



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:53 PM GMT

PDB ID : 3K6S  
Title : Structure of integrin alphaXbeta2 ectodomain  
Authors : Xie, C.; Zhu, J.; Chen, X.; Mi, L.; Nishida, N.; Springer, T.A.  
Deposited on : 2009-10-09  
Resolution : 3.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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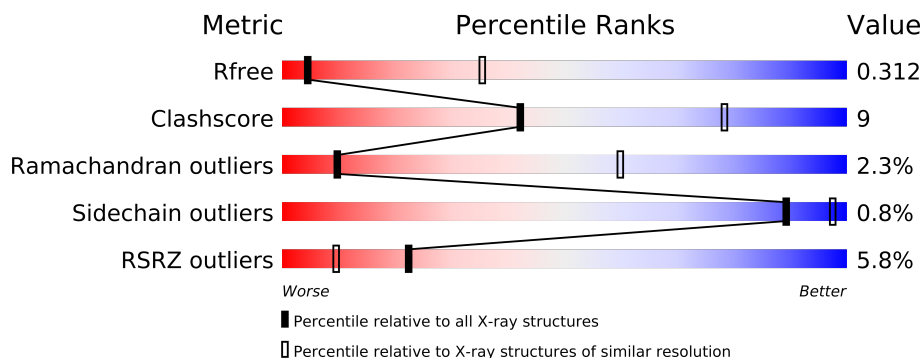
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.50 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))
$R_{free}$	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1095	
1	C	1095	
1	E	1095	
1	G	1095	
2	B	687	
2	D	687	
2	F	687	
2	H	687	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	NAG	A	3678	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	NAG	C	3678	-	X
6	NAG	D	3094	-	X
6	NAG	G	3678	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 50187 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Integrin alpha-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1082	Total	C	N	O	S	0	0	0
			8392	5304	1454	1596	38			
1	C	885	Total	C	N	O	S	0	0	0
			6825	4311	1182	1298	34			
1	E	884	Total	C	N	O	S	0	0	0
			6819	4308	1181	1296	34			
1	G	885	Total	C	N	O	S	0	0	0
			6825	4311	1182	1298	34			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	GLY	-	EXPRESSION TAG	UNP P20702
A	1086	CYS	-	EXPRESSION TAG	UNP P20702
A	1087	GLY	-	EXPRESSION TAG	UNP P20702
A	1088	GLY	-	EXPRESSION TAG	UNP P20702
A	1089	LEU	-	EXPRESSION TAG	UNP P20702
A	1090	GLU	-	EXPRESSION TAG	UNP P20702
A	1091	ASN	-	EXPRESSION TAG	UNP P20702
A	1092	LEU	-	EXPRESSION TAG	UNP P20702
A	1093	TYR	-	EXPRESSION TAG	UNP P20702
A	1094	PHE	-	EXPRESSION TAG	UNP P20702
A	1095	GLN	-	EXPRESSION TAG	UNP P20702
C	1085	GLY	-	EXPRESSION TAG	UNP P20702
C	1086	CYS	-	EXPRESSION TAG	UNP P20702
C	1087	GLY	-	EXPRESSION TAG	UNP P20702
C	1088	GLY	-	EXPRESSION TAG	UNP P20702
C	1089	LEU	-	EXPRESSION TAG	UNP P20702
C	1090	GLU	-	EXPRESSION TAG	UNP P20702
C	1091	ASN	-	EXPRESSION TAG	UNP P20702
C	1092	LEU	-	EXPRESSION TAG	UNP P20702
C	1093	TYR	-	EXPRESSION TAG	UNP P20702
C	1094	PHE	-	EXPRESSION TAG	UNP P20702

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1095	GLN	-	EXPRESSION TAG	UNP P20702
E	1085	GLY	-	EXPRESSION TAG	UNP P20702
E	1086	CYS	-	EXPRESSION TAG	UNP P20702
E	1087	GLY	-	EXPRESSION TAG	UNP P20702
E	1088	GLY	-	EXPRESSION TAG	UNP P20702
E	1089	LEU	-	EXPRESSION TAG	UNP P20702
E	1090	GLU	-	EXPRESSION TAG	UNP P20702
E	1091	ASN	-	EXPRESSION TAG	UNP P20702
E	1092	LEU	-	EXPRESSION TAG	UNP P20702
E	1093	TYR	-	EXPRESSION TAG	UNP P20702
E	1094	PHE	-	EXPRESSION TAG	UNP P20702
E	1095	GLN	-	EXPRESSION TAG	UNP P20702
G	1085	GLY	-	EXPRESSION TAG	UNP P20702
G	1086	CYS	-	EXPRESSION TAG	UNP P20702
G	1087	GLY	-	EXPRESSION TAG	UNP P20702
G	1088	GLY	-	EXPRESSION TAG	UNP P20702
G	1089	LEU	-	EXPRESSION TAG	UNP P20702
G	1090	GLU	-	EXPRESSION TAG	UNP P20702
G	1091	ASN	-	EXPRESSION TAG	UNP P20702
G	1092	LEU	-	EXPRESSION TAG	UNP P20702
G	1093	TYR	-	EXPRESSION TAG	UNP P20702
G	1094	PHE	-	EXPRESSION TAG	UNP P20702
G	1095	GLN	-	EXPRESSION TAG	UNP P20702

- Molecule 2 is a protein called Integrin beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			
2	D	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			
2	F	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			
2	H	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	678	ASP	-	EXPRESSION TAG	UNP P05107
B	679	GLY	-	EXPRESSION TAG	UNP P05107
B	680	CYS	-	EXPRESSION TAG	UNP P05107

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Chain	Residue	Modelled	Actual	Comment	Reference
B	681	GLY	-	EXPRESSION TAG	UNP P05107
B	682	GLU	-	EXPRESSION TAG	UNP P05107
B	684	LEU	-	EXPRESSION TAG	UNP P05107
B	685	TYR	-	EXPRESSION TAG	UNP P05107
B	686	PHE	-	EXPRESSION TAG	UNP P05107
B	687	GLN	-	EXPRESSION TAG	UNP P05107
D	678	ASP	-	EXPRESSION TAG	UNP P05107
D	679	GLY	-	EXPRESSION TAG	UNP P05107
D	680	CYS	-	EXPRESSION TAG	UNP P05107
D	681	GLY	-	EXPRESSION TAG	UNP P05107
D	682	GLU	-	EXPRESSION TAG	UNP P05107
D	684	LEU	-	EXPRESSION TAG	UNP P05107
D	685	TYR	-	EXPRESSION TAG	UNP P05107
D	686	PHE	-	EXPRESSION TAG	UNP P05107
D	687	GLN	-	EXPRESSION TAG	UNP P05107
F	678	ASP	-	EXPRESSION TAG	UNP P05107
F	679	GLY	-	EXPRESSION TAG	UNP P05107
F	680	CYS	-	EXPRESSION TAG	UNP P05107
F	681	GLY	-	EXPRESSION TAG	UNP P05107
F	682	GLU	-	EXPRESSION TAG	UNP P05107
F	684	LEU	-	EXPRESSION TAG	UNP P05107
F	685	TYR	-	EXPRESSION TAG	UNP P05107
F	686	PHE	-	EXPRESSION TAG	UNP P05107
F	687	GLN	-	EXPRESSION TAG	UNP P05107
H	678	ASP	-	EXPRESSION TAG	UNP P05107
H	679	GLY	-	EXPRESSION TAG	UNP P05107
H	680	CYS	-	EXPRESSION TAG	UNP P05107
H	681	GLY	-	EXPRESSION TAG	UNP P05107
H	682	GLU	-	EXPRESSION TAG	UNP P05107
H	684	LEU	-	EXPRESSION TAG	UNP P05107
H	685	TYR	-	EXPRESSION TAG	UNP P05107
H	686	PHE	-	EXPRESSION TAG	UNP P05107
H	687	GLN	-	EXPRESSION TAG	UNP P05107

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

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

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	GLY	-	EXPRESSION TAG	UNP P20702
A	1086	CYS	-	EXPRESSION TAG	UNP P20702
A	1087	GLY	-	EXPRESSION TAG	UNP P20702
A	1088	GLY	-	EXPRESSION TAG	UNP P20702
A	1089	LEU	-	EXPRESSION TAG	UNP P20702
A	1090	GLU	-	EXPRESSION TAG	UNP P20702
A	1091	ASN	-	EXPRESSION TAG	UNP P20702
A	1092	LEU	-	EXPRESSION TAG	UNP P20702
A	1093	TYR	-	EXPRESSION TAG	UNP P20702
A	1094	PHE	-	EXPRESSION TAG	UNP P20702
A	1095	GLN	-	EXPRESSION TAG	UNP P20702
A	1085	GLY	-	EXPRESSION TAG	UNP P20702
A	1086	CYS	-	EXPRESSION TAG	UNP P20702
A	1087	GLY	-	EXPRESSION TAG	UNP P20702
A	1088	GLY	-	EXPRESSION TAG	UNP P20702
A	1089	LEU	-	EXPRESSION TAG	UNP P20702
A	1090	GLU	-	EXPRESSION TAG	UNP P20702
A	1091	ASN	-	EXPRESSION TAG	UNP P20702
A	1092	LEU	-	EXPRESSION TAG	UNP P20702
A	1093	TYR	-	EXPRESSION TAG	UNP P20702
A	1094	PHE	-	EXPRESSION TAG	UNP P20702
A	1095	GLN	-	EXPRESSION TAG	UNP P20702
C	1085	GLY	-	EXPRESSION TAG	UNP P20702
C	1086	CYS	-	EXPRESSION TAG	UNP P20702
C	1087	GLY	-	EXPRESSION TAG	UNP P20702
C	1088	GLY	-	EXPRESSION TAG	UNP P20702
C	1089	LEU	-	EXPRESSION TAG	UNP P20702

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1090	GLU	-	EXPRESSION TAG	UNP P20702
C	1091	ASN	-	EXPRESSION TAG	UNP P20702
C	1092	LEU	-	EXPRESSION TAG	UNP P20702
C	1093	TYR	-	EXPRESSION TAG	UNP P20702
C	1094	PHE	-	EXPRESSION TAG	UNP P20702
C	1095	GLN	-	EXPRESSION TAG	UNP P20702
C	1085	GLY	-	EXPRESSION TAG	UNP P20702
C	1086	CYS	-	EXPRESSION TAG	UNP P20702
C	1087	GLY	-	EXPRESSION TAG	UNP P20702
C	1088	GLY	-	EXPRESSION TAG	UNP P20702
C	1089	LEU	-	EXPRESSION TAG	UNP P20702
C	1090	GLU	-	EXPRESSION TAG	UNP P20702
C	1091	ASN	-	EXPRESSION TAG	UNP P20702
C	1092	LEU	-	EXPRESSION TAG	UNP P20702
C	1093	TYR	-	EXPRESSION TAG	UNP P20702
C	1094	PHE	-	EXPRESSION TAG	UNP P20702
C	1095	GLN	-	EXPRESSION TAG	UNP P20702
C	1085	GLY	-	EXPRESSION TAG	UNP P20702
C	1086	CYS	-	EXPRESSION TAG	UNP P20702
C	1087	GLY	-	EXPRESSION TAG	UNP P20702
C	1088	GLY	-	EXPRESSION TAG	UNP P20702
C	1089	LEU	-	EXPRESSION TAG	UNP P20702
C	1090	GLU	-	EXPRESSION TAG	UNP P20702
C	1091	ASN	-	EXPRESSION TAG	UNP P20702
C	1092	LEU	-	EXPRESSION TAG	UNP P20702
C	1093	TYR	-	EXPRESSION TAG	UNP P20702
C	1094	PHE	-	EXPRESSION TAG	UNP P20702
C	1095	GLN	-	EXPRESSION TAG	UNP P20702
E	1085	GLY	-	EXPRESSION TAG	UNP P20702
E	1086	CYS	-	EXPRESSION TAG	UNP P20702
E	1087	GLY	-	EXPRESSION TAG	UNP P20702
E	1088	GLY	-	EXPRESSION TAG	UNP P20702
E	1089	LEU	-	EXPRESSION TAG	UNP P20702
E	1090	GLU	-	EXPRESSION TAG	UNP P20702
E	1091	ASN	-	EXPRESSION TAG	UNP P20702
E	1092	LEU	-	EXPRESSION TAG	UNP P20702
E	1093	TYR	-	EXPRESSION TAG	UNP P20702
E	1094	PHE	-	EXPRESSION TAG	UNP P20702
E	1095	GLN	-	EXPRESSION TAG	UNP P20702
E	1085	GLY	-	EXPRESSION TAG	UNP P20702
E	1086	CYS	-	EXPRESSION TAG	UNP P20702
E	1087	GLY	-	EXPRESSION TAG	UNP P20702

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1088	GLY	-	EXPRESSION TAG	UNP P20702
E	1089	LEU	-	EXPRESSION TAG	UNP P20702
E	1090	GLU	-	EXPRESSION TAG	UNP P20702
E	1091	ASN	-	EXPRESSION TAG	UNP P20702
E	1092	LEU	-	EXPRESSION TAG	UNP P20702
E	1093	TYR	-	EXPRESSION TAG	UNP P20702
E	1094	PHE	-	EXPRESSION TAG	UNP P20702
E	1095	GLN	-	EXPRESSION TAG	UNP P20702
G	1085	GLY	-	EXPRESSION TAG	UNP P20702
G	1086	CYS	-	EXPRESSION TAG	UNP P20702
G	1087	GLY	-	EXPRESSION TAG	UNP P20702
G	1088	GLY	-	EXPRESSION TAG	UNP P20702
G	1089	LEU	-	EXPRESSION TAG	UNP P20702
G	1090	GLU	-	EXPRESSION TAG	UNP P20702
G	1091	ASN	-	EXPRESSION TAG	UNP P20702
G	1092	LEU	-	EXPRESSION TAG	UNP P20702
G	1093	TYR	-	EXPRESSION TAG	UNP P20702
G	1094	PHE	-	EXPRESSION TAG	UNP P20702
G	1095	GLN	-	EXPRESSION TAG	UNP P20702
G	1085	GLY	-	EXPRESSION TAG	UNP P20702
G	1086	CYS	-	EXPRESSION TAG	UNP P20702
G	1087	GLY	-	EXPRESSION TAG	UNP P20702
G	1088	GLY	-	EXPRESSION TAG	UNP P20702
G	1089	LEU	-	EXPRESSION TAG	UNP P20702
G	1090	GLU	-	EXPRESSION TAG	UNP P20702
G	1091	ASN	-	EXPRESSION TAG	UNP P20702
G	1092	LEU	-	EXPRESSION TAG	UNP P20702
G	1093	TYR	-	EXPRESSION TAG	UNP P20702
G	1094	PHE	-	EXPRESSION TAG	UNP P20702
G	1095	GLN	-	EXPRESSION TAG	UNP P20702

