



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:03 PM GMT

PDB ID : 3SM5
Title : Influenza hemagglutinin in complex with a neutralizing antibody
Authors : Whittle, J.R.R.; Harrison, S.C.
Deposited on : 2011-06-27
Resolution : 3.19 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

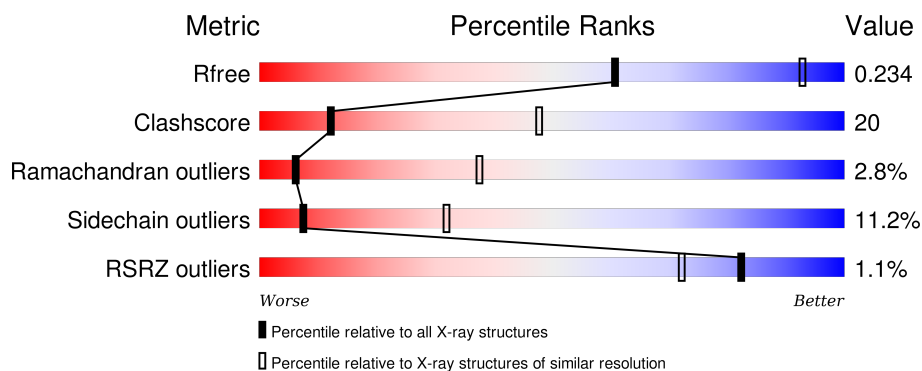
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	327	<div> <div>2%</div> <div> <div>61%</div> <div>32%</div> <div>6%</div> </div> </div>
1	C	327	<div> <div>61%</div> <div>31%</div> <div>6%</div> </div>
1	E	327	<div> <div>58%</div> <div>34%</div> <div>6%</div> </div>
2	B	182	<div> <div>2%</div> <div> <div>50%</div> <div>34%</div> <div>10%</div> <div>5%</div> </div> </div>
2	D	182	<div> <div>5%</div> <div> <div>48%</div> <div>36%</div> <div>10%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	182	
3	H	227	
3	I	227	
3	J	227	
4	L	211	
4	M	211	
4	N	211	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	E	351	X	-	-	-
9	SO4	C	334	-	-	X	-
9	SO4	C	340	-	-	X	-
9	SO4	C	343	-	-	-	X
9	SO4	E	335	-	-	-	X
9	SO4	E	342	-	-	-	X
9	SO4	E	344	-	-	X	-
9	SO4	E	346	-	-	-	X
9	SO4	I	229	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22009 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	323	Total	C	N	O	S	0	0	0
			2535	1597	441	486	11			
1	C	323	Total	C	N	O	S	0	0	0
			2535	1597	441	486	11			
1	E	323	Total	C	N	O	S	0	0	0
			2535	1597	441	486	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLU	-	EXPRESSION TAG	UNP A7UPX0
C	4	GLU	-	EXPRESSION TAG	UNP A7UPX0
E	4	GLU	-	EXPRESSION TAG	UNP A7UPX0

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1391	871	238	275	7			
2	D	173	Total	C	N	O	S	0	0	0
			1391	871	238	275	7			
2	F	173	Total	C	N	O	S	0	0	0
			1391	871	238	275	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	677	ARG	-	EXPRESSION TAG	UNP C5H943
B	678	SER	-	EXPRESSION TAG	UNP C5H943
B	679	LEU	-	EXPRESSION TAG	UNP C5H943
B	680	VAL	-	EXPRESSION TAG	UNP C5H943
B	681	PRO	-	EXPRESSION TAG	UNP C5H943

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Chain	Residue	Modelled	Actual	Comment	Reference
B	682	ARG	-	EXPRESSION TAG	UNP C5H943
D	677	ARG	-	EXPRESSION TAG	UNP C5H943
D	678	SER	-	EXPRESSION TAG	UNP C5H943
D	679	LEU	-	EXPRESSION TAG	UNP C5H943
D	680	VAL	-	EXPRESSION TAG	UNP C5H943
D	681	PRO	-	EXPRESSION TAG	UNP C5H943
D	682	ARG	-	EXPRESSION TAG	UNP C5H943
F	677	ARG	-	EXPRESSION TAG	UNP C5H943
F	678	SER	-	EXPRESSION TAG	UNP C5H943
F	679	LEU	-	EXPRESSION TAG	UNP C5H943
F	680	VAL	-	EXPRESSION TAG	UNP C5H943
F	681	PRO	-	EXPRESSION TAG	UNP C5H943
F	682	ARG	-	EXPRESSION TAG	UNP C5H943

- Molecule 3 is a protein called CH65, heavy chain, Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	221	Total	C	N	O	S	0	0	0
			1673	1059	278	328	8			
3	I	221	Total	C	N	O	S	0	0	0
			1673	1059	278	328	8			
3	J	221	Total	C	N	O	S	0	0	0
			1673	1059	278	328	8			

- Molecule 4 is a protein called CH65, light chain, Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	210	Total	C	N	O	S	0	0	0
			1565	973	269	318	5			
4	M	210	Total	C	N	O	S	0	0	0
			1565	973	269	318	5			
4	N	210	Total	C	N	O	S	0	0	0
			1565	973	269	318	5			

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

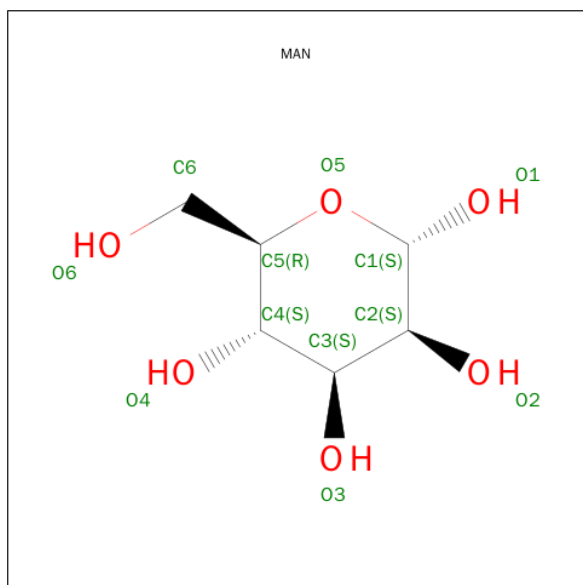
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	A	2	Total	C	N	O	0	0
			28	16	2	10		

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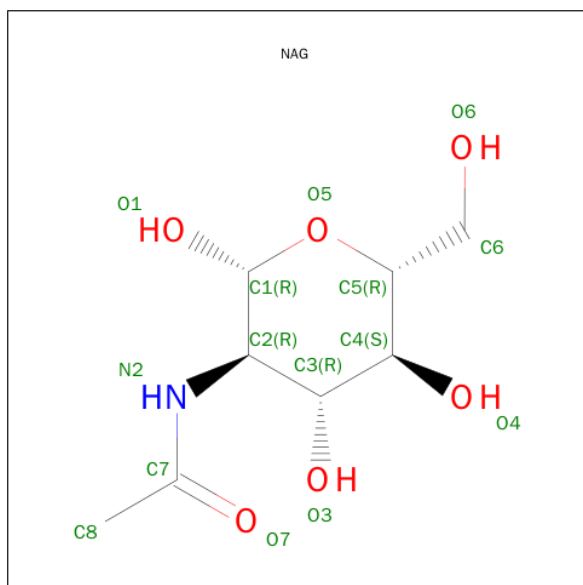
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	2	Total	C	N	O	0	0
			28	16	2	10		
5	C	2	Total	C	N	O	0	0
			28	16	2	10		
5	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

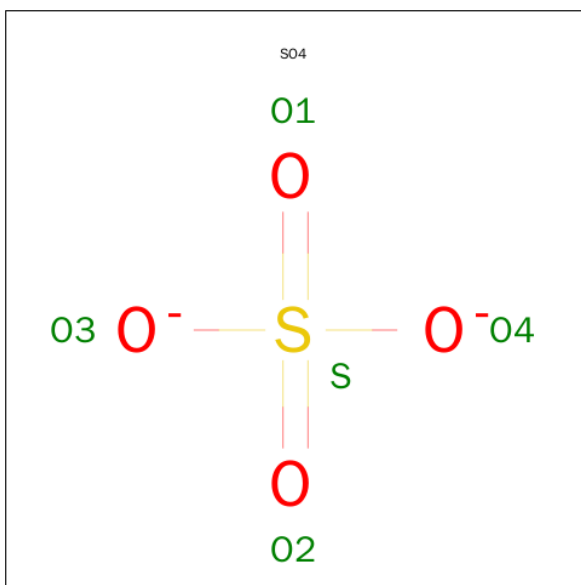


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1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

- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	H	1	Total	O	S	0	0
			5	4	1		
9	J	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	I	1	Total	O	S	0	0
			5	4	1		
9	H	1	Total	O	S	0	0
			5	4	1		
9	I	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	N	1	Total	O	S	0	0
			5	4	1		
9	J	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total 5	O 4	S 1	0	0
9	C	1	Total 5	O 4	S 1	0	0
9	E	1	Total 5	O 4	S 1	0	0
9	E	1	Total 5	O 4	S 1	0	0
9	A	1	Total 5	O 4	S 1	0	0
9	H	1	Total 5	O 4	S 1	0	0
9	N	1	Total 5	O 4	S 1	0	0
9	L	1	Total 5	O 4	S 1	0	0
9	E	1	Total 5	O 4	S 1	0	0
9	A	1	Total 5	O 4	S 1	0	0
9	M	1	Total 5	O 4	S 1	0	0
9	C	1	Total 5	O 4	S 1	0	0
9	A	1	Total 5	O 4	S 1	0	0
9	C	1	Total 5	O 4	S 1	0	0
9	I	1	Total 5	O 4	S 1	0	0
9	E	1	Total 5	O 4	S 1	0	0
9	E	1	Total 5	O 4	S 1	0	0
9	E	1	Total 5	O 4	S 1	0	0
9	L	1	Total 5	O 4	S 1	0	0
9	N	1	Total 5	O 4	S 1	0	0
9	A	1	Total 5	O 4	S 1	0	0

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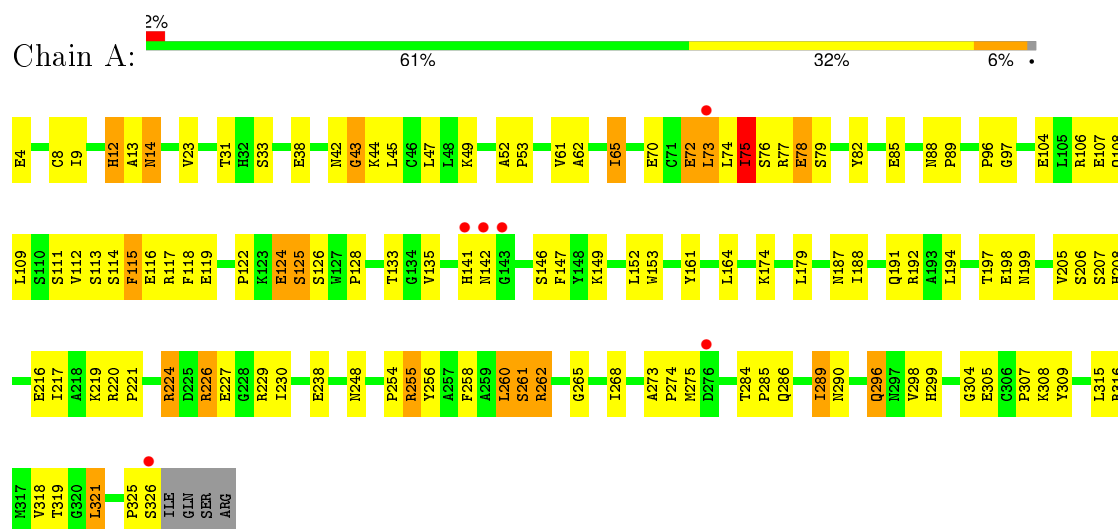
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	I	1	Total	O	S	0	0
			5	4	1		
9	I	1	Total	O	S	0	0
			5	4	1		

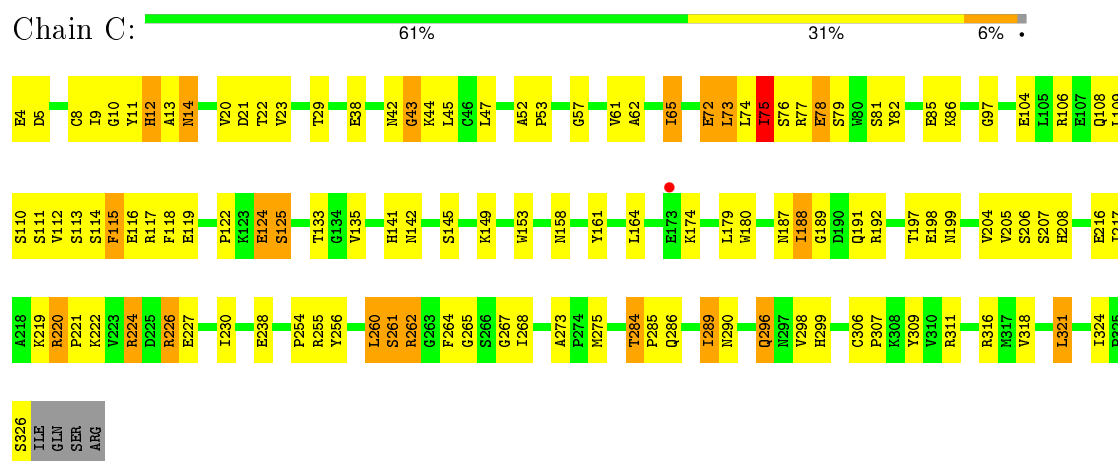
3 Residue-property plots [i](#)

