6	14,14,15	0.53	0	15,19,21	0.92	1 (6%)
6	NAG	C	403	6	14,14,15	0.47	0	15,19,21	0.71	0
6	BMA	C	404	6	11,11,12	0.76	0	14,15,17	0.68	0
6	NAG	E	402	1,6	14,14,15	0.52	0	15,19,21	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	E	403	6	14,14,15	0.54	0	15,19,21	1.07	1 (6%)
6	BMA	E	404	6	11,11,12	0.71	0	14,15,17	0.74	0
6	NAG	G	402	1,6	14,14,15	0.53	0	15,19,21	0.78	0
6	NAG	G	403	6	14,14,15	0.60	0	15,19,21	1.06	2 (13%)
6	BMA	G	404	6	11,11,12	0.71	0	14,15,17	0.70	0
6	NAG	I	402	1,6	14,14,15	0.51	0	15,19,21	0.92	1 (6%)
6	NAG	I	403	6	14,14,15	0.58	0	15,19,21	1.21	1 (6%)
6	BMA	I	404	6	11,11,12	1.05	2 (18%)	14,15,17	1.54	2 (14%)
6	NAG	K	402	1,6	14,14,15	0.52	0	15,19,21	0.61	0
6	NAG	K	403	6	14,14,15	0.60	0	15,19,21	1.26	1 (6%)
6	BMA	K	404	6	11,11,12	0.81	0	14,15,17	0.72	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
6	NAG	A	402	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	403	6	-	0/6/23/26	0/1/1/1
6	BMA	A	404	6	-	0/2/19/22	0/1/1/1
6	NAG	C	402	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	403	6	-	0/6/23/26	0/1/1/1
6	BMA	C	404	6	-	0/2/19/22	0/1/1/1
6	NAG	E	402	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	403	6	-	0/6/23/26	0/1/1/1
6	BMA	E	404	6	-	0/2/19/22	0/1/1/1
6	NAG	G	402	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	403	6	-	0/6/23/26	0/1/1/1
6	BMA	G	404	6	-	0/2/19/22	0/1/1/1
6	NAG	I	402	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	403	6	-	1/6/23/26	0/1/1/1
6	BMA	I	404	6	-	0/2/19/22	0/1/1/1
6	NAG	K	402	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	403	6	-	0/6/23/26	0/1/1/1
6	BMA	K	404	6	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	404	BMA	C1-C2	2.33	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	404	BMA	C2-C3	2.44	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	402	NAG	C2-N2-C7	-2.42	119.93	123.04
6	A	402	NAG	O4-C4-C3	-2.41	104.91	110.34
6	C	402	NAG	C2-N2-C7	-2.32	120.06	123.04
6	G	403	NAG	C4-C3-C2	2.07	114.45	111.23
6	I	402	NAG	C1-O5-C5	2.17	115.00	112.25
6	A	402	NAG	C1-O5-C5	2.26	115.12	112.25
6	G	403	NAG	C3-C4-C5	2.56	114.67	110.20
6	I	404	BMA	O5-C1-C2	2.60	115.08	110.86
6	A	403	NAG	C4-C3-C2	2.82	115.61	111.23
6	E	403	NAG	C4-C3-C2	2.84	115.64	111.23
6	I	403	NAG	C4-C3-C2	3.28	116.33	111.23
6	K	403	NAG	C4-C3-C2	3.32	116.39	111.23