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			61	34	2	25		

There are 11 discrepancies between the modelled and reference sequences:

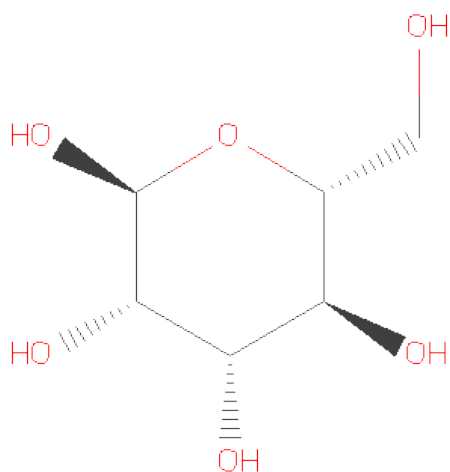
Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	GLY	-	EXPRESSION TAG	UNP P20702
A	1086	CYS	-	EXPRESSION TAG	UNP P20702

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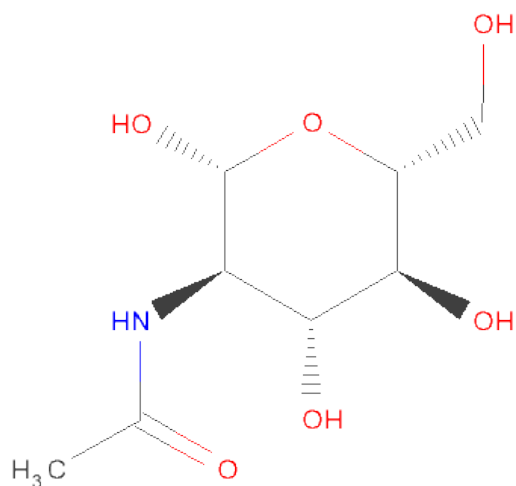
Chain	Residue	Modelled	Actual	Comment	Reference
A	1087	GLY	-	EXPRESSION TAG	UNP P20702
A	1088	GLY	-	EXPRESSION TAG	UNP P20702
A	1089	LEU	-	EXPRESSION TAG	UNP P20702
A	1090	GLU	-	EXPRESSION TAG	UNP P20702
A	1091	ASN	-	EXPRESSION TAG	UNP P20702
A	1092	LEU	-	EXPRESSION TAG	UNP P20702
A	1093	TYR	-	EXPRESSION TAG	UNP P20702
A	1094	PHE	-	EXPRESSION TAG	UNP P20702
A	1095	GLN	-	EXPRESSION TAG	UNP P20702

- Molecule 5 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	3	Total Ca 3 3	0	0
7	D	1	Total Ca 1 1	0	0
7	E	3	Total Ca 3 3	0	0
7	H	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0
7	C	3	Total Ca 3 3	0	0
7	A	3	Total Ca 3 3	0	0
7	F	1	Total Ca 1 1	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Mg 1 1	0	0

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

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

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1085	GLY	-	EXPRESSION TAG	UNP P20702
E	1086	CYS	-	EXPRESSION TAG	UNP P20702
E	1087	GLY	-	EXPRESSION TAG	UNP P20702
E	1088	GLY	-	EXPRESSION TAG	UNP P20702
E	1089	LEU	-	EXPRESSION TAG	UNP P20702
E	1090	GLU	-	EXPRESSION TAG	UNP P20702
E	1091	ASN	-	EXPRESSION TAG	UNP P20702
E	1092	LEU	-	EXPRESSION TAG	UNP P20702
E	1093	TYR	-	EXPRESSION TAG	UNP P20702

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1094	PHE	-	EXPRESSION TAG	UNP P20702
E	1095	GLN	-	EXPRESSION TAG	UNP P20702
G	1085	GLY	-	EXPRESSION TAG	UNP P20702
G	1086	CYS	-	EXPRESSION TAG	UNP P20702
G	1087	GLY	-	EXPRESSION TAG	UNP P20702
G	1088	GLY	-	EXPRESSION TAG	UNP P20702
G	1089	LEU	-	EXPRESSION TAG	UNP P20702
G	1090	GLU	-	EXPRESSION TAG	UNP P20702
G	1091	ASN	-	EXPRESSION TAG	UNP P20702
G	1092	LEU	-	EXPRESSION TAG	UNP P20702
G	1093	TYR	-	EXPRESSION TAG	UNP P20702
G	1094	PHE	-	EXPRESSION TAG	UNP P20702
G	1095	GLN	-	EXPRESSION TAG	UNP P20702

- Molecule 10 is water.

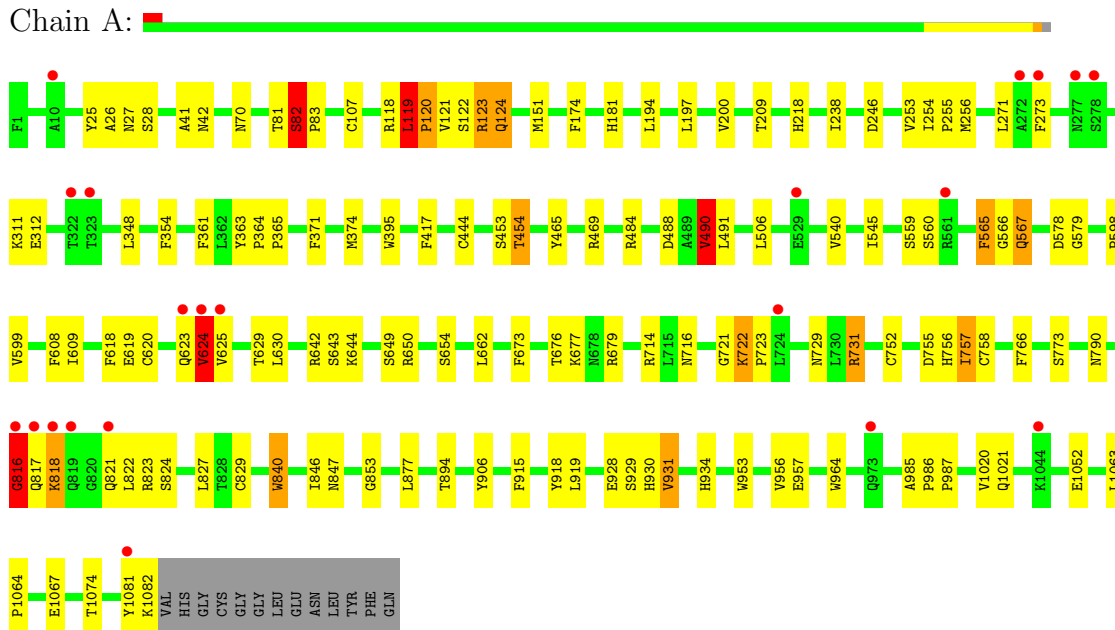
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	3	Total O 3 3	0	0

### 3 Residue-property plots

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.

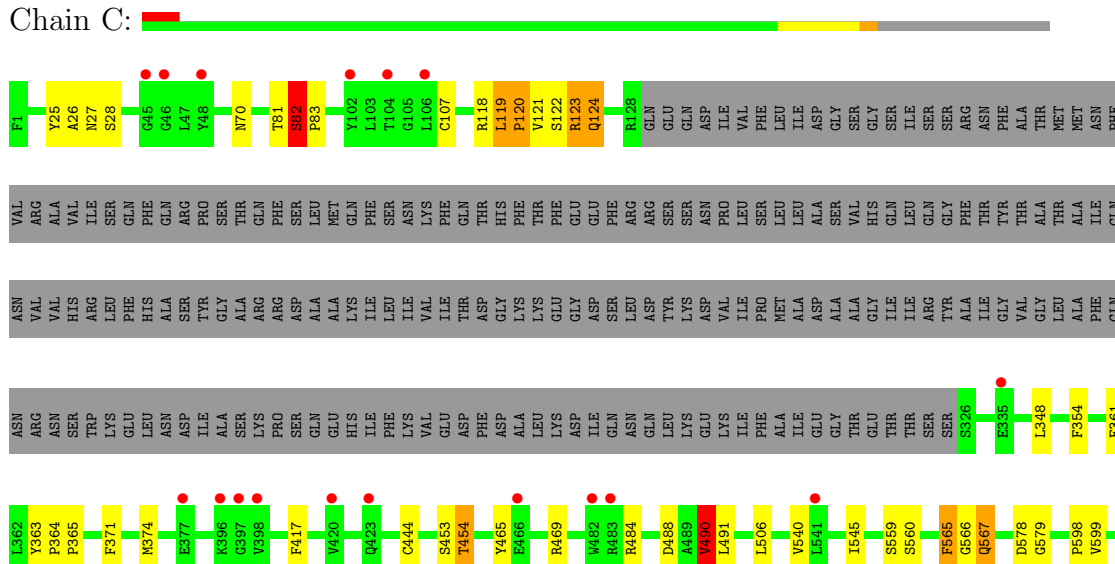
#### • Molecule 1: Integrin alpha-X

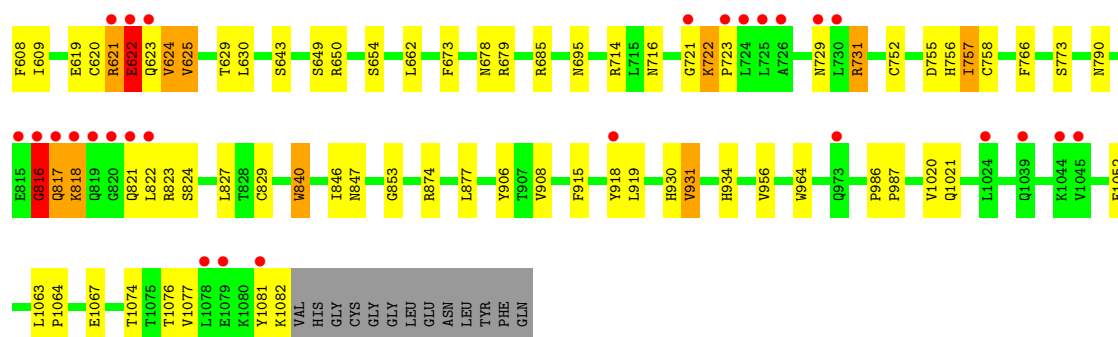
Chain A:



#### • Molecule 1: Integrin alpha-X

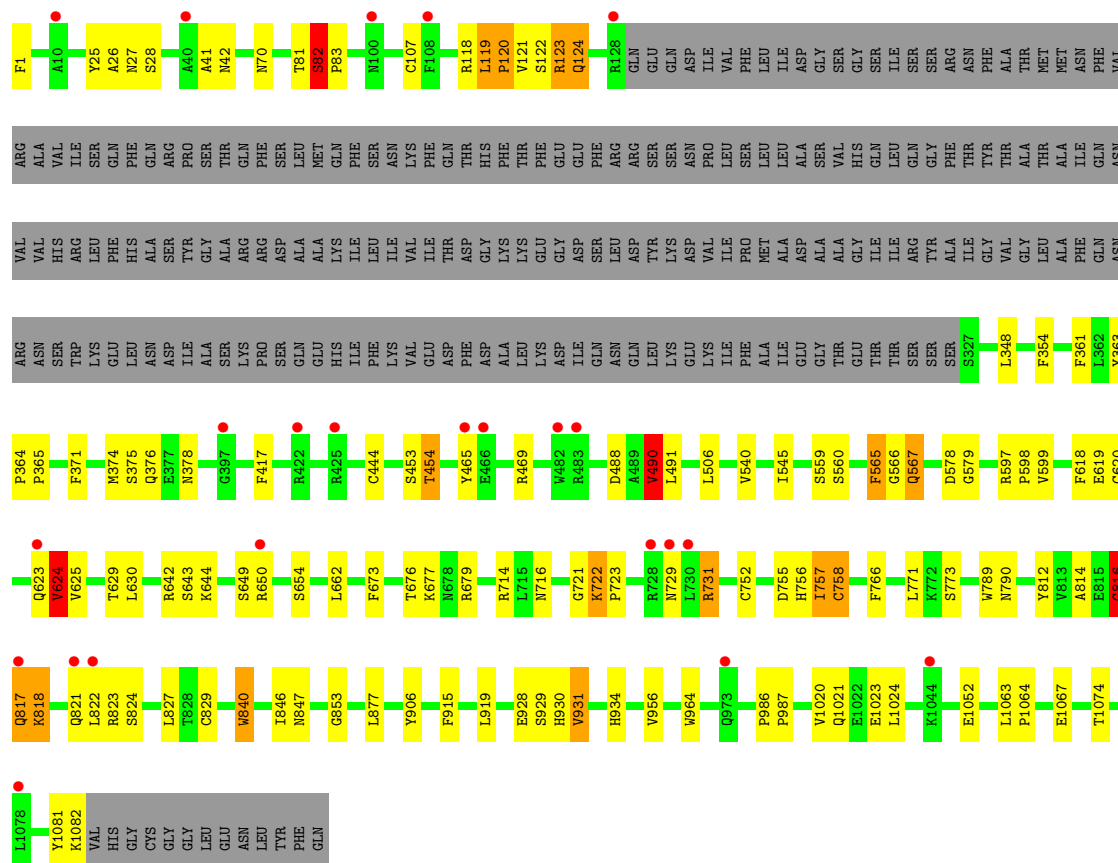
Chain C:





