



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 07:52 PM GMT

PDB ID : 1FV3  
Title : THE HC FRAGMENT OF TETANUS TOXIN COMPLEXED WITH AN ANALOGUE OF ITS GANGLIOSIDE RECEPTOR GT1B  
Authors : Fotinou, C.; Emsley, P.; Black, I.; Ando, H.; Ishida, H.; Kiso, M.; Sinha, K.A.; Fairweather, N.F.; Isaacs, N.W.  
Deposited on : 2000-09-18  
Resolution : 2.30 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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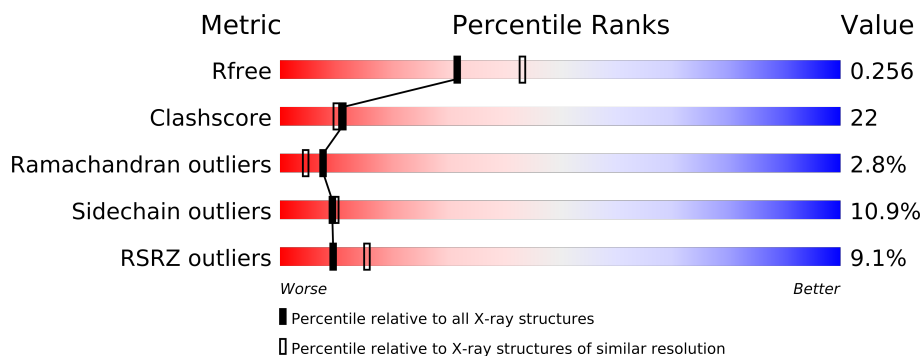
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	472	
1	B	472	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	CEQ	A	8[A]	-	X
4	CEQ	A	8[B]	-	X
4	CEQ	B	8[A]	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7786 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 TETANUS TOXIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	1	0
			3652	2336	612	694	10			
1	B	451	Total	C	N	O	S	0	0	0
			3648	2334	611	693	10			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	844	MET	-	SEE REMARK 999	? P04958
A	845	GLY	-	SEE REMARK 999	? P04958
A	846	SER	-	SEE REMARK 999	? P04958
A	847	SER	-	SEE REMARK 999	? P04958
A	848	HIS	-	SEE REMARK 999	? P04958
A	849	HIS	-	SEE REMARK 999	? P04958
A	850	HIS	-	SEE REMARK 999	? P04958
A	851	HIS	-	SEE REMARK 999	? P04958
A	852	HIS	-	SEE REMARK 999	? P04958
A	853	HIS	-	SEE REMARK 999	? P04958
A	854	SER	-	SEE REMARK 999	? P04958
A	855	SER	-	SEE REMARK 999	? P04958
A	856	GLY	-	SEE REMARK 999	? P04958
A	857	LEU	-	SEE REMARK 999	? P04958
A	858	VAL	-	SEE REMARK 999	? P04958
A	859	PRO	-	SEE REMARK 999	? P04958
A	860	ARG	-	SEE REMARK 999	? P04958
A	861	GLY	-	SEE REMARK 999	? P04958
A	862	SER	-	SEE REMARK 999	? P04958
A	863	HIS	-	SEE REMARK 999	? P04958
A	864	MET	-	SEE REMARK 999	? P04958
B	844	MET	-	SEE REMARK 999	? P04958
B	845	GLY	-	SEE REMARK 999	? P04958
B	846	SER	-	SEE REMARK 999	? P04958
B	847	SER	-	SEE REMARK 999	? P04958

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Chain	Residue	Modelled	Actual	Comment	Reference
B	848	HIS	-	SEE REMARK 999	? P04958
B	849	HIS	-	SEE REMARK 999	? P04958
B	850	HIS	-	SEE REMARK 999	? P04958
B	851	HIS	-	SEE REMARK 999	? P04958
B	852	HIS	-	SEE REMARK 999	? P04958
B	853	HIS	-	SEE REMARK 999	? P04958
B	854	SER	-	SEE REMARK 999	? P04958
B	855	SER	-	SEE REMARK 999	? P04958
B	856	GLY	-	SEE REMARK 999	? P04958
B	857	LEU	-	SEE REMARK 999	? P04958
B	858	VAL	-	SEE REMARK 999	? P04958
B	859	PRO	-	SEE REMARK 999	? P04958
B	860	ARG	-	SEE REMARK 999	? P04958
B	861	GLY	-	SEE REMARK 999	? P04958
B	862	SER	-	SEE REMARK 999	? P04958
B	863	HIS	-	SEE REMARK 999	? P04958
B	864	MET	-	SEE REMARK 999	? P04958

- Molecule 2 is a polymer of unknown type called SUGAR (GLC-GAL-NGA-GAL-NAN-SLB-NAN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	7	Total	C	N	O	0	0
			108	59	4	45		
2	B	7	Total	C	N	O	0	0
			108	59	4	45		

There are 42 discrepancies between the modelled and reference sequences:

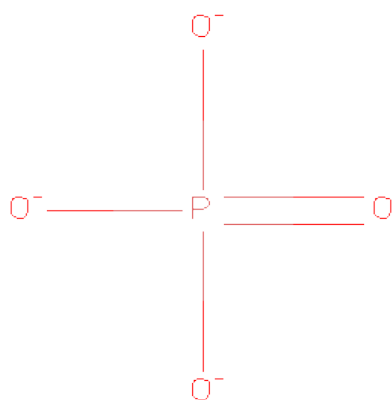
Chain	Residue	Modelled	Actual	Comment	Reference
A	844	MET	-	SEE REMARK 999	? P04958
A	845	GLY	-	SEE REMARK 999	? P04958
A	846	SER	-	SEE REMARK 999	? P04958
A	847	SER	-	SEE REMARK 999	? P04958
A	848	HIS	-	SEE REMARK 999	? P04958
A	849	HIS	-	SEE REMARK 999	? P04958
A	850	HIS	-	SEE REMARK 999	? P04958
A	851	HIS	-	SEE REMARK 999	? P04958
A	852	HIS	-	SEE REMARK 999	? P04958
A	853	HIS	-	SEE REMARK 999	? P04958
A	854	SER	-	SEE REMARK 999	? P04958
A	855	SER	-	SEE REMARK 999	? P04958