6	I	404	BMA	C1-C2-C3	4.01	114.28	109.54

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	403	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	402	NAG	1	0
6	G	403	NAG	1	0
6	K	402	NAG	1	0
6	K	403	NAG	1	0

5.6 Ligand geometry ⓘ

12 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
5	NAG	A	401	1	14,14,15	0.41	0	15,19,21	1.21	1 (6%)
5	NAG	B	201	2	14,14,15	0.53	0	15,19,21	0.84	1 (6%)
5	NAG	C	401	1	14,14,15	0.49	0	15,19,21	1.30	1 (6%)
5	NAG	D	201	2	14,14,15	0.50	0	15,19,21	0.66	0
5	NAG	E	401	1	14,14,15	0.56	0	15,19,21	1.00	1 (6%)
5	NAG	F	201	2	14,14,15	0.51	0	15,19,21	1.11	1 (6%)
5	NAG	G	401	1	14,14,15	0.63	0	15,19,21	0.63	0
5	NAG	H	201	2	14,14,15	0.47	0	15,19,21	0.73	0
5	NAG	I	401	1	14,14,15	0.53	0	15,19,21	1.11	1 (6%)
5	NAG	J	201	2	14,14,15	0.44	0	15,19,21	0.80	0
5	NAG	K	401	1	14,14,15	0.53	0	15,19,21	1.51	1 (6%)
5	NAG	L	201	2	14,14,15	0.46	0	15,19,21	2.45	3 (20%)

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
5	NAG	A	401	1	-	0/6/23/26	0/1/1/1
5	NAG	B	201	2	-	0/6/23/26	0/1/1/1
5	NAG	C	401	1	-	0/6/23/26	0/1/1/1
5	NAG	D	201	2	-	0/6/23/26	0/1/1/1
5	NAG	E	401	1	-	2/6/23/26	0/1/1/1
5	NAG	F	201	2	-	0/6/23/26	0/1/1/1
5	NAG	G	401	1	-	0/6/23/26	0/1/1/1
5	NAG	H	201	2	-	0/6/23/26	0/1/1/1
5	NAG	I	401	1	-	0/6/23/26	0/1/1/1
5	NAG	J	201	2	-	0/6/23/26	0/1/1/1
5	NAG	K	401	1	-	2/6/23/26	0/1/1/1
5	NAG	L	201	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	B	201	NAG	C1-O5-C5	2.12	114.93	112.25
5	L	201	NAG	O3-C3-C2	2.22	113.52	109.11
5	E	401	NAG	C1-O5-C5	2.73	115.71	112.25
5	L	201	NAG	C2-N2-C7	2.83	126.68	123.04
5	F	201	NAG	C1-O5-C5	3.62	116.85	112.25
5	I	401	NAG	C1-O5-C5	3.77	117.04	112.25
5	A	401	NAG	C1-O5-C5	3.82	117.09	112.25
5	C	401	NAG	C1-O5-C5	4.64	118.13	112.25
5	K	401	NAG	C1-O5-C5	4.99	118.58	112.25
5	L	201	NAG	C1-O5-C5	8.52	123.06	112.25

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	401	NAG	C8-C7-N2-C2
5	K	401	NAG	O7-C7-N2-C2
5	K	401	NAG	C8-C7-N2-C2
5	E	401	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	201	NAG	1	0
5	H	201	NAG	1	0
5	L	201	NAG	1	0

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	325/331 (98%)	0.60	19 (5%) 26 21	43, 86, 149, 213	0
1	C	325/331 (98%)	0.42	20 (6%) 24 19	31, 71, 134, 219	0
1	E	325/331 (98%)	0.48	14 (4%) 39 32	37, 74, 129, 199	0