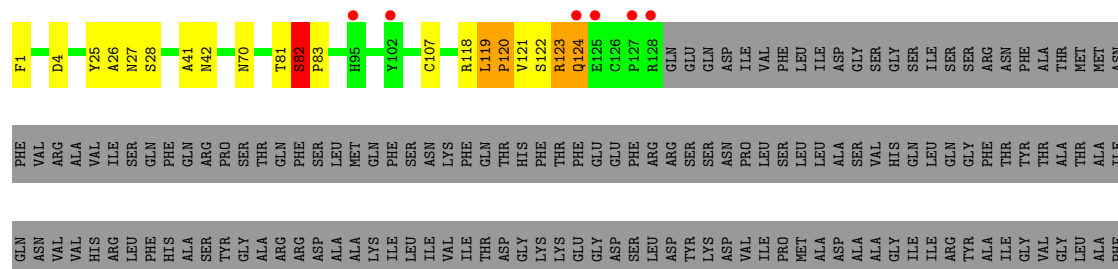
• Molecule 1: Integrin alpha-X

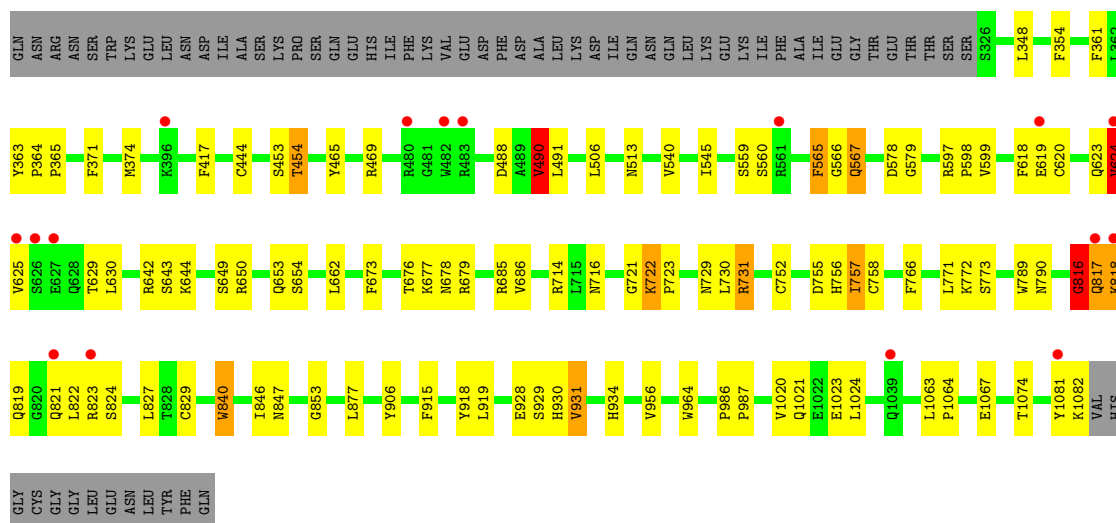
Chain E:



• Molecule 1: Integrin alpha-X

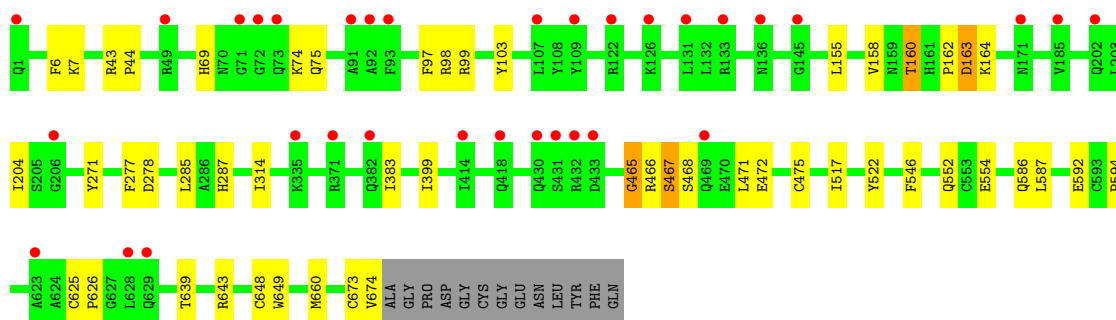
Chain G:





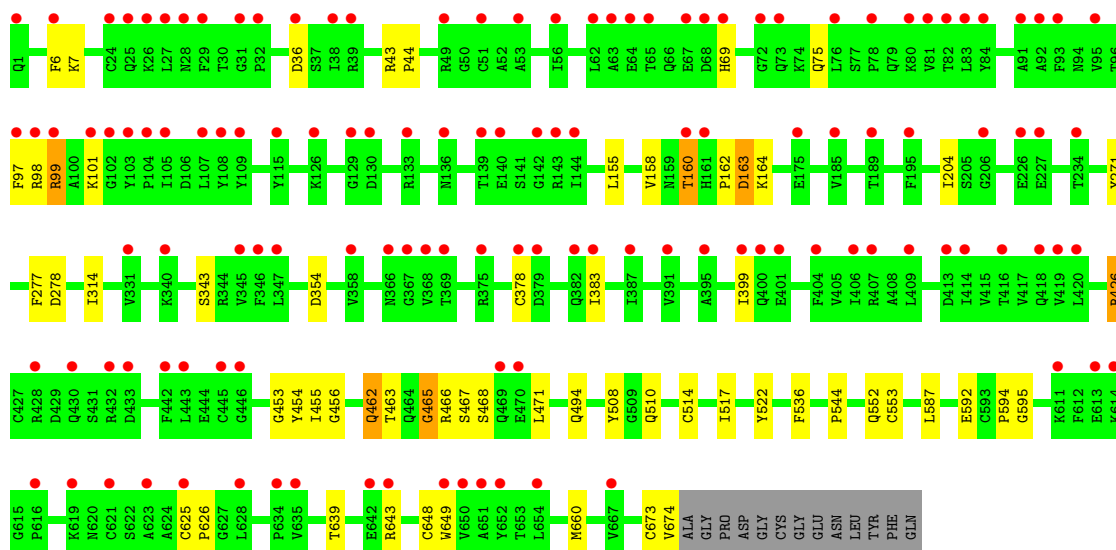
• Molecule 2: Integrin beta-2

Chain B:



• Molecule 2: Integrin beta-2

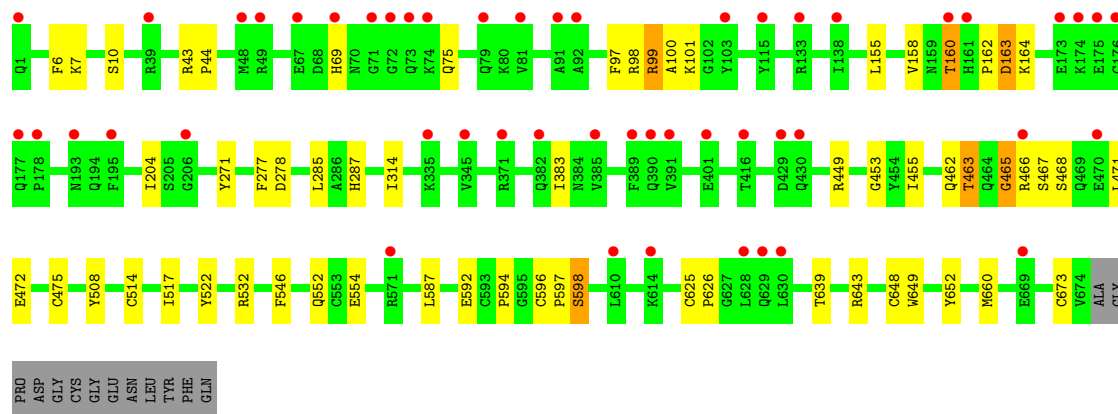
Chain D:



• Molecule 2: Integrin beta-2

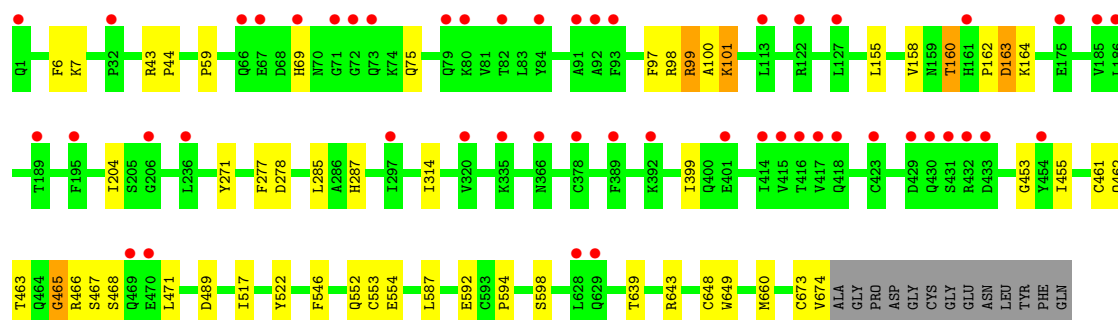


Chain F:



- Molecule 2: Integrin beta-2

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.09Å 163.56Å 536.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 3.50 48.61 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.61-3.50) 100.0 (48.61-3.50)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.297 , 0.335 0.280 , 0.312	Depositor DCC
$R_{free}$ test set	1531 reflections (1.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	80.7	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 135.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 147305 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	50187	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.23	0/8579	0.44	1/11652 (0.0%)
1	C	0.24	0/6980	0.46	0/9494
1	E	0.23	0/6974	0.45	0/9486
1	G	0.24	0/6980	0.45	0/9494
2	B	0.22	0/5280	0.41	0/7129
2	D	0.24	0/5280	0.43	0/7129
2	F	0.23	0/5280	0.42	0/7129
2	H	0.23	0/5280	0.42	0/7129
All	All	0.23	0/50633	0.44	1/68642 (0.0%)

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
1	A	0	10
1	C	0	11
1	E	0	10
1	G	0	11
2	B	0	2
2	D	0	3
2	F	0	2
2	H	0	3
3	C	1	0
4	A	2	0
9	E	2	0
9	G	2	0
All	All	7	52

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	LEU	C-N-CD	-5.77	107.90	120.60

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	3373	NAG	C1
4	A	3375	MAN	C1
3	C	3373	NAG	C1
9	E	3373	NAG	C1
9	E	3375	MAN	C1
9	G	3373	NAG	C1
9	G	3375	MAN	C1