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

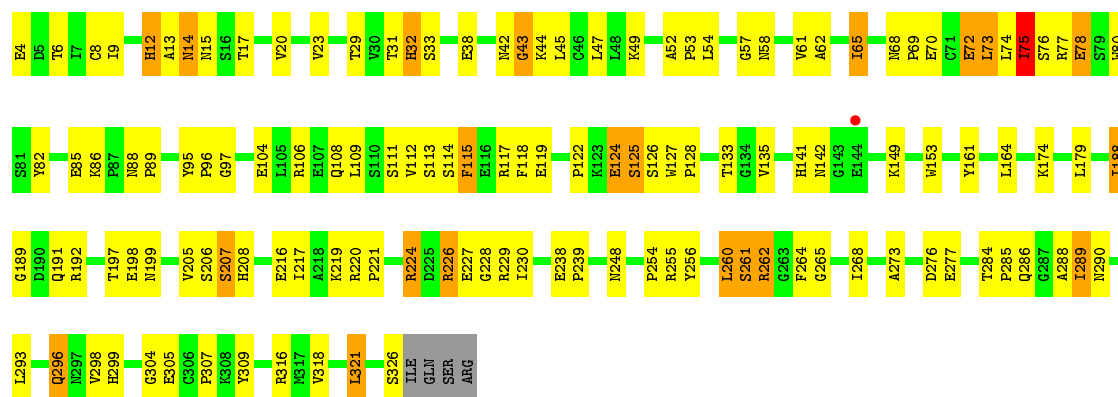


• Molecule 1: Hemagglutinin

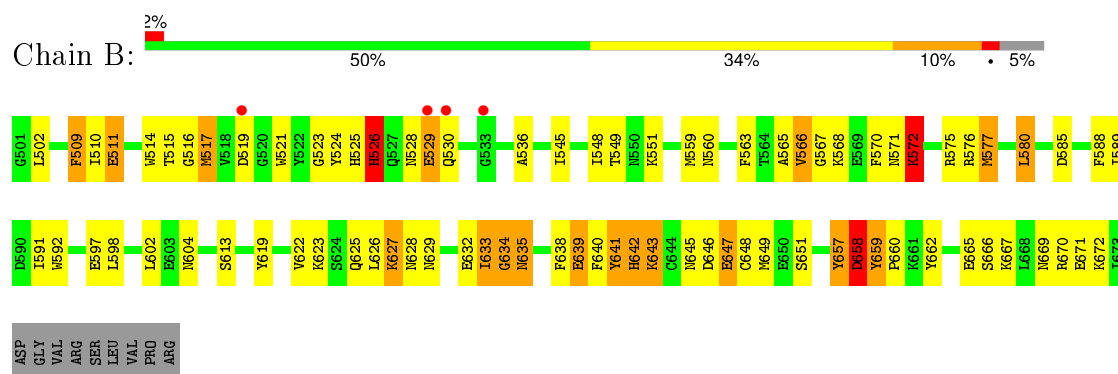


• Molecule 1: Hemagglutinin

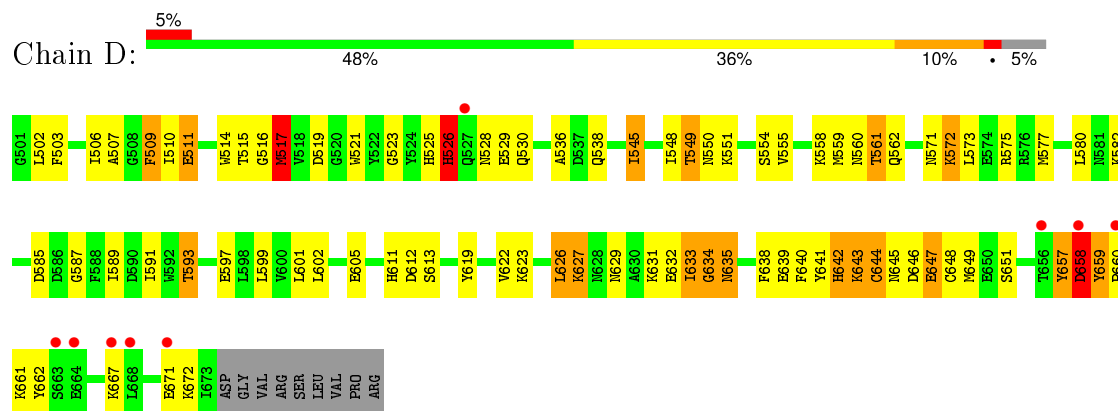




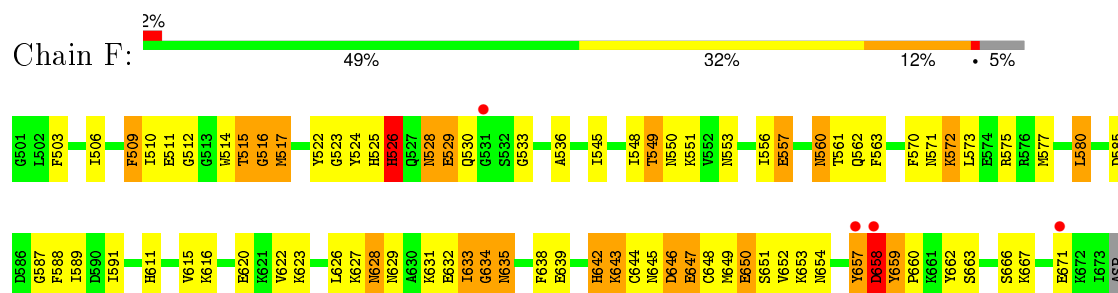
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin

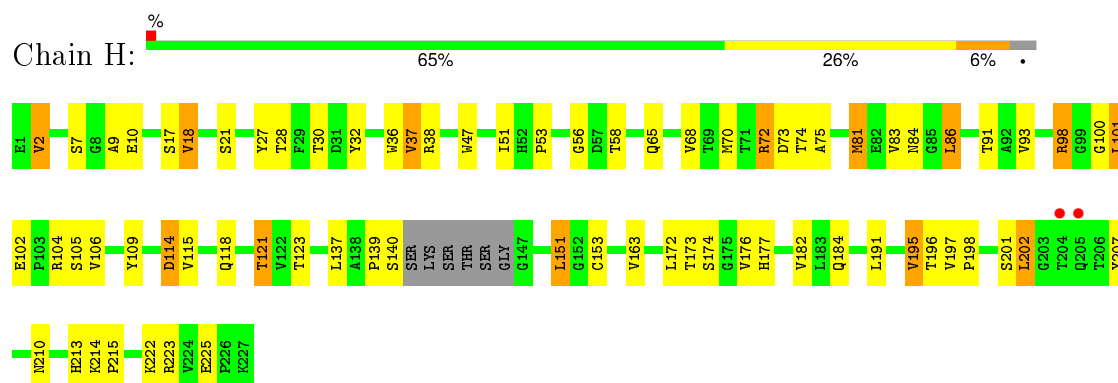


• Molecule 2: Hemagglutinin

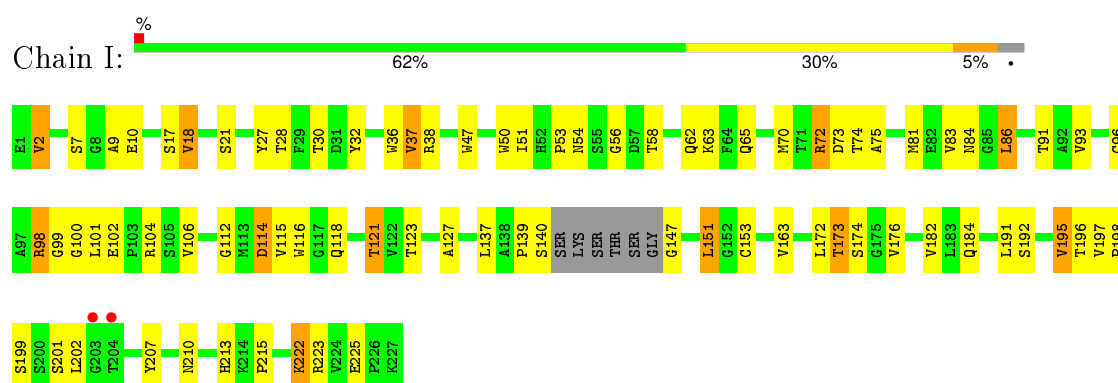


GLY
VAL
ARG
SER
LEU
PRO
ARG

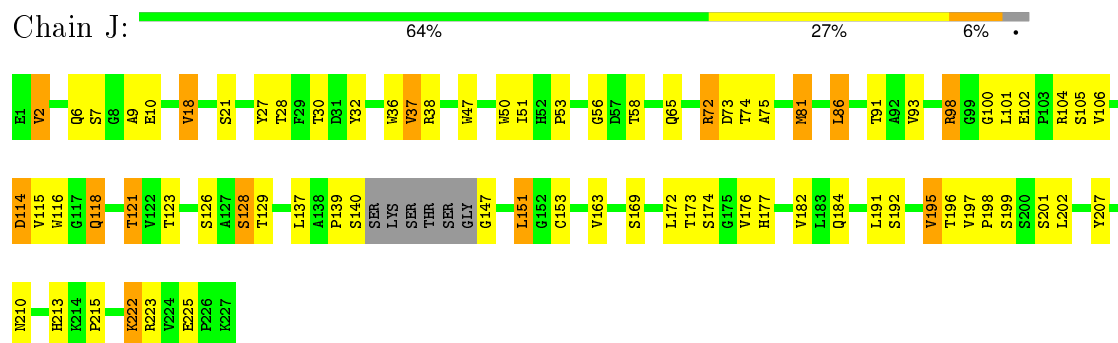
- Molecule 3: CH65, heavy chain, Fab fragment



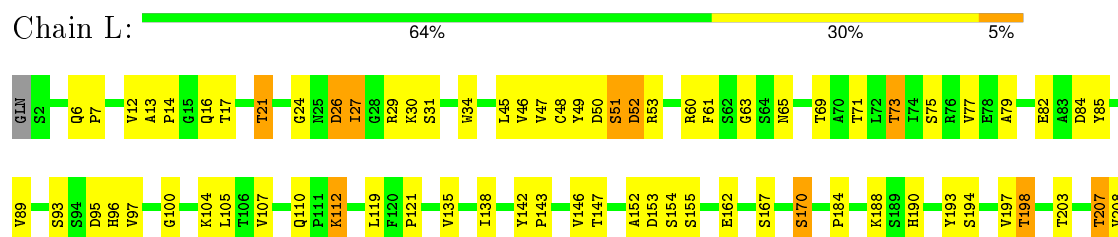
- Molecule 3: CH65, heavy chain, Fab fragment



- Molecule 3: CH65, heavy chain, Fab fragment

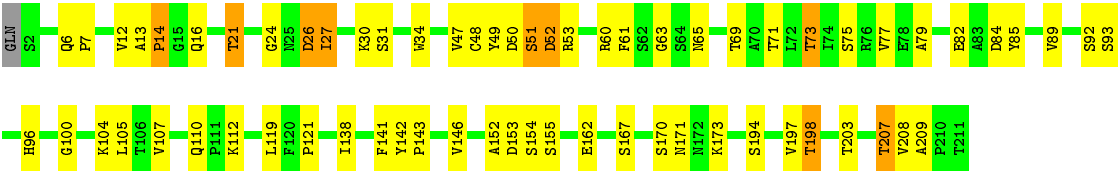


- Molecule 4: CH65, light chain, Fab fragment

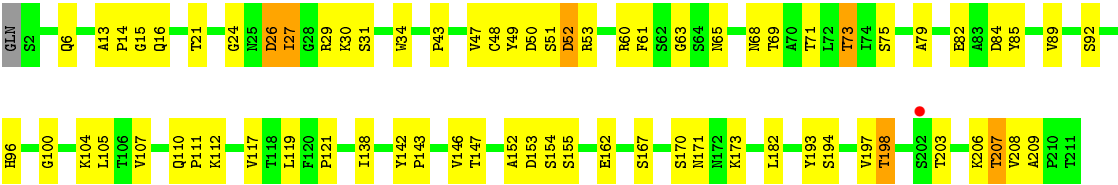




● Molecule 4: CH65, light chain, Fab fragment



● Molecule 4: CH65, light chain, Fab fragment



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	154.98Å 191.84Å 332.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.09 – 3.19 30.09 – 3.19	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.09-3.19) 92.4 (30.09-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.211 , 0.249 0.196 , 0.234	Depositor DCC
R_{free} test set	1869 reflections (2.47%)	DCC
Wilson B-factor (Å ²)	80.3	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 80373 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22009	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: SO4, BMA, NAG, MAN

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	0.46	0/2601	0.62	0/3540
1	C	0.47	0/2601	0.62	0/3540
1	E	0.47	0/2601	0.61	0/3540
2	B	0.45	0/1418	0.65	0/1905
2	D	0.47	0/1418	0.63	0/1905
2	F	0.51	0/1418	0.67	0/1905
3	H	0.51	0/1718	0.65	0/2347
3	I	0.51	0/1718	0.65	0/2347
3	J	0.54	0/1718	0.64	0/2347
4	L	0.45	0/1603	0.60	0/2192
4	M	0.45	0/1603	0.60	0/2192
4	N	0.46	0/1603	0.61	0/2192
All	All	0.48	0/22020	0.63	0/29952