1	G	325/331 (98%)	0.48	19 (5%) 26 21	60, 104, 146, 175	0
1	I	325/331 (98%)	0.55	43 (13%) 4 3	65, 109, 151, 202	0
1	K	325/331 (98%)	0.43	28 (8%) 13 10	62, 100, 134, 148	0
2	B	171/176 (97%)	0.59	13 (7%) 17 14	43, 107, 161, 207	0
2	D	171/176 (97%)	0.71	13 (7%) 17 14	33, 109, 150, 171	0
2	F	171/176 (97%)	0.55	12 (7%) 19 16	37, 102, 155, 189	0
2	H	171/176 (97%)	0.90	28 (16%) 2 2	58, 102, 152, 206	0
2	J	171/176 (97%)	0.83	20 (11%) 6 5	53, 109, 154, 177	0
2	L	171/176 (97%)	0.73	18 (10%) 8 7	46, 99, 139, 172	0
3	M	227/231 (98%)	0.44	18 (7%) 15 12	49, 90, 151, 210	0
3	O	124/231 (53%)	0.72	17 (13%) 4 3	62, 113, 148, 161	0
3	Q	227/231 (98%)	1.26	55 (24%) 1 1	67, 135, 212, 241	0
3	S	124/231 (53%)	0.84	20 (16%) 3 2	100, 143, 179, 191	0
3	U	124/231 (53%)	1.14	22 (17%) 2 1	98, 141, 183, 213	0
3	W	124/231 (53%)	0.68	18 (14%) 3 3	101, 132, 164, 180	0
4	N	213/217 (98%)	0.40	18 (8%) 13 10	46, 77, 116, 156	0
4	P	110/217 (50%)	0.81	20 (18%) 2 1	73, 119, 158, 165	0
4	R	213/217 (98%)	1.03	52 (24%) 1 1	80, 156, 205, 251	0
4	T	110/217 (50%)	1.13	29 (26%) 1 1	113, 160, 179, 215	0
4	V	110/217 (50%)	1.80	39 (35%) 0 1	137, 171, 215, 247	0
4	X	110/217 (50%)	1.04	29 (26%) 1 1	112, 148, 185, 222	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4792/5730 (83%)	0.70	584 (12%) 5 4	31, 106, 176, 251	0

All (584) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	V	89	ALA	16.4
3	Q	130	SER	13.9
3	Q	129	LYS	12.3
1	A	264(A)	GLY	12.1
3	Q	126	PRO	10.4
4	V	90	ALA	10.2
4	V	21	ILE	10.1
3	U	93	ALA	9.6
4	V	22	SER	8.9
4	V	86	TYR	8.6
4	R	2	PRO	8.2
4	T	86	TYR	8.0
1	G	264(A)	GLY	7.7
3	Q	132	SER	7.2
3	U	18	LEU	7.2
4	V	82	ASP	7.0
3	Q	119	PRO	6.9
1	E	79	LEU	6.8
2	H	1	GLY	6.7
4	V	36	TYR	6.6
3	Q	184	VAL	6.5
4	V	19[A]	VAL	6.4
3	S	100(F)	TYR	6.0
3	U	112	SER	6.0
3	Q	127	SER	6.0
3	Q	138	LEU	5.9
4	V	34	ASN	5.8
3	U	17	SER	5.8
4	X	19[A]	VAL	5.7
4	V	13	GLY	5.6
3	Q	100(F)	TYR	5.6
4	X	106(A)	LEU	5.4
4	V	20	THR	5.4
1	C	114	SER	5.3
1	K	302	ILE	5.3
1	I	210	ASN	5.3
2	L	64	THR	5.3

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Mol	Chain	Res	Type	RSRZ
3	Q	194	TYR	5.2
4	X	62	PHE	5.2
3	Q	131	THR	5.2
3	O	10	GLY	5.1
4	V	75	ILE	5.1
4	X	75	ILE	5.1
4	V	80	SER	5.0
4	N	104	LEU	5.0
1	G	280	LYS	5.0
4	V	97[A]	VAL	5.0
4	R	191	TYR	5.0
4	V	37	GLN	4.9
4	T	106(A)	LEU	4.9
3	O	82	MET	4.9
4	T	97[A]	VAL	4.9