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ARG	Peptide
1	A	119	LEU	Peptide
1	A	488	ASP	Peptide
1	A	490	VAL	Peptide
1	A	624	VAL	Peptide
1	A	625	VAL	Peptide
1	A	816	GLY	Peptide
1	A	82	SER	Peptide
1	A	821	GLN	Peptide
1	A	824	SER	Peptide
2	B	160	THR	Peptide
2	B	163	ASP	Peptide
1	C	118	ARG	Peptide
1	C	488	ASP	Peptide
1	C	490	VAL	Peptide
1	C	621	ARG	Peptide
1	C	622	GLU	Peptide
1	C	625	VAL	Peptide
1	C	816	GLY	Peptide
1	C	817	GLN	Peptide
1	C	82	SER	Peptide
1	C	821	GLN	Peptide
1	C	824	SER	Peptide
2	D	160	THR	Peptide
2	D	163	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	D	462	GLN	Peptide
1	E	118	ARG	Peptide
1	E	488	ASP	Peptide
1	E	490	VAL	Peptide
1	E	624	VAL	Peptide
1	E	625	VAL	Peptide
1	E	816	GLY	Peptide
1	E	817	GLN	Peptide
1	E	82	SER	Peptide
1	E	821	GLN	Peptide
1	E	824	SER	Peptide
2	F	160	THR	Peptide
2	F	163	ASP	Peptide
1	G	118	ARG	Peptide
1	G	488	ASP	Peptide
1	G	490	VAL	Peptide
1	G	624	VAL	Peptide
1	G	625	VAL	Peptide
1	G	816	GLY	Peptide
1	G	817	GLN	Peptide
1	G	819	GLN	Peptide
1	G	82	SER	Peptide
1	G	821	GLN	Peptide
1	G	824	SER	Peptide
2	H	160	THR	Peptide
2	H	163	ASP	Peptide
2	H	99	ARG	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8392	0	180	89	0
1	C	6825	0	134	81	0
1	E	6819	0	129	78	0
1	G	6825	0	134	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5184	0	174	33	0
2	D	5184	0	174	40	0
2	F	5184	0	174	40	0
2	H	5184	0	174	33	0
3	A	56	0	50	0	0
3	C	84	0	75	3	0
3	E	56	0	50	1	0
3	G	56	0	50	1	0
4	A	61	0	52	9	0
5	A	11	0	10	4	0
6	A	28	0	25	0	0
6	B	14	0	13	0	0
6	C	28	0	25	1	0
6	D	14	0	13	0	0
6	E	28	0	25	0	0
6	F	14	0	13	0	0
6	G	28	0	24	1	0
6	H	14	0	13	0	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
7	C	3	0	0	0	0
7	D	1	0	0	0	0
7	E	3	0	0	0	0
7	F	1	0	0	0	0
7	G	3	0	0	0	0
7	H	1	0	0	0	0
8	A	1	0	0	0	0
9	E	39	0	34	5	0
9	G	39	0	34	6	0
10	A	3	0	0	0	0
All	All	50187	0	1779	470	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (470) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:455:ILE:CG2	2:D:494:GLN:NE2	2.36	0.89
4:A:3377:MAN:H4	5:A:3378:MAN:C1	2.02	0.88
1:G:816:GLY:O	1:G:818:LYS:N	2.13	0.82
1:A:985:ALA:CB	1:C:621:ARG:CD	2.57	0.82
9:G:3374:NAG:O3	9:G:3375:MAN:H2	1.79	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:816:GLY:O	1:E:818:LYS:N	2.12	0.82
9:E:3374:NAG:O3	9:E:3375:MAN:H2	1.80	0.82
1:A:985:ALA:CB	1:C:621:ARG:CB	2.59	0.81
1:A:119:LEU:O	1:A:363:TYR:CE1	2.35	0.80
4:A:3374:NAG:O3	4:A:3375:MAN:H2	1.81	0.79
1:G:597:ARG:HB3	1:G:731:ARG:O	1.83	0.79
1:G:597:ARG:HD2	1:G:731:ARG:O	1.86	0.76
1:A:484:ARG:CD	2:B:594:PRO:HG2	2.15	0.76
1:A:957:GLU:CB	1:C:621:ARG:NH2	2.50	0.75
1:A:816:GLY:O	1:A:818:LYS:N	2.20	0.74
1:A:395:TRP:CZ2	1:A:1021:GLN:OE1	2.42	0.73
1:G:119:LEU:O	1:G:363:TYR:CE1	2.41	0.73
1:E:119:LEU:O	1:E:363:TYR:CE1	2.41	0.73
1:C:119:LEU:O	1:C:363:TYR:CE1	2.41	0.72
4:A:3377:MAN:C4	5:A:3378:MAN:C1	2.67	0.72
2:F:455:ILE:CG1	2:F:463:THR:HG23	2.19	0.72
2:H:100:ALA:O	2:H:101:LYS:HB2	1.90	0.72
1:G:598:PRO:CG	1:G:650:ARG:NH1	2.54	0.70
1:A:953:TRP:CH2	1:C:755:ASP:HA	2.26	0.70
2:F:472:GLU:HA	2:F:475:CYS:CB	2.23	0.69
1:E:756:HIS:O	1:E:757:ILE:HG22	1.94	0.68
1:A:953:TRP:CZ2	1:C:755:ASP:HA	2.29	0.67
1:C:816:GLY:O	1:C:818:LYS:N	2.28	0.67
1:G:756:HIS:O	1:G:757:ILE:HG22	1.96	0.66
2:F:455:ILE:CG1	2:F:463:THR:CG2	2.76	0.64
2:B:468:SER:HB2	2:B:471:LEU:HG	1.81	0.63
1:A:756:HIS:O	1:A:757:ILE:HG22	1.98	0.63
2:D:468:SER:HB2	2:D:471:LEU:HG	1.81	0.62
1:G:119:LEU:N	1:G:120:PRO:CA	2.62	0.62
1:A:953:TRP:CE2	1:C:755:ASP:HB2	2.35	0.62
1:C:756:HIS:O	1:C:757:ILE:HG22	1.99	0.62
2:H:468:SER:HB2	2:H:471:LEU:HG	1.82	0.62
2:F:468:SER:HB2	2:F:471:LEU:HG	1.81	0.61
1:C:119:LEU:N	1:C:120:PRO:CA	2.63	0.61
4:A:3377:MAN:O3	5:A:3378:MAN:C1	2.48	0.61
9:G:3374:NAG:C3	9:G:3375:MAN:H2	2.30	0.61
2:B:522:TYR:CD1	2:B:552:GLN:HA	2.36	0.61
1:E:119:LEU:N	1:E:120:PRO:CA	2.63	0.61
1:A:1052:GLU:OE1	1:C:756:HIS:HA	2.00	0.61
2:F:508:TYR:CZ	2:F:514:CYS:HB3	2.36	0.61
1:E:599:VAL:HG23	1:E:599:VAL:O	2.01	0.60
1:C:721:GLY:C	1:C:723:PRO:CD	2.70	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:522:TYR:CD1	2:F:552:GLN:HA	2.36	0.60
1:E:721:GLY:C	1:E:723:PRO:CD	2.70	0.60
1:G:721:GLY:C	1:G:723:PRO:CD	2.70	0.60
1:A:721:GLY:C	1:A:723:PRO:CD	2.70	0.60
9:E:3374:NAG:C3	9:E:3375:MAN:H2	2.32	0.59
1:G:599:VAL:HG23	1:G:599:VAL:O	2.01	0.59
2:D:162:PRO:O	2:D:164:LYS:N	2.35	0.59
2:F:162:PRO:O	2:F:164:LYS:N	2.35	0.59
2:B:162:PRO:O	2:B:164:LYS:N	2.35	0.59
1:E:919:LEU:O	2:F:643:ARG:NH1	2.35	0.59
1:G:722:LYS:N	1:G:723:PRO:CD	2.66	0.58
1:A:599:VAL:HG23	1:A:599:VAL:O	2.01	0.58
2:H:162:PRO:O	2:H:164:LYS:N	2.36	0.58
1:C:599:VAL:O	1:C:599:VAL:HG23	2.01	0.58
1:A:119:LEU:N	1:A:120:PRO:CA	2.66	0.58
1:C:722:LYS:N	1:C:723:PRO:CD	2.66	0.58
1:E:722:LYS:N	1:E:723:PRO:CD	2.66	0.58
2:B:468:SER:HB2	2:B:471:LEU:CG	2.34	0.58
2:D:468:SER:HB2	2:D:471:LEU:CG	2.34	0.58
1:C:484:ARG:NH2	1:C:1021:GLN:CA	2.67	0.58
2:H:468:SER:HB2	2:H:471:LEU:CG	2.34	0.58
1:A:953:TRP:CE2	1:C:755:ASP:CB	2.87	0.58
2:H:455:ILE:CG1	2:H:463:THR:HG23	2.34	0.58
1:A:722:LYS:N	1:A:723:PRO:CD	2.67	0.57
2:F:453:GLY:O	2:F:462:GLN:HG3	2.05	0.57
1:G:598:PRO:HG3	1:G:650:ARG:NH1	2.19	0.57
2:D:6:PHE:CE1	2:D:536:PHE:CB	2.88	0.57
2:F:468:SER:HB2	2:F:471:LEU:CG	2.34	0.57
1:A:756:HIS:HA	1:C:1052:GLU:OE1	2.04	0.57
2:D:456:GLY:CA	2:D:494:GLN:OE1	2.53	0.56
1:C:755:ASP:O	1:C:756:HIS:HB3	2.05	0.56
1:G:1:PHE:CE2	1:G:599:VAL:HG11	2.40	0.56
1:E:598:PRO:HB3	1:E:650:ARG:NH1	2.20	0.56
1:G:598:PRO:HB3	1:G:650:ARG:NH1	2.21	0.56
1:G:597:ARG:HG3	1:G:731:ARG:CG	2.36	0.56
1:A:490:VAL:CG1	1:A:491:LEU:N	2.69	0.55
1:G:490:VAL:CG1	1:G:491:LEU:N	2.68	0.55
1:A:81:THR:O	1:A:82:SER:C	2.45	0.55
1:C:619:GLU:O	1:C:620:CYS:SG	2.65	0.54
1:C:650:ARG:CD	1:C:729:ASN:CB	2.86	0.54
1:C:81:THR:O	1:C:82:SER:C	2.45	0.54
1:A:986:PRO:CB	1:A:987:PRO:CD	2.86	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:592:GLU:O	2:B:594:PRO:HD3	2.08	0.54
1:C:490:VAL:CG1	1:C:491:LEU:N	2.68	0.54
2:H:455:ILE:CG1	2:H:463:THR:CG2	2.86	0.54
1:E:490:VAL:CG1	1:E:491:LEU:N	2.68	0.54
1:G:816:GLY:O	1:G:818:LYS:CA	2.56	0.54
4:A:3373:NAG:H3	4:A:3374:NAG:N2	2.22	0.53
1:E:81:THR:O	1:E:82:SER:C	2.45	0.53
1:G:81:THR:O	1:G:82:SER:C	2.46	0.53
1:E:81:THR:O	1:E:82:SER:O	2.26	0.53
2:H:453:GLY:O	2:H:462:GLN:HG3	2.07	0.53
2:D:454:TYR:CE2	2:D:462:GLN:HG3	2.43	0.53
9:E:3373:NAG:H3	9:E:3374:NAG:N2	2.23	0.53
1:A:81:THR:O	1:A:82:SER:O	2.27	0.53
1:E:756:HIS:CG	1:E:756:HIS:O	2.61	0.53
1:C:986:PRO:CB	1:C:987:PRO:CD	2.87	0.53
1:A:650:ARG:CD	1:A:729:ASN:CB	2.87	0.53
1:G:756:HIS:CG	1:G:756:HIS:O	2.62	0.52
1:E:789:TRP:CZ2	1:G:771:LEU:O	2.61	0.52
2:F:592:GLU:O	2:F:594:PRO:HD3	2.09	0.52
1:E:986:PRO:CB	1:E:987:PRO:CD	2.87	0.52
2:H:592:GLU:O	2:H:594:PRO:HD3	2.09	0.52
1:E:82:SER:CB	1:E:83:PRO:CD	2.88	0.52
1:G:598:PRO:CB	1:G:650:ARG:NH1	2.73	0.52
1:A:82:SER:CB	1:A:83:PRO:CD	2.88	0.52
1:E:619:GLU:O	1:E:620:CYS:SG	2.68	0.52
9:G:3373:NAG:H3	9:G:3374:NAG:N2	2.24	0.52
2:D:592:GLU:O	2:D:594:PRO:HD3	2.09	0.52
1:C:81:THR:O	1:C:82:SER:O	2.27	0.52
2:H:75:GLN:CD	2:H:98:ARG:O	2.48	0.52
1:G:619:GLU:O	1:G:620:CYS:SG	2.67	0.52
1:G:650:ARG:CD	1:G:729:ASN:CB	2.88	0.52
1:C:82:SER:CB	1:C:83:PRO:CD	2.88	0.52
2:D:508:TYR:CZ	2:D:514:CYS:HB3	2.45	0.52
1:C:364:PRO:CB	1:C:365:PRO:CD	2.89	0.51
1:G:986:PRO:CB	1:G:987:PRO:CD	2.87	0.51
4:A:3374:NAG:C3	4:A:3375:MAN:H2	2.39	0.51
2:F:508:TYR:CE1	2:F:514:CYS:HB3	2.46	0.51
1:E:650:ARG:CD	1:E:729:ASN:CB	2.88	0.51
2:D:75:GLN:CD	2:D:98:ARG:O	2.49	0.51
1:C:756:HIS:O	1:C:756:HIS:CG	2.63	0.51
2:B:522:TYR:CE1	2:B:552:GLN:HA	2.45	0.51
2:F:522:TYR:CE1	2:F:552:GLN:HA	2.46	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:546:PHE:CE2	2:B:554:GLU:HG2	2.46	0.51
1:G:623:GLN:O	1:G:624:VAL:CG2	2.59	0.51
1:C:685:ARG:CZ	1:G:685:ARG:NH2	2.74	0.51
1:G:364:PRO:CB	1:G:365:PRO:CD	2.89	0.51
1:E:121:VAL:CG1	1:E:121:VAL:O	2.59	0.51
1:C:919:LEU:CD1	2:D:643:ARG:NH1	2.74	0.51
1:G:81:THR:O	1:G:82:SER:O	2.28	0.51
1:G:82:SER:CB	1:G:83:PRO:CD	2.88	0.51
1:A:122:SER:O	1:A:123:ARG:C	2.50	0.51
1:G:121:VAL:CG1	1:G:121:VAL:O	2.59	0.51
1:A:364:PRO:CB	1:A:365:PRO:CD	2.88	0.50
1:C:623:GLN:O	1:C:624:VAL:CG2	2.58	0.50
1:A:311:LYS:CG	1:A:312:GLU:N	2.74	0.50
2:B:75:GLN:CD	2:B:98:ARG:O	2.49	0.50
1:G:465:TYR:CG	1:G:469:ARG:CG	2.94	0.50
1:C:121:VAL:O	1:C:121:VAL:CG1	2.59	0.50
2:B:546:PHE:CD2	2:B:554:GLU:O	2.64	0.50
1:E:122:SER:O	1:E:123:ARG:C	2.50	0.50
1:A:623:GLN:O	1:A:624:VAL:CG2	2.58	0.50
1:C:716:ASN:C	1:C:716:ASN:OD1	2.50	0.50
1:E:364:PRO:CB	1:E:365:PRO:CD	2.89	0.50
3:C:3373:NAG:H3	3:C:3374:NAG:N2	2.27	0.50
1:C:908:VAL:CG1	2:D:595:GLY:HA3	2.41	0.50
1:E:716:ASN:OD1	1:E:716:ASN:C	2.50	0.50
2:H:673:CYS:O	2:H:674:VAL:C	2.50	0.50
1:A:121:VAL:O	1:A:121:VAL:CG1	2.59	0.50
1:E:465:TYR:CG	1:E:469:ARG:CG	2.94	0.50
1:G:122:SER:O	1:G:123:ARG:C	2.50	0.50
1:A:756:HIS:O	1:A:756:HIS:CG	2.64	0.50
1:C:465:TYR:CG	1:C:469:ARG:CG	2.94	0.50
2:F:100:ALA:C	2:F:101:LYS:HG3	2.32	0.50
2:F:75:GLN:CD	2:F:98:ARG:O	2.49	0.50
1:C:685:ARG:NH2	1:G:685:ARG:CZ	2.75	0.49
1:G:716:ASN:OD1	1:G:716:ASN:C	2.50	0.49
1:E:623:GLN:O	1:E:624:VAL:CG2	2.60	0.49
1:A:465:TYR:CG	1:A:469:ARG:CG	2.94	0.49
1:E:766:PHE:CZ	1:E:877:LEU:CD1	2.95	0.49
1:A:766:PHE:CZ	1:A:877:LEU:CD1	2.95	0.49
1:C:598:PRO:HB3	1:C:650:ARG:NH1	2.27	0.49
1:A:174:PHE:CG	1:A:174:PHE:O	2.65	0.49
1:A:716:ASN:OD1	1:A:716:ASN:C	2.49	0.49
1:A:444:CYS:CB	1:A:506:LEU:CD1	2.91	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:426:ARG:CZ	2:D:426:ARG:CB	2.91	0.49
1:E:755:ASP:O	1:E:756:HIS:HB3	2.12	0.49
2:D:465:GLY:O	2:D:466:ARG:HG2	2.13	0.49
1:E:816:GLY:O	1:E:818:LYS:CA	2.61	0.49
1:G:597:ARG:NH2	1:G:730:LEU:CD1	2.76	0.49
1:G:26:ALA:O	1:G:28:SER:N	2.45	0.49
2:F:465:GLY:O	2:F:466:ARG:HG2	2.13	0.49
2:D:522:TYR:CD1	2:D:552:GLN:HA	2.48	0.49
2:H:522:TYR:CD1	2:H:552:GLN:HA	2.48	0.48
1:G:766:PHE:CZ	1:G:877:LEU:CD1	2.95	0.48
1:E:453:SER:O	1:E:454:THR:C	2.51	0.48
1:C:766:PHE:CZ	1:C:877:LEU:CD1	2.95	0.48
1:C:122:SER:O	1:C:123:ARG:C	2.50	0.48
1:A:934:HIS:ND1	1:A:1074:THR:CG2	2.77	0.48
1:C:26:ALA:O	1:C:28:SER:N	2.46	0.48
1:E:26:ALA:O	1:E:28:SER:N	2.46	0.48
1:A:26:ALA:O	1:A:28:SER:N	2.46	0.48
1:C:444:CYS:CB	1:C:506:LEU:CD1	2.91	0.48
1:A:559:SER:O	1:A:560:SER:C	2.52	0.48
1:A:354:PHE:CG	4:A:3373:NAG:H62	2.48	0.48
1:C:453:SER:O	1:C:454:THR:C	2.51	0.48
1:A:254:ILE:N	1:A:255:PRO:CD	2.76	0.48
1:G:444:CYS:CB	1:G:506:LEU:CD1	2.91	0.48
1:G:559:SER:O	1:G:560:SER:C	2.52	0.48
1:A:755:ASP:O	1:A:756:HIS:HB3	2.14	0.48
1:G:934:HIS:ND1	1:G:1074:THR:CG2	2.76	0.48
1:C:934:HIS:ND1	1:C:1074:THR:CG2	2.76	0.48
1:E:444:CYS:CB	1:E:506:LEU:CD1	2.91	0.48
1:A:181:HIS:CE1	1:A:200:VAL:CG1	2.96	0.48
2:F:10:SER:CB	2:F:449:ARG:CZ	2.91	0.48
1:G:453:SER:O	1:G:454:THR:C	2.51	0.48
1:C:559:SER:O	1:C:560:SER:C	2.52	0.48
1:G:25:TYR:O	1:G:26:ALA:C	2.52	0.48
2:H:465:GLY:O	2:H:466:ARG:HG2	2.13	0.48
1:E:559:SER:O	1:E:560:SER:C	2.52	0.48
1:G:354:PHE:CG	9:G:3373:NAG:H62	2.49	0.48
1:E:598:PRO:CB	1:E:650:ARG:NH1	2.77	0.47
1:A:453:SER:O	1:A:454:THR:C	2.52	0.47