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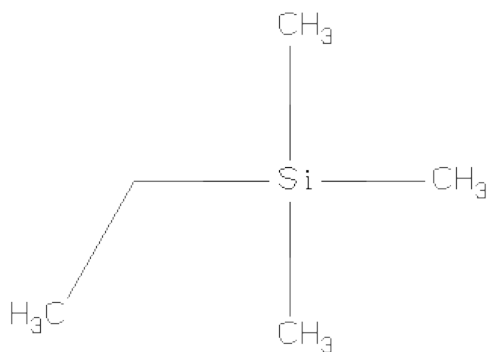
Chain	Residue	Modelled	Actual	Comment	Reference
A	856	GLY	-	SEE REMARK 999	? P04958
A	857	LEU	-	SEE REMARK 999	? P04958
A	858	VAL	-	SEE REMARK 999	? P04958
A	859	PRO	-	SEE REMARK 999	? P04958
A	860	ARG	-	SEE REMARK 999	? P04958
A	861	GLY	-	SEE REMARK 999	? P04958
A	862	SER	-	SEE REMARK 999	? P04958
A	863	HIS	-	SEE REMARK 999	? P04958
A	864	MET	-	SEE REMARK 999	? P04958
B	844	MET	-	SEE REMARK 999	? P04958
B	845	GLY	-	SEE REMARK 999	? P04958
B	846	SER	-	SEE REMARK 999	? P04958
B	847	SER	-	SEE REMARK 999	? P04958
B	848	HIS	-	SEE REMARK 999	? P04958
B	849	HIS	-	SEE REMARK 999	? P04958
B	850	HIS	-	SEE REMARK 999	? P04958
B	851	HIS	-	SEE REMARK 999	? P04958
B	852	HIS	-	SEE REMARK 999	? P04958
B	853	HIS	-	SEE REMARK 999	? P04958
B	854	SER	-	SEE REMARK 999	? P04958
B	855	SER	-	SEE REMARK 999	? P04958
B	856	GLY	-	SEE REMARK 999	? P04958
B	857	LEU	-	SEE REMARK 999	? P04958
B	858	VAL	-	SEE REMARK 999	? P04958
B	859	PRO	-	SEE REMARK 999	? P04958
B	860	ARG	-	SEE REMARK 999	? P04958
B	861	GLY	-	SEE REMARK 999	? P04958
B	862	SER	-	SEE REMARK 999	? P04958
B	863	HIS	-	SEE REMARK 999	? P04958
B	864	MET	-	SEE REMARK 999	? P04958

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ETHYL-TRIMETHYL-SILANE (three-letter code: CEQ) (formula:  $C_5H_{14}Si$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	Si	0	1
			12	10	2		
4	B	1	Total	C	Si	0	1
			12	10	2		

- Molecule 5 is water.

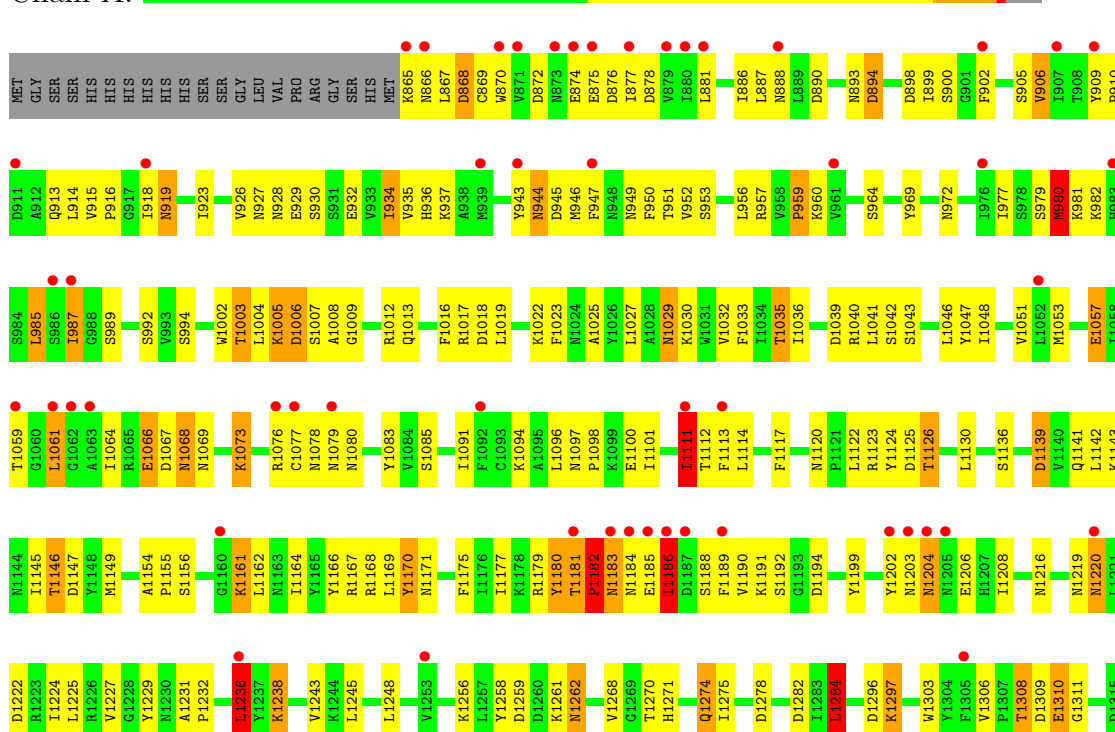
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total 87	O 87	0	0
5	B	154	Total 154	O 154	0	0

### 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.

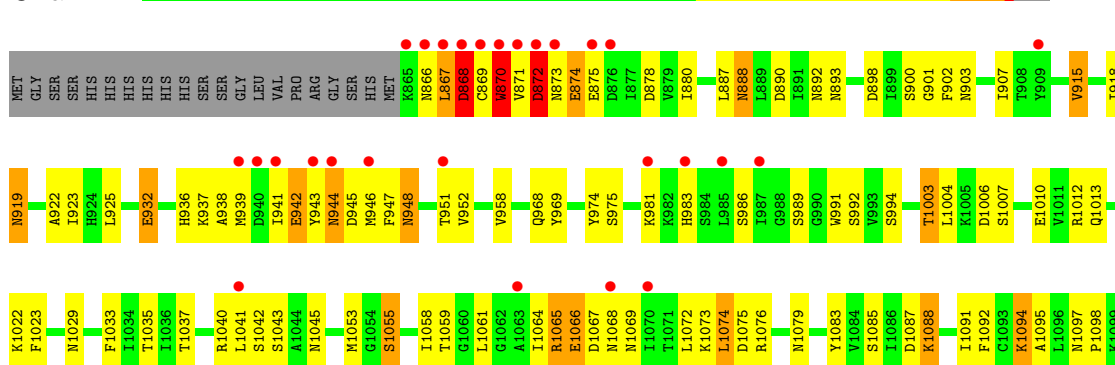
#### • Molecule 1: TETANUS TOXIN HEAVY CHAIN