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	351	NAG	C1

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	2535	0	2441	112	0
1	C	2535	0	2438	119	0
1	E	2535	0	2440	111	0
2	B	1391	0	1316	93	0
2	D	1391	0	1316	112	0
2	F	1391	0	1316	109	0
3	H	1673	0	1606	48	0
3	I	1673	0	1606	50	0
3	J	1673	0	1606	42	0
4	L	1565	0	1513	60	0
4	M	1565	0	1513	47	0
4	N	1565	0	1513	49	0
5	A	56	0	50	3	0
5	C	56	0	50	2	0
5	E	28	0	25	3	0
6	A	11	0	10	0	0
7	A	28	0	26	2	0
7	C	42	0	39	0	0
7	E	42	0	39	4	0
8	E	39	0	34	7	0
9	A	30	0	0	1	0
9	C	45	0	0	6	0
9	E	60	0	0	4	0
9	H	15	0	0	1	0
9	I	25	0	0	1	0
9	J	10	0	0	0	0
9	L	10	0	0	1	0
9	M	5	0	0	0	0
9	N	15	0	0	1	0
All	All	22009	0	20897	851	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (851) 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)
2:D:519:ASP:HB2	2:D:536:ALA:HB3	1.45	0.97
1:E:77:ARG:NH1	9:E:344:SO4:O4	1.99	0.96
3:H:18:VAL:HG22	3:H:86:LEU:HD21	1.47	0.95
1:E:70:GLU:HG3	8:E:331:NAG:HN2	1.31	0.95
2:D:642:HIS:O	2:D:642:HIS:ND1	2.01	0.94
1:C:321:LEU:HB3	2:D:611:HIS:CD2	2.04	0.92
1:C:78:GLU:O	1:C:114:SER:HA	1.71	0.90
3:I:18:VAL:HG22	3:I:86:LEU:HD21	1.52	0.89
1:A:114:SER:OG	1:A:174:LYS:NZ	2.06	0.88
2:D:622:VAL:HG12	2:D:638:PHE:CE1	2.08	0.88
2:D:530:GLN:NE2	2:D:645:ASN:HD21	1.71	0.88
2:F:526:HIS:O	2:F:526:HIS:ND1	2.06	0.88
2:D:577:MET:HG3	2:F:577:MET:HE3	1.56	0.88
1:E:114:SER:OG	1:E:174:LYS:NZ	2.07	0.87
1:A:78:GLU:O	1:A:114:SER:HA	1.73	0.87
1:A:70:GLU:HG3	5:A:331:NAG:HN2	1.40	0.86
3:J:18:VAL:HG22	3:J:86:LEU:HD21	1.53	0.86
2:B:526:HIS:O	2:B:526:HIS:ND1	2.08	0.86
4:L:198:THR:HB	4:L:203:THR:OG1	1.76	0.85
1:E:78:GLU:O	1:E:114:SER:HA	1.74	0.85
1:C:114:SER:OG	1:C:174:LYS:NZ	2.11	0.84
1:A:23:VAL:HG22	2:B:602:LEU:HD12	1.59	0.84
4:N:79:ALA:HA	4:N:107:VAL:HG11	1.59	0.84
1:C:9:ILE:HD12	2:D:619:TYR:HA	1.60	0.83
4:M:79:ALA:HA	4:M:107:VAL:HG11	1.60	0.83
2:B:570:PHE:CE1	2:B:577:MET:HG2	2.13	0.82
1:E:248:ASN:HD22	7:E:341:NAG:H82	1.44	0.82
4:L:146:VAL:HG11	4:L:197:VAL:HG13	1.59	0.82
2:B:597:GLU:OE1	2:D:558:LYS:NZ	2.10	0.82
2:D:511:GLU:OE2	2:D:511:GLU:HA	1.80	0.81
1:A:107:GLU:OE2	2:B:568:LYS:NZ	2.13	0.81
2:F:529:GLU:OE2	2:F:530:GLN:HG3	1.79	0.81
4:L:79:ALA:HA	4:L:107:VAL:HG11	1.63	0.80
3:H:198:PRO:O	3:H:201:SER:OG	2.00	0.80
4:N:146:VAL:HG11	4:N:197:VAL:HG13	1.64	0.80
3:H:197:VAL:HB	3:H:198:PRO:HD2	1.64	0.80
4:M:146:VAL:HG11	4:M:197:VAL:HG13	1.65	0.79
2:D:623:LYS:HB2	2:D:638:PHE:HZ	1.46	0.79
2:D:529:GLU:OE2	2:D:530:GLN:HG3	1.82	0.79
1:C:224:ARG:NH2	5:C:331:NAG:O3	2.17	0.78
1:A:23:VAL:CG2	2:B:602:LEU:HD12	2.13	0.77
4:M:198:THR:HB	4:M:203:THR:OG1	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ILE:HD11	1:A:298:VAL:HG21	1.68	0.76
2:F:648:CYS:O	2:F:651:SER:HB3	1.87	0.75
4:L:121:PRO:HB3	4:L:208:VAL:HG11	1.68	0.75
1:E:189:GLY:HA3	4:N:92:SER:O	1.87	0.75
2:D:526:HIS:HD2	2:D:649:MET:HG3	1.52	0.75
4:L:30:LYS:HD3	4:L:89:VAL:HG11	1.69	0.75
2:F:642:HIS:ND1	2:F:642:HIS:O	2.18	0.75
4:M:121:PRO:HB3	4:M:208:VAL:HG11	1.67	0.74
2:D:622:VAL:HG12	2:D:638:PHE:HE1	1.50	0.74
1:E:112:VAL:HG11	1:E:115:PHE:HB3	1.68	0.74
2:B:662:TYR:O	2:B:666:SER:OG	2.03	0.74
2:F:509:PHE:HD1	2:F:509:PHE:O	1.71	0.74
2:D:623:LYS:HB2	2:D:638:PHE:CZ	2.23	0.74
2:F:645:ASN:C	2:F:647:GLU:H	1.90	0.74
1:E:197:THR:HG22	1:E:199:ASN:H	1.52	0.74
3:J:197:VAL:HB	3:J:198:PRO:HD2	1.70	0.73
1:C:23:VAL:HG11	2:F:551:LYS:HE2	1.70	0.73
1:C:324:ILE:HD11	2:D:507:ALA:HB2	1.70	0.73
1:C:11:TYR:CZ	2:D:506:ILE:HG23	2.24	0.73
4:L:170:SER:OG	9:L:212:SO4:O4	2.07	0.73
1:A:112:VAL:HG11	1:A:115:PHE:HB3	1.70	0.73
3:I:176:VAL:HG22	3:I:195:VAL:HG12	1.71	0.73
4:N:30:LYS:HD3	4:N:89:VAL:HG11	1.70	0.73
1:E:8:CYS:HB2	2:F:525:HIS:HB3	1.69	0.73
1:C:197:THR:HG22	1:C:199:ASN:H	1.54	0.72
3:I:197:VAL:HB	3:I:198:PRO:HD2	1.71	0.72
2:F:526:HIS:HD1	2:F:526:HIS:C	1.91	0.72
3:J:198:PRO:O	3:J:201:SER:OG	2.06	0.72
2:B:642:HIS:ND1	2:B:642:HIS:O	2.22	0.72
4:N:198:THR:HB	4:N:203:THR:OG1	1.90	0.72
2:B:632:GLU:HG2	2:B:638:PHE:HE2	1.53	0.72
2:F:510:ILE:O	2:F:512:GLY:N	2.23	0.72
1:C:112:VAL:HG11	1:C:115:PHE:HB3	1.70	0.71
2:B:519:ASP:HB2	2:B:536:ALA:HB3	1.72	0.71
2:F:642:HIS:CE1	2:F:662:TYR:CD1	2.79	0.71
3:J:176:VAL:HG22	3:J:195:VAL:HG12	1.71	0.71
3:I:2:VAL:HG12	3:I:27:TYR:HD2	1.56	0.71
4:N:121:PRO:HB3	4:N:208:VAL:HG11	1.71	0.71
3:I:198:PRO:O	3:I:201:SER:OG	2.06	0.70
3:I:176:VAL:HG22	3:I:195:VAL:CG1	2.20	0.70
4:M:30:LYS:HD3	4:M:89:VAL:HG11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:THR:HG22	1:A:199:ASN:H	1.55	0.70
1:C:12:HIS:ND1	1:C:13:ALA:N	2.39	0.70
2:D:526:HIS:CD2	2:D:649:MET:HG3	2.27	0.70
1:C:9:ILE:HD11	2:D:622:VAL:HG21	1.74	0.70
2:D:530:GLN:NE2	2:D:645:ASN:ND2	2.40	0.70
2:B:577:MET:HB2	2:D:577:MET:HE1	1.75	0.69
2:D:545:ILE:O	2:D:549:THR:HB	1.91	0.69
1:A:43:GLY:HA2	1:A:286:GLN:O	1.92	0.69
1:C:289:ILE:HD11	1:C:298:VAL:HG21	1.74	0.69
1:C:306:CYS:O	2:D:561:THR:HG21	1.93	0.69
2:F:649:MET:O	2:F:651:SER:N	2.25	0.69
3:J:176:VAL:HG22	3:J:195:VAL:CG1	2.22	0.69
2:B:514:TRP:HE3	2:B:517:MET:HE2	1.56	0.69
2:D:519:ASP:HB2	2:D:536:ALA:CB	2.21	0.68
1:E:224:ARG:HH22	8:E:331:NAG:H83	1.58	0.68
1:A:8:CYS:HB2	2:B:525:HIS:HB3	1.73	0.68
2:D:623:LYS:HD2	2:D:632:GLU:OE2	1.94	0.68
2:D:622:VAL:HG12	2:D:638:PHE:CD1	2.29	0.68
1:A:187:ASN:ND2	4:L:93:SER:HA	2.08	0.68
2:B:571:ASN:HB2	2:B:572:LYS:HE3	1.75	0.68
2:D:577:MET:HG3	2:F:577:MET:CE	2.24	0.68
1:C:219:LYS:HE3	1:C:227:GLU:OE2	1.94	0.68
1:E:77:ARG:HA	9:E:344:SO4:O4	1.94	0.68
1:A:42:ASN:O	1:A:44:LYS:N	2.27	0.68
2:D:509:PHE:O	2:D:509:PHE:HD1	1.76	0.68
2:B:667:LYS:O	2:B:671:GLU:HG2	1.93	0.67
4:M:194:SER:HB3	4:M:207:THR:HB	1.76	0.67
4:L:146:VAL:CG1	4:L:197:VAL:HG13	2.25	0.67
1:E:289:ILE:HD11	1:E:298:VAL:HG21	1.75	0.67
1:E:42:ASN:O	1:E:44:LYS:N	2.28	0.67
2:B:509:PHE:O	2:B:635:ASN:HB3	1.94	0.67
4:N:194:SER:HB3	4:N:207:THR:HB	1.75	0.67
1:E:4:GLU:HB2	2:F:639:GLU:OE2	1.95	0.67
2:D:633:ILE:HD13	2:D:639:GLU:HB2	1.75	0.67
1:C:311:ARG:NH1	2:F:560:ASN:OD1	2.28	0.67
1:A:106:ARG:HB3	1:A:268:ILE:HD12	1.77	0.67
3:H:2:VAL:HG12	3:H:27:TYR:HD2	1.59	0.66
1:E:12:HIS:ND1	1:E:13:ALA:N	2.43	0.66
2:D:657:TYR:O	2:D:658:ASP:HB2	1.94	0.66
1:E:262:ARG:HH11	1:E:262:ARG:HA	1.61	0.66
1:C:104:GLU:O	1:C:108:GLN:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:HIS:ND1	1:A:13:ALA:N	2.43	0.66
3:I:98:ARG:HD3	3:I:114:ASP:OD2	1.95	0.66
1:A:262:ARG:HA	1:A:262:ARG:HH11	1.61	0.66
3:H:98:ARG:HD3	3:H:114:ASP:OD2	1.96	0.66
2:F:644:CYS:HB2	2:F:648:CYS:HB3	1.76	0.66
1:E:43:GLY:HA2	1:E:286:GLN:O	1.96	0.66
1:C:321:LEU:HB3	2:D:611:HIS:HD2	1.61	0.65
2:F:645:ASN:C	2:F:647:GLU:N	2.49	0.65
1:C:43:GLY:HA2	1:C:286:GLN:O	1.96	0.65
1:A:119:GLU:HG3	1:A:256:TYR:CZ	2.32	0.65
2:F:645:ASN:O	2:F:648:CYS:N	2.30	0.65
4:N:146:VAL:CG1	4:N:197:VAL:HG13	2.26	0.65
1:C:124:GLU:O	1:C:125:SER:HB3	1.97	0.65
3:J:98:ARG:HD3	3:J:114:ASP:OD2	1.97	0.65
4:L:6:GLN:OE1	4:L:100:GLY:HA3	1.96	0.64
1:C:191:GLN:HB2	1:C:217:ILE:HD11	1.80	0.64
2:D:517:MET:SD	2:D:523:GLY:HA3	2.37	0.64
1:A:304:GLY:HA2	2:B:563:PHE:CD1	2.33	0.64
3:H:176:VAL:HG22	3:H:195:VAL:HG12	1.78	0.64
1:C:262:ARG:HA	1:C:262:ARG:HH11	1.63	0.64
2:B:502:LEU:HD12	2:D:613:SER:CB	2.27	0.64
2:B:633:ILE:O	2:B:635:ASN:N	2.28	0.64
1:C:106:ARG:HB3	1:C:268:ILE:HD12	1.80	0.64
1:C:81:SER:HG	1:C:82:TYR:HD2	1.46	0.64
2:F:645:ASN:O	2:F:647:GLU:N	2.30	0.64
1:E:104:GLU:O	1:E:108:GLN:HG3	1.96	0.64
1:E:106:ARG:HB3	1:E:268:ILE:HD12	1.80	0.64
3:J:2:VAL:HG12	3:J:27:TYR:HD2	1.63	0.63
1:A:104:GLU:O	1:A:108:GLN:HG3	1.97	0.63
2:F:526:HIS:C	2:F:526:HIS:ND1	2.49	0.63
1:C:42:ASN:O	1:C:44:LYS:N	2.31	0.63
1:C:119:GLU:HG3	1:C:256:TYR:CE1	2.34	0.63
2:F:649:MET:C	2:F:651:SER:H	1.99	0.63
2:B:572:LYS:H	2:B:572:LYS:HD3	1.64	0.63
1:C:189:GLY:HA3	4:M:92:SER:O	1.99	0.63
2:D:642:HIS:CE1	2:D:662:TYR:CD1	2.86	0.63
2:F:509:PHE:O	2:F:509:PHE:CD1	2.52	0.62
1:E:73:LEU:HD11	1:E:117:ARG:HD3	1.81	0.62
1:E:73:LEU:HD11	1:E:117:ARG:CD	2.29	0.62
4:M:73:THR:HG22	4:M:73:THR:O	1.98	0.62
1:A:73:LEU:HD11	1:A:117:ARG:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLU:HB3	1:A:74:LEU:CD2	2.29	0.62
2:F:642:HIS:O	2:F:643:LYS:O	2.17	0.62
2:F:571:ASN:HB2	2:F:572:LYS:HE3	1.81	0.62
2:F:585:ASP:O	2:F:589:ILE:HG13	1.99	0.62
2:D:509:PHE:CD1	2:D:510:ILE:HG13	2.35	0.62
1:E:191:GLN:HB2	1:E:217:ILE:HD11	1.82	0.62
4:N:6:GLN:OE1	4:N:100:GLY:HA3	1.99	0.62
1:A:309:TYR:CD2	2:B:589:ILE:HD13	2.34	0.62
2:F:644:CYS:HB2	2:F:648:CYS:SG	2.40	0.62
4:M:146:VAL:CG1	4:M:197:VAL:HG13	2.29	0.62
1:C:72:GLU:HB3	1:C:74:LEU:CD2	2.30	0.62
1:C:158:ASN:HB3	3:I:54:ASN:HD22	1.65	0.62
3:H:176:VAL:HG22	3:H:195:VAL:CG1	2.30	0.62
1:A:73:LEU:HD11	1:A:117:ARG:CD	2.30	0.62
4:M:6:GLN:OE1	4:M:100:GLY:HA3	2.00	0.61
4:L:119:LEU:HD23	4:L:208:VAL:HG23	1.82	0.61
2:D:667:LYS:O	2:D:671:GLU:HG2	2.00	0.61
1:A:191:GLN:HB2	1:A:217:ILE:HD11	1.81	0.61
1:C:187:ASN:ND2	4:M:93:SER:HA	2.14	0.61
1:C:9:ILE:CD1	2:D:619:TYR:HA	2.28	0.61
1:A:304:GLY:HA2	2:B:563:PHE:CE1	2.35	0.61
2:D:629:ASN:ND2	2:D:659:TYR:HD2	1.98	0.61
2:B:519:ASP:HB2	2:B:536:ALA:CB	2.30	0.61
2:F:523:GLY:HA3	2:F:536:ALA:HA	1.83	0.61
4:L:194:SER:HB3	4:L:207:THR:HB	1.83	0.61
1:A:106:ARG:HB3	1:A:268:ILE:CD1	2.30	0.61
1:E:106:ARG:HB3	1:E:268:ILE:CD1	2.31	0.60
2:F:553:ASN:O	2:F:557:GLU:HB3	2.01	0.60
3:H:32:TYR:CD1	3:H:100:GLY:HA2	2.37	0.60
1:C:197:THR:HG22	1:C:199:ASN:N	2.17	0.60
2:B:645:ASN:ND2	2:B:646:ASP:H	1.99	0.60
5:E:351:NAG:H61	5:E:352:NAG:N2	2.16	0.60
3:H:98:ARG:NH2	9:H:229:SO4:O3	2.35	0.60
2:F:556:ILE:HG22	2:F:557:GLU:N	2.15	0.60
1:E:219:LYS:HE3	1:E:227:GLU:OE2	2.02	0.60
1:A:119:GLU:HG3	1:A:256:TYR:CE1	2.35	0.60
1:C:119:GLU:HG3	1:C:256:TYR:CZ	2.37	0.60
2:B:623:LYS:HD2	2:B:632:GLU:OE2	2.01	0.60
2:F:633:ILE:CG1	2:F:634:GLY:H	2.14	0.60
2:B:648:CYS:O	2:B:651:SER:HB3	2.01	0.60
3:I:102:GLU:O	4:M:49:TYR:OH	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:198:PRO:HG2	3:H:201:SER:OG	2.02	0.60
4:M:6:GLN:NE2	4:M:85:TYR:O	2.35	0.60
1:E:296:GLN:HB2	1:E:307:PRO:HB2	1.84	0.60
1:A:219:LYS:HE3	1:A:227:GLU:OE2	2.02	0.60
2:D:599:LEU:O	2:D:599:LEU:HG	2.01	0.60
1:E:197:THR:HG22	1:E:199:ASN:N	2.16	0.59
1:A:318:VAL:HG12	2:B:604:ASN:OD1	2.01	0.59
1:A:224:ARG:NH2	5:A:331:NAG:O3	2.36	0.59
1:A:289:ILE:CD1	1:A:298:VAL:HG21	2.30	0.59
1:C:106:ARG:HB3	1:C:268:ILE:CD1	2.33	0.59
4:L:6:GLN:NE2	4:L:85:TYR:O	2.35	0.59
2:F:629:ASN:OD1	2:F:659:TYR:HD2	1.85	0.59
1:A:315:LEU:HD21	2:B:597:GLU:HG2	1.85	0.59
3:J:53:PRO:O	3:J:72:ARG:NH1	2.36	0.59
2:F:644:CYS:HB2	2:F:648:CYS:CB	2.32	0.59
1:A:197:THR:HG22	1:A:199:ASN:N	2.17	0.59
5:E:351:NAG:H61	5:E:352:NAG:C7	2.33	0.59
2:F:659:TYR:HD1	2:F:660:PRO:HD3	1.67	0.59
2:F:616:LYS:O	2:F:620:GLU:HG2	2.02	0.59
3:J:32:TYR:CD1	3:J:100:GLY:HA2	2.38	0.59
2:F:633:ILE:HG13	2:F:634:GLY:N	2.18	0.59
1:E:72:GLU:HB3	1:E:74:LEU:CD2	2.32	0.58
1:C:97:GLY:HA3	1:C:230:ILE:O	2.02	0.58
1:C:324:ILE:CD1	2:D:507:ALA:HB2	2.32	0.58
4:N:73:THR:O	4:N:73:THR:HG22	2.03	0.58
2:D:658:ASP:O	2:D:661:LYS:HB3	2.04	0.58
1:C:321:LEU:N	1:C:321:LEU:HD23	2.19	0.58
2:B:567:GLY:O	2:B:568:LYS:HE2	2.04	0.58
1:C:316:ARG:NH2	9:C:340:SO4:O2	2.33	0.58
4:L:73:THR:O	4:L:73:THR:HG22	2.02	0.58
1:A:4:GLU:HB2	2:B:639:GLU:OE2	2.03	0.58
3:I:114:ASP:HB2	3:I:115:VAL:HG23	1.86	0.58
1:E:119:GLU:HG3	1:E:256:TYR:CZ	2.38	0.58
1:C:73:LEU:HD11	1:C:117:ARG:CD	2.34	0.57
1:E:321:LEU:N	1:E:321:LEU:HD23	2.19	0.57
4:M:110:GLN:OE1	4:M:142:TYR:CD1	2.57	0.57
2:B:629:ASN:OD1	2:B:659:TYR:HD2	1.87	0.57
1:C:153:TRP:CH2	3:I:106:VAL:HG11	2.39	0.57
2:F:649:MET:O	2:F:652:VAL:N	2.36	0.57
2:B:529:GLU:OE2	2:B:530:GLN:HG3	2.04	0.57
4:M:53:ARG:HD3	4:M:61:PHE:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:296:GLN:CB	1:E:307:PRO:HB2	2.34	0.57
4:N:68:ASN:HB2	9:N:213:SO4:O4	2.03	0.57
1:A:72:GLU:HB3	1:A:74:LEU:HD21	1.87	0.57
4:N:50:ASP:OD1	4:N:65:ASN:ND2	2.37	0.57
3:I:73:ASP:O	3:I:75:ALA:N	2.36	0.57
1:C:296:GLN:HB2	1:C:307:PRO:HB2	1.86	0.57
2:F:623:LYS:HD2	2:F:632:GLU:OE2	2.04	0.57
1:A:153:TRP:CH2	3:H:106:VAL:HG11	2.40	0.57
3:H:114:ASP:HB2	3:H:115:VAL:HG23	1.85	0.57
1:E:119:GLU:HG3	1:E:256:TYR:CE1	2.40	0.57
1:A:97:GLY:HA3	1:A:230:ILE:O	2.05	0.57
2:D:514:TRP:HE3	2:D:517:MET:HE2	1.70	0.57
2:F:509:PHE:O	2:F:635:ASN:HB3	2.05	0.57
2:B:629:ASN:CG	2:B:659:TYR:HD2	2.07	0.56
1:A:296:GLN:HB2	1:A:307:PRO:HB2	1.86	0.56
4:N:53:ARG:HD3	4:N:61:PHE:O	2.05	0.56
1:C:296:GLN:CB	1:C:307:PRO:HB2	2.35	0.56
1:E:38:GLU:OE1	1:E:290:ASN:HB3	2.05	0.56
1:A:226:ARG:HH12	4:L:29:ARG:HH21	1.53	0.56
4:L:53:ARG:HD3	4:L:61:PHE:O	2.05	0.56
2:D:530:GLN:HE21	2:D:645:ASN:ND2	2.03	0.56
1:E:124:GLU:O	1:E:125:SER:HB3	2.05	0.56
1:A:8:CYS:HB2	2:B:525:HIS:CB	2.35	0.56
2:D:585:ASP:O	2:D:589:ILE:HG13	2.05	0.56
3:H:184:GLN:HG2	4:L:162:GLU:HG3	1.87	0.56
3:H:53:PRO:O	3:H:72:ARG:NH1	2.38	0.56
3:J:7:SER:HB3	3:J:21:SER:HB3	1.88	0.56
2:D:526:HIS:ND1	2:D:526:HIS:O	2.38	0.56