1:E:934:HIS:ND1	1:E:1074:THR:CG2	2.76	0.47
1:A:662:LEU:CD1	1:A:673:PHE:CE1	2.97	0.47
1:E:598:PRO:CG	1:E:650:ARG:NH1	2.77	0.47
2:D:453:GLY:O	2:D:463:THR:HG23	2.13	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:840:TRP:CD1	1:C:840:TRP:N	2.83	0.47
1:E:566:GLY:O	1:E:567:GLN:C	2.53	0.47
1:C:906:TYR:CE2	1:C:1067:GLU:OE1	2.68	0.47
1:G:906:TYR:CE2	1:G:1067:GLU:OE1	2.68	0.47
1:A:906:TYR:CE2	1:A:1067:GLU:OE1	2.68	0.47
2:B:465:GLY:O	2:B:466:ARG:HG2	2.13	0.47
2:D:343:SER:O	2:D:378:CYS:O	2.33	0.47
1:G:662:LEU:CD1	1:G:673:PHE:CE1	2.98	0.47
1:C:566:GLY:O	1:C:567:GLN:C	2.53	0.47
1:A:618:PHE:CD2	1:A:619:GLU:N	2.82	0.47
1:E:25:TYR:O	1:E:26:ALA:C	2.52	0.47
1:A:253:VAL:CG2	1:A:254:ILE:N	2.78	0.47
3:G:3716:NAG:H4	3:G:3717:NAG:H2	1.70	0.47
1:A:840:TRP:CD1	1:A:840:TRP:N	2.83	0.47
2:D:43:ARG:N	2:D:44:PRO:CD	2.78	0.47
1:E:662:LEU:CD1	1:E:673:PHE:CE1	2.97	0.47
1:A:953:TRP:NE1	1:C:755:ASP:HB2	2.30	0.47
1:A:25:TYR:O	1:A:26:ALA:C	2.52	0.47
1:G:840:TRP:CD1	1:G:840:TRP:N	2.83	0.47
1:C:119:LEU:CD2	1:C:124:GLN:NE2	2.78	0.47
1:E:597:ARG:HB3	1:E:731:ARG:O	2.14	0.47
2:D:522:TYR:CE1	2:D:552:GLN:HA	2.49	0.47
1:E:119:LEU:CD2	1:E:124:GLN:NE2	2.78	0.47
2:H:43:ARG:N	2:H:44:PRO:CD	2.78	0.47
1:E:840:TRP:CD1	1:E:840:TRP:N	2.83	0.47
1:C:662:LEU:CD1	1:C:673:PHE:CE1	2.98	0.47
2:B:98:ARG:O	2:B:99:ARG:C	2.53	0.46
1:A:566:GLY:O	1:A:567:GLN:C	2.53	0.46
1:E:906:TYR:CE2	1:E:1067:GLU:OE1	2.68	0.46
1:G:119:LEU:CD2	1:G:124:GLN:NE2	2.78	0.46
2:F:465:GLY:O	2:F:466:ARG:CG	2.63	0.46
1:A:619:GLU:O	1:A:620:CYS:SG	2.73	0.46
2:F:43:ARG:N	2:F:44:PRO:CD	2.78	0.46
1:E:354:PHE:CG	9:E:3373:NAG:H62	2.50	0.46
2:F:643:ARG:NH2	2:F:649:TRP:CZ2	2.84	0.46
2:H:461:CYS:SG	2:H:466:ARG:CD	3.04	0.46
1:E:1052:GLU:OE1	1:G:756:HIS:HA	2.16	0.46
2:F:597:PRO:O	2:F:598:SER:CB	2.63	0.46
1:A:598:PRO:HB3	1:A:650:ARG:NH1	2.31	0.46
1:E:618:PHE:CD2	1:E:619:GLU:N	2.84	0.46
1:A:119:LEU:CD2	1:A:124:GLN:NE2	2.78	0.46
1:G:827:LEU:CD1	1:G:829:CYS:SG	3.04	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:99:ARG:NH1	2:D:101:LYS:O	2.49	0.46
2:B:43:ARG:N	2:B:44:PRO:CD	2.78	0.46
1:A:894:THR:O	1:C:874:ARG:NH2	2.48	0.46
1:C:25:TYR:CG	1:C:26:ALA:N	2.84	0.46
1:A:25:TYR:CG	1:A:26:ALA:N	2.84	0.46
1:C:827:LEU:CD1	1:C:829:CYS:SG	3.04	0.46
2:D:465:GLY:O	2:D:466:ARG:CG	2.64	0.46
2:H:465:GLY:O	2:H:466:ARG:CG	2.64	0.46
1:A:752:CYS:SG	1:A:758:CYS:N	2.89	0.46
1:G:1063:LEU:N	1:G:1064:PRO:CD	2.79	0.46
1:E:827:LEU:CD1	1:E:829:CYS:SG	3.04	0.46
1:A:354:PHE:CE2	4:A:3373:NAG:O5	2.69	0.45
1:C:1063:LEU:N	1:C:1064:PRO:CD	2.79	0.45
1:A:827:LEU:CD1	1:A:829:CYS:SG	3.04	0.45
2:H:643:ARG:NH2	2:H:649:TRP:CZ2	2.84	0.45
2:B:673:CYS:O	2:B:674:VAL:C	2.54	0.45
1:E:789:TRP:NE1	1:G:772:LYS:CB	2.79	0.45
2:B:465:GLY:O	2:B:466:ARG:CG	2.64	0.45
2:B:643:ARG:NH2	2:B:649:TRP:CZ2	2.85	0.45
2:D:271:TYR:CG	2:D:271:TYR:O	2.69	0.45
2:F:271:TYR:O	2:F:271:TYR:CG	2.69	0.45
1:E:25:TYR:CG	1:E:26:ALA:N	2.85	0.45
1:A:565:PHE:CD2	1:A:565:PHE:O	2.69	0.45
1:A:218:HIS:NE2	1:A:256:MET:SD	2.90	0.45
1:C:816:GLY:O	1:C:818:LYS:CA	2.65	0.45
1:C:25:TYR:O	1:C:26:ALA:C	2.52	0.45
1:G:566:GLY:O	1:G:567:GLN:C	2.53	0.45
1:E:565:PHE:O	1:E:565:PHE:CD2	2.69	0.45
1:E:629:THR:CG2	1:E:630:LEU:N	2.80	0.45
1:C:354:PHE:CG	3:C:3373:NAG:H62	2.51	0.45
2:D:673:CYS:O	2:D:674:VAL:C	2.55	0.45
2:F:546:PHE:CD2	2:F:554:GLU:O	2.69	0.45
1:G:629:THR:CG2	1:G:630:LEU:N	2.80	0.45
2:H:100:ALA:O	2:H:101:LYS:CB	2.62	0.45
2:H:552:GLN:HG3	2:H:553:CYS:H	1.82	0.45
1:E:1063:LEU:N	1:E:1064:PRO:CD	2.79	0.45
1:C:565:PHE:O	1:C:565:PHE:CD2	2.69	0.45
1:A:1063:LEU:N	1:A:1064:PRO:CD	2.79	0.45
1:G:25:TYR:CG	1:G:26:ALA:N	2.84	0.45
1:A:629:THR:CG2	1:A:630:LEU:N	2.79	0.45
4:A:3377:MAN:C3	5:A:3378:MAN:C1	2.95	0.44
1:E:752:CYS:SG	1:E:758:CYS:N	2.90	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:587:LEU:N	2:D:587:LEU:CD1	2.80	0.44
2:D:36:ASP:N	2:D:510:GLN:NE2	2.65	0.44
2:D:98:ARG:O	2:D:99:ARG:C	2.56	0.44
2:D:643:ARG:NH2	2:D:649:TRP:CZ2	2.85	0.44
1:G:565:PHE:O	1:G:565:PHE:CD2	2.70	0.44
1:E:354:PHE:CE2	9:E:3373:NAG:O5	2.70	0.44
2:F:75:GLN:CG	2:F:98:ARG:O	2.66	0.44
2:B:271:TYR:O	2:B:271:TYR:CG	2.70	0.44
2:D:75:GLN:CG	2:D:98:ARG:O	2.66	0.44
2:H:522:TYR:CE1	2:H:552:GLN:HA	2.53	0.44
1:C:629:THR:CG2	1:C:630:LEU:N	2.80	0.44
2:H:271:TYR:CG	2:H:271:TYR:O	2.70	0.44
1:G:4:ASP:OD2	1:G:597:ARG:NH2	2.51	0.44
2:H:75:GLN:CG	2:H:98:ARG:O	2.65	0.44
1:A:953:TRP:CD2	1:C:755:ASP:HB3	2.52	0.44
1:A:816:GLY:O	1:A:818:LYS:CA	2.66	0.44
1:A:1081:TYR:O	1:A:1082:LYS:HB2	2.18	0.44
2:B:75:GLN:CG	2:B:98:ARG:O	2.66	0.44
2:B:99:ARG:O	2:B:383:ILE:O	2.36	0.44
1:G:822:LEU:CG	1:G:823:ARG:N	2.81	0.44
2:D:277:PHE:CE1	2:D:278:ASP:O	2.71	0.44
2:B:587:LEU:CD1	2:B:587:LEU:N	2.80	0.44
2:F:98:ARG:O	2:F:99:ARG:C	2.57	0.43
2:H:461:CYS:SG	2:H:466:ARG:NE	2.91	0.43
1:E:789:TRP:CZ2	1:G:772:LYS:CA	3.00	0.43
2:H:277:PHE:CE1	2:H:278:ASP:O	2.71	0.43
2:B:277:PHE:CE1	2:B:278:ASP:O	2.71	0.43
1:G:354:PHE:CE2	9:G:3373:NAG:O5	2.71	0.43
1:E:597:ARG:HA	1:E:598:PRO:HD3	1.88	0.43
2:D:552:GLN:HG3	2:D:553:CYS:H	1.83	0.43
1:A:361:PHE:CE2	1:A:371:PHE:CE1	3.06	0.43
1:C:731:ARG:CG	1:C:731:ARG:O	2.67	0.43
2:H:587:LEU:N	2:H:587:LEU:CD1	2.80	0.43
1:C:930:HIS:O	1:C:931:VAL:C	2.57	0.43
2:D:354:ASP:O	2:D:544:PRO:CB	2.66	0.43
2:B:466:ARG:O	2:B:467:SER:CB	2.65	0.43
2:F:587:LEU:N	2:F:587:LEU:CD1	2.80	0.43
1:E:1:PHE:CE2	1:E:599:VAL:HG11	2.54	0.43
2:F:75:GLN:O	2:F:97:PHE:CD1	2.72	0.43
2:B:6:PHE:CG	2:B:7:LYS:N	2.86	0.43
1:E:771:LEU:O	1:G:789:TRP:CZ2	2.71	0.43
1:A:790:ASN:O	1:A:853:GLY:O	2.36	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:361:PHE:CE2	1:E:371:PHE:CE1	3.07	0.43
1:E:565:PHE:C	1:E:565:PHE:CD2	2.92	0.43
1:E:930:HIS:O	1:E:931:VAL:C	2.57	0.43
1:A:822:LEU:CG	1:A:823:ARG:N	2.81	0.43
1:E:790:ASN:O	1:E:853:GLY:O	2.36	0.43
1:A:484:ARG:NH1	2:B:586:GLN:NE2	2.67	0.43
2:F:277:PHE:CE1	2:F:278:ASP:O	2.71	0.43
1:G:1081:TYR:O	1:G:1082:LYS:HB2	2.18	0.43
2:H:6:PHE:CG	2:H:7:LYS:N	2.86	0.43
2:B:75:GLN:O	2:B:97:PHE:CD1	2.72	0.43
2:F:6:PHE:CG	2:F:7:LYS:N	2.86	0.43
1:C:790:ASN:O	1:C:853:GLY:O	2.37	0.43
1:G:513:ASN:CB	1:G:599:VAL:HG21	2.49	0.43
2:H:75:GLN:O	2:H:97:PHE:CD1	2.72	0.43
1:G:618:PHE:CD2	1:G:619:GLU:N	2.87	0.43
2:D:75:GLN:O	2:D:97:PHE:CD1	2.72	0.43
1:A:930:HIS:O	1:A:931:VAL:C	2.57	0.43
1:G:790:ASN:O	1:G:853:GLY:O	2.36	0.43
1:G:755:ASP:O	1:G:756:HIS:HB3	2.18	0.42
1:E:107:CYS:SG	1:E:348:LEU:CD2	3.07	0.42
1:G:361:PHE:CE2	1:G:371:PHE:CE1	3.06	0.42
1:C:361:PHE:CE2	1:C:371:PHE:CE1	3.06	0.42
2:D:6:PHE:CG	2:D:7:LYS:N	2.87	0.42
1:A:194:LEU:CD2	1:A:197:LEU:CD1	2.97	0.42
1:A:151:MET:SD	1:A:238:ILE:CG2	3.08	0.42
1:C:565:PHE:C	1:C:565:PHE:CD2	2.92	0.42
1:G:930:HIS:O	1:G:931:VAL:C	2.57	0.42
1:E:374:MET:SD	1:E:417:PHE:CZ	3.13	0.42
2:H:648:CYS:SG	2:H:673:CYS:N	2.92	0.42
1:A:731:ARG:O	1:A:731:ARG:CG	2.66	0.42
1:C:107:CYS:SG	1:C:348:LEU:CD2	3.08	0.42
1:E:41:ALA:O	1:E:42:ASN:C	2.58	0.42
1:E:731:ARG:CG	1:E:731:ARG:O	2.67	0.42
1:C:491:LEU:CD1	1:C:545:ILE:CG1	2.98	0.42
1:G:565:PHE:C	1:G:565:PHE:CD2	2.93	0.42
1:C:695:ASN:O	1:G:686:VAL:CG1	2.67	0.42
1:G:41:ALA:O	1:G:42:ASN:C	2.58	0.42
1:E:822:LEU:CG	1:E:823:ARG:N	2.82	0.42
1:G:107:CYS:SG	1:G:348:LEU:CD2	3.08	0.42
1:E:491:LEU:CD1	1:E:545:ILE:CG1	2.98	0.42
2:F:466:ARG:HE	2:F:466:ARG:HB3	1.81	0.42
1:C:1081:TYR:O	1:C:1082:LYS:HB2	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:822:LEU:CG	1:C:823:ARG:N	2.81	0.42
1:E:816:GLY:C	1:E:818:LYS:N	2.73	0.42
1:C:1020:VAL:O	1:C:1021:GLN:CB	2.68	0.42
1:A:565:PHE:CD2	1:A:565:PHE:C	2.92	0.42
1:A:374:MET:SD	1:A:417:PHE:CZ	3.13	0.42
2:B:74:LYS:CD	2:B:103:TYR:OH	2.68	0.42
1:G:374:MET:SD	1:G:417:PHE:CZ	3.12	0.42
1:C:622:GLU:C	1:C:623:GLN:CG	2.88	0.42
1:G:918:TYR:O	1:G:919:LEU:C	2.58	0.42
1:A:918:TYR:O	1:A:919:LEU:C	2.58	0.42
2:H:546:PHE:CD2	2:H:554:GLU:HG2	2.55	0.42
2:F:648:CYS:SG	2:F:673:CYS:N	2.93	0.42
1:A:1020:VAL:O	1:A:1021:GLN:CB	2.68	0.42
2:H:468:SER:HB2	2:H:471:LEU:HD12	2.01	0.42
1:E:491:LEU:CD2	1:E:545:ILE:O	2.68	0.42
1:C:630:LEU:CD2	1:G:653:GLN:OE1	2.67	0.42
3:E:3716:NAG:H4	3:E:3717:NAG:H2	1.69	0.42
1:C:630:LEU:CD2	1:G:653:GLN:CB	2.98	0.41
1:C:374:MET:SD	1:C:417:PHE:CZ	3.13	0.41
1:G:597:ARG:CG	1:G:731:ARG:CG	2.99	0.41
2:F:508:TYR:CE1	2:F:514:CYS:CB	3.03	0.41
1:G:491:LEU:CD2	1:G:545:ILE:O	2.69	0.41
2:D:155:LEU:N	2:D:160:THR:CG2	2.84	0.41
1:G:678:ASN:ND2	6:G:3678:NAG:C7	2.79	0.41
2:H:468:SER:HB2	2:H:471:LEU:CD1	2.51	0.41
1:A:491:LEU:CD1	1:A:545:ILE:CG1	2.98	0.41
1:E:1020:VAL:O	1:E:1021:GLN:CB	2.68	0.41
1:A:107:CYS:SG	1:A:348:LEU:CD2	3.08	0.41
9:G:3374:NAG:HO3	9:G:3375:MAN:H2	1.83	0.41
1:G:731:ARG:O	1:G:731:ARG:CG	2.68	0.41
2:D:468:SER:HB2	2:D:471:LEU:HD12	2.01	0.41
1:A:491:LEU:CD2	1:A:545:ILE:O	2.68	0.41
1:C:354:PHE:CE2	3:C:3373:NAG:O5	2.73	0.41
1:A:662:LEU:CD1	1:A:673:PHE:CZ	3.04	0.41
1:A:41:ALA:O	1:A:42:ASN:C	2.59	0.41
1:G:752:CYS:SG	1:G:758:CYS:N	2.93	0.41
2:F:468:SER:HB2	2:F:471:LEU:CD1	2.50	0.41
2:D:99:ARG:O	2:D:383:ILE:O	2.39	0.41
1:E:374:MET:O	1:E:375:SER:OG	2.39	0.41
2:H:155:LEU:N	2:H:160:THR:CG2	2.84	0.41
2:B:285:LEU:C	2:B:287:HIS:N	2.74	0.41
2:B:468:SER:HB2	2:B:471:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:468:SER:HB2	2:D:471:LEU:CD1	2.51	0.41
1:G:491:LEU:CD1	1:G:545:ILE:CG1	2.98	0.41
1:C:752:CYS:SG	1:C:758:CYS:N	2.94	0.41
2:B:648:CYS:SG	2:B:673:CYS:N	2.94	0.41
2:H:546:PHE:CE2	2:H:554:GLU:HG2	2.56	0.41
1:E:676:THR:O	1:E:677:LYS:CB	2.69	0.41
1:E:1081:TYR:O	1:E:1082:LYS:HB2	2.20	0.41
2:B:468:SER:HB2	2:B:471:LEU:HD12	2.02	0.41
2:F:468:SER:HB2	2:F:471:LEU:HD12	2.01	0.41
1:A:181:HIS:CG	1:A:200:VAL:CG2	3.04	0.41
1:G:662:LEU:CD1	1:G:673:PHE:CZ	3.04	0.41
2:D:648:CYS:SG	2:D:673:CYS:N	2.94	0.41
1:G:928:GLU:CG	1:G:929:SER:N	2.84	0.41
2:B:472:GLU:HA	2:B:475:CYS:CB	2.50	0.41
1:G:1020:VAL:O	1:G:1021:GLN:CB	2.68	0.41
2:F:155:LEU:N	2:F:160:THR:CG2	2.83	0.41
1:E:1023:GLU:O	1:E:1024:LEU:C	2.60	0.41
2:H:285:LEU:C	2:H:287:HIS:N	2.74	0.41
1:G:1023:GLU:O	1:G:1024:LEU:C	2.59	0.41
1:E:642:ARG:O	1:E:644:LYS:N	2.54	0.41
1:C:662:LEU:CD1	1:C:673:PHE:CZ	3.04	0.40
2:B:155:LEU:N	2:B:160:THR:CG2	2.84	0.40
1:A:271:LEU:C	1:A:273:PHE:N	2.75	0.40
2:B:625:CYS:N	2:B:626:PRO:CD	2.84	0.40
1:G:642:ARG:O	1:G:644:LYS:N	2.54	0.40
1:A:928:GLU:CG	1:A:929:SER:N	2.85	0.40
1:E:376:GLN:C	1:E:378:ASN:N	2.75	0.40
1:E:662:LEU:CD1	1:E:673:PHE:CZ	3.04	0.40
2:F:596:CYS:HA	2:F:597:PRO:HD3	1.85	0.40
2:F:532:ARG:CD	2:F:554:GLU:HG3	2.51	0.40
2:F:285:LEU:C	2:F:287:HIS:N	2.74	0.40
1:E:812:TYR:CE2	1:E:814:ALA:CB	3.04	0.40
2:F:625:CYS:N	2:F:626:PRO:CD	2.85	0.40
2:F:99:ARG:O	2:F:383:ILE:O	2.39	0.40
2:D:522:TYR:CD2	2:D:522:TYR:C	2.95	0.40
1:C:678:ASN:ND2	6:C:3678:NAG:C7	2.78	0.40
1:G:676:THR:O	1:G:677:LYS:CB	2.69	0.40
1:C:918:TYR:O	1:C:919:LEU:C	2.58	0.40
1:C:608:PHE:O	1:C:609:ILE:C	2.59	0.40
1:A:642:ARG:O	1:A:644:LYS:N	2.54	0.40
1:C:1076:THR:CG2	1:C:1077:VAL:N	2.85	0.40
1:A:676:THR:O	1:A:677:LYS:CB	2.69	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:625:CYS:N	2:D:626:PRO:CD	2.84	0.40
1:A:608:PHE:O	1:A:609:ILE:C	2.59	0.40
1:E:928:GLU:CG	1:E:929:SER:N	2.84	0.40