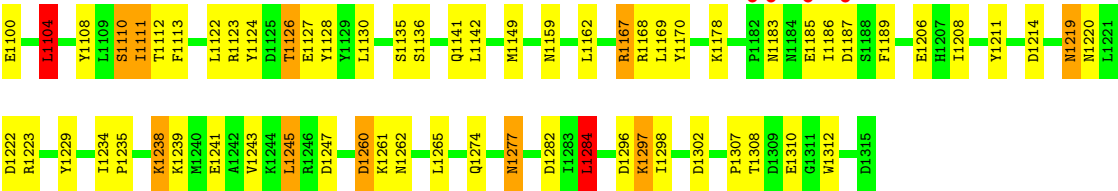
Chain A:



#### • Molecule 1: TETANUS TOXIN HEAVY CHAIN

Chain B:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.31Å 53.07Å 118.28Å 90.00° 89.78° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.00-2.30) 96.5 (29.93-2.30)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.237 , 0.306 0.228 , 0.256	Depositor DCC
$R_{free}$ test set	1543 reflections (3.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.7	Xtriage
Anisotropy	0.846	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 97.4	EDS
Estimated twinning fraction	0.225 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.29$ , $\langle L^2 \rangle = 0.13$	Xtriage
Outliers	0 of 49640 reflections	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	7786	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: BGC, NGA, PO4, SIA, GAL, CEQ, SLB

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	0.76	0/3740	1.07	20/5076 (0.4%)
1	B	0.94	1/3731 (0.0%)	1.13	19/5064 (0.4%)
All	All	0.85	1/7471 (0.0%)	1.10	39/10140 (0.4%)

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	1
2	B	1	0
All	All	1	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1229	TYR	CD2-CE2	-5.04	1.31	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1075	ASP	CB-CG-OD2	9.21	126.59	118.30
1	B	1222	ASP	CB-CG-OD2	8.71	126.14	118.30
1	B	1087	ASP	CB-CG-OD2	7.70	125.23	118.30
1	B	1104	LEU	CB-CG-CD1	-7.20	98.77	111.00
1	B	1282	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	945	ASP	CB-CG-OD2	6.91	124.52	118.30
1	A	1183	ASN	N-CA-C	6.88	129.57	111.00
1	A	980	MET	CB-CG-SD	-6.70	92.31	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1309	ASP	CB-CG-OD2	6.63	124.26	118.30
1	B	1260	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	872	ASP	CB-CG-OD2	6.58	124.22	118.30
1	B	1302	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	1067	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	868	ASP	CB-CG-OD2	6.24	123.91	118.30
1	A	1282	ASP	CB-CG-OD2	6.07	123.76	118.30
1	B	915	VAL	CB-CA-C	-5.99	100.03	111.40
1	B	1247	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	878	ASP	CB-CG-OD2	5.85	123.57	118.30
1	B	945	ASP	CB-CG-OD2	5.85	123.56	118.30
1	B	872	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	1222	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	1214	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	876	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	1125	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	898	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	878	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	890	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	1284	LEU	CA-CB-CG	5.57	128.11	115.30
1	B	1110	SER	N-CA-C	5.46	125.75	111.00
1	B	1104	LEU	CA-CB-CG	5.45	127.83	115.30
1	B	1296	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	1284	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	1168	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	894	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	1236	LEU	CA-CB-CG	-5.17	103.41	115.30
1	A	1186	ILE	CB-CA-C	-5.14	101.31	111.60
1	A	1216	ASN	N-CA-CB	5.10	119.79	110.60
1	A	1139	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	868	ASP	CB-CG-OD2	5.03	122.83	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	7	SIA	C2

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1182	PRO	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	3652	0	3592	170	0
1	B	3648	0	3588	150	1
2	A	108	0	87	7	0
2	B	108	0	87	10	0
3	B	5	0	0	2	0
4	A	12	0	0	0	0
4	B	12	0	0	0	0
5	A	87	0	0	4	0
5	B	154	0	0	2	0
All	All	7786	0	7354	333	1

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 22.