1:E:113:SER:OG	1:E:261:SER:HB3	2.05	0.56
2:F:649:MET:C	2:F:651:SER:N	2.59	0.56
4:M:119:LEU:HD23	4:M:208:VAL:HG23	1.86	0.56
1:C:73:LEU:HD11	1:C:117:ARG:HD3	1.86	0.56
2:D:629:ASN:ND2	2:D:659:TYR:HB2	2.20	0.56
1:C:289:ILE:CD1	1:C:298:VAL:HG21	2.36	0.56
2:F:628:ASN:H	2:F:628:ASN:HD22	1.54	0.55
1:A:296:GLN:CB	1:A:307:PRO:HB2	2.35	0.55
3:J:128:SER:O	3:J:129:THR:C	2.44	0.55
4:N:119:LEU:HD23	4:N:208:VAL:HG23	1.88	0.55
1:C:316:ARG:NH1	9:C:340:SO4:O2	2.39	0.55
1:C:72:GLU:HB3	1:C:74:LEU:HD21	1.88	0.55
1:A:113:SER:OG	1:A:261:SER:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:HIS:O	1:A:142:ASN:HB2	2.07	0.55
1:C:5:ASP:O	2:D:640:PHE:HB2	2.06	0.55
2:F:650:GLU:O	2:F:654:ASN:ND2	2.40	0.55
2:B:657:TYR:O	2:B:658:ASP:HB2	2.06	0.55
2:F:657:TYR:O	2:F:658:ASP:HB2	2.05	0.55
1:A:124:GLU:O	1:A:125:SER:HB3	2.06	0.55
1:A:308:LYS:HG2	2:B:592:TRP:CE2	2.42	0.55
1:C:115:PHE:HB2	1:C:260:LEU:CB	2.37	0.55
1:C:286:GLN:NE2	1:C:298:VAL:HG12	2.22	0.55
2:D:629:ASN:CG	2:D:659:TYR:HD2	2.10	0.55
1:C:4:GLU:HB2	2:D:639:GLU:OE2	2.07	0.54
2:B:514:TRP:CE3	2:B:517:MET:HE2	2.39	0.54
1:A:62:ALA:HA	1:A:65:ILE:HD11	1.89	0.54
2:F:629:ASN:CG	2:F:659:TYR:HD2	2.10	0.54
1:E:97:GLY:HA3	1:E:230:ILE:O	2.08	0.54
1:E:141:HIS:O	1:E:142:ASN:HB2	2.06	0.54
1:C:9:ILE:HD11	2:D:622:VAL:CG2	2.38	0.54
4:L:60:ARG:HD2	4:L:75:SER:O	2.07	0.54
2:D:519:ASP:CB	2:D:536:ALA:HB3	2.28	0.54
2:D:645:ASN:OD1	2:D:647:GLU:HB2	2.07	0.54
2:D:509:PHE:O	2:D:509:PHE:CD1	2.59	0.54
1:C:4:GLU:CD	2:D:643:LYS:HD3	2.27	0.54
3:J:93:VAL:HG22	3:J:121:THR:HG23	1.89	0.54
4:L:142:TYR:CD2	4:L:143:PRO:HA	2.43	0.54
1:A:62:ALA:O	1:A:65:ILE:HD12	2.07	0.54
4:N:153:ASP:C	4:N:155:SER:H	2.11	0.54
3:I:7:SER:HB3	3:I:21:SER:HB3	1.90	0.54
2:B:632:GLU:HG2	2:B:638:PHE:CE2	2.40	0.54
4:M:50:ASP:OD1	4:M:65:ASN:ND2	2.38	0.54
4:N:34:TRP:HB2	4:N:47:VAL:HB	1.90	0.54
3:H:2:VAL:HG12	3:H:27:TYR:CD2	2.41	0.54
1:A:153:TRP:CZ2	3:H:106:VAL:HG11	2.43	0.54
3:J:184:GLN:HG2	4:N:162:GLU:HG3	1.90	0.54
2:B:645:ASN:OD1	2:B:647:GLU:HB2	2.08	0.53
3:I:184:GLN:HG2	4:M:162:GLU:HG3	1.89	0.53
2:F:633:ILE:HG13	2:F:634:GLY:H	1.73	0.53
1:A:179:LEU:O	1:A:254:PRO:HB3	2.07	0.53
1:E:224:ARG:NH2	8:E:331:NAG:O3	2.41	0.53
2:D:633:ILE:HG13	2:D:634:GLY:H	1.73	0.53
1:C:286:GLN:HE21	1:C:298:VAL:HG12	1.74	0.53
2:B:509:PHE:C	2:B:509:PHE:CD1	2.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:73:ASP:O	3:J:75:ALA:N	2.34	0.53
2:D:575:ARG:NH2	1:E:264:PHE:CE1	2.77	0.53
1:A:4:GLU:CD	2:B:643:LYS:HD3	2.29	0.53
1:E:289:ILE:CD1	1:E:298:VAL:HG21	2.37	0.53
3:J:56:GLY:O	3:J:58:THR:HG23	2.09	0.53
2:D:633:ILE:HG13	2:D:634:GLY:N	2.23	0.53
1:A:255:ARG:NH2	9:A:336:SO4:O3	2.42	0.53
4:L:153:ASP:C	4:L:155:SER:H	2.12	0.53
2:D:530:GLN:HE22	2:D:645:ASN:HD21	1.51	0.53
2:F:659:TYR:N	2:F:660:PRO:CD	2.72	0.53
4:L:34:TRP:HB2	4:L:47:VAL:HB	1.89	0.53
1:A:115:PHE:HB2	1:A:260:LEU:CB	2.38	0.52
2:B:671:GLU:O	2:B:672:LYS:HD3	2.09	0.52
3:J:198:PRO:HG2	3:J:201:SER:OG	2.09	0.52
2:D:629:ASN:ND2	2:D:659:TYR:CD2	2.78	0.52
8:E:331:NAG:H83	8:E:331:NAG:O3	2.08	0.52
2:B:530:GLN:NE2	2:B:645:ASN:HD21	2.08	0.52
3:H:93:VAL:HG22	3:H:121:THR:HG23	1.91	0.52
2:F:667:LYS:O	2:F:671:GLU:HG2	2.09	0.52
3:I:2:VAL:HG12	3:I:27:TYR:CD2	2.39	0.52
4:L:50:ASP:OD1	4:L:65:ASN:ND2	2.41	0.52
1:C:62:ALA:HA	1:C:65:ILE:HD11	1.91	0.52
1:E:45:LEU:CD2	1:E:273:ALA:HB3	2.38	0.52
4:N:30:LYS:O	4:N:31:SER:HB3	2.10	0.52
1:A:74:LEU:O	1:A:76:SER:N	2.43	0.52
2:F:514:TRP:HE3	2:F:517:MET:HE2	1.74	0.52
1:E:115:PHE:HB2	1:E:260:LEU:CB	2.39	0.52
3:I:198:PRO:HG2	3:I:201:SER:OG	2.09	0.52
2:B:657:TYR:O	2:B:658:ASP:CB	2.57	0.52
1:C:45:LEU:CD2	1:C:273:ALA:HB3	2.40	0.52
1:A:286:GLN:NE2	1:A:298:VAL:HG12	2.24	0.52
1:E:74:LEU:O	1:E:76:SER:N	2.42	0.52
4:N:152:ALA:O	4:N:153:ASP:HB2	2.09	0.52
4:M:34:TRP:HB2	4:M:47:VAL:HB	1.90	0.52
3:I:32:TYR:CD1	3:I:100:GLY:HA2	2.43	0.52
2:B:517:MET:SD	2:B:523:GLY:HA3	2.50	0.52
2:D:671:GLU:HB2	2:D:672:LYS:HE2	1.92	0.52
3:I:191:LEU:C	3:I:191:LEU:HD12	2.29	0.52
4:M:51:SER:HB3	4:M:63:GLY:O	2.10	0.52
4:M:60:ARG:HD2	4:M:75:SER:O	2.10	0.52
1:C:75:ILE:HD12	1:C:75:ILE:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:642:HIS:CG	2:D:642:HIS:O	2.62	0.52
3:J:114:ASP:HB2	3:J:115:VAL:HG23	1.92	0.52
4:N:60:ARG:HD2	4:N:75:SER:O	2.10	0.52
2:B:577:MET:SD	2:D:577:MET:HE1	2.50	0.52
1:C:141:HIS:O	1:C:142:ASN:HB2	2.09	0.52
1:E:62:ALA:HA	1:E:65:ILE:HD11	1.92	0.52
4:L:30:LYS:HD3	4:L:89:VAL:CG1	2.39	0.51
2:B:642:HIS:O	2:B:643:LYS:O	2.28	0.51
2:D:651:SER:OG	2:D:657:TYR:HA	2.10	0.51
3:H:36:TRP:CG	3:H:81:MET:HG3	2.45	0.51
2:F:629:ASN:OD1	2:F:659:TYR:CD2	2.64	0.51
3:I:173:THR:HG23	9:I:232:SO4:O4	2.11	0.51
1:E:226:ARG:HH12	4:N:29:ARG:HH21	1.57	0.51
1:A:38:GLU:OE1	1:A:290:ASN:HB3	2.09	0.51
1:C:38:GLU:OE1	1:C:290:ASN:HB3	2.11	0.51
4:L:146:VAL:HG11	4:L:197:VAL:CG1	2.37	0.51
2:F:629:ASN:ND2	2:F:659:TYR:HD2	2.08	0.51
1:A:133:THR:O	1:A:135:VAL:HG13	2.10	0.51
1:A:286:GLN:HE21	1:A:298:VAL:HG12	1.75	0.51
2:B:645:ASN:C	2:B:647:GLU:H	2.14	0.51
2:F:623:LYS:HB2	2:F:638:PHE:CZ	2.46	0.51
1:A:45:LEU:CD2	1:A:273:ALA:HB3	2.40	0.51
2:B:670:ARG:C	2:B:672:LYS:H	2.14	0.51
1:E:72:GLU:HB3	1:E:74:LEU:HD21	1.92	0.51
3:J:36:TRP:CG	3:J:81:MET:HG3	2.44	0.51
1:A:42:ASN:O	1:A:43:GLY:C	2.49	0.51
3:I:53:PRO:O	3:I:72:ARG:NH1	2.43	0.51
1:C:113:SER:OG	1:C:261:SER:HB3	2.11	0.51
2:D:633:ILE:CG1	2:D:634:GLY:H	2.24	0.51
2:F:509:PHE:C	2:F:509:PHE:CD1	2.84	0.51
1:A:262:ARG:NH2	2:F:575:ARG:HH12	2.09	0.51
2:B:629:ASN:OD1	2:B:659:TYR:CD2	2.64	0.51
1:E:115:PHE:CD1	1:E:115:PHE:C	2.84	0.51
4:N:6:GLN:NE2	4:N:85:TYR:O	2.44	0.51
4:L:82:GLU:HG3	4:L:105:LEU:O	2.11	0.51
2:D:645:ASN:ND2	2:D:646:ASP:H	2.09	0.51
3:I:36:TRP:CG	3:I:81:MET:HG3	2.45	0.51
1:C:311:ARG:N	2:D:593:THR:OG1	2.43	0.50
4:N:110:GLN:HB2	4:N:111:PRO:CD	2.40	0.50
4:M:153:ASP:C	4:M:155:SER:H	2.14	0.50
3:H:56:GLY:O	3:H:58:THR:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:THR:O	1:E:135:VAL:HG13	2.12	0.50
2:F:528:ASN:OD1	2:F:646:ASP:N	2.45	0.50
3:I:163:VAL:CG1	3:I:191:LEU:HD21	2.42	0.50
4:N:82:GLU:HG3	4:N:105:LEU:O	2.11	0.50
4:N:51:SER:HB3	4:N:63:GLY:O	2.10	0.50
3:H:191:LEU:HD12	3:H:191:LEU:C	2.32	0.50
1:E:8:CYS:O	2:F:524:TYR:HA	2.12	0.50
2:F:525:HIS:O	2:F:533:GLY:O	2.30	0.50
2:B:645:ASN:ND2	2:B:646:ASP:N	2.60	0.50
1:C:133:THR:O	1:C:135:VAL:HG13	2.11	0.50
2:F:549:THR:HG22	2:F:550:ASN:N	2.27	0.50
1:E:179:LEU:O	1:E:254:PRO:HB3	2.11	0.50
2:D:629:ASN:OD1	2:D:659:TYR:HD2	1.95	0.50
2:B:659:TYR:N	2:B:660:PRO:CD	2.75	0.50
2:F:632:GLU:HG2	2:F:638:PHE:HE2	1.76	0.50
4:N:13:ALA:O	4:N:16:GLN:HB2	2.12	0.50
1:A:285:PRO:HG2	1:A:299:HIS:CE1	2.47	0.50
1:C:179:LEU:O	1:C:254:PRO:HB3	2.12	0.50
1:E:58:ASN:ND2	7:E:361:NAG:C7	2.75	0.49
2:D:642:HIS:O	2:D:643:LYS:O	2.31	0.49
2:F:645:ASN:OD1	2:F:647:GLU:HB2	2.12	0.49
3:J:2:VAL:HG12	3:J:27:TYR:CD2	2.46	0.49
1:C:119:GLU:CD	1:C:122:PRO:HA	2.32	0.49
1:C:226:ARG:HD3	9:C:334:SO4:O2	2.12	0.49
1:E:286:GLN:NE2	1:E:298:VAL:HG12	2.27	0.49
4:M:142:TYR:CD2	4:M:143:PRO:HA	2.48	0.49
1:C:220:ARG:HB3	1:C:221:PRO:HD2	1.93	0.49
3:H:73:ASP:O	3:H:74:THR:HB	2.13	0.49
4:M:30:LYS:O	4:M:31:SER:HB3	2.12	0.49
1:A:9:ILE:O	2:B:510:ILE:HD13	2.12	0.49
1:A:248:ASN:HD22	7:A:341:NAG:H82	1.78	0.49
2:D:528:ASN:ND2	2:D:644:CYS:O	2.37	0.49
2:F:522:TYR:OH	2:F:611:HIS:ND1	2.32	0.49
2:D:506:ILE:HG13	2:D:612:ASP:HA	1.93	0.49
4:L:152:ALA:O	4:L:153:ASP:HB2	2.12	0.49
4:M:13:ALA:O	4:M:16:GLN:HB2	2.13	0.49
3:I:93:VAL:HG22	3:I:121:THR:HG23	1.94	0.49
3:H:7:SER:HB3	3:H:21:SER:HB3	1.94	0.49
2:B:575:ARG:NH2	1:C:264:PHE:CE1	2.81	0.49
8:E:332:NAG:H4	8:E:333:BMA:O2	2.13	0.49
1:A:325:PRO:HB3	2:B:515:THR:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PHE:CD1	1:A:115:PHE:C	2.85	0.49
2:F:628:ASN:N	2:F:628:ASN:HD22	2.11	0.49
1:E:62:ALA:O	1:E:65:ILE:HD12	2.13	0.49
1:E:153:TRP:CZ2	3:J:106:VAL:HG11	2.47	0.49
4:L:30:LYS:O	4:L:31:SER:HB3	2.13	0.49
1:C:226:ARG:HA	9:C:334:SO4:O2	2.13	0.49
3:H:102:GLU:O	4:L:49:TYR:OH	2.25	0.48
2:F:528:ASN:ND2	2:F:644:CYS:O	2.45	0.48
4:M:146:VAL:HG11	4:M:197:VAL:CG1	2.41	0.48
2:D:645:ASN:ND2	2:D:646:ASP:N	2.61	0.48
2:F:530:GLN:NE2	2:F:645:ASN:HD21	2.12	0.48
1:C:115:PHE:C	1:C:115:PHE:CD1	2.85	0.48
1:A:8:CYS:O	2:B:524:TYR:HA	2.13	0.48
4:M:152:ALA:O	4:M:153:ASP:HB2	2.12	0.48
4:N:112:LYS:N	4:N:112:LYS:HD3	2.28	0.48
1:E:164:LEU:HD12	1:E:164:LEU:O	2.13	0.48
3:J:104:ARG:HH11	3:J:104:ARG:HG2	1.79	0.48
3:J:191:LEU:HD12	3:J:191:LEU:C	2.33	0.48
5:A:331:NAG:O3	5:A:332:NAG:H62	2.13	0.48
2:F:644:CYS:CB	2:F:648:CYS:SG	3.01	0.48
2:B:642:HIS:ND1	2:B:642:HIS:C	2.66	0.48
1:A:194:LEU:HD23	3:H:109:TYR:CD2	2.49	0.48
1:C:164:LEU:O	1:C:164:LEU:HD12	2.13	0.48
3:H:213:HIS:CD2	3:H:215:PRO:HD2	2.48	0.48
2:D:551:LYS:O	2:D:554:SER:N	2.46	0.48
3:I:197:VAL:HG11	3:I:207:TYR:CE1	2.48	0.48
1:C:115:PHE:O	1:C:115:PHE:HD1	1.97	0.48
4:N:153:ASP:O	4:N:155:SER:N	2.47	0.48
1:E:53:PRO:HB3	1:E:82:TYR:CE2	2.49	0.48
3:J:116:TRP:CZ3	4:N:43:PRO:HG2	2.49	0.48
2:F:528:ASN:CB	2:F:646:ASP:OD1	2.61	0.48
1:C:23:VAL:HG12	2:F:551:LYS:HB2	1.96	0.48
2:B:576:ARG:HB2	1:C:104:GLU:OE2	2.14	0.48
2:D:571:ASN:HB2	2:D:572:LYS:HE3	1.95	0.48
1:A:149:LYS:HD3	1:A:149:LYS:HA	1.70	0.48
1:C:11:TYR:CE1	2:D:506:ILE:HG23	2.49	0.48
1:C:153:TRP:CZ2	3:I:106:VAL:HG11	2.49	0.48
2:F:622:VAL:HG12	2:F:638:PHE:CE1	2.49	0.48
3:I:104:ARG:HH11	3:I:104:ARG:HG2	1.78	0.48
2:D:631:LYS:HE3	2:D:633:ILE:HG22	1.97	0.47
4:M:7:PRO:HD2	4:M:21:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:LEU:HD21	7:E:371:NAG:H62	1.95	0.47
4:M:30:LYS:HD3	4:M:89:VAL:CG1	2.42	0.47
1:C:222:LYS:NZ	4:M:26:ASP:OD1	2.48	0.47
3:J:51:ILE:HG23	3:J:51:ILE:O	2.14	0.47
3:H:182:VAL:O	3:H:182:VAL:HG13	2.14	0.47
2:D:509:PHE:CD1	2:D:509:PHE:C	2.87	0.47
2:B:509:PHE:CD1	2:B:510:ILE:HG13	2.50	0.47
2:F:623:LYS:HB2	2:F:638:PHE:HZ	1.78	0.47
2:D:631:LYS:O	2:D:631:LYS:HG3	2.14	0.47
4:N:30:LYS:HD3	4:N:89:VAL:CG1	2.40	0.47
2:B:509:PHE:C	2:B:509:PHE:HD1	2.16	0.47
1:C:62:ALA:O	1:C:65:ILE:HD12	2.14	0.47
1:E:70:GLU:HG3	8:E:331:NAG:N2	2.14	0.47
2:B:577:MET:SD	2:D:577:MET:CE	3.03	0.47
4:L:198:THR:HB	4:L:203:THR:HG1	1.76	0.47
4:N:138:ILE:HG12	4:N:197:VAL:HG21	1.97	0.47
1:E:31:THR:HG23	1:E:321:LEU:O	2.15	0.47
2:F:514:TRP:C	2:F:516:GLY:N	2.68	0.47
4:L:48:CYS:O	4:L:52:ASP:HB2	2.14	0.47
4:L:51:SER:HB3	4:L:63:GLY:O	2.14	0.47
3:H:83:VAL:HG12	3:H:86:LEU:HD13	1.96	0.47
1:C:23:VAL:HG22	2:D:602:LEU:HD12	1.97	0.47
2:D:659:TYR:N	2:D:660:PRO:CD	2.78	0.47
1:E:206:SER:C	1:E:208:HIS:H	2.17	0.47
2:B:511:GLU:OE2	2:B:511:GLU:HA	2.14	0.47
1:A:321:LEU:HD21	2:B:521:TRP:CD1	2.50	0.47
4:N:208:VAL:HG12	4:N:209:ALA:N	2.30	0.47
1:C:119:GLU:OE2	1:C:122:PRO:HA	2.14	0.47
3:I:223:ARG:HD2	3:I:225:GLU:OE2	2.14	0.47
3:J:18:VAL:HG22	3:J:86:LEU:CD2	2.37	0.47
4:N:146:VAL:HG11	4:N:197:VAL:CG1	2.41	0.47
1:C:115:PHE:O	1:C:115:PHE:CD1	2.68	0.47
1:C:296:GLN:O	1:C:309:TYR:HA	2.15	0.47
4:L:153:ASP:O	4:L:155:SER:N	2.48	0.47
3:H:163:VAL:CG1	3:H:191:LEU:HD21	2.45	0.47
4:N:48:CYS:O	4:N:52:ASP:HB2	2.15	0.47
2:B:585:ASP:O	2:B:589:ILE:HG13	2.14	0.46
3:J:163:VAL:CG1	3:J:191:LEU:HD21	2.45	0.46
3:I:37:VAL:HB	3:I:47:TRP:HA	1.97	0.46
1:A:286:GLN:H	1:A:286:GLN:HG2	1.40	0.46
3:J:197:VAL:HG11	3:J:207:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ARG:HB3	1:A:221:PRO:HD2	1.97	0.46
4:L:208:VAL:HG12	4:L:209:ALA:N	2.30	0.46
1:E:309:TYR:CD2	2:F:589:ILE:HD13	2.51	0.46
3:H:223:ARG:HD2	3:H:225:GLU:OE2	2.16	0.46
3:I:9:ALA:C	3:I:10:GLU:HG2	2.35	0.46
2:B:588:PHE:CE1	2:F:587:GLY:HA3	2.51	0.46
1:C:8:CYS:HB2	2:D:525:HIS:HB3	1.97	0.46
3:H:51:ILE:HG23	3:H:51:ILE:O	2.14	0.46
3:I:56:GLY:O	3:I:58:THR:HG23	2.14	0.46
2:D:622:VAL:CG1	2:D:638:PHE:CE1	2.92	0.46
3:J:30:THR:HA	3:J:53:PRO:HB2	1.97	0.46
3:H:30:THR:HA	3:H:53:PRO:HB2	1.97	0.46
2:B:526:HIS:CD2	2:B:649:MET:HG3	2.51	0.46
2:D:503:PHE:N	2:D:612:ASP:OD1	2.47	0.46
1:C:12:HIS:HE1	1:C:14:ASN:HB3	1.79	0.46
1:E:220:ARG:HB3	1:E:221:PRO:HD2	1.98	0.46
2:B:628:ASN:HD22	2:B:670:ARG:CZ	2.29	0.46
4:L:194:SER:HB2	4:L:207:THR:HG22	1.97	0.46
3:H:73:ASP:O	3:H:75:ALA:N	2.38	0.46
3:I:139:PRO:O	3:I:140:SER:C	2.54	0.46
1:A:53:PRO:HB3	1:A:82:TYR:CE2	2.50	0.46
3:H:104:ARG:HG2	3:H:104:ARG:HH11	1.79	0.46
1:A:65:ILE:HG22	1:A:258:PHE:CE1	2.51	0.46
2:F:580:LEU:HD22	2:F:580:LEU:O	2.15	0.46
2:D:626:LEU:O	2:D:627:LYS:C	2.54	0.46
2:B:622:VAL:HG12	2:B:638:PHE:CE1	2.51	0.46
1:E:42:ASN:O	1:E:43:GLY:C	2.53	0.46
1:C:124:GLU:O	1:C:125:SER:CB	2.63	0.46
2:D:503:PHE:CE1	2:D:613:SER:HB2	2.50	0.46
1:E:304:GLY:HA2	2:F:563:PHE:CD1	2.51	0.46
3:J:182:VAL:O	3:J:182:VAL:HG13	2.16	0.46
3:J:37:VAL:HB	3:J:47:TRP:HA	1.98	0.46
1:E:286:GLN:HE21	1:E:298:VAL:HG12	1.81	0.46
4:L:13:ALA:O	4:L:16:GLN:HB2	2.15	0.46
2:B:645:ASN:HD22	2:B:646:ASP:H	1.64	0.45
1:E:15:ASN:OD1	5:E:351:NAG:N2	2.49	0.45
1:E:206:SER:O	1:E:208:HIS:N	2.48	0.45