4	R	106(A)	LEU	4.9
2	J	117	ASN	4.9
3	U	81	GLN	4.8
2	L	21	TRP	4.8
4	T	82	ASP	4.8
2	D	138	PHE	4.8
3	M	131	THR	4.7
2	L	24	TYR	4.7
3	Q	183	THR	4.7
3	Q	142	VAL	4.7
4	V	33	VAL	4.7
1	G	301	THR	4.7
2	H	4	GLY	4.7
4	R	185	TRP	4.6
4	R	28	ILE	4.6
4	V	88	CYS	4.6
2	F	157	TYR	4.6
4	V	98	PHE	4.6
4	T	2	PRO	4.6
3	O	9	GLY	4.6
3	M	132	SER	4.6
2	H	64	THR	4.6
4	X	14	SER	4.6
3	W	112	SER	4.5
3	Q	128	SER	4.5
2	L	1	GLY	4.5
1	A	9	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
4	T	47[A]	LEU	4.4
2	D	141	TYR	4.4
4	R	125	LEU	4.4
4	R	133	VAL	4.4
2	D	143	LYS	4.4
2	J	23	GLY	4.4
3	S	36	TRP	4.4
4	R	90	ALA	4.4
3	Q	144	ASP	4.4
2	H	72[A]	ASN	4.3
4	R	118	PHE	4.3
3	S	9	GLY	4.3
3	W	78	LEU	4.3
4	R	193	CYS	4.3
4	T	104	LEU	4.3
3	S	100(H)	PRO	4.3
4	P	106(A)	LEU	4.3
4	X	47[A]	LEU	4.3
3	Q	182	VAL	4.3
1	A	302	ILE	4.2
4	V	44	PRO	4.2
2	H	62	GLN	4.2
3	S	90	TYR	4.2
1	I	302	ILE	4.2
2	F	17	MET	4.2
2	B	144	CYS	4.2
4	X	78[A]	LEU	4.2
3	U	45	LEU	4.2
3	O	11	VAL	4.2
4	R	107	GLY	4.1
4	V	73	LEU	4.1
4	X	86	TYR	4.1
4	R	19[A]	VAL	4.1
4	X	73	LEU	4.1
4	T	40	PRO	4.1
2	H	65	ALA	4.1
4	X	18	ARG	4.0
2	D	140	PHE	4.0
1	I	304	GLU	4.0
4	N	91	TRP	4.0
4	V	35	TRP	4.0
2	J	140	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	302	ILE	4.0
2	B	140	PHE	4.0
1	G	54[A]	LEU	4.0
4	V	83	GLU	4.0
3	O	82(A)	ASN	4.0
1	I	16	GLY	4.0
3	Q	143	LYS	3.9
4	X	21	ILE	3.9
1	G	302	ILE	3.9
4	R	106	VAL	3.9
2	B	72[A]	ASN	3.9
2	D	1	GLY	3.9
4	R	146	VAL	3.9
1	A	264	SER	3.9
3	Q	207	VAL	3.8
2	B	67	GLY	3.8
4	X	13	GLY	3.8
3	Q	120	SER	3.8
4	R	174	ALA	3.8
4	V	2	PRO	3.8
3	Q	214	LYS	3.8
1	G	279	THR	3.8
4	V	106	VAL	3.7
4	R	132	LEU	3.7
4	R	129	LYS	3.7
1	E	80	LEU	3.7
2	J	66	VAL	3.7
3	Q	159	LEU	3.7
3	W	18	LEU	3.7
1	A	13	ILE	3.7
3	U	34	MET	3.7
3	O	18	LEU	3.7
3	Q	185	PRO	3.7
3	U	48	VAL	3.7
4	P	2	PRO	3.7
4	V	106(A)	LEU	3.7
2	J	27	GLN	3.7
1	K	264(A)	GLY	3.7
4	R	98	PHE	3.6
3	Q	67	PHE	3.6
4	V	104	LEU	3.6
2	D	144	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
2	J	67	GLY	3.6
2	F	64	THR	3.6
1	K	257	ALA	3.6
2	B	134	GLY	3.6
4	T	91	TRP	3.6
4	N	51	LEU	3.6
4	N	142	GLY	3.6
3	Q	51	ILE	3.6
1	G	288	ILE	3.5
1	I	79	LEU	3.5
3	M	100(F)	TYR	3.5
3	Q	188	SER	3.5
4	N	47[A]	LEU	3.5
4	P	47[A]	LEU	3.5
4	V	28	ILE	3.5
3	Q	125	ALA	3.5
3	S	103	TRP	3.5
2	H	140	PHE	3.5
3	W	45	LEU	3.5
4	P	73	LEU	3.5
4	V	47[A]	LEU	3.5
3	S	105	GLN	3.5