All (333) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1145:ILE:H	1:A:1145:ILE:HD12	1.14	1.07
1:A:985:LEU:O	1:A:985:LEU:HD22	1.54	1.06
1:B:1064:ILE:O	1:B:1064:ILE:HG22	1.68	0.93
1:B:1111:ILE:HD12	1:B:1112:THR:H	1.33	0.92
1:B:1124:TYR:O	1:B:1126:THR:HG22	1.72	0.88
1:A:1297:LYS:HE3	1:A:1297:LYS:O	1.79	0.83
1:A:959:PRO:HA	1:A:1029:ASN:HB3	1.61	0.82
1:B:871:VAL:HG22	1:B:872:ASP:H	1.43	0.82
2:B:6:SLB:C8	2:B:7:SIA:O1B	2.26	0.79
1:A:1145:ILE:H	1:A:1145:ILE:CD1	1.88	0.79
1:B:871:VAL:HG23	1:B:874:GLU:HB3	1.65	0.78
1:A:932:GLU:HB3	1:A:1073:LYS:HB2	1.64	0.78
1:B:1219:ASN:O	1:B:1220:ASN:HB3	1.84	0.78
1:B:932:GLU:HB3	1:B:1073:LYS:HB2	1.66	0.78
1:B:946:MET:HE3	1:B:1065:ARG:HG2	1.65	0.76
1:B:939:MET:HA	1:B:943:TYR:HE1	1.49	0.76
1:B:1123:ARG:HB2	1:B:1126:THR:HG21	1.69	0.73
1:A:980:MET:CE	1:A:987:ILE:HG21	2.18	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1161:LYS:N	1:A:1161:LYS:HD3	2.04	0.72
1:B:1023:PHE:CD1	1:B:1167:ARG:HD2	2.25	0.72
1:B:888:ASN:HD22	1:B:888:ASN:C	1.93	0.71
1:A:926:VAL:HG12	1:A:927:ASN:H	1.53	0.71
1:B:936:HIS:HA	1:B:1069:ASN:HD22	1.55	0.71
1:B:874:GLU:HG3	1:B:875:GLU:N	2.05	0.71
1:A:1035:THR:HG23	1:A:1047:TYR:HB2	1.73	0.70
1:A:1261:LYS:HG3	1:A:1261:LYS:O	1.90	0.70
1:A:985:LEU:CD2	1:A:985:LEU:O	2.37	0.69
1:A:980:MET:HE2	1:A:987:ILE:HG21	1.73	0.69
1:B:1111:ILE:HD12	1:B:1112:THR:N	2.05	0.69
1:A:1124:TYR:O	1:A:1126:THR:HG22	1.93	0.69
1:B:871:VAL:HG23	1:B:874:GLU:CB	2.22	0.69
1:A:909:TYR:HB3	1:A:910:PRO:HD2	1.75	0.69
1:A:1145:ILE:N	1:A:1145:ILE:HD12	1.99	0.68
1:A:1262:ASN:O	1:A:1262:ASN:ND2	2.26	0.68
1:B:944:ASN:ND2	1:B:946:MET:HB2	2.09	0.68
1:A:1111:ILE:HD12	1:A:1111:ILE:H	1.57	0.67
1:A:1155:PRO:HB2	1:A:1168:ARG:HD3	1.76	0.67
1:B:874:GLU:HG3	1:B:875:GLU:HG2	1.76	0.67
1:B:1010:GLU:HG2	1:B:1061:LEU:HD23	1.77	0.67
1:A:1012:ARG:HD2	1:A:1057:GLU:O	1.95	0.66
1:B:936:HIS:HA	1:B:1069:ASN:ND2	2.10	0.66
1:B:915:VAL:HG23	1:B:922:ALA:HB3	1.77	0.66
1:B:1277:ASN:OD1	1:B:1277:ASN:C	2.34	0.66
1:A:1229:TYR:HB3	1:A:1236:LEU:HD13	1.77	0.65
1:A:1297:LYS:HE3	1:A:1297:LYS:HA	1.79	0.65
1:B:1260:ASP:O	1:B:1261:LYS:HD3	1.96	0.65
1:B:1064:ILE:CG2	1:B:1064:ILE:O	2.42	0.64
1:A:1270:THR:O	2:A:4:GAL:H61	1.97	0.64
1:B:871:VAL:HG23	1:B:874:GLU:HG2	1.78	0.64
1:B:918:ILE:HA	5:B:1397:HOH:O	1.95	0.64
1:A:972:ASN:ND2	1:A:1078:ASN:H	1.94	0.64
1:B:868:ASP:O	1:B:869:CYS:SG	2.56	0.64
1:A:1006:ASP:O	1:A:1006:ASP:OD1	2.16	0.63
1:A:919:ASN:O	1:A:919:ASN:ND2	2.32	0.63
1:A:869:CYS:SG	1:A:870:TRP:HE3	2.21	0.63
1:B:918:ILE:HD12	1:B:919:ASN:N	2.14	0.62
1:A:1208:ILE:HD13	1:A:1238:LYS:HG2	1.81	0.62
1:A:1142:LEU:HD13	1:A:1227:VAL:HG21	1.81	0.62
1:A:1047:TYR:CE1	1:A:1101:ILE:CD1	2.83	0.62
1:B:890:ASP:OD2	1:B:892:ASN:ND2	2.33	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:870:TRP:HE3	1:B:870:TRP:N	1.97	0.62
1:A:1112:THR:HG23	1:A:1113:PHE:HD1	1.65	0.62
1:B:1219:ASN:O	1:B:1220:ASN:CB	2.48	0.61
1:B:1310:GLU:O	1:B:1310:GLU:HG3	2.00	0.61
1:B:947:PHE:O	1:B:1040:ARG:HG3	2.00	0.61
1:B:981:LYS:HA	1:B:1067:ASP:HB2	1.83	0.61
2:A:5:SIA:H7	2:A:5:SIA:O10	2.01	0.61
1:B:900:SER:O	1:B:902:PHE:N	2.34	0.61
1:B:871:VAL:CG2	1:B:874:GLU:HG2	2.30	0.60
1:B:925:LEU:HD13	1:B:1073:LYS:HA	1.83	0.60
1:B:938:ALA:N	1:B:942:GLU:OE2	2.34	0.60
1:A:894:ASP:N	5:A:1390:HOH:O	2.33	0.60
1:A:1224:ILE:HD13	1:A:1275:ILE:HD11	1.82	0.60
1:A:1122:LEU:HD11	1:A:1177:ILE:HD12	1.83	0.60
1:A:1114:LEU:HD21	1:A:1192:SER:HB2	1.83	0.60
1:B:983:HIS:HB2	1:B:986:SER:O	2.01	0.60
1:B:871:VAL:HG22	1:B:872:ASP:N	2.15	0.60
1:B:918:ILE:HD12	1:B:918:ILE:C	2.22	0.60
1:A:1022:LYS:HZ2	1:A:1164:ILE:HB	1.67	0.59
1:B:1094:LYS:HG3	1:B:1095:ALA:O	2.02	0.59
1:A:1142:LEU:HD11	1:A:1227:VAL:HB	1.82	0.59
1:A:1139:ASP:OD2	1:A:1154:ALA:HB2	2.03	0.59
2:A:5:SIA:H7	2:A:5:SIA:C10	2.33	0.58