4:L:119:LEU:CD2	4:L:208:VAL:HG23	2.44	0.45
4:M:208:VAL:HG12	4:M:209:ALA:N	2.31	0.45
1:C:53:PRO:HB3	1:C:82:TYR:CE2	2.50	0.45
1:E:119:GLU:CD	1:E:122:PRO:HA	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:68:VAL:HG22	3:H:83:VAL:HG22	1.97	0.45
1:E:248:ASN:HD22	7:E:341:NAG:C8	2.22	0.45
1:E:6:THR:O	2:F:649:MET:HE3	2.15	0.45
1:C:12:HIS:HB2	2:D:521:TRP:HA	1.99	0.45
1:E:72:GLU:OE1	1:E:72:GLU:HA	2.16	0.45
2:B:509:PHE:O	2:B:509:PHE:HD1	1.99	0.45
1:C:61:VAL:HG23	1:C:85:GLU:OE1	2.16	0.45
3:H:70:MET:HG2	3:H:81:MET:HG2	1.98	0.45
1:E:75:ILE:N	1:E:75:ILE:HD12	2.32	0.45
1:A:116:GLU:HG3	1:A:116:GLU:O	2.15	0.45
2:F:570:PHE:CE1	2:F:577:MET:HG2	2.51	0.45
2:F:662:TYR:O	2:F:666:SER:OG	2.31	0.45
2:F:616:LYS:O	2:F:616:LYS:HG3	2.15	0.45
1:E:188:ILE:O	1:E:192:ARG:HG3	2.16	0.45
3:H:37:VAL:HB	3:H:47:TRP:HA	1.98	0.45
1:E:238:GLU:H	1:E:238:GLU:CD	2.20	0.45
4:M:104:LYS:HE3	4:M:104:LYS:HB3	1.85	0.45
3:J:102:GLU:O	4:N:49:TYR:OH	2.26	0.45
2:B:580:LEU:HD13	2:F:580:LEU:HD11	1.98	0.45
3:I:213:HIS:CD2	3:I:215:PRO:HD2	2.52	0.45
3:J:222:LYS:HA	3:J:222:LYS:HD3	1.74	0.45
1:E:286:GLN:HG2	1:E:286:GLN:H	1.36	0.45
4:L:26:ASP:HB3	4:L:29:ARG:HG2	1.98	0.45
1:A:321:LEU:N	1:A:321:LEU:HD23	2.32	0.45
2:B:551:LYS:HE3	1:E:23:VAL:HG11	1.97	0.45
4:N:104:LYS:HE3	4:N:104:LYS:HB3	1.82	0.45
2:D:657:TYR:HE2	2:D:659:TYR:CB	2.30	0.45
4:L:16:GLN:HB3	4:L:17:THR:H	1.61	0.45
2:D:591:ILE:HD13	2:F:591:ILE:HG21	1.99	0.45
4:L:7:PRO:HD2	4:L:21:THR:O	2.16	0.45
2:F:629:ASN:ND2	2:F:659:TYR:HB2	2.31	0.45
2:F:626:LEU:O	2:F:627:LYS:C	2.55	0.45
3:J:223:ARG:HD2	3:J:225:GLU:OE2	2.16	0.45
2:D:509:PHE:O	2:D:635:ASN:HB3	2.17	0.44
2:B:640:PHE:C	2:B:642:HIS:H	2.19	0.44
2:D:593:THR:O	2:D:597:GLU:HG3	2.17	0.44
1:A:248:ASN:HD22	7:A:341:NAG:C8	2.29	0.44
2:B:521:TRP:CZ3	2:B:545:ILE:HG13	2.53	0.44
4:M:171:ASN:OD1	4:M:173:LYS:HB2	2.17	0.44
3:J:213:HIS:CD2	3:J:215:PRO:HD2	2.51	0.44
1:A:238:GLU:CD	1:A:238:GLU:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:HD12	1:A:164:LEU:O	2.17	0.44
2:F:650:GLU:OE2	2:F:653:LYS:HD2	2.17	0.44
4:L:24:GLY:C	4:L:27:ILE:HD13	2.37	0.44
3:J:139:PRO:O	3:J:140:SER:C	2.56	0.44
1:C:116:GLU:O	1:C:116:GLU:HG3	2.17	0.44
4:L:112:LYS:N	4:L:112:LYS:CD	2.81	0.44
2:F:644:CYS:CB	2:F:648:CYS:HG	2.31	0.44
2:B:523:GLY:HA3	2:B:536:ALA:HA	1.98	0.44
2:D:659:TYR:HD1	2:D:660:PRO:HD3	1.81	0.44
1:C:76:SER:HB3	9:C:343:SO4:O2	2.17	0.44
4:L:27:ILE:HG22	4:L:65:ASN:OD1	2.17	0.44
1:C:206:SER:C	1:C:208:HIS:H	2.21	0.44
1:C:10:GLY:N	2:D:514:TRP:CH2	2.85	0.44
2:D:510:ILE:O	2:D:511:GLU:C	2.56	0.44
3:H:197:VAL:HB	3:H:198:PRO:CD	2.42	0.44
4:N:26:ASP:HB3	4:N:29:ARG:HG2	1.98	0.44
4:M:82:GLU:HG3	4:M:105:LEU:O	2.17	0.44
2:D:587:GLY:HA3	2:F:588:PHE:CE1	2.53	0.44
1:E:119:GLU:OE2	1:E:122:PRO:HA	2.18	0.44
4:N:24:GLY:C	4:N:27:ILE:HD13	2.38	0.44
1:E:88:ASN:O	1:E:89:PRO:C	2.55	0.44
2:D:538:GLN:HA	2:D:538:GLN:OE1	2.18	0.44
2:D:506:ILE:N	2:D:612:ASP:OD2	2.47	0.44
4:N:194:SER:HB3	4:N:207:THR:CB	2.45	0.44
1:A:12:HIS:HE1	1:A:14:ASN:HB3	1.82	0.44
1:A:119:GLU:CD	1:A:122:PRO:HA	2.38	0.44
1:C:45:LEU:HB2	1:C:275:MET:HA	1.99	0.44
1:E:226:ARG:HD3	9:E:336:SO4:O2	2.17	0.44
3:J:91:THR:HG23	3:J:123:THR:HA	2.00	0.44
1:C:42:ASN:O	1:C:43:GLY:C	2.56	0.44
2:F:628:ASN:HD21	2:F:659:TYR:HE2	1.66	0.44
4:M:24:GLY:C	4:M:27:ILE:HD13	2.38	0.44
4:L:152:ALA:HB2	4:L:193:TYR:CE2	2.53	0.44
2:F:515:THR:O	2:F:516:GLY:O	2.36	0.44
2:D:502:LEU:HG	2:F:503:PHE:CZ	2.53	0.44
1:E:115:PHE:HD1	1:E:115:PHE:O	2.01	0.44
2:B:571:ASN:HB2	2:B:572:LYS:CE	2.47	0.44
1:A:206:SER:C	1:A:208:HIS:H	2.21	0.44
4:M:112:LYS:HG2	4:M:112:LYS:H	1.68	0.44
2:D:526:HIS:HB2	2:D:649:MET:HE3	1.99	0.43
1:C:286:GLN:H	1:C:286:GLN:HG2	1.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:629:ASN:N	2:F:629:ASN:OD1	2.51	0.43
3:I:182:VAL:O	3:I:182:VAL:HG13	2.17	0.43
1:A:23:VAL:HG11	2:D:551:LYS:HE2	1.99	0.43
4:M:153:ASP:O	4:M:155:SER:N	2.52	0.43
1:A:321:LEU:CD2	2:B:521:TRP:CD1	3.01	0.43
1:E:304:GLY:HA2	2:F:563:PHE:CE1	2.52	0.43
1:A:61:VAL:HG23	1:A:85:GLU:OE1	2.18	0.43
2:D:631:LYS:HE2	2:D:639:GLU:HG2	1.99	0.43
2:F:634:GLY:O	2:F:635:ASN:O	2.36	0.43
2:D:549:THR:HG22	2:D:550:ASN:N	2.33	0.43
2:F:514:TRP:CE3	2:F:517:MET:HE2	2.52	0.43
2:F:545:ILE:O	2:F:549:THR:HB	2.18	0.43
4:L:146:VAL:HG12	4:L:147:THR:N	2.33	0.43
3:I:73:ASP:O	3:I:74:THR:HB	2.18	0.43
2:D:644:CYS:HB2	2:D:648:CYS:SG	2.59	0.43
1:A:31:THR:HG23	1:A:321:LEU:O	2.19	0.43
2:B:665:GLU:O	2:B:669:ASN:ND2	2.46	0.43
4:M:138:ILE:HG12	4:M:197:VAL:HG21	2.01	0.43
1:E:197:THR:HG23	9:E:339:SO4:O2	2.18	0.43
4:N:142:TYR:CD2	4:N:143:PRO:HA	2.53	0.43
1:E:57:GLY:O	1:E:86:LYS:HG2	2.19	0.43
3:H:9:ALA:C	3:H:10:GLU:HG2	2.39	0.43
3:I:83:VAL:HG12	3:I:86:LEU:HD13	2.01	0.43
1:A:115:PHE:HD1	1:A:115:PHE:O	2.01	0.43
1:A:45:LEU:HB2	1:A:275:MET:HA	2.01	0.43
1:C:79:SER:HB3	1:C:113:SER:O	2.18	0.43
4:M:119:LEU:CD2	4:M:208:VAL:HG23	2.49	0.43
1:A:296:GLN:O	1:A:309:TYR:HA	2.19	0.43
3:J:9:ALA:C	3:J:10:GLU:HG2	2.38	0.43
2:D:631:LYS:HG2	2:D:639:GLU:HB3	2.01	0.43
1:A:115:PHE:CD1	1:A:115:PHE:O	2.72	0.43
2:B:572:LYS:H	2:B:572:LYS:CD	2.30	0.43
1:C:188:ILE:O	1:C:192:ARG:HG3	2.19	0.43
5:C:341:NAG:O3	5:C:342:NAG:O5	2.34	0.43
1:C:110:SER:OG	1:C:267:GLY:N	2.52	0.43
1:C:238:GLU:H	1:C:238:GLU:CD	2.22	0.43
3:I:30:THR:HA	3:I:53:PRO:HB2	2.00	0.43
3:I:147:GLY:O	3:I:199:SER:OG	2.35	0.43
1:A:88:ASN:O	1:A:89:PRO:C	2.57	0.43
4:L:142:TYR:CD2	4:L:143:PRO:CA	3.02	0.43
1:C:164:LEU:HD12	1:C:164:LEU:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:514:TRP:CE3	2:B:517:MET:CE	3.02	0.42
1:A:72:GLU:OE1	1:A:72:GLU:HA	2.19	0.42
1:E:31:THR:C	1:E:32:HIS:ND1	2.72	0.42
1:A:53:PRO:O	1:A:77:ARG:NH2	2.48	0.42
3:H:139:PRO:O	3:H:140:SER:C	2.57	0.42
2:D:601:LEU:HA	2:D:601:LEU:HD23	1.76	0.42
1:C:180:TRP:CE2	1:C:204:VAL:HG21	2.54	0.42
4:M:141:PHE:CE2	4:M:146:VAL:HG23	2.55	0.42
1:A:9:ILE:HD12	2:B:619:TYR:HA	2.01	0.42
1:C:311:ARG:NH2	2:F:562:GLN:HG3	2.34	0.42
1:A:273:ALA:HA	1:A:274:PRO:HD2	1.85	0.42
2:D:523:GLY:CA	2:D:536:ALA:HA	2.49	0.42
4:M:48:CYS:O	4:M:52:ASP:HB2	2.18	0.42
1:E:115:PHE:CD1	1:E:115:PHE:O	2.72	0.42
2:F:659:TYR:CD1	2:F:660:PRO:HD3	2.51	0.42
2:F:516:GLY:O	2:F:517:MET:C	2.58	0.42
3:H:36:TRP:CD2	3:H:81:MET:HG3	2.55	0.42
2:F:631:LYS:CG	2:F:639:GLU:HB3	2.50	0.42
3:J:36:TRP:CD2	3:J:81:MET:HG3	2.54	0.42
2:B:545:ILE:O	2:B:549:THR:HB	2.20	0.42
1:C:206:SER:O	1:C:208:HIS:N	2.52	0.42
1:E:20:VAL:HG11	1:E:318:VAL:HB	2.02	0.42
3:I:51:ILE:HG23	3:I:51:ILE:O	2.18	0.42
4:L:190:HIS:CD2	4:L:190:HIS:N	2.88	0.42
4:L:104:LYS:HE3	4:L:104:LYS:HB3	1.91	0.42
1:E:224:ARG:HH22	8:E:331:NAG:C8	2.27	0.42
1:C:23:VAL:CG1	2:F:551:LYS:HE2	2.46	0.42
1:A:206:SER:O	1:A:208:HIS:N	2.53	0.42
3:H:91:THR:HG23	3:H:123:THR:HA	2.01	0.42
4:N:117:VAL:O	4:N:206:LYS:HE3	2.20	0.42
1:E:96:PRO:HB2	1:E:229:ARG:CD	2.48	0.42
2:D:642:HIS:ND1	2:D:642:HIS:C	2.70	0.42
1:C:289:ILE:HD13	1:C:289:ILE:HA	1.71	0.42
1:C:61:VAL:HG21	1:C:106:ARG:HG2	2.01	0.42
1:C:53:PRO:O	1:C:77:ARG:NH2	2.52	0.42
4:N:152:ALA:HB2	4:N:193:TYR:CE2	2.55	0.42
1:C:75:ILE:HD12	1:C:75:ILE:H	1.83	0.42
2:B:521:TRP:HZ3	2:B:545:ILE:N	2.18	0.42
1:A:319:THR:HB	2:B:548:ILE:HG21	2.01	0.42
1:E:149:LYS:HD3	1:E:149:LYS:HA	1.71	0.42
2:D:632:GLU:HG2	2:D:638:PHE:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:146:VAL:HG12	4:N:147:THR:N	2.35	0.42
4:L:119:LEU:HD12	4:L:135:VAL:O	2.20	0.42
2:D:671:GLU:C	2:D:672:LYS:HD3	2.40	0.42
4:M:50:ASP:OD1	4:M:65:ASN:CB	2.68	0.42
3:I:70:MET:HG2	3:I:81:MET:HG2	2.02	0.42
3:I:91:THR:HG23	3:I:123:THR:HA	2.00	0.42
1:E:47:LEU:HD22	1:E:52:ALA:CB	2.50	0.42
1:E:47:LEU:HD22	1:E:52:ALA:HB2	2.01	0.42
3:H:101:LEU:HD11	4:L:45:LEU:HD21	2.01	0.42
2:B:565:ALA:O	2:B:566:VAL:C	2.58	0.42
1:C:158:ASN:HB3	3:I:54:ASN:ND2	2.33	0.42
3:I:222:LYS:HD3	3:I:222:LYS:HA	1.72	0.42
2:F:506:ILE:HD11	2:F:615:VAL:HG21	2.01	0.42
4:L:121:PRO:HB3	4:L:208:VAL:CG1	2.46	0.42
2:B:623:LYS:HB2	2:B:638:PHE:HZ	1.85	0.42
4:N:50:ASP:OD1	4:N:65:ASN:CB	2.68	0.42
1:A:96:PRO:HB2	1:A:229:ARG:CD	2.50	0.42
4:L:138:ILE:HG12	4:L:197:VAL:HG21	2.01	0.41
1:A:309:TYR:HD2	2:B:589:ILE:HD13	1.85	0.41
3:I:36:TRP:CD2	3:I:81:MET:HG3	2.55	0.41
4:L:184:PRO:O	4:L:188:LYS:HD3	2.20	0.41
1:E:285:PRO:HG2	1:E:299:HIS:CE1	2.55	0.41
1:A:192:ARG:NH1	4:L:95:ASP:OD2	2.52	0.41
1:A:152:LEU:HA	1:A:152:LEU:HD23	1.89	0.41
1:A:33:SER:OG	1:A:316:ARG:HD3	2.20	0.41
3:H:17:SER:OG	3:H:84:ASN:HA	2.19	0.41
2:B:526:HIS:HD2	2:B:649:MET:HG3	1.85	0.41
2:F:642:HIS:C	2:F:642:HIS:ND1	2.73	0.41
1:E:228:GLY:O	1:E:229:ARG:HD3	2.20	0.41
3:J:147:GLY:O	3:J:199:SER:OG	2.36	0.41
1:A:47:LEU:HD22	1:A:52:ALA:HB2	2.01	0.41
4:M:12:VAL:HG11	4:M:77:VAL:HG21	2.02	0.41
3:I:116:TRP:N	3:I:116:TRP:CD1	2.88	0.41
1:A:146:SER:OG	1:A:147:PHE:N	2.51	0.41
3:H:201:SER:O	3:H:202:LEU:O	2.38	0.41
4:N:31:SER:OG	4:N:49:TYR:HD1	2.02	0.41
1:E:8:CYS:HB2	2:F:525:HIS:CB	2.43	0.41
1:C:197:THR:HG23	9:C:337:SO4:O2	2.20	0.41
1:A:226:ARG:NH1	4:L:29:ARG:HH21	2.16	0.41
1:A:79:SER:HB3	1:A:113:SER:O	2.21	0.41
4:L:46:VAL:HG23	4:L:47:VAL:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:13:ALA:O	4:M:14:PRO:O	2.38	0.41
2:B:591:ILE:HG21	2:F:591:ILE:HD13	2.02	0.41
4:N:171:ASN:OD1	4:N:173:LYS:HB2	2.20	0.41
1:A:187:ASN:HD22	4:L:93:SER:HA	1.84	0.41
2:F:631:LYS:HG3	2:F:639:GLU:HB3	2.02	0.41
2:F:562:GLN:HE21	2:F:562:GLN:HB3	1.71	0.41
2:F:629:ASN:ND2	2:F:659:TYR:CD2	2.87	0.41
1:E:61:VAL:HG23	1:E:85:GLU:OE1	2.20	0.41
1:E:9:ILE:O	2:F:510:ILE:HD13	2.20	0.41
3:J:184:GLN:HE21	3:J:184:GLN:HB2	1.73	0.41
3:I:36:TRP:CZ3	3:I:96:CYS:HB3	2.55	0.41
1:E:54:LEU:HD13	1:E:80:TRP:CE3	2.56	0.41
1:E:68:ASN:HA	1:E:69:PRO:HD3	1.87	0.41
2:D:642:HIS:O	2:D:643:LYS:C	2.58	0.41
3:H:201:SER:O	3:H:202:LEU:C	2.59	0.41
2:B:588:PHE:CZ	2:F:587:GLY:HA3	2.56	0.41
3:I:17:SER:OG	3:I:84:ASN:HA	2.21	0.41
1:A:75:ILE:HD12	1:A:75:ILE:N	2.35	0.41
1:A:289:ILE:HA	1:A:289:ILE:HD13	1.72	0.41
1:A:226:ARG:HH12	4:L:29:ARG:NH2	2.15	0.41
1:E:226:ARG:NH1	4:N:29:ARG:HH21	2.18	0.41
4:L:31:SER:OG	4:L:49:TYR:HD1	2.03	0.41
1:E:288:ALA:O	1:E:289:ILE:HD13	2.21	0.41
3:I:30:THR:O	3:I:54:ASN:HB2	2.20	0.41
4:N:153:ASP:C	4:N:155:SER:N	2.73	0.41
1:C:220:ARG:HH21	1:E:207:SER:N	2.18	0.41
3:H:47:TRP:CG	4:L:97:VAL:HB	2.56	0.41
1:E:238:GLU:HB2	1:E:239:PRO:HD2	2.03	0.41
3:I:62:GLN:O	3:I:63:LYS:C	2.59	0.41
3:I:99:GLY:HA2	3:I:112:GLY:O	2.21	0.41
1:C:149:LYS:HD3	1:C:149:LYS:HA	1.74	0.41
1:E:276:ASP:CG	1:E:277:GLU:H	2.25	0.41
1:C:11:TYR:CE2	2:D:506:ILE:HG23	2.56	0.41
4:N:119:LEU:CD2	4:N:208:VAL:HG23	2.51	0.41
1:E:95:TYR:HA	1:E:96:PRO:HD2	1.93	0.41
4:L:12:VAL:HG11	4:L:77:VAL:HG21	2.03	0.41
4:M:194:SER:HB2	4:M:207:THR:HG22	2.03	0.40
2:F:572:LYS:CD	2:F:572:LYS:H	2.35	0.40
1:C:296:GLN:HB3	1:C:307:PRO:HB2	2.04	0.40
4:M:27:ILE:HG22	4:M:65:ASN:OD1	2.21	0.40
3:H:214:LYS:N	3:H:215:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:SER:C	1:E:208:HIS:N	2.75	0.40
3:I:199:SER:H	3:I:199:SER:HG	1.67	0.40
1:E:33:SER:OG	1:E:316:ARG:HD3	2.21	0.40
2:D:632:GLU:HG2	2:D:638:PHE:CE2	2.56	0.40
1:E:6:THR:O	2:F:649:MET:CE	2.69	0.40
1:C:74:LEU:O	1:C:76:SER:N	2.54	0.40
3:J:73:ASP:O	3:J:74:THR:HB	2.21	0.40
3:J:6:GLN:N	3:J:118:GLN:OE1	2.31	0.40
1:C:22:THR:HB	2:D:605:GLU:OE1	2.20	0.40
1:C:285:PRO:HG2	1:C:299:HIS:CE1	2.56	0.40
2:F:530:GLN:NE2	2:F:645:ASN:ND2	2.69	0.40
3:H:197:VAL:HG11	3:H:207:TYR:CE1	2.56	0.40
1:C:284:THR:HG21	1:C:289:ILE:HG12	2.04	0.40
1:E:296:GLN:HB3	1:E:307:PRO:HB2	2.03	0.40
4:L:50:ASP:OD1	4:L:65:ASN:CB	2.69	0.40
2:B:626:LEU:O	2:B:627:LYS:C	2.59	0.40
1:C:47:LEU:HD22	1:C:52:ALA:HB2	2.03	0.40
2:D:517:MET:CG	2:D:536:ALA:HB2	2.51	0.40
4:M:194:SER:HB3	4:M:207:THR:CB	2.47	0.40
1:A:119:GLU:OE2	1:A:122:PRO:HA	2.22	0.40
1:E:49:LYS:HE2	1:E:305:GLU:CD	2.42	0.40
1:C:57:GLY:O	1:C:86:LYS:HG2	2.21	0.40
1:A:126:SER:C	1:A:128:PRO:HD3	2.41	0.40
2:B:634:GLY:O	2:B:635:ASN:O	2.39	0.40
1:E:12:HIS:HE1	1:E:14:ASN:HB3	1.86	0.40
2:B:669:ASN:H	2:B:669:ASN:ND2	2.18	0.40
1:A:49:LYS:HE2	1:A:305:GLU:CD	2.42	0.40
1:E:126:SER:C	1:E:128:PRO:HD3	2.41	0.40
1:E:127:TRP:N	1:E:128:PRO:HD3	2.37	0.40
1:C:20:VAL:HG11	1:C:318:VAL:HB	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/327 (98%)	285 (89%)	29 (9%)	7 (2%)	8	45
1	C	321/327 (98%)	286 (89%)	27 (8%)	8 (2%)	7	41
1	E	321/327 (98%)	284 (88%)	30 (9%)	7 (2%)	8	45
2	B	171/182 (94%)	129 (75%)	28 (16%)	14 (8%)	1	7
2	D	171/182 (94%)	133 (78%)	26 (15%)	12 (7%)	1	10
2	F	171/182 (94%)	135 (79%)	23 (14%)	13 (8%)	1	9
3	H	217/227 (96%)	197 (91%)	18 (8%)	2 (1%)	21	67
3	I	217/227 (96%)	198 (91%)	16 (7%)	3 (1%)	14	57
3	J	217/227 (96%)	196 (90%)	19 (9%)	2 (1%)	21	67
4	L	208/211 (99%)	186 (89%)	19 (9%)	3 (1%)	14	57
4	M	208/211 (99%)	189 (91%)	16 (8%)	3 (1%)	14	57
4	N	208/211 (99%)	189 (91%)	16 (8%)	3 (1%)	14	57
All	All	2751/2841 (97%)	2407 (88%)	267 (10%)	77 (3%)	6	37