2	H	112	ASP	3.5
2	J	144	CYS	3.5
3	Q	137	ALA	3.5
3	Q	121	VAL	3.5
4	V	87	TYR	3.5
1	C	13	ILE	3.5
3	W	36	TRP	3.5
1	A	288	ILE	3.4
1	K	260	LEU	3.4
4	N	19[A]	VAL	3.4
1	I	301	THR	3.4
3	M	189	LEU	3.4
3	Q	161	SER	3.4
3	M	140[A]	CYS	3.4
4	V	11	ALA	3.4
4	T	78[A]	LEU	3.4
4	R	12	SER	3.4
4	V	12	SER	3.4
4	T	99	GLY	3.4
3	S	38	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
2	L	153	ARG	3.4
1	A	25	THR	3.4
1	A	303	GLY	3.3
3	W	34	MET	3.3
1	I	61	LEU	3.3
2	H	117	ASN	3.3
2	L	66	VAL	3.3
4	R	149	LYS	3.3
3	Q	177	SER	3.3
3	Q	154	TRP	3.3
2	B	1	GLY	3.3
2	L	23	GLY	3.3
2	H	114	ASN	3.3
3	Q	50	VAL	3.3
4	T	35	TRP	3.3
3	O	82(C)	LEU	3.3
4	N	105	THR	3.3
1	I	15	ILE	3.3
4	X	35	TRP	3.3
3	Q	2	VAL	3.3
4	P	13	GLY	3.3
3	W	93	ALA	3.3
2	B	23	GLY	3.3
1	C	302	ILE	3.3
2	F	67	GLY	3.3
1	A	11	ASP	3.3
2	J	114	ASN	3.2
3	Q	133	GLY	3.2
4	P	105	THR	3.2
2	D	35	ALA	3.2
2	J	106	ARG	3.2
2	J	17	MET	3.2
1	I	51	LEU	3.2
4	T	21	ILE	3.2
3	O	103	TRP	3.2
3	Q	112	SER	3.2
1	C	79	LEU	3.2
2	H	148	CYS	3.2
1	K	58	PRO	3.2
4	R	104	LEU	3.2
4	R	192	SER	3.2
3	Q	145	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
4	P	80	SER	3.1
4	X	22	SER	3.1
4	N	35	TRP	3.1
1	K	219	ALA	3.1
4	P	86	TYR	3.1
2	H	8	GLY	3.1
2	H	113	SER	3.1
2	J	32	SER	3.1
3	Q	82(C)	LEU	3.1
3	Q	59	TYR	3.1
4	R	21	ILE	3.1
1	A	24	ASP	3.1
4	P	82	ASP	3.1
4	X	48	ILE	3.1
3	U	82	MET	3.1
2	H	109	ASP	3.1
3	Q	155	ASN	3.1
4	N	106	VAL	3.1
3	U	20	LEU	3.1
1	C	264(A)	GLY	3.1
3	Q	8	GLY	3.1
1	I	214[A]	THR	3.1
4	R	175	SER	3.1
4	P	3	VAL	3.1
4	R	195	VAL	3.1
1	I	69	TRP	3.0
4	R	148	TRP	3.0
4	R	105	THR	3.0
4	T	33	VAL	3.0
3	S	82(C)	LEU	3.0
1	C	115	VAL	3.0
2	B	17	MET	3.0
3	S	82	MET	3.0
4	P	35	TRP	3.0
4	R	117	LEU	3.0
4	P	21	ILE	3.0
1	C	289	ASN	2.9
4	T	19[A]	VAL	2.9
4	N	86	TYR	2.9
4	R	178	LEU	2.9
2	H	66	VAL	2.9
2	B	62	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
3	W	37	VAL	2.9
1	I	264(A)	GLY	2.9
4	R	155	VAL	2.9
4	T	46	LEU	2.9
4	R	13	GLY	2.9
4	R	83	GLU	2.9
2	L	144	CYS	2.9
2	H	67	GLY	2.9
4	R	207	ALA	2.9
3	O	80	LEU	2.9
4	T	88	CYS	2.9
2	H	21	TRP	2.8
4	T	23	CYS	2.8
2	J	26	HIS	2.8
4	R	116	THR	2.8
2	F	66	VAL	2.8
3	U	90	TYR	2.8
1	I	260	LEU	2.8
4	X	12	SER	2.8
3	W	48	VAL	2.8
2	L	157	TYR	2.8
4	X	64	GLY	2.8
4	X	90	ALA	2.8
1	K	152	LEU	2.8
4	R	78[A]	LEU	2.8
3	S	27	PHE	2.8
4	P	98	PHE	2.8
4	R	22	SER	2.8
1	I	71	LEU	2.8
3	Q	211	VAL	2.8
4	V	3	VAL	2.8
2	B	66	VAL	2.8