There are no symmetry-related clashes.

## 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	1080/1095 (99%)	839 (78%)	215 (20%)	26 (2%)	9	59
1	C	881/1095 (80%)	663 (75%)	194 (22%)	24 (3%)	8	56
1	E	880/1095 (80%)	665 (76%)	190 (22%)	25 (3%)	8	55
1	G	881/1095 (80%)	666 (76%)	191 (22%)	24 (3%)	8	56
2	B	672/687 (98%)	514 (76%)	147 (22%)	11 (2%)	14	68
2	D	672/687 (98%)	515 (77%)	145 (22%)	12 (2%)	13	65
2	F	672/687 (98%)	514 (76%)	145 (22%)	13 (2%)	12	64
2	H	672/687 (98%)	512 (76%)	146 (22%)	14 (2%)	11	62
All	All	6410/7128 (90%)	4888 (76%)	1373 (21%)	149 (2%)	10	60

All (149) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	A	120	PRO
1	A	757	ILE
1	C	82	SER
1	C	757	ILE
1	E	82	SER
1	E	757	ILE
1	E	817	GLN
1	G	82	SER

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Mol	Chain	Res	Type
1	G	757	ILE
1	G	817	GLN
2	H	99	ARG
1	A	27	ASN
1	A	490	VAL
1	A	624	VAL
1	A	817	GLN
1	A	818	LYS
1	A	847	ASN
1	A	931	VAL
1	A	956	VAL
2	B	163	ASP
2	B	465	GLY
1	C	27	ASN
1	C	490	VAL
1	C	818	LYS
1	C	847	ASN
1	C	931	VAL
1	C	956	VAL
2	D	163	ASP
2	D	465	GLY
1	E	27	ASN
1	E	490	VAL
1	E	624	VAL
1	E	818	LYS
1	E	847	ASN
1	E	931	VAL
1	E	956	VAL
2	F	163	ASP
2	F	465	GLY
1	G	27	ASN
1	G	490	VAL
1	G	624	VAL
1	G	847	ASN
1	G	931	VAL
1	G	956	VAL
2	H	101	LYS
2	H	163	ASP
2	H	465	GLY
1	A	649	SER
2	B	158	VAL
2	B	314	ILE

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Mol	Chain	Res	Type
2	B	467	SER
1	C	649	SER
1	C	817	GLN
2	D	158	VAL
2	D	314	ILE
2	D	467	SER
1	E	649	SER
2	F	158	VAL
2	F	314	ILE
2	F	467	SER
1	G	649	SER
1	G	818	LYS
2	H	158	VAL
2	H	314	ILE
2	H	467	SER
1	A	70	ASN
1	A	123	ARG
1	A	124	GLN
1	A	209	THR
1	A	246	ASP
1	A	643	SER
1	A	654	SER
2	B	69	HIS
1	C	123	ARG
1	C	124	GLN
1	C	454	THR
1	C	624	VAL
1	C	643	SER
1	C	654	SER
1	C	816	GLY
2	D	69	HIS
1	E	123	ARG
1	E	124	GLN
1	E	454	THR
1	E	654	SER
1	E	758	CYS
2	F	69	HIS
2	F	463	THR
1	G	123	ARG
1	G	124	GLN
1	G	643	SER
1	G	654	SER

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Mol	Chain	Res	Type
2	H	69	HIS
1	A	454	THR
1	A	579	GLY
1	A	816	GLY
2	B	639	THR
1	C	70	ASN
1	C	579	GLY
2	D	99	ARG
1	E	70	ASN
1	E	579	GLY
1	E	643	SER
1	E	722	LYS
2	F	99	ARG
2	F	639	THR
1	G	70	ASN
1	G	454	THR
1	G	579	GLY
2	H	639	THR
1	A	722	LYS
1	A	773	SER
2	B	660	MET
1	C	722	LYS
1	C	773	SER
2	D	639	THR
2	D	660	MET
1	E	773	SER
1	E	816	GLY
2	F	652	TYR
2	F	660	MET
1	G	722	LYS
1	G	773	SER
1	G	816	GLY
2	H	660	MET
1	A	540	VAL
1	C	540	VAL
1	C	846	ILE
1	E	540	VAL
1	E	846	ILE
1	G	540	VAL
1	A	846	ILE
1	G	846	ILE
2	H	59	PRO

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Mol	Chain	Res	Type
2	B	517	ILE
2	D	517	ILE
2	F	517	ILE
2	H	399	ILE
2	H	517	ILE
2	B	204	ILE
2	B	399	ILE
2	D	204	ILE
2	D	399	ILE
2	F	204	ILE
2	H	204	ILE
1	C	120	PRO
1	E	120	PRO
1	G	120	PRO

### 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	924/934 (99%)	914 (99%)	10 (1%)	84	96
1	C	754/934 (81%)	742 (98%)	12 (2%)	75	95
1	E	753/934 (81%)	743 (99%)	10 (1%)	80	96
1	G	754/934 (81%)	744 (99%)	10 (1%)	80	96
2	B	583/592 (98%)	583 (100%)	0	100	100
2	D	583/592 (98%)	582 (100%)	1 (0%)	96	99
2	F	583/592 (98%)	582 (100%)	1 (0%)	96	99
2	H	583/592 (98%)	581 (100%)	2 (0%)	96	99
All	All	5517/6104 (90%)	5471 (99%)	46 (1%)	89	97

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	565	PHE
1	A	567	GLN

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Mol	Chain	Res	Type
1	A	578	ASP
1	A	679	ARG
1	A	714	ARG
1	A	731	ARG
1	A	840	TRP
1	A	915	PHE
1	A	964	TRP
1	C	119	LEU
1	C	565	PHE
1	C	567	GLN
1	C	578	ASP
1	C	622	GLU
1	C	625	VAL
1	C	679	ARG
1	C	714	ARG
1	C	731	ARG
1	C	840	TRP
1	C	915	PHE
1	C	964	TRP
2	D	426	ARG
1	E	119	LEU
1	E	565	PHE
1	E	567	GLN
1	E	578	ASP
1	E	679	ARG
1	E	714	ARG
1	E	731	ARG
1	E	840	TRP
1	E	915	PHE
1	E	964	TRP
2	F	598	SER
1	G	119	LEU
1	G	565	PHE
1	G	567	GLN
1	G	578	ASP
1	G	679	ARG
1	G	714	ARG
1	G	731	ARG
1	G	840	TRP
1	G	915	PHE
1	G	964	TRP
2	H	489	ASP

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Mol	Chain	Res	Type
2	H	598	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	462	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