1:B:1239:LYS:NZ	1:B:1262:ASN:OD1	2.26	0.58
1:A:1297:LYS:HE3	1:A:1297:LYS:CA	2.33	0.58
1:A:935:VAL:O	1:A:1069:ASN:HA	2.02	0.58
1:B:968:GLN:HG3	1:B:969:TYR:CE2	2.38	0.58
1:A:1111:ILE:HD12	1:A:1111:ILE:N	2.19	0.58
1:B:991:TRP:HB3	1:B:1004:LEU:HD23	1.85	0.58
1:A:1098:PRO:HA	1:A:1101:ILE:HB	1.86	0.57
1:B:871:VAL:HG23	1:B:874:GLU:CG	2.33	0.57
1:A:1297:LYS:CE	1:A:1297:LYS:O	2.52	0.57
2:B:1:BGC:H6C1	2:B:2:GAL:H1	1.86	0.57
1:A:909:TYR:HB3	1:A:910:PRO:CD	2.34	0.57
1:B:1277:ASN:OD1	1:B:1277:ASN:O	2.23	0.57
1:B:1037:THR:OG1	1:B:1045:ASN:HB2	2.04	0.56
1:A:1259:ASP:OD1	1:A:1259:ASP:C	2.44	0.56
1:A:1018:ASP:OD2	1:A:1027:LEU:N	2.34	0.56
1:B:1169:LEU:HD12	1:B:1312:TRP:CD1	2.41	0.56
1:B:1023:PHE:CE1	1:B:1167:ARG:HD2	2.41	0.56
1:B:1178:LYS:HE3	1:B:1206:GLU:OE1	2.06	0.56
1:B:1241:GLU:HG2	1:B:1243:VAL:HG13	1.86	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:992:SER:OG	1:A:1003:THR:HG23	2.06	0.55
1:A:1130:LEU:HD22	1:A:1303:TRP:CE3	2.42	0.55
1:A:1036:ILE:HD11	1:A:1046:LEU:HD13	1.88	0.55
1:A:1145:ILE:O	1:A:1146:THR:HB	2.05	0.55
2:B:3:NGA:H1	2:B:6:SLB:C1	2.36	0.55
1:A:980:MET:HE3	1:A:987:ILE:HG21	1.89	0.55
1:B:1310:GLU:O	1:B:1310:GLU:CG	2.55	0.55
1:B:1010:GLU:HG2	1:B:1061:LEU:CD2	2.37	0.55
1:B:887:LEU:HD12	1:B:898:ASP:OD1	2.06	0.55
1:A:1111:ILE:HG13	1:A:1248:LEU:HD11	1.88	0.55
1:B:892:ASN:O	1:B:893:ASN:HB2	2.06	0.55
1:A:1143:LYS:HB3	1:A:1147:ASP:HB3	1.89	0.54
1:A:913:GLN:C	1:A:914:LEU:HD23	2.28	0.54
1:A:1035:THR:CG2	1:A:1047:TYR:HB2	2.37	0.54
1:A:1006:ASP:C	1:A:1006:ASP:OD1	2.46	0.54
1:A:979:SER:O	1:A:1066:GLU:HB2	2.07	0.54
1:A:1164:ILE:O	1:A:1164:ILE:HG13	2.06	0.54
1:A:952:VAL:HG22	1:A:1091:ILE:HD13	1.89	0.54
1:B:974:TYR:O	1:B:994:SER:HB2	2.06	0.54
1:B:1003:THR:HB	1:B:1013:GLN:HE21	1.72	0.54
1:B:1110:SER:O	1:B:1112:THR:N	2.41	0.54
1:A:1096:LEU:HA	1:A:1100:GLU:OE1	2.08	0.54
1:A:1202:TYR:O	1:A:1203:ASN:HB2	2.08	0.54
1:B:1042:SER:OG	1:B:1043:SER:N	2.40	0.54
1:A:1122:LEU:HD12	1:A:1190:VAL:HG21	1.89	0.53
1:A:893:ASN:O	1:A:894:ASP:HB2	2.08	0.53
1:A:1208:ILE:CD1	1:A:1238:LYS:HG2	2.37	0.53
1:A:1061:LEU:HD23	1:A:1061:LEU:N	2.24	0.53
1:A:937:LYS:NZ	1:A:1066:GLU:OE1	2.41	0.53
1:A:1048:ILE:HD12	1:A:1053:MET:HG3	1.91	0.53
1:A:906:VAL:HA	1:A:934:ILE:O	2.09	0.53
1:B:1083:TYR:OH	1:B:1310:GLU:HG2	2.08	0.53
1:A:1123:ARG:NH2	1:A:1189:PHE:CE2	2.77	0.53
1:A:969:TYR:CD2	1:A:1079:ASN:HB2	2.44	0.53
1:B:1123:ARG:HB2	1:B:1126:THR:CG2	2.35	0.53
1:B:870:TRP:CE3	1:B:870:TRP:N	2.77	0.53
1:A:980:MET:O	1:A:980:MET:HG2	2.09	0.53
1:B:1023:PHE:CE2	1:B:1136:SER:HB2	2.44	0.52
1:A:1162:LEU:O	1:A:1164:ILE:HG23	2.09	0.52
1:A:989:SER:O	1:A:1066:GLU:HB3	2.09	0.52
1:B:1097:ASN:HB2	1:B:1098:PRO:HD2	1.91	0.52
1:A:1023:PHE:CE2	1:A:1136:SER:HB2	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:887:LEU:HD23	1:A:1091:ILE:HG13	1.92	0.52
1:A:1155:PRO:O	1:A:1168:ARG:HG3	2.10	0.52
1:A:1180:TYR:OH	1:A:1238:LYS:NZ	2.40	0.52
1:B:939:MET:HA	1:B:943:TYR:CE1	2.39	0.52
1:B:1088:LYS:HG2	1:B:1108:TYR:CE1	2.44	0.52
1:A:1111:ILE:H	1:A:1111:ILE:CD1	2.19	0.52
2:A:1:BGC:H6C1	2:A:2:GAL:H1	1.89	0.52
1:A:1141:GLN:HG3	1:A:1142:LEU:N	2.25	0.52
1:A:1145:ILE:O	1:A:1146:THR:CB	2.58	0.51
1:B:946:MET:CE	1:B:1065:ARG:HG2	2.38	0.51
1:B:1169:LEU:HD12	1:B:1312:TRP:NE1	2.24	0.51
1:B:1067:ASP:C	1:B:1069:ASN:H	2.12	0.51
1:B:952:VAL:O	1:B:1035:THR:HA	2.10	0.51
1:A:950:PHE:HZ	1:A:1004:LEU:HD21	1.75	0.51
1:B:1169:LEU:HD12	1:B:1312:TRP:CE2	2.46	0.51
1:B:888:ASN:ND2	1:B:888:ASN:C	2.64	0.51
1:B:1076:ARG:HG3	1:B:1076:ARG:HH21	1.75	0.51
1:B:936:HIS:CD2	1:B:1069:ASN:HD21	2.29	0.51
1:A:1271:HIS:HE1	2:A:3:NGA:O4	1.93	0.51
2:B:6:SLB:H8	2:B:7:SIA:O1B	2.08	0.51
1:A:926:VAL:HG12	1:A:927:ASN:N	2.25	0.51
1:A:906:VAL:HG13	1:A:935:VAL:HG13	1.92	0.51
1:B:1065:ARG:HB3	1:B:1065:ARG:CZ	2.41	0.50