2	F	27	GLN	2.8
1	K	194	LEU	2.8
3	S	20	LEU	2.8
3	M	198	VAL	2.8
1	C	10	GLY	2.8
1	I	13	ILE	2.8
3	O	20	LEU	2.8
3	W	27	PHE	2.8
3	W	79	TYR	2.7
4	R	23	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
3	S	80	LEU	2.7
4	X	50[A]	SER	2.7
2	H	3	PHE	2.7
3	U	82(A)	ASN	2.7
2	H	139	GLU	2.7
4	X	97[A]	VAL	2.7
4	V	91	TRP	2.7
1	K	282	GLN	2.7
3	M	196[A]	CYS	2.7
4	P	88	CYS	2.7
3	U	12	VAL	2.7
3	U	98[A]	MET	2.7
2	F	23	GLY	2.7
2	H	106	ARG	2.7
2	J	113	SER	2.7
4	R	14	SER	2.7
1	E	115	VAL	2.7
1	K	54[A]	LEU	2.7
3	Q	169[A]	VAL	2.7
4	T	36	TYR	2.7
3	U	49	ALA	2.7
4	T	90	ALA	2.7
4	T	73	LEU	2.7
2	F	21	TRP	2.7
3	Q	100(A)	TYR	2.7
4	T	89	ALA	2.7
4	P	104	LEU	2.6
3	U	100(F)	TYR	2.6
1	G	264	SER	2.6
3	U	86	ASP	2.6
3	Q	18	LEU	2.6
1	I	118	PHE	2.6
1	I	9	PRO	2.6
2	D	64	THR	2.6
4	T	4	LEU	2.6
1	K	15	ILE	2.6
1	K	86	TYR	2.6
2	L	36	ALA	2.6
3	S	82(A)	ASN	2.6
4	V	4	LEU	2.6
2	L	106	ARG	2.6
1	C	214[A]	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	211	ARG	2.6
3	W	50	VAL	2.6
1	E	211	ARG	2.5
4	N	73	LEU	2.5
4	N	33	VAL	2.5
4	R	86	TYR	2.5
2	H	116	ARG	2.5
4	X	104	LEU	2.5
2	D	21	TRP	2.5
3	U	15	ARG	2.5
3	W	100(F)	TYR	2.5
3	Q	118	GLY	2.5
4	R	75	ILE	2.5
1	E	212	ARG	2.5
1	I	125(A)	LYS	2.5
1	I	152	LEU	2.5
1	C	262	ARG	2.5
2	D	142	HIS	2.5
3	W	100(A)	TYR	2.5
3	U	8	GLY	2.5
3	U	100(H)	PRO	2.5
3	S	58	TYR	2.5
2	F	144	CYS	2.5
1	A	265	SER	2.5
3	O	36	TRP	2.5
4	R	73	LEU	2.5
4	T	50[A]	SER	2.5
1	G	16	GLY	2.5
2	B	63	PHE	2.5
2	B	143	LYS	2.5
2	L	4	GLY	2.5
1	C	323	ILE	2.5
2	L	140	PHE	2.5
3	Q	196[A]	CYS	2.5
1	K	191	GLN	2.5
1	K	16	GLY	2.5
3	O	100(H)	PRO	2.5
2	D	126	LEU	2.5
3	S	50	VAL	2.5
4	N	78[A]	LEU	2.5
1	I	52	CYS	2.4
4	P	14	SER	2.4

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Mol	Chain	Res	Type	RSRZ
4	T	20	THR	2.4
4	R	47[A]	LEU	2.4
4	T	3	VAL	2.4
4	R	89	ALA	2.4
1	E	199	ASP	2.4
3	Q	60	ALA	2.4
2	L	35	ALA	2.4
1	I	17	TYR	2.4
3	S	91	TYR	2.4
4	R	111	ALA	2.4
3	O	90	TYR	2.4
1	K	9	PRO	2.4
1	G	281	CYS	2.4
1	I	154	LEU	2.4
2	J	102	LEU	2.4
1	I	288	ILE	2.4
3	Q	195	ILE	2.4
4	R	91	TRP	2.4
3	S	8	GLY	2.4
1	A	318	THR	2.4
3	U	100(A)	TYR	2.4
3	M	159	LEU	2.4
1	K	303	GLY	2.4
1	K	245	PHE	2.4
3	M	80	LEU	2.4
3	M	194	TYR	2.4
4	T	11	ALA	2.4
1	K	118	PHE	2.4
3	M	163	VAL	2.4
1	E	61	LEU	2.3
1	K	18	HIS	2.3
1	G	86	TYR	2.3
1	I	191	GLN	2.3
3	Q	208	ASP	2.3
3	O	19[A]	ARG	2.3
1	I	305	CYS	2.3
4	T	44	PRO	2.3