29 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
3	NAG	A	3042	1,3	12,14,15	0.68	1 (8%)	15,19,21	0.84	1 (6%)
3	NAG	A	3043	3	12,14,15	0.66	0	15,19,21	1.06	1 (6%)
4	NAG	A	3373	1,4	12,14,15	0.67	1 (8%)	15,19,21	1.25	2 (13%)
4	NAG	A	3374	4	12,14,15	0.70	1 (8%)	15,19,21	1.39	2 (13%)
4	MAN	A	3375	4	10,11,12	0.65	0	11,15,17	2.31	4 (36%)
4	MAN	A	3376	4	10,11,12	0.81	1 (10%)	11,15,17	1.21	1 (9%)
4	MAN	A	3377	4	10,11,12	0.89	1 (10%)	11,15,17	1.65	3 (27%)
3	NAG	A	3716	1,3	12,14,15	0.72	1 (8%)	15,19,21	0.97	1 (6%)
3	NAG	A	3717	3	12,14,15	0.67	1 (8%)	15,19,21	0.79	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	3042	1,3	12,14,15	0.70	1 (8%)	15,19,21	0.86	1 (6%)
3	NAG	C	3043	3	12,14,15	0.70	1 (8%)	15,19,21	1.01	1 (6%)
3	NAG	C	3373	1,3	12,14,15	0.64	0	15,19,21	1.28	2 (13%)
3	NAG	C	3374	3	12,14,15	0.67	0	15,19,21	0.98	0
3	NAG	C	3716	1,3	12,14,15	0.63	0	15,19,21	1.02	1 (6%)
3	NAG	C	3717	3	12,14,15	0.67	1 (8%)	15,19,21	0.81	0
3	NAG	E	3042	1,3	12,14,15	0.70	1 (8%)	15,19,21	0.88	1 (6%)
3	NAG	E	3043	3	12,14,15	0.69	1 (8%)	15,19,21	1.09	1 (6%)
9	NAG	E	3373	1,9	12,14,15	0.65	0	15,19,21	1.23	2 (13%)
9	NAG	E	3374	9	12,14,15	0.70	1 (8%)	15,19,21	1.34	2 (13%)
9	MAN	E	3375	9	10,11,12	0.69	0	11,15,17	2.01	2 (18%)
3	NAG	E	3716	1,3	12,14,15	0.66	0	15,19,21	1.10	1 (6%)
3	NAG	E	3717	3	12,14,15	0.70	1 (8%)	15,19,21	0.77	0
3	NAG	G	3042	1,3	12,14,15	0.68	1 (8%)	15,19,21	0.90	1 (6%)
3	NAG	G	3043	3	12,14,15	0.68	1 (8%)	15,19,21	1.02	1 (6%)
9	NAG	G	3373	1,9	12,14,15	0.65	0	15,19,21	1.26	2 (13%)
9	NAG	G	3374	9	12,14,15	0.69	1 (8%)	15,19,21	1.36	1 (6%)
9	MAN	G	3375	9	10,11,12	0.71	0	11,15,17	2.00	2 (18%)
3	NAG	G	3716	1,3	12,14,15	0.68	0	15,19,21	1.23	1 (6%)
3	NAG	G	3717	3	12,14,15	0.69	1 (8%)	15,19,21	0.73	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	3043	3	-	0/6/23/26	0/1/1/1
4	NAG	A	3373	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	3374	4	-	0/6/23/26	0/1/1/1
4	MAN	A	3375	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	3376	4	-	0/2/19/22	0/1/1/1
4	MAN	A	3377	4	-	0/2/19/22	0/1/1/1
3	NAG	A	3716	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	3717	3	-	0/6/23/26	0/1/1/1
3	NAG	C	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	3043	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	3373	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	3374	3	-	0/6/23/26	0/1/1/1
3	NAG	C	3716	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	3717	3	-	0/6/23/26	0/1/1/1
3	NAG	E	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	3043	3	-	0/6/23/26	0/1/1/1
9	NAG	E	3373	1,9	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	E	3374	9	-	0/6/23/26	0/1/1/1
9	MAN	E	3375	9	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	E	3716	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	3717	3	-	0/6/23/26	0/1/1/1
3	NAG	G	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	3043	3	-	0/6/23/26	0/1/1/1
9	NAG	G	3373	1,9	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	G	3374	9	-	0/6/23/26	0/1/1/1
9	MAN	G	3375	9	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	G	3716	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	3717	3	-	0/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3716	NAG	O5-C5	-2.19	1.41	1.45
9	E	3374	NAG	O5-C5	-2.17	1.41	1.45
9	G	3374	NAG	O5-C5	-2.16	1.41	1.45
4	A	3377	MAN	O5-C5	-2.15	1.41	1.45
4	A	3374	NAG	O5-C5	-2.15	1.41	1.45
3	E	3717	NAG	O5-C5	-2.13	1.41	1.45
3	C	3042	NAG	O5-C5	-2.12	1.41	1.45
3	C	3043	NAG	O5-C5	-2.11	1.41	1.45
3	G	3717	NAG	O5-C5	-2.11	1.41	1.45
3	G	3043	NAG	O5-C5	-2.08	1.41	1.45
4	A	3376	MAN	O5-C5	-2.06	1.41	1.45
3	E	3042	NAG	O5-C5	-2.06	1.41	1.45
3	A	3042	NAG	O5-C5	-2.04	1.41	1.45
3	E	3043	NAG	O5-C5	-2.03	1.41	1.45
3	C	3717	NAG	O5-C5	-2.02	1.41	1.45
3	G	3042	NAG	O5-C5	-2.02	1.41	1.45
3	A	3717	NAG	O5-C5	-2.02	1.41	1.45
4	A	3373	NAG	O5-C5	-2.01	1.41	1.45

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	3375	MAN	O5-C5-C6	5.25	112.49	106.98
9	G	3375	MAN	O5-C5-C6	5.10	112.33	106.98
4	A	3375	MAN	O5-C5-C6	4.11	111.29	106.98
4	A	3375	MAN	C4-C3-C2	-3.98	105.16	110.50
4	A	3375	MAN	O3-C3-C2	3.81	116.91	109.94
9	G	3375	MAN	C4-C3-C2	-3.58	105.70	110.50
9	E	3375	MAN	C4-C3-C2	-3.42	105.91	110.50
3	G	3716	NAG	C3-C2-N2	-3.39	106.60	111.76
4	A	3377	MAN	O5-C5-C4	-3.28	106.49	110.65
4	A	3376	MAN	O5-C5-C6	3.19	110.33	106.98
3	C	3373	NAG	O5-C5-C6	3.06	110.20	106.98
9	G	3374	NAG	O4-C4-C3	3.01	117.11	110.35
9	G	3373	NAG	O5-C5-C6	2.99	110.11	106.98
3	E	3043	NAG	O5-C5-C6	2.97	110.10	106.98
4	A	3373	NAG	O5-C5-C6	2.96	110.08	106.98
9	E	3374	NAG	O4-C4-C3	2.93	116.91	110.35
3	E	3716	NAG	C3-C2-N2	-2.91	107.34	111.76
4	A	3374	NAG	O4-C4-C3	2.90	116.86	110.35
3	A	3043	NAG	O5-C5-C6	2.88	110.00	106.98
9	E	3373	NAG	O5-C5-C6	2.84	109.96	106.98
4	A	3377	MAN	C6-C5-C4	-2.80	106.24	113.00
3	A	3716	NAG	C3-C2-N2	-2.78	107.53	111.76
3	G	3043	NAG	O5-C5-C6	2.64	109.75	106.98
3	G	3042	NAG	O5-C5-C6	2.60	109.71	106.98
3	E	3042	NAG	O5-C5-C6	2.57	109.68	106.98
3	C	3043	NAG	O5-C5-C6	2.49	109.60	106.98
3	C	3042	NAG	O5-C5-C6	2.45	109.55	106.98
9	E	3373	NAG	C3-C2-N2	-2.45	108.04	111.76
9	G	3373	NAG	C3-C2-N2	-2.42	108.07	111.76
3	C	3716	NAG	C3-C2-N2	-2.41	108.09	111.76
3	A	3042	NAG	O5-C5-C6	2.40	109.50	106.98
4	A	3375	MAN	C3-C4-C5	-2.35	106.01	110.20
4	A	3373	NAG	C3-C2-N2	-2.33	108.21	111.76
3	C	3373	NAG	C3-C2-N2	-2.26	108.32	111.76
4	A	3374	NAG	O5-C5-C4	2.25	113.50	110.65
4	A	3377	MAN	C4-C3-C2	-2.13	107.64	110.50
9	E	3374	NAG	O5-C5-C4	2.11	113.33	110.65

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	E	3375	MAN	C1
9	E	3373	NAG	C1

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Mol	Chain	Res	Type	Atom
9	G	3375	MAN	C1
3	C	3373	NAG	C1
4	A	3373	NAG	C1
9	G	3373	NAG	C1
4	A	3375	MAN	C1

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 17 are monoatomic - leaving 13 for Mogul analysis.

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	MAN	A	3378	-	10,11,12	1.08	1 (10%)	11,15,17	1.92	2 (18%)
6	NAG	A	3678	1	12,14,15	0.65	0	15,19,21	0.77	0
6	NAG	A	3880	1	12,14,15	0.56	0	15,19,21	0.82	0
6	NAG	B	3094	2	12,14,15	0.64	0	15,19,21	0.88	1 (6%)
6	NAG	C	3678	1	12,14,15	0.63	0	15,19,21	0.75	1 (6%)
6	NAG	C	3880	1	12,14,15	0.56	0	15,19,21	0.79	0
6	NAG	D	3094	2	12,14,15	0.68	0	15,19,21	0.86	1 (6%)
6	NAG	E	3678	1	12,14,15	0.65	0	15,19,21	0.73	0
6	NAG	E	3880	1	12,14,15	0.56	0	15,19,21	0.80	0
6	NAG	F	3094	2	12,14,15	0.66	0	15,19,21	0.94	1 (6%)
6	NAG	G	3678	1	12,14,15	0.66	0	15,19,21	0.77	1 (6%)
6	NAG	G	3880	1	12,14,15	0.57	0	15,19,21	0.79	0
6	NAG	H	3094	2	12,14,15	0.66	0	15,19,21	0.88	1 (6%)

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	MAN	A	3378	-	-	0/2/19/22	0/1/1/1
6	NAG	A	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	A	3880	1	-	0/6/23/26	0/1/1/1
6	NAG	B	3094	2	-	0/6/23/26	0/1/1/1
6	NAG	C	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	C	3880	1	-	0/6/23/26	0/1/1/1
6	NAG	D	3094	2	-	0/6/23/26	0/1/1/1
6	NAG	E	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	E	3880	1	-	0/6/23/26	0/1/1/1
6	NAG	F	3094	2	-	0/6/23/26	0/1/1/1
6	NAG	G	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	G	3880	1	-	0/6/23/26	0/1/1/1
6	NAG	H	3094	2	-	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	A	3378	MAN	O5-C5	-2.58	1.40	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3378	MAN	C3-C4-C5	4.79	118.76	110.20
6	F	3094	NAG	O5-C5-C6	2.95	110.07	106.98
6	B	3094	NAG	O5-C5-C6	2.62	109.73	106.98
6	H	3094	NAG	O5-C5-C6	2.58	109.69	106.98
6	D	3094	NAG	O5-C5-C6	2.47	109.58	106.98
5	A	3378	MAN	O3-C3-C2	2.32	114.18	109.94
6	G	3678	NAG	O5-C5-C6	2.03	109.11	106.98
6	C	3678	NAG	O5-C5-C6	2.02	109.10	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	1082/1095 (98%)	0.14	21 (1%) 64 32	61, 153, 256, 362	0
1	C	885/1095 (80%)	0.34	44 (4%) 28 12	67, 172, 280, 410	0
1	E	884/1095 (80%)	0.16	23 (2%) 53 24	65, 157, 266, 337	0
1	G	885/1095 (80%)	0.13	22 (2%) 54 25	74, 150, 266, 342	0
2	B	674/687 (98%)	0.41	33 (4%) 28 12	100, 205, 286, 421	2 (0%)
2	D	674/687 (98%)	0.96	129 (19%) 2 2	107, 229, 313, 416	2 (0%)
2	F	674/687 (98%)	0.50	50 (7%) 14 7	98, 207, 289, 374	2 (0%)
2	H	674/687 (98%)	0.51	50 (7%) 14 7	100, 210, 293, 390	2 (0%)
All	All	6432/7128 (90%)	0.36	372 (5%) 22 9	61, 185, 283, 421	8 (0%)