1:A:969:TYR:CE2	1:A:1079:ASN:HB2	2.46	0.50
1:A:1199:TYR:CD2	1:A:1206:GLU:HB3	2.45	0.50
1:A:1047:TYR:HA	1:A:1051:VAL:O	2.10	0.50
1:A:972:ASN:HD21	1:A:1077:CYS:HA	1.76	0.50
2:A:5:SIA:C7	2:A:5:SIA:O10	2.59	0.50
1:B:1220:ASN:ND2	1:B:1220:ASN:O	2.44	0.50
1:A:1186:ILE:H	1:A:1186:ILE:HD13	1.77	0.50
1:A:1022:LYS:NZ	1:A:1164:ILE:HB	2.27	0.50
1:B:932:GLU:HB3	1:B:1073:LYS:CD	2.42	0.50
1:A:1297:LYS:HE3	1:A:1297:LYS:C	2.31	0.49
1:B:869:CYS:HB2	1:B:1094:LYS:HB3	1.93	0.49
1:A:1122:LEU:HD12	1:A:1190:VAL:CG2	2.42	0.49
1:B:992:SER:OG	1:B:1003:THR:HG23	2.11	0.49
1:B:1219:ASN:ND2	2:B:3:NGA:O4	2.42	0.49
1:B:1169:LEU:CD1	1:B:1312:TRP:CE2	2.96	0.49
1:A:972:ASN:HD21	1:A:1078:ASN:H	1.59	0.49
1:B:1074:LEU:N	1:B:1074:LEU:HD23	2.27	0.49
1:A:1039:ASP:OD2	1:A:1039:ASP:C	2.49	0.49
1:B:1110:SER:OG	1:B:1110:SER:O	2.20	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:969:TYR:CD2	1:B:1079:ASN:HB2	2.47	0.49
1:A:985:LEU:C	1:A:985:LEU:HD22	2.31	0.49
1:B:874:GLU:HG3	1:B:875:GLU:H	1.77	0.49
1:B:1007:SER:OG	1:B:1065:ARG:HG3	2.12	0.49
1:B:1123:ARG:CB	1:B:1126:THR:HG21	2.41	0.49
1:B:1067:ASP:OD2	1:B:1069:ASN:HB2	2.13	0.49
1:A:1047:TYR:CZ	1:A:1101:ILE:HD12	2.48	0.48
1:A:947:PHE:O	1:A:1040:ARG:HG3	2.13	0.48
1:B:1297:LYS:HG2	1:B:1298:ILE:HG13	1.94	0.48
1:B:937:LYS:HG2	1:B:942:GLU:OE1	2.13	0.48
1:A:1169:LEU:O	1:A:1170:TYR:HB2	2.14	0.48
1:B:946:MET:O	1:B:1040:ARG:NH1	2.36	0.48
1:B:872:ASP:O	1:B:873:ASN:ND2	2.47	0.48
1:A:1061:LEU:HD23	1:A:1061:LEU:H	1.79	0.48
1:B:1088:LYS:HD2	1:B:1088:LYS:N	2.29	0.48
1:B:918:ILE:O	1:B:919:ASN:HB2	2.13	0.48
1:B:1067:ASP:C	1:B:1069:ASN:N	2.67	0.47
1:A:1225:LEU:HD11	1:A:1268:VAL:HG13	1.96	0.47
1:B:1111:ILE:CD1	1:B:1112:THR:N	2.75	0.47
1:A:1179:ARG:NH1	1:A:1179:ARG:HG3	2.30	0.47
1:B:1128:TYR:HE1	1:B:1307:PRO:HG3	1.79	0.47
1:A:1139:ASP:OD2	1:A:1154:ALA:CB	2.63	0.47
2:B:1:BGC:H6C1	2:B:2:GAL:C1	2.44	0.47
1:A:1271:HIS:CE1	2:A:3:NGA:O4	2.68	0.47
1:B:1128:TYR:CE1	1:B:1307:PRO:HG3	2.49	0.47
1:A:1274[B]:GLN:NE2	1:A:1278:ASP:O	2.45	0.47
1:A:1130:LEU:HD12	1:A:1175:PHE:CZ	2.50	0.47
1:A:1256:LYS:HD3	1:A:1258:TYR:CZ	2.49	0.47
1:A:923:ILE:O	1:A:1085:SER:HA	2.15	0.47
1:A:951:THR:HG21	1:A:1096:LEU:HD12	1.95	0.47
1:A:957:ARG:NH1	1:A:1120:ASN:HD21	2.13	0.47
1:B:874:GLU:CG	1:B:875:GLU:N	2.77	0.47
2:B:6:SLB:C7	2:B:7:SIA:O1B	2.63	0.47
1:A:1175:PHE:CD1	1:A:1175:PHE:N	2.83	0.47
1:B:1141:GLN:HG3	1:B:1142:LEU:N	2.30	0.47
1:A:1130:LEU:HA	1:A:1130:LEU:HD23	1.70	0.47
1:B:1211:TYR:CE1	1:B:1223:ARG:HB3	2.50	0.47
1:B:989:SER:OG	1:B:1006:ASP:C	2.54	0.46
1:A:1003:THR:HB	1:A:1013:GLN:HG2	1.97	0.46
1:A:956:LEU:HD12	1:A:957:ARG:H	1.81	0.46
1:B:869:CYS:C	1:B:870:TRP:HE3	2.19	0.46
1:A:1297:LYS:CE	1:A:1297:LYS:HA	2.45	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1179:ARG:HG3	1:A:1179:ARG:HH11	1.80	0.46
1:A:1170:TYR:CE1	1:A:1308:THR:HA	2.51	0.46
1:B:1223:ARG:NH1	1:B:1265:LEU:O	2.49	0.46
1:A:928:ASN:O	1:A:930:SER:N	2.49	0.46
1:B:918:ILE:CD1	1:B:918:ILE:C	2.83	0.46
1:B:941:ILE:HG22	1:B:941:ILE:O	2.15	0.46
1:B:868:ASP:CG	1:B:869:CYS:H	2.19	0.46
1:A:1047:TYR:CE1	1:A:1101:ILE:HD12	2.51	0.46
1:A:914:LEU:N	1:A:914:LEU:HD23	2.31	0.46
1:B:1297:LYS:HE2	1:B:1298:ILE:CD1	2.46	0.46
1:B:1012:ARG:HA	1:B:1012:ARG:HD3	1.61	0.46
2:B:6:SLB:H7	2:B:7:SIA:O1B	2.16	0.45
1:B:981:LYS:HG2	1:B:983:HIS:CE1	2.51	0.45
1:B:1243:VAL:HG21	1:B:1245:LEU:HD22	1.98	0.45
1:A:877:ILE:O	1:A:881:LEU:HG	2.16	0.45
2:B:3:NGA:H1	2:B:6:SLB:O1A	2.16	0.45
1:B:907:ILE:HG12	1:B:936:HIS:HE1	1.82	0.45
1:A:951:THR:HG21	1:A:1096:LEU:CD1	2.46	0.45
1:B:952:VAL:HG22	1:B:1091:ILE:HD13	1.98	0.45
1:A:1191:LYS:HB2	1:A:1194:ASP:OD1	2.17	0.45
1:B:1149:MET:HB2	1:B:1284:LEU:HG	1.99	0.45
1:B:944:ASN:HD22	1:B:946:MET:HB2	1.82	0.45
1:B:1260:ASP:OD1	1:B:1260:ASP:N	2.49	0.45