4	P	78[A]	LEU	2.3
1	E	16	GLY	2.3
1	E	264(A)	GLY	2.3
2	H	71	ASN	2.3
3	Q	98[A]	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	313	LYS	2.3
1	E	54[A]	LEU	2.3
4	N	75	ILE	2.3
4	P	106	VAL	2.3
1	G	84	TRP	2.3
1	I	277	CYS	2.3
1	I	282	GLN	2.3
1	C	267	ILE	2.3
3	W	24	ALA	2.3
2	L	17	MET	2.3
1	I	212	ARG	2.3
2	D	22	TYR	2.3
2	B	149	MET	2.3
3	M	34	MET	2.3
1	G	154	LEU	2.3
2	L	138	PHE	2.3
3	M	29	PHE	2.3
1	E	210	ASN	2.3
4	N	97[A]	VAL	2.3
2	F	22	TYR	2.3
2	D	30	GLN	2.3
1	I	265	SER	2.3
1	G	104	ASP	2.2
1	I	55	GLY	2.2
4	R	150	ALA	2.2
1	C	324	PRO	2.2
1	E	59	LEU	2.2
1	K	288	ILE	2.2
1	A	214[A]	THR	2.2
4	X	103	LYS	2.2
1	C	51	LEU	2.2
3	Q	176	TYR	2.2
1	I	50	LYS	2.2
3	O	93	ALA	2.2
4	N	83	GLU	2.2
1	I	213	PHE	2.2
4	N	64	GLY	2.2
4	X	98	PHE	2.2
4	X	9	SER	2.2
2	J	118	LEU	2.2
3	S	45	LEU	2.2
4	X	51	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	66[A]	ILE	2.2
2	H	157	TYR	2.2
4	R	140	TYR	2.2
4	X	87	TYR	2.2
3	Q	100(H)	PRO	2.2
1	C	15	ILE	2.2
3	M	182	VAL	2.2
3	U	7	SER	2.2
3	S	24	ALA	2.2
4	R	131	THR	2.2
2	H	2	LEU	2.2
1	I	54[A]	LEU	2.2
4	V	14	SER	2.2
4	N	32	THR	2.2
1	I	220	ARG	2.2
1	A	304	GLU	2.1
4	V	45	LYS	2.1
1	G	57	ALA	2.1
4	V	62	PHE	2.1
2	J	1	GLY	2.1
2	J	64	THR	2.1
2	F	62	GLN	2.1
3	O	27	PHE	2.1
3	W	20	LEU	2.1
2	H	107	THR	2.1
2	H	126	LEU	2.1
3	M	150	VAL	2.1
1	I	281	CYS	2.1
4	X	82	ASP	2.1
1	K	59	LEU	2.1
4	P	89	ALA	2.1
1	K	252	ILE	2.1
4	X	83	GLU	2.1
4	R	141	PRO	2.1
4	R	182	PRO	2.1
4	X	36	TYR	2.1
1	I	14	CYS	2.1
1	C	87	ILE	2.1
1	I	270	SER	2.1
3	W	91	TYR	2.1
4	R	186	LYS	2.1
2	H	5	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	M	136	ALA	2.1
2	J	29	GLU	2.1
3	M	36	TRP	2.1
4	R	25	GLY	2.1
3	O	112	SER	2.1
2	L	67	GLY	2.1
3	M	100(H)	PRO	2.1
1	A	198	ALA	2.1
3	Q	156	SER	2.1
1	E	119	GLU	2.1
2	F	29	GLU	2.1
1	K	153	TRP	2.1
1	I	209	TYR	2.1
1	A	216	GLU	2.1
4	T	12	SER	2.1
2	H	63	PHE	2.1
1	K	168	TYR	2.1
1	G	304	GLU	2.1
3	W	103	TRP	2.1
4	V	105	THR	2.1
1	A	215	PRO	2.1
1	G	58	PRO	2.1
1	I	303	GLY	2.1
3	Q	212	GLU	2.1
1	K	123	ILE	2.0
2	J	18	ILE	2.0
1	C	61	LEU	2.0
1	I	102	PHE	2.0
2	L	126	LEU	2.0
1	C	127	TRP	2.0
1	K	69	TRP	2.0
1	K	119	GLU	2.0
1	A	15	ILE	2.0
1	I	268	ILE	2.0
1	C	112	LEU	2.0
4	V	51	LEU	2.0
1	G	225	ASP	2.0
1	K	127	TRP	2.0
3	Q	47	TRP	2.0
1	G	277	CYS	2.0
1	I	179	LEU	2.0