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ILE
2	B	643	LYS
1	C	125	SER
2	D	526	HIS
2	D	627	LYS
2	D	643	LYS
1	E	75	ILE
1	E	125	SER
2	F	511	GLU
2	F	643	LYS
2	F	646	ASP
2	F	650	GLU
1	A	43	GLY
1	A	125	SER
1	A	262	ARG
1	A	265	GLY
2	B	572	LYS
2	B	627	LYS
2	B	634	GLY

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Mol	Chain	Res	Type
2	B	658	ASP
1	C	43	GLY
1	C	75	ILE
1	C	262	ARG
1	C	265	GLY
2	D	511	GLU
2	D	516	GLY
1	E	43	GLY
1	E	262	ARG
1	E	265	GLY
2	F	516	GLY
2	F	517	MET
2	F	633	ILE
3	H	151	LEU
3	H	202	LEU
3	I	151	LEU
3	I	202	LEU
3	J	151	LEU
3	J	202	LEU
4	L	154	SER
4	M	154	SER
1	A	14	ASN
2	B	511	GLU
2	B	517	MET
2	B	635	ASN
2	B	641	TYR
2	B	657	TYR
1	C	14	ASN
1	C	207	SER
2	D	626	LEU
2	D	633	ILE
2	D	635	ASN
2	D	657	TYR
1	E	207	SER
2	F	657	TYR
2	F	658	ASP
4	N	154	SER
1	A	207	SER
2	B	633	ILE
2	D	517	MET
2	D	658	ASP
1	E	14	ASN