1:B:1110:SER:OG	1:B:1112:THR:HG22	2.16	0.45
1:A:1030:LYS:HE3	1:A:1117:PHE:CZ	2.52	0.45
1:B:1045:ASN:OD1	1:B:1055:SER:HB3	2.17	0.45
1:B:1211:TYR:CD1	1:B:1223:ARG:HB3	2.52	0.45
1:B:1033:PHE:CE2	1:B:1035:THR:CG2	2.99	0.45
1:B:1185:GLU:HG3	1:B:1185:GLU:O	2.16	0.45
1:A:1039:ASP:OD2	1:A:1041:LEU:N	2.45	0.44
1:B:1297:LYS:HE2	1:B:1298:ILE:HD12	2.00	0.44
1:A:1231:ALA:HA	1:A:1232:PRO:HD2	1.86	0.44
1:A:1149:MET:CB	1:A:1284:LEU:HG	2.47	0.44
1:A:1002:TRP:O	1:A:1013:GLN:HG2	2.18	0.44
1:A:1022:LYS:HZ1	1:A:1164:ILE:CG2	2.31	0.44
1:A:1083:TYR:OH	1:A:1310:GLU:HB2	2.17	0.44
1:A:1261:LYS:O	1:A:1262:ASN:OD1	2.35	0.44
1:B:1159:ASN:ND2	1:B:1162:LEU:HD12	2.32	0.44
1:B:1065:ARG:HB2	3:B:301:PO4:O2	2.18	0.44
1:A:951:THR:HA	1:A:1036:ILE:O	2.18	0.44
1:A:1036:ILE:CD1	1:A:1046:LEU:HD13	2.47	0.44
1:A:943:TYR:O	1:A:944:ASN:C	2.55	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1033:PHE:HD2	5:A:1352:HOH:O	1.99	0.44
1:B:869:CYS:O	1:B:871:VAL:N	2.45	0.43
1:A:886:ILE:HA	1:A:902:PHE:HE1	1.82	0.43
1:A:1097:ASN:O	1:A:1100:GLU:HB2	2.18	0.43
1:A:953:SER:HA	1:A:1035:THR:HA	2.01	0.43
1:A:1261:LYS:O	1:A:1262:ASN:CG	2.56	0.43
1:B:1012:ARG:HH21	1:B:1058:ILE:HA	1.83	0.43
1:A:915:VAL:HB	1:A:916:PRO:HD2	1.99	0.43
1:A:1122:LEU:CD1	1:A:1190:VAL:HG21	2.49	0.43
1:B:871:VAL:CG2	1:B:872:ASP:H	2.22	0.43
1:B:939:MET:O	5:B:1417:HOH:O	2.21	0.43
1:A:1117:PHE:HB2	1:A:1306:VAL:HG22	2.01	0.43
1:A:1005:LYS:HE3	1:A:1009:GLY:HA2	2.00	0.43
1:B:1065:ARG:O	1:B:1066:GLU:O	2.37	0.43
1:A:886:ILE:HA	1:A:902:PHE:CE1	2.54	0.43
1:A:1079:ASN:C	1:A:1079:ASN:OD1	2.57	0.42
1:A:1219:ASN:O	1:A:1220:ASN:CB	2.66	0.42
1:A:937:LYS:HE2	1:A:1068:ASN:HA	2.01	0.42
1:A:1016:PHE:CE1	1:A:1053:MET:HE2	2.54	0.42
1:B:1110:SER:O	1:B:1112:THR:HG22	2.20	0.42
1:A:1124:TYR:CE1	1:A:1177:ILE:HG22	2.54	0.42
1:A:1149:MET:HB3	1:A:1284:LEU:HG	2.01	0.42
1:B:1041:LEU:HA	1:B:1041:LEU:HD23	1.80	0.42
1:B:1234:ILE:HA	1:B:1235:PRO:HD3	1.79	0.42
1:A:1181:THR:HA	1:A:1182:PRO:HD3	1.84	0.42
1:A:1124:TYR:CZ	1:A:1179:ARG:HG2	2.55	0.42
1:A:1017:ARG:HA	1:A:1017:ARG:HD2	1.93	0.42
1:B:1072:LEU:HD12	1:B:1072:LEU:N	2.34	0.42
1:B:867:LEU:O	1:B:948:ASN:ND2	2.52	0.42
1:B:923:ILE:O	1:B:1085:SER:HA	2.19	0.41
1:A:1122:LEU:HD11	1:A:1177:ILE:CD1	2.48	0.41
1:B:1208:ILE:HD11	1:B:1238:LYS:HD3	2.01	0.41
1:A:869:CYS:SG	1:A:870:TRP:CE3	3.08	0.41
1:A:1022:LYS:HZ1	1:A:1164:ILE:HG22	1.86	0.41
1:A:865:LYS:HG3	1:A:868:ASP:OD2	2.21	0.41
1:B:871:VAL:HG11	1:B:880:ILE:CG2	2.51	0.41
1:A:888:ASN:HB3	1:A:899:ILE:HG13	2.02	0.41
1:A:909:TYR:CB	1:A:910:PRO:CD	2.97	0.41
1:A:1006:ASP:O	1:A:1008:ALA:N	2.54	0.41
1:B:903:ASN:HD22	1:B:903:ASN:N	2.19	0.41
1:B:969:TYR:CG	1:B:1079:ASN:HB2	2.56	0.41
1:A:1169:LEU:O	1:A:1170:TYR:CB	2.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1113:PHE:HE2	1:B:1189:PHE:CB	2.33	0.41
1:B:902:PHE:O	1:B:903:ASN:HB2	2.20	0.41
1:B:1022:LYS:HD3	1:B:1022:LYS:HA	1.74	0.41
1:A:1156:SER:HB2	5:A:1319:HOH:O	2.20	0.41
1:A:1097:ASN:N	1:A:1100:GLU:OE1	2.48	0.40
1:B:1033:PHE:CE2	1:B:1104:LEU:HD13	2.56	0.40
1:A:899:ILE:C	1:A:900:SER:O	2.57	0.40
1:A:960:LYS:HE2	1:A:1166:TYR:CZ	2.56	0.40
1:A:959:PRO:HB3	1:A:1311:GLY:HA2	2.03	0.40
1:B:944:ASN:HD22	1:B:944:ASN:HA	1.62	0.40
1:A:913:GLN:O	1:A:914:LEU:HD23	2.20	0.40
1:A:1203:ASN:O	1:A:1204:ASN:CB	2.69	0.40
1:A:867:LEU:HA	1:A:867:LEU:HD23	1.94	0.40
1:B:1170:TYR:CE1	1:B:1308:THR:HA	2.56	0.40
1:B:951:THR:HB	1:B:1092:PHE:HB2	2.03	0.40
1:B:1067:ASP:O	1:B:1069:ASN:N	2.55	0.40
2:B:1:BGC:C6	2:B:2:GAL:H1	2.51	0.40
1:A:868:ASP:OD1	1:A:949:ASN:ND2	2.46	0.40
1:B:1007:SER:HG	3:B:301:PO4:P	2.44	0.40
1:B:1097:ASN:ND2	1:B:1100:GLU:CD	2.75	0.40
1:A:936:HIS:NE2	5:A:1387:HOH:O	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:873:ASN:O	1:B:1127:GLU:OE1[1_565]	2.17	0.03