4	P	23	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	J	20	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	PCA	N	1	8/9	0.68	0.26	-	172,194,204,208	0
4	PCA	P	1	8/9	0.70	0.60	-	124,132,163,169	0
4	PCA	R	1	8/9	0.41	0.53	-	203,208,217,222	0
3	PCA	M	1	8/9	0.69	0.29	-	120,132,139,146	0
4	PCA	T	1	8/9	0.71	0.33	-	193,201,222,228	0
4	PCA	V	1	8/9	0.58	0.34	-	206,209,213,215	0
4	PCA	X	1	8/9	0.66	0.41	-	207,212,215,218	0
3	PCA	U	1	8/9	0.89	0.15	-	170,178,182,187	0
3	PCA	O	1	8/9	0.84	0.14	-	151,153,157,160	0
3	PCA	S	1	8/9	0.55	0.37	-	199,209,211,212	0
3	PCA	W	1	8/9	0.91	0.14	-	195,198,202,208	0
3	PCA	Q	1	8/9	0.74	0.56	-	155,160,163,164	0

6.3 Carbohydrates [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	K	402	14/15	0.94	0.23	0.20	65,106,114,116	0
6	NAG	E	402	14/15	0.90	0.22	0.14	50,70,80,81	0
6	NAG	A	402	14/15	0.90	0.30	0.11	99,109,118,126	0
6	NAG	C	402	14/15	0.92	0.23	-0.14	62,79,94,98	0
6	NAG	G	402	14/15	0.94	0.15	-0.87	78,90,99,99	0
6	NAG	I	402	14/15	0.93	0.13	-1.14	78,102,106,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	BMA	K	404	11/12	0.87	0.21	-	122,132,138,140	0
6	BMA	E	404	11/12	0.68	0.46	-	122,134,154,160	0
6	BMA	I	404	11/12	0.89	0.28	-	99,117,171,172	0
6	BMA	C	404	11/12	0.86	0.23	-	83,104,113,124	0
6	NAG	E	403	14/15	0.91	0.20	-	67,77,90,107	0
6	BMA	A	404	11/12	0.82	0.14	-	101,127,129,135	0
6	NAG	I	403	14/15	0.91	0.16	-	100,126,130,138	0
6	NAG	G	403	14/15	0.93	0.14	-	108,124,132,133	0
6	NAG	K	403	14/15	0.90	0.20	-	116,120,133,135	0
6	NAG	A	403	14/15	0.89	0.32	-	107,118,131,133	0
6	BMA	G	404	11/12	0.84	0.20	-	114,120,128,131	0
6	NAG	C	403	14/15	0.89	0.20	-	96,100,107,110	0

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	D	201	14/15	0.77	0.27	-	139,164,173,176	0
5	NAG	A	401	14/15	0.74	0.39	-	152,185,198,200	0
5	NAG	B	201	14/15	0.71	0.41	-	153,170,177,180	0
5	NAG	K	401	14/15	0.87	0.25	-	116,156,174,182	0
5	NAG	E	401	14/15	0.75	0.26	-	186,209,213,218	0
5	NAG	C	401	14/15	0.76	0.28	-	151,163,173,176	0
5	NAG	L	201	14/15	0.78	0.38	-	140,174,180,183	0
5	NAG	I	401	14/15	0.58	0.58	-	179,188,220,226	0
5	NAG	J	201	14/15	0.64	0.44	-	122,141,152,153	0
5	NAG	H	201	14/15	0.74	0.38	-	135,152,165,168	0
5	NAG	F	201	14/15	0.59	0.33	-	163,181,186,191	0
5	NAG	G	401	14/15	0.81	0.19	-	175,184,195,196	0

6.5 Other polymers ⓘ

There are no such residues in this entry.