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Mol	Chain	Res	Type
2	F	557	GLU
2	F	634	GLY
2	F	635	ASN
3	I	127	ALA
2	B	526	HIS
1	C	145	SER
2	F	526	HIS
4	L	51	SER
4	M	14	PRO
4	M	51	SER
4	N	14	PRO
2	B	516	GLY
4	L	14	PRO
2	D	634	GLY
4	N	15	GLY
2	B	566	VAL

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	283/287 (99%)	257 (91%)	26 (9%)	11	41
1	C	283/287 (99%)	254 (90%)	29 (10%)	9	36
1	E	283/287 (99%)	254 (90%)	29 (10%)	9	36
2	B	148/157 (94%)	130 (88%)	18 (12%)	6	27
2	D	148/157 (94%)	125 (84%)	23 (16%)	3	15
2	F	148/157 (94%)	130 (88%)	18 (12%)	6	27
3	H	184/190 (97%)	158 (86%)	26 (14%)	4	20
3	I	184/190 (97%)	159 (86%)	25 (14%)	5	22
3	J	184/190 (97%)	153 (83%)	31 (17%)	2	13
4	L	177/178 (99%)	162 (92%)	15 (8%)	13	47
4	M	177/178 (99%)	164 (93%)	13 (7%)	17	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	N	177/178 (99%)	163 (92%)	14 (8%)	15 53
All	All	2376/2436 (98%)	2109 (89%)	267 (11%)	7 32

All (267) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	65	ILE
1	A	72	GLU
1	A	73	LEU
1	A	75	ILE
1	A	78	GLU
1	A	109	LEU
1	A	111	SER
1	A	115	PHE
1	A	118	PHE
1	A	124	GLU
1	A	161	TYR
1	A	188	ILE
1	A	198	GLU
1	A	205	VAL
1	A	216	GLU
1	A	224	ARG
1	A	226	ARG
1	A	255	ARG
1	A	260	LEU
1	A	261	SER
1	A	284	THR
1	A	289	ILE
1	A	296	GLN
1	A	321	LEU
1	A	326	SER
2	B	509	PHE
2	B	526	HIS
2	B	528	ASN
2	B	529	GLU
2	B	559	MET
2	B	560	ASN
2	B	572	LYS
2	B	577	MET
2	B	580	LEU
2	B	598	LEU

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Mol	Chain	Res	Type
2	B	613	SER
2	B	625	GLN
2	B	639	GLU
2	B	641	TYR
2	B	642	HIS
2	B	647	GLU
2	B	658	ASP
2	B	659	TYR
1	C	12	HIS
1	C	21	ASP
1	C	29	THR
1	C	65	ILE
1	C	72	GLU
1	C	73	LEU
1	C	75	ILE
1	C	78	GLU
1	C	109	LEU
1	C	111	SER
1	C	115	PHE
1	C	118	PHE
1	C	124	GLU
1	C	161	TYR
1	C	188	ILE
1	C	198	GLU
1	C	205	VAL
1	C	216	GLU
1	C	220	ARG
1	C	224	ARG
1	C	226	ARG
1	C	255	ARG
1	C	260	LEU
1	C	261	SER
1	C	284	THR
1	C	289	ILE
1	C	296	GLN
1	C	321	LEU
1	C	326	SER
2	D	509	PHE
2	D	515	THR
2	D	517	MET
2	D	526	HIS
2	D	545	ILE

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Mol	Chain	Res	Type
2	D	548	ILE
2	D	549	THR
2	D	555	VAL
2	D	559	MET
2	D	560	ASN
2	D	561	THR
2	D	562	GLN
2	D	572	LYS
2	D	573	LEU
2	D	580	LEU
2	D	582	LYS
2	D	593	THR
2	D	641	TYR
2	D	642	HIS
2	D	644	CYS
2	D	647	GLU
2	D	658	ASP
2	D	659	TYR
1	E	12	HIS
1	E	17	THR
1	E	29	THR
1	E	32	HIS
1	E	65	ILE
1	E	72	GLU
1	E	73	LEU
1	E	75	ILE
1	E	78	GLU
1	E	109	LEU
1	E	111	SER
1	E	115	PHE
1	E	118	PHE
1	E	124	GLU
1	E	161	TYR
1	E	188	ILE
1	E	198	GLU
1	E	205	VAL
1	E	216	GLU
1	E	224	ARG
1	E	226	ARG
1	E	255	ARG
1	E	260	LEU
1	E	261	SER

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Mol	Chain	Res	Type
1	E	284	THR
1	E	289	ILE
1	E	296	GLN
1	E	321	LEU
1	E	326	SER
2	F	509	PHE
2	F	515	THR
2	F	526	HIS
2	F	528	ASN
2	F	529	GLU
2	F	548	ILE
2	F	549	THR
2	F	560	ASN
2	F	561	THR
2	F	572	LYS
2	F	573	LEU
2	F	580	LEU
2	F	628	ASN
2	F	642	HIS
2	F	647	GLU
2	F	658	ASP
2	F	659	TYR
2	F	663	SER
3	H	2	VAL
3	H	18	VAL
3	H	28	THR
3	H	37	VAL
3	H	38	ARG
3	H	65	GLN
3	H	72	ARG
3	H	81	MET
3	H	86	LEU
3	H	98	ARG
3	H	101	LEU
3	H	105	SER
3	H	114	ASP
3	H	118	GLN
3	H	121	THR
3	H	137	LEU
3	H	151	LEU
3	H	153	CYS
3	H	172	LEU

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Mol	Chain	Res	Type
3	H	173	THR
3	H	174	SER
3	H	177	HIS
3	H	195	VAL
3	H	196	THR
3	H	210	ASN
3	H	222	LYS
3	I	2	VAL
3	I	18	VAL
3	I	28	THR
3	I	37	VAL
3	I	38	ARG
3	I	50	TRP
3	I	65	GLN
3	I	72	ARG
3	I	86	LEU
3	I	98	ARG
3	I	101	LEU
3	I	114	ASP
3	I	118	GLN
3	I	121	THR
3	I	137	LEU
3	I	151	LEU
3	I	153	CYS
3	I	172	LEU
3	I	173	THR
3	I	174	SER
3	I	192	SER
3	I	195	VAL
3	I	196	THR
3	I	210	ASN
3	I	222	LYS
3	J	2	VAL
3	J	18	VAL
3	J	28	THR
3	J	37	VAL
3	J	38	ARG
3	J	50	TRP
3	J	65	GLN
3	J	72	ARG
3	J	81	MET
3	J	86	LEU

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Mol	Chain	Res	Type
3	J	98	ARG
3	J	101	LEU
3	J	105	SER
3	J	114	ASP
3	J	118	GLN
3	J	121	THR
3	J	126	SER
3	J	128	SER
3	J	137	LEU
3	J	151	LEU
3	J	153	CYS
3	J	169	SER
3	J	172	LEU
3	J	173	THR
3	J	174	SER
3	J	177	HIS
3	J	192	SER
3	J	195	VAL
3	J	196	THR
3	J	210	ASN
3	J	222	LYS
4	L	21	THR
4	L	26	ASP
4	L	27	ILE
4	L	52	ASP
4	L	69	THR
4	L	71	THR
4	L	73	THR
4	L	84	ASP
4	L	96	HIS
4	L	110	GLN
4	L	112	LYS
4	L	167	SER
4	L	170	SER
4	L	198	THR
4	L	207	THR
4	M	21	THR
4	M	26	ASP
4	M	27	ILE
4	M	52	ASP
4	M	69	THR
4	M	71	THR

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Mol	Chain	Res	Type
4	M	73	THR
4	M	84	ASP
4	M	96	HIS
4	M	167	SER
4	M	170	SER
4	M	198	THR
4	M	207	THR
4	N	21	THR
4	N	26	ASP
4	N	27	ILE
4	N	52	ASP
4	N	69	THR
4	N	71	THR
4	N	73	THR
4	N	84	ASP
4	N	96	HIS
4	N	167	SER
4	N	170	SER
4	N	182	LEU
4	N	198	THR
4	N	207	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	286	GLN
2	B	530	GLN
2	B	628	ASN
2	B	645	ASN
2	B	654	ASN
2	B	669	ASN
1	C	187	ASN
1	C	286	GLN
2	D	530	GLN
1	E	286	GLN
2	F	530	GLN
2	F	628	ASN
2	F	645	ASN
3	I	54	ASN
4	L	190	HIS
4	M	190	HIS

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Mol	Chain	Res	Type
4	N	190	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

13 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$
5	NAG	A	331	1,5	14,14,15	0.61	0	15,19,21	0.96	0
5	NAG	A	332	5	14,14,15	0.57	0	15,19,21	1.75	4 (26%)
5	NAG	A	371	1,5	14,14,15	0.52	0	15,19,21	0.90	1 (6%)
5	NAG	A	372	5	14,14,15	0.55	0	15,19,21	0.89	1 (6%)
5	NAG	C	331	1,5	14,14,15	0.44	0	15,19,21	2.42	2 (13%)
5	NAG	C	332	5	14,14,15	0.63	0	15,19,21	1.43	3 (20%)
5	NAG	C	341	1,5	14,14,15	0.42	0	15,19,21	1.48	3 (20%)
5	NAG	C	342	5	14,14,15	0.55	0	15,19,21	2.11	2 (13%)
8	NAG	E	331	1,8	14,14,15	0.64	0	15,19,21	1.05	1 (6%)
8	NAG	E	332	8	14,14,15	0.72	0	15,19,21	1.53	4 (26%)
8	BMA	E	333	8	11,11,12	0.64	0	14,15,17	2.38	3 (21%)
5	NAG	E	351	1,5	14,14,15	0.80	1 (7%)	15,19,21	1.84	2 (13%)
5	NAG	E	352	5	14,14,15	0.65	0	15,19,21	2.26	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	331	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	332	5	-	1/6/23/26	0/1/1/1
5	NAG	A	371	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	372	5	-	1/6/23/26	0/1/1/1
5	NAG	C	331	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	332	5	-	0/6/23/26	0/1/1/1
5	NAG	C	341	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	342	5	-	0/6/23/26	0/1/1/1
8	NAG	E	331	1,8	-	0/6/23/26	0/1/1/1
8	NAG	E	332	8	-	0/6/23/26	0/1/1/1
8	BMA	E	333	8	-	0/2/19/22	1/1/1/1
5	NAG	E	351	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	E	352	5	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	351	NAG	C1-C2	2.31	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	341	NAG	C4-C3-C2	-2.90	106.72	111.23
8	E	332	NAG	O7-C7-C8	-2.85	116.83	122.06
5	C	331	NAG	C6-C5-C4	-2.63	106.52	113.02
5	C	341	NAG	C3-C4-C5	-2.61	105.65	110.20
5	C	332	NAG	O7-C7-C8	-2.41	117.64	122.06
5	C	332	NAG	C4-C3-C2	2.05	114.42	111.23
5	A	332	NAG	C3-C4-C5	2.07	113.80	110.20
8	E	332	NAG	O7-C7-N2	2.11	126.17	121.86
8	E	333	BMA	O2-C2-C1	2.20	113.62	109.21
8	E	332	NAG	O4-C4-C3	2.21	115.31	110.34
5	A	372	NAG	C2-N2-C7	2.30	126.00	123.04
5	C	341	NAG	O5-C5-C6	2.33	112.40	107.35
5	A	371	NAG	C4-C3-C2	2.48	115.08	111.23
5	A	332	NAG	O5-C5-C6	2.55	112.88	107.35
5	E	352	NAG	C8-C7-N2	2.56	121.01	116.11
5	E	351	NAG	C2-N2-C7	2.65	126.44	123.04
5	C	332	NAG	C2-N2-C7	2.81	126.65	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	331	NAG	C1-O5-C5	2.86	115.88	112.25
8	E	332	NAG	C2-N2-C7	3.29	127.27	123.04
5	A	332	NAG	C1-O5-C5	3.70	116.95	112.25
8	E	333	BMA	C1-C2-C3	4.05	114.33	109.54
5	A	332	NAG	C2-N2-C7	4.28	128.54	123.04
5	E	352	NAG	C1-O5-C5	4.77	118.30	112.25
5	C	342	NAG	C2-N2-C7	5.05	129.53	123.04
5	C	342	NAG	C1-O5-C5	5.51	119.24	112.25
5	E	352	NAG	C2-N2-C7	5.82	130.51	123.04
5	E	351	NAG	C1-O5-C5	5.83	119.65	112.25
8	E	333	BMA	C1-O5-C5	6.91	121.01	112.25
5	C	331	NAG	C1-O5-C5	8.27	122.74	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	351	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	332	NAG	O7-C7-N2-C2
5	A	372	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	333	BMA	C1-C2-C3-C4-C5-O5

10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	331	NAG	3	0
5	A	332	NAG	1	0
5	C	331	NAG	1	0
5	C	341	NAG	1	0
5	C	342	NAG	1	0
8	E	331	NAG	6	0
8	E	332	NAG	1	0
8	E	333	BMA	1	0
5	E	351	NAG	3	0
5	E	352	NAG	2	0