All (372) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	817	GLN	10.3
2	B	72	GLY	8.6
2	H	72	GLY	8.3
2	D	92	ALA	8.2
2	B	92	ALA	8.0
1	C	817	GLN	7.5
1	C	818	LYS	7.5
2	F	175	GLU	7.3
2	D	63	ALA	7.2
2	D	91	ALA	6.7
2	F	176	CYS	6.5
1	G	817	GLN	6.1
1	C	821	GLN	5.9
2	F	92	ALA	5.8
2	D	32	PRO	5.8
2	H	73	GLN	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	820	GLY	5.7
1	G	818	LYS	5.6
2	F	91	ALA	5.6
1	G	127	PRO	5.4
2	D	175	GLU	5.4
1	C	1044	LYS	5.3
2	D	83	LEU	5.2
2	F	629	GLN	5.2
1	E	128	ARG	4.9
2	D	76	LEU	4.9
1	C	721	GLY	4.8
2	H	432	ARG	4.8
2	D	144	ILE	4.8
1	C	730	LEU	4.7
2	H	469	GLN	4.6
2	F	161	HIS	4.6
2	B	432	ARG	4.5
2	D	105	ILE	4.5
1	G	128	ARG	4.5
1	A	818	LYS	4.5
2	D	68	ASP	4.4
1	C	819	GLN	4.4
1	A	1044	LYS	4.4
1	C	102	TYR	4.3
2	B	73	GLN	4.3
2	D	109	TYR	4.2
1	A	623	GLN	4.2
2	D	379	ASP	4.1
2	D	62	LEU	4.1
1	C	482	TRP	4.1
1	E	482	TRP	4.1
2	D	161	HIS	4.0
2	D	369	THR	4.0
1	A	816	GLY	4.0
2	D	104	PRO	4.0
2	D	399	ILE	4.0
2	D	400	GLN	3.9
1	C	726	ALA	3.9
1	A	821	GLN	3.9
2	D	97	PHE	3.9
2	F	177	GLN	3.9
2	D	24	CYS	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	1	GLN	3.9
2	F	345	VAL	3.9
2	F	1	GLN	3.9
2	B	91	ALA	3.9
1	C	1078	LEU	3.8
2	D	407	ARG	3.8
2	D	433	ASP	3.8
2	D	443	LEU	3.8
2	D	133	ARG	3.8
2	H	416	THR	3.8
1	A	819	GLN	3.8
1	C	106	LEU	3.8
2	D	445	CYS	3.8
2	D	82	THR	3.8
2	D	401	GLU	3.8
2	H	32	PRO	3.7
1	G	627	GLU	3.7
1	E	483	ARG	3.7
2	D	67	GLU	3.7
2	D	189	THR	3.7
2	D	650	VAL	3.7
1	C	1079	GLU	3.7
2	H	80	LYS	3.7
2	D	432	ARG	3.6
2	H	433	ASP	3.6
2	B	133	ARG	3.6
2	B	382	GLN	3.6
1	E	821	GLN	3.6
2	H	401	GLU	3.6
1	C	396	LYS	3.6
1	C	816	GLY	3.5
2	B	71	GLY	3.5
2	D	409	LEU	3.5
2	F	72	GLY	3.5
2	D	65	THR	3.5
1	C	723	PRO	3.5
1	A	323	THR	3.5
2	F	115	TYR	3.5
1	C	1081	TYR	3.5
2	B	433	ASP	3.5
2	H	206	GLY	3.5
1	G	823	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	39	ARG	3.5
2	D	382	GLN	3.4
1	G	483	ARG	3.4
2	F	669	GLU	3.4
2	B	431	SER	3.4
1	G	396	LYS	3.4
2	D	80	LYS	3.3
2	D	628	LEU	3.3
2	D	69	HIS	3.3
2	H	92	ALA	3.3
2	F	335	LYS	3.3
2	D	38	ILE	3.2
2	F	49	ARG	3.2
2	D	56	ILE	3.2
2	B	469	GLN	3.2
2	D	391	VAL	3.2
2	D	446	GLY	3.2
2	B	430	GLN	3.2
2	H	470	GLU	3.2
2	H	629	GLN	3.1
1	E	817	GLN	3.1
2	D	419	VAL	3.1
2	D	367	GLY	3.1
2	H	417	VAL	3.1
2	B	206	GLY	3.1
2	H	454	TYR	3.1
2	B	1	GLN	3.1
2	F	133	ARG	3.1
2	D	93	PHE	3.0
2	D	227	GLU	3.0
1	E	729	ASN	3.0
2	F	416	THR	3.0
2	D	143	ARG	3.0
2	D	378	CYS	3.0
2	H	67	GLU	3.0
1	C	420	VAL	3.0
2	D	98	ARG	3.0
2	H	1	GLN	3.0
2	D	625	CYS	2.9
1	E	422	ARG	2.9
2	D	635	VAL	2.9
2	D	126	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	626	SER	2.9
2	B	628	LEU	2.9
1	C	466	GLU	2.9
1	C	623	GLN	2.9
2	H	430	GLN	2.9
1	C	815	GLU	2.9
1	E	1044	LYS	2.9
2	D	107	LEU	2.9
1	C	822	LEU	2.9
2	D	375	ARG	2.9
2	D	6	PHE	2.9
1	A	277	ASN	2.9
2	D	613	GLU	2.9
2	H	431	SER	2.9
2	D	64	GLU	2.9
1	C	104	THR	2.9
1	E	973	GLN	2.9
2	F	371	ARG	2.8
1	G	619	GLU	2.8
2	D	226	GLU	2.8
2	D	51	CYS	2.8
1	A	625	VAL	2.8
2	D	101	LYS	2.8
2	D	614	LYS	2.8
2	H	71	GLY	2.8
2	D	28	ASN	2.7
2	F	48	MET	2.7
2	H	335	LYS	2.7
1	G	102	TYR	2.7
1	C	398	VAL	2.7
2	H	418	GLN	2.7
2	D	383	ILE	2.7
2	H	423	CYS	2.7
1	E	397	GLY	2.7
1	G	124	GLN	2.7
2	H	93	PHE	2.7
2	H	389	PHE	2.7
1	G	561	ARG	2.7
1	G	624	VAL	2.7
1	A	278	SER	2.7
1	G	482	TRP	2.7
1	A	724	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	730	LEU	2.7
2	D	470	GLU	2.7
2	H	378	CYS	2.6
1	G	625	VAL	2.6
2	D	469	GLN	2.6
2	H	91	ALA	2.6
1	E	623	GLN	2.6
2	D	430	GLN	2.6
2	F	630	LEU	2.6
2	D	416	THR	2.6
2	F	430	GLN	2.6
2	D	115	TYR	2.6
2	F	39	ARG	2.6
2	D	99	ARG	2.6
2	H	236	LEU	2.6
2	H	185	VAL	2.6
2	D	136	ASN	2.6
1	E	40	ALA	2.6
2	F	390	GLN	2.6
2	D	634	PRO	2.5
1	C	48	TYR	2.5
2	D	81	VAL	2.5
2	D	49	ARG	2.5
2	B	136	ASN	2.5
2	F	628	LEU	2.5
1	C	729	ASN	2.5
2	F	382	GLN	2.5
2	D	84	TYR	2.5
2	H	189	THR	2.5
2	D	29	PHE	2.5
1	E	466	GLU	2.5
2	H	297	ILE	2.5
2	D	103	TYR	2.5
2	F	470	GLU	2.5
2	H	127	LEU	2.5
2	D	623	ALA	2.5
1	E	728	ARG	2.5
1	C	397	GLY	2.5
2	D	129	GLY	2.5
1	C	725	LEU	2.4
2	D	331	VAL	2.4
2	F	178	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	377	GLU	2.4
1	C	541	LEU	2.4
2	D	651	ALA	2.4
2	D	345	VAL	2.4
2	F	81	VAL	2.4
2	F	138	ILE	2.4
2	F	193	ASN	2.4
2	F	69	HIS	2.4
1	A	624	VAL	2.4
2	D	27	LEU	2.4
2	D	413	ASP	2.4
2	D	406	ILE	2.4
2	F	385	VAL	2.4
2	D	78	PRO	2.4
2	D	95	VAL	2.4
2	B	629	GLN	2.4
2	B	49	ARG	2.3
1	C	46	GLY	2.3
2	B	107	LEU	2.3
2	B	131	LEU	2.3
1	A	973	GLN	2.3
1	C	973	GLN	2.3
2	B	185	VAL	2.3
2	D	654	LEU	2.3
2	H	82	THR	2.3
2	D	53	ALA	2.3
1	G	95	HIS	2.3
2	D	185	VAL	2.3
2	H	79	GLN	2.3
2	H	628	LEU	2.3
2	D	404	PHE	2.3
2	H	414	ILE	2.3
2	F	103	TYR	2.3
1	G	821	GLN	2.3
2	D	102	GLY	2.3
1	A	272	ALA	2.3
2	D	108	TYR	2.3
2	D	31	GLY	2.3
2	B	122	ARG	2.3
2	D	142	GLY	2.3
1	A	322	THR	2.3
2	D	621	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	71	GLY	2.3
1	A	1081	TYR	2.3
2	B	145	GLY	2.3
2	B	335	LYS	2.3
1	C	1045	VAL	2.3
2	D	347	LEU	2.3
2	D	366	ASN	2.3
2	F	160	THR	2.3
2	D	667	VAL	2.2
2	H	195	PHE	2.2
2	B	414	ILE	2.2
1	G	480	ARG	2.2
2	F	466	ARG	2.2
2	H	320	VAL	2.2
2	F	391	VAL	2.2
2	B	371	ARG	2.2
2	F	79	GLN	2.2
2	H	84	TYR	2.2
1	C	1024	LEU	2.2
2	H	69	HIS	2.2
2	F	67	GLU	2.2
1	C	45	GLY	2.2
2	H	429	ASP	2.2
1	C	335	GLU	2.2
2	B	171	ASN	2.2
2	D	160	THR	2.2
2	D	642	GLU	2.2
2	H	161	HIS	2.2
2	F	195	PHE	2.2
1	G	125	GLU	2.2
2	D	234	THR	2.2
2	F	206	GLY	2.2
1	G	1081	TYR	2.2
2	B	93	PHE	2.2
2	D	206	GLY	2.2
2	D	73	GLN	2.2
2	D	652	TYR	2.2
2	D	340	LYS	2.2
2	D	36	ASP	2.2
2	D	368	VAL	2.1
1	C	483	ARG	2.1
2	H	122	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	126	LYS	2.1
2	D	358	VAL	2.1
2	D	395	ALA	2.1
2	H	175	GLU	2.1
1	E	100	ASN	2.1
2	D	195	PHE	2.1
2	H	415	VAL	2.1
1	E	425	ARG	2.1
1	C	423	GLN	2.1
1	C	621	ARG	2.1
2	D	418	GLN	2.1
1	E	108	PHE	2.1
1	G	1039	GLN	2.1
2	D	346	PHE	2.1
2	D	140	GLU	2.1
2	F	174	LYS	2.1
1	E	650	ARG	2.1
2	D	387	ILE	2.1
2	F	610	LEU	2.1
2	B	202	GLN	2.1
2	F	73	GLN	2.1
1	C	1039	GLN	2.1
2	B	418	GLN	2.1
2	B	623	ALA	2.1
2	D	420	LEU	2.1
2	D	611	LYS	2.1
2	D	130	ASP	2.1
2	D	442	PHE	2.1
2	D	72	GLY	2.1
2	D	139	THR	2.1
2	D	616	PRO	2.1
2	F	173	GLU	2.1
2	D	619	LYS	2.1
1	E	10	ALA	2.1
2	H	186	LEU	2.1
2	D	26	LYS	2.1
1	A	561	ARG	2.1
2	D	414	ILE	2.1
2	F	571	ARG	2.0
2	D	649	TRP	2.0
2	F	429	ASP	2.0
2	F	401	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	392	LYS	2.0
1	E	465	TYR	2.0
1	E	1078	LEU	2.0
2	D	643	ARG	2.0
1	C	622	GLU	2.0
2	D	25	GLN	2.0
2	F	74	LYS	2.0
2	F	614	LYS	2.0
2	H	66	GLN	2.0
1	A	273	PHE	2.0
1	A	10	ALA	2.0
2	H	366	ASN	2.0
1	C	724	LEU	2.0
1	E	822	LEU	2.0
2	D	428	ARG	2.0
1	C	918	TYR	2.0
2	B	109	TYR	2.0
2	H	113	LEU	2.0
1	A	529	GLU	2.0
2	F	389	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	C	3374	14/15	0.63	20.14	136,238,359,434	0
4	NAG	A	3373	14/15	0.32	1.41	136,261,376,443	0
4	NAG	A	3374	14/15	0.31	1.22	91,240,362,435	0
3	NAG	C	3373	14/15	0.47	1.02	198,292,381,425	0
3	NAG	G	3716	14/15	0.24	0.93	77,188,300,303	0
9	NAG	E	3373	14/15	0.42	0.90	146,324,390,464	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	C	3716	14/15	0.18	0.69	60,167,211,249	0
9	NAG	G	3373	14/15	0.34	0.54	106,265,384,401	0
9	NAG	G	3374	14/15	0.44	0.45	136,261,326,367	0
9	NAG	E	3374	14/15	0.33	0.44	201,279,352,410	0
4	MAN	A	3377	11/12	0.23	0.38	99,256,308,331	0
3	NAG	E	3716	14/15	0.21	0.06	49,184,277,297	0
3	NAG	E	3042	14/15	0.41	-0.36	198,249,285,287	0
3	NAG	G	3042	14/15	0.26	-0.39	193,244,274,279	0
3	NAG	C	3042	14/15	0.23	-0.47	150,232,327,335	0
3	NAG	A	3716	14/15	0.18	-0.93	28,156,272,274	0
3	NAG	A	3042	14/15	0.17	-1.07	133,175,235,244	0
4	MAN	A	3375	11/12	0.16	-2.86	140,207,283,324	0
3	NAG	C	3717	14/15	0.76	-	224,297,342,395	0
3	NAG	C	3043	14/15	0.31	-	179,305,351,363	0
9	MAN	G	3375	11/12	0.31	-	173,208,309,351	0
9	MAN	E	3375	11/12	0.25	-	171,251,305,311	0
4	MAN	A	3376	11/12	0.22	-	114,259,296,316	0
3	NAG	E	3043	14/15	0.55	-	183,310,366,378	0
3	NAG	G	3043	14/15	0.26	-	176,248,297,317	0
3	NAG	G	3717	14/15	0.31	-	192,216,305,376	0
3	NAG	A	3043	14/15	0.23	-	80,233,327,333	0
3	NAG	E	3717	14/15	0.21	-	117,240,280,337	0
3	NAG	A	3717	14/15	0.30	-	185,218,319,381	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	G	3678	14/15	0.50	6.99	132,218,244,251	0
6	NAG	C	3678	14/15	0.39	5.10	125,245,317,319	0
6	NAG	A	3678	14/15	0.49	4.52	117,269,324,327	0
6	NAG	G	3880	14/15	0.28	1.48	84,176,236,252	0
5	MAN	A	3378	11/12	0.31	0.35	171,186,272,293	0
6	NAG	C	3880	14/15	0.24	0.33	60,171,245,293	0
6	NAG	E	3678	14/15	0.21	-0.28	104,227,276,317	0
6	NAG	D	3094	14/15	0.69	-0.39	189,258,296,299	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	E	3880	14/15	0.18	-0.58	80,160,189,194	0
6	NAG	H	3094	14/15	0.41	-0.60	148,232,292,297	0
6	NAG	F	3094	14/15	0.29	-0.71	124,217,266,291	0
6	NAG	B	3094	14/15	0.31	-0.81	107,197,277,325	0
7	CA	C	2007	1/1	0.11	-1.05	206,206,206,206	0
6	NAG	A	3880	14/15	0.19	-1.06	105,143,196,220	0
7	CA	C	2006	1/1	0.13	-1.14	125,125,125,125	0
7	CA	C	2005	1/1	0.05	-1.26	200,200,200,200	0
7	CA	A	2005	1/1	0.10	-1.41	145,145,145,145	0
7	CA	F	2002	1/1	0.10	-1.44	578,578,578,578	0
7	CA	D	2002	1/1	0.14	-1.52	547,547,547,547	0
8	MG	A	2009	1/1	0.10	-1.53	367,367,367,367	0
7	CA	E	2005	1/1	0.09	-1.53	176,176,176,176	0
7	CA	B	2002	1/1	0.09	-1.64	535,535,535,535	0
7	CA	E	2006	1/1	0.10	-1.67	137,137,137,137	0
7	CA	H	2002	1/1	0.09	-1.69	510,510,510,510	0
7	CA	A	2007	1/1	0.05	-1.70	181,181,181,181	0
7	CA	G	2005	1/1	0.07	-1.93	139,139,139,139	0
7	CA	E	2007	1/1	0.13	-2.13	188,188,188,188	0
7	CA	A	2006	1/1	0.11	-2.32	107,107,107,107	0
7	CA	G	2007	1/1	0.08	-2.55	150,150,150,150	0
7	CA	G	2006	1/1	0.07	-2.76	95,95,95,95	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.