5.6 Ligand geometry ⓘ

52 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	$\# Z > 2$
6	MAN	A	333	-	11,11,12	0.65	0	14,15,17	0.68	0
9	SO4	A	334	-	4,4,4	0.08	0	6,6,6	0.30	0
9	SO4	A	335	-	4,4,4	0.12	0	6,6,6	0.37	0
9	SO4	A	336	-	4,4,4	0.14	0	6,6,6	0.20	0
9	SO4	A	337	-	4,4,4	0.13	0	6,6,6	0.23	0
9	SO4	A	338	-	4,4,4	0.10	0	6,6,6	0.12	0
9	SO4	A	339	-	4,4,4	0.14	0	6,6,6	0.19	0
7	NAG	A	341	1	14,14,15	0.43	0	15,19,21	2.26	2 (13%)
7	NAG	A	361	1	14,14,15	0.55	0	15,19,21	1.19	2 (13%)
9	SO4	C	333	-	4,4,4	0.13	0	6,6,6	0.40	0
9	SO4	C	334	-	4,4,4	0.39	0	6,6,6	0.76	0
9	SO4	C	335	-	4,4,4	0.14	0	6,6,6	0.22	0
9	SO4	C	336	-	4,4,4	0.11	0	6,6,6	0.29	0
9	SO4	C	337	-	4,4,4	0.19	0	6,6,6	0.43	0
9	SO4	C	338	-	4,4,4	0.16	0	6,6,6	0.31	0
9	SO4	C	339	-	4,4,4	0.19	0	6,6,6	0.08	0
9	SO4	C	340	-	4,4,4	0.38	0	6,6,6	0.58	0
9	SO4	C	343	-	4,4,4	0.48	0	6,6,6	0.33	0
7	NAG	C	351	1	14,14,15	0.74	1 (7%)	15,19,21	1.80	2 (13%)
7	NAG	C	361	1	14,14,15	0.59	0	15,19,21	1.06	2 (13%)
7	NAG	C	371	1	14,14,15	0.64	0	15,19,21	1.42	2 (13%)
9	SO4	E	334	-	4,4,4	0.16	0	6,6,6	0.32	0
9	SO4	E	335	-	4,4,4	0.13	0	6,6,6	0.19	0
9	SO4	E	336	-	4,4,4	0.24	0	6,6,6	0.23	0
9	SO4	E	337	-	4,4,4	0.23	0	6,6,6	0.25	0
9	SO4	E	338	-	4,4,4	0.12	0	6,6,6	0.18	0
9	SO4	E	339	-	4,4,4	0.19	0	6,6,6	0.19	0
9	SO4	E	340	-	4,4,4	0.16	0	6,6,6	0.15	0
7	NAG	E	341	1	14,14,15	0.51	0	15,19,21	2.71	3 (20%)
9	SO4	E	342	-	4,4,4	0.09	0	6,6,6	0.23	0
9	SO4	E	343	-	4,4,4	0.14	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	E	344	-	4,4,4	0.24	0	6,6,6	0.28	0
9	SO4	E	345	-	4,4,4	0.38	0	6,6,6	0.12	0
9	SO4	E	346	-	4,4,4	0.52	0	6,6,6	0.66	0
7	NAG	E	361	1	14,14,15	0.57	0	15,19,21	0.84	0
7	NAG	E	371	1	14,14,15	0.56	0	15,19,21	1.12	2 (13%)
9	SO4	H	228	-	4,4,4	0.26	0	6,6,6	0.37	0
9	SO4	H	229	-	4,4,4	0.16	0	6,6,6	0.34	0
9	SO4	H	230	-	4,4,4	0.19	0	6,6,6	0.25	0
9	SO4	I	228	-	4,4,4	0.11	0	6,6,6	0.23	0
9	SO4	I	229	-	4,4,4	0.09	0	6,6,6	0.27	0
9	SO4	I	230	-	4,4,4	0.19	0	6,6,6	0.17	0
9	SO4	I	231	-	4,4,4	0.15	0	6,6,6	0.36	0
9	SO4	I	232	-	4,4,4	0.27	0	6,6,6	0.52	0
9	SO4	J	228	-	4,4,4	0.29	0	6,6,6	0.71	0
9	SO4	J	229	-	4,4,4	0.25	0	6,6,6	0.55	0
9	SO4	L	212	-	4,4,4	0.11	0	6,6,6	0.16	0
9	SO4	L	213	-	4,4,4	0.13	0	6,6,6	0.24	0
9	SO4	M	212	-	4,4,4	0.12	0	6,6,6	0.26	0
9	SO4	N	212	-	4,4,4	0.18	0	6,6,6	0.36	0
9	SO4	N	213	-	4,4,4	0.11	0	6,6,6	0.48	0
9	SO4	N	214	-	4,4,4	0.18	0	6,6,6	0.34	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	MAN	A	333	-	-	0/2/19/22	0/1/1/1
9	SO4	A	334	-	-	0/0/0/0	0/0/0/0
9	SO4	A	335	-	-	0/0/0/0	0/0/0/0
9	SO4	A	336	-	-	0/0/0/0	0/0/0/0
9	SO4	A	337	-	-	0/0/0/0	0/0/0/0
9	SO4	A	338	-	-	0/0/0/0	0/0/0/0
9	SO4	A	339	-	-	0/0/0/0	0/0/0/0
7	NAG	A	341	1	-	0/6/23/26	0/1/1/1
7	NAG	A	361	1	-	2/6/23/26	0/1/1/1
9	SO4	C	333	-	-	0/0/0/0	0/0/0/0
9	SO4	C	334	-	-	0/0/0/0	0/0/0/0
9	SO4	C	335	-	-	0/0/0/0	0/0/0/0
9	SO4	C	336	-	-	0/0/0/0	0/0/0/0
9	SO4	C	337	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SO4	C	338	-	-	0/0/0/0	0/0/0/0
9	SO4	C	339	-	-	0/0/0/0	0/0/0/0
9	SO4	C	340	-	-	0/0/0/0	0/0/0/0
9	SO4	C	343	-	-	0/0/0/0	0/0/0/0
7	NAG	C	351	1	-	0/6/23/26	0/1/1/1
7	NAG	C	361	1	-	0/6/23/26	0/1/1/1
7	NAG	C	371	1	-	0/6/23/26	0/1/1/1
9	SO4	E	334	-	-	0/0/0/0	0/0/0/0
9	SO4	E	335	-	-	0/0/0/0	0/0/0/0
9	SO4	E	336	-	-	0/0/0/0	0/0/0/0
9	SO4	E	337	-	-	0/0/0/0	0/0/0/0
9	SO4	E	338	-	-	0/0/0/0	0/0/0/0
9	SO4	E	339	-	-	0/0/0/0	0/0/0/0
9	SO4	E	340	-	-	0/0/0/0	0/0/0/0
7	NAG	E	341	1	-	0/6/23/26	0/1/1/1
9	SO4	E	342	-	-	0/0/0/0	0/0/0/0
9	SO4	E	343	-	-	0/0/0/0	0/0/0/0
9	SO4	E	344	-	-	0/0/0/0	0/0/0/0
9	SO4	E	345	-	-	0/0/0/0	0/0/0/0
9	SO4	E	346	-	-	0/0/0/0	0/0/0/0
7	NAG	E	361	1	-	0/6/23/26	0/1/1/1
7	NAG	E	371	1	-	0/6/23/26	0/1/1/1
9	SO4	H	228	-	-	0/0/0/0	0/0/0/0
9	SO4	H	229	-	-	0/0/0/0	0/0/0/0
9	SO4	H	230	-	-	0/0/0/0	0/0/0/0
9	SO4	I	228	-	-	0/0/0/0	0/0/0/0
9	SO4	I	229	-	-	0/0/0/0	0/0/0/0
9	SO4	I	230	-	-	0/0/0/0	0/0/0/0
9	SO4	I	231	-	-	0/0/0/0	0/0/0/0
9	SO4	I	232	-	-	0/0/0/0	0/0/0/0
9	SO4	J	228	-	-	0/0/0/0	0/0/0/0
9	SO4	J	229	-	-	0/0/0/0	0/0/0/0
9	SO4	L	212	-	-	0/0/0/0	0/0/0/0
9	SO4	L	213	-	-	0/0/0/0	0/0/0/0
9	SO4	M	212	-	-	0/0/0/0	0/0/0/0
9	SO4	N	212	-	-	0/0/0/0	0/0/0/0
9	SO4	N	213	-	-	0/0/0/0	0/0/0/0
9	SO4	N	214	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	351	NAG	C1-C2	2.23	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	341	NAG	C4-C3-C2	-5.16	103.21	111.23
7	A	341	NAG	C4-C3-C2	-4.44	104.33	111.23
7	C	351	NAG	C4-C3-C2	2.00	114.34	111.23
7	C	361	NAG	O5-C5-C6	2.07	111.83	107.35
7	C	361	NAG	C1-O5-C5	2.07	114.87	112.25
7	E	371	NAG	O5-C5-C6	2.22	112.16	107.35
7	C	371	NAG	C2-N2-C7	2.22	125.90	123.04
7	A	361	NAG	C2-N2-C7	2.23	125.90	123.04
7	E	371	NAG	C4-C3-C2	2.41	114.98	111.23
7	E	341	NAG	O3-C3-C2	2.68	114.41	109.11
7	A	361	NAG	O5-C5-C6	3.00	113.85	107.35
7	C	371	NAG	C1-O5-C5	3.56	116.77	112.25
7	C	351	NAG	C1-O5-C5	6.22	120.14	112.25
7	A	341	NAG	C1-O5-C5	6.74	120.80	112.25
7	E	341	NAG	C1-O5-C5	7.78	122.12	112.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	361	NAG	C8-C7-N2-C2
7	A	361	NAG	O7-C7-N2-C2

There are no ring outliers.

16 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	336	SO4	1	0
7	A	341	NAG	2	0
9	C	334	SO4	2	0
9	C	337	SO4	1	0
9	C	340	SO4	2	0
9	C	343	SO4	1	0
9	E	336	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	339	SO4	1	0
7	E	341	NAG	2	0
9	E	344	SO4	2	0
7	E	361	NAG	1	0
7	E	371	NAG	1	0
9	H	229	SO4	1	0
9	I	232	SO4	1	0
9	L	212	SO4	1	0
9	N	213	SO4	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	323/327 (98%)	-0.15	6 (1%) 70 55	70, 90, 118, 146	0
1	C	323/327 (98%)	-0.12	1 (0%) 94 93	67, 88, 115, 145	0
1	E	323/327 (98%)	-0.17	1 (0%) 94 93	66, 87, 116, 144	0
2	B	173/182 (95%)	-0.10	4 (2%) 64 49	63, 102, 143, 158	0
2	D	173/182 (95%)	0.01	9 (5%) 31 18	55, 101, 150, 170	0
2	F	173/182 (95%)	-0.11	4 (2%) 64 49	60, 92, 146, 168	0
3	H	221/227 (97%)	-0.18	2 (0%) 85 78	61, 79, 111, 133	0
3	I	221/227 (97%)	-0.25	2 (0%) 85 78	61, 78, 114, 134	0
3	J	221/227 (97%)	-0.20	0 100 100	58, 77, 112, 134	0
4	L	210/211 (99%)	-0.11	0 100 100	70, 92, 113, 136	0
4	M	210/211 (99%)	-0.15	0 100 100	68, 90, 112, 134	0
4	N	210/211 (99%)	-0.21	1 (0%) 91 87	68, 88, 110, 133	0
All	All	2781/2841 (97%)	-0.15	30 (1%) 82 72	55, 87, 127, 170	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	LEU	3.9
2	B	530	GLN	3.9
3	I	203	GLY	3.8
2	D	658	ASP	3.7
3	I	204	THR	3.5
2	D	671	GLU	3.4
2	D	667	LYS	3.3
2	D	664	GLU	3.0
1	A	326	SER	2.9
2	F	657	TYR	2.9
1	E	144	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	671	GLU	2.8
1	A	141	HIS	2.7
1	A	143	GLY	2.7
2	D	660	PRO	2.7
1	C	173	GLU	2.6
2	B	519	ASP	2.5
4	N	202	SER	2.4
2	D	668	LEU	2.4
1	A	142	ASN	2.4
1	A	276	ASP	2.3
2	D	527	GLN	2.4
3	H	204	THR	2.3
2	F	531	GLY	2.3
2	F	658	ASP	2.3
2	B	533	GLY	2.3
2	D	656	THR	2.3
2	B	529	GLU	2.2
3	H	205	GLN	2.1
2	D	663	SER	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](#)

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
5	NAG	A	331	14/15	0.93	0.29	0.69	78,106,119,130	0
5	NAG	C	331	14/15	0.97	0.24	0.56	71,92,110,125	0
8	NAG	E	331	14/15	0.95	0.22	0.30	68,93,116,121	0
5	NAG	C	341	14/15	0.79	0.42	-	120,144,153,168	0
5	NAG	C	332	14/15	0.85	0.27	-	100,128,146,150	0
5	NAG	A	332	14/15	0.90	0.39	-	87,114,129,133	0
5	NAG	E	352	14/15	0.80	0.26	-	115,143,154,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	NAG	E	332	14/15	0.84	0.34	-	100,116,137,142	0
5	NAG	A	371	14/15	0.90	0.35	-	82,143,163,164	0
5	NAG	E	351	14/15	0.89	0.15	-	108,132,146,146	0
5	NAG	C	342	14/15	0.77	0.59	-	113,162,168,172	0
5	NAG	A	372	14/15	0.75	0.54	-	136,162,181,182	0
8	BMA	E	333	11/12	0.82	0.34	-	89,122,134,135	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
9	SO4	E	335	5/5	0.91	0.28	2.99	106,110,129,145	0
9	SO4	E	346	5/5	0.73	0.28	2.96	102,122,137,161	0
9	SO4	I	229	5/5	0.90	0.30	2.57	106,113,139,152	0
9	SO4	E	342	5/5	0.82	0.29	2.36	128,128,162,175	0
9	SO4	C	343	5/5	0.89	0.33	2.04	117,121,150,159	0
9	SO4	N	214	5/5	0.84	0.21	0.74	122,124,156,171	0
9	SO4	E	336	5/5	0.97	0.21	0.46	68,82,98,102	0
9	SO4	J	229	5/5	0.89	0.26	0.33	92,110,126,145	0
9	SO4	I	231	5/5	0.97	0.17	0.26	64,82,90,92	0
9	SO4	A	338	5/5	0.94	0.17	0.17	113,121,146,148	0
9	SO4	I	232	5/5	0.89	0.18	-0.15	95,119,139,139	0
9	SO4	C	334	5/5	0.95	0.19	-0.18	73,76,97,106	0
9	SO4	A	335	5/5	0.97	0.16	-0.68	55,88,102,103	0
9	SO4	L	212	5/5	0.95	0.15	-0.83	105,113,134,149	0
9	SO4	H	228	5/5	0.96	0.12	-1.22	73,78,88,102	0
9	SO4	C	333	5/5	0.97	0.16	-1.33	79,87,105,109	0
9	SO4	J	228	5/5	0.96	0.10	-1.56	67,74,78,113	0
9	SO4	A	334	5/5	0.97	0.10	-3.05	93,95,122,127	0
9	SO4	E	334	5/5	0.96	0.10	-3.44	95,98,112,118	0
9	SO4	M	212	5/5	0.90	0.27	-	117,120,132,144	0
7	NAG	C	361	14/15	0.82	0.38	-	116,147,153,158	0
9	SO4	C	336	5/5	0.91	0.28	-	100,112,135,145	0
7	NAG	C	371	14/15	0.72	0.42	-	83,131,148,149	0
9	SO4	A	337	5/5	0.94	0.35	-	106,115,143,149	0
9	SO4	C	338	5/5	0.89	0.28	-	109,117,134,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	SO4	L	213	5/5	0.95	0.40	-	118,126,151,151	0
9	SO4	E	343	5/5	0.94	0.19	-	124,134,162,163	0
6	MAN	A	333	11/12	0.75	0.31	-	110,121,146,150	0
9	SO4	H	230	5/5	0.89	0.27	-	126,130,147,157	0
9	SO4	I	230	5/5	0.88	0.30	-	124,151,160,166	0
7	NAG	E	371	14/15	0.74	0.40	-	91,124,140,144	0
9	SO4	E	344	5/5	0.96	0.14	-	111,113,129,135	0
9	SO4	E	339	5/5	0.91	0.38	-	116,119,140,143	0
9	SO4	E	338	5/5	0.92	0.12	-	113,116,144,149	0
9	SO4	C	335	5/5	0.93	0.15	-	113,119,122,139	0
9	SO4	C	340	5/5	0.78	0.34	-	106,121,139,155	0
9	SO4	C	337	5/5	0.80	0.33	-	114,131,160,169	0
9	SO4	C	339	5/5	0.80	0.42	-	118,178,179,184	0
9	SO4	N	213	5/5	0.93	0.33	-	114,121,137,145	0
9	SO4	I	228	5/5	0.93	0.27	-	84,112,118,141	0
7	NAG	E	361	14/15	0.84	0.25	-	111,128,141,143	0
9	SO4	A	336	5/5	0.87	0.17	-	115,130,154,164	0
7	NAG	E	341	14/15	0.81	0.42	-	113,129,137,139	0
9	SO4	A	339	5/5	0.94	0.26	-	123,125,138,158	0
9	SO4	E	337	5/5	0.92	0.22	-	102,102,121,141	0
9	SO4	E	345	5/5	0.91	0.40	-	122,123,146,154	0
9	SO4	H	229	5/5	0.86	0.30	-	96,110,138,149	0
7	NAG	A	361	14/15	0.83	0.33	-	116,142,148,148	0
9	SO4	N	212	5/5	0.82	0.28	-	115,125,146,164	0
7	NAG	C	351	14/15	0.71	0.45	-	120,155,173,173	0
9	SO4	E	340	5/5	0.87	0.31	-	118,135,172,174	0
7	NAG	A	341	14/15	0.83	0.51	-	120,133,141,144	0

6.5 Other polymers [i](#)

There are no such residues in this entry.