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	450/472 (95%)	399 (89%)	38 (8%)	13 (3%)	7	4
1	B	449/472 (95%)	396 (88%)	41 (9%)	12 (3%)	8	5
All	All	899/944 (95%)	795 (88%)	79 (9%)	25 (3%)	8	4

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	929	GLU
1	A	1025	ALA
1	A	1182	PRO
1	B	870	TRP
1	B	1066	GLU
1	B	1111	ILE
1	A	1111	ILE
1	A	1180	TYR
1	B	868	ASP
1	B	872	ASP
1	B	901	GLY
1	B	919	ASN
1	B	1187	ASP
1	A	981	LYS
1	A	1007	SER
1	B	1183	ASN
1	A	874	GLU
1	A	919	ASN
1	B	1029	ASN
1	A	866	ASN
1	A	944	ASN
1	A	1042	SER
1	A	1170	TYR
1	B	948	ASN
1	B	1219	ASN

### 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	408/425 (96%)	350 (86%)	58 (14%)	5	4
1	B	407/425 (96%)	375 (92%)	32 (8%)	18	21
All	All	815/850 (96%)	725 (89%)	90 (11%)	9	10

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	875	GLU
1	A	905	SER
1	A	906	VAL
1	A	918	ILE
1	A	934	ILE
1	A	946	MET
1	A	959	PRO
1	A	964	SER
1	A	977	ILE
1	A	980	MET
1	A	982	LYS
1	A	985	LEU
1	A	987	ILE
1	A	994	SER
1	A	1003	THR
1	A	1005	LYS
1	A	1006	ASP
1	A	1019	LEU
1	A	1029	ASN
1	A	1032	VAL
1	A	1035	THR
1	A	1043	SER
1	A	1057	GLU
1	A	1059	THR
1	A	1061	LEU
1	A	1064	ILE
1	A	1066	GLU
1	A	1068	ASN
1	A	1073	LYS
1	A	1076	ARG
1	A	1080	ASN
1	A	1094	LYS
1	A	1111	ILE
1	A	1126	THR
1	A	1146	THR
1	A	1161	LYS
1	A	1167	ARG
1	A	1171	ASN
1	A	1181	THR
1	A	1183	ASN
1	A	1184	ASN
1	A	1185	GLU
1	A	1186	ILE

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Mol	Chain	Res	Type
1	A	1188	SER
1	A	1204	ASN
1	A	1220	ASN
1	A	1236	LEU
1	A	1238	LYS
1	A	1243	VAL
1	A	1245	LEU
1	A	1262	ASN
1	A	1274[A]	GLN
1	A	1274[B]	GLN
1	A	1284	LEU
1	A	1296	ASP
1	A	1297	LYS
1	A	1308	THR
1	A	1310	GLU
1	B	866	ASN
1	B	867	LEU
1	B	870	TRP
1	B	874	GLU
1	B	888	ASN
1	B	932	GLU
1	B	942	GLU
1	B	944	ASN
1	B	958	VAL
1	B	975	SER
1	B	1003	THR
1	B	1053	MET
1	B	1055	SER
1	B	1059	THR
1	B	1065	ARG
1	B	1068	ASN
1	B	1074	LEU
1	B	1088	LYS
1	B	1094	LYS
1	B	1104	LEU
1	B	1122	LEU
1	B	1126	THR
1	B	1130	LEU
1	B	1135	SER
1	B	1167	ARG
1	B	1186	ILE
1	B	1238	LYS

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Mol	Chain	Res	Type
1	B	1245	LEU
1	B	1274	GLN
1	B	1277	ASN
1	B	1284	LEU
1	B	1297	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	903	ASN
1	A	972	ASN
1	A	1045	ASN
1	A	1171	ASN
1	A	1184	ASN
1	A	1220	ASN
1	B	873	ASN
1	B	892	ASN
1	B	903	ASN
1	B	928	ASN
1	B	936	HIS
1	B	944	ASN
1	B	1013	GLN
1	B	1029	ASN
1	B	1068	ASN
1	B	1069	ASN
1	B	1078	ASN
1	B	1216	ASN
1	B	1220	ASN
1	B	1274	GLN
1	B	1293	HIS

### 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 ⓘ

14 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$
2	BGC	A	1	2,4	11,11,12	1.29	1 (9%)	11,15,17	1.67	3 (27%)
2	GAL	A	2	2	10,10,12	1.32	1 (10%)	8,13,17	1.02	1 (12%)
2	NGA	A	3	2	13,14,15	0.94	1 (7%)	14,19,21	1.08	1 (7%)
2	GAL	A	4	2	11,11,12	0.69	0	10,15,17	1.11	1 (10%)
2	SIA	A	5	2	21,21,21	4.87	3 (14%)	31,31,31	4.23	12 (38%)
2	SLB	A	6	2	21,21,21	1.60	3 (14%)	31,31,31	2.27	15 (48%)
2	SIA	A	7	2	20,20,21	4.16	1 (5%)	23,28,31	1.99	2 (8%)
2	BGC	B	1	2,4	11,11,12	0.84	0	11,15,17	1.96	4 (36%)
2	GAL	B	2	2	10,10,12	1.59	2 (20%)	8,13,17	1.46	1 (12%)
2	NGA	B	3	2	13,14,15	0.74	0	14,19,21	1.52	2 (14%)
2	GAL	B	4	2	11,11,12	1.36	3 (27%)	10,15,17	0.93	1 (10%)
2	SIA	B	5	2	21,21,21	4.78	4 (19%)	31,31,31	3.60	11 (35%)
2	SLB	B	6	2	21,21,21	1.77	3 (14%)	31,31,31	3.44	18 (58%)
2	SIA	B	7	-	20,20,21	3.61	3 (15%)	23,28,31	2.35	7 (30%)

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
2	BGC	A	1	2,4	-	0/2/18/22	0/1/1/1
2	GAL	A	2	2	-	0/2/15/22	0/1/1/1
2	NGA	A	3	2	-	0/6/22/26	0/1/1/1
2	GAL	A	4	2	-	0/2/18/22	0/1/1/1
2	SIA	A	5	2	-	0/20/38/38	0/1/1/1
2	SLB	A	6	2	-	0/20/38/38	0/1/1/1
2	SIA	A	7	2	-	0/15/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	B	1	2,4	-	0/2/18/22	0/1/1/1
2	GAL	B	2	2	-	0/2/15/22	0/1/1/1
2	NGA	B	3	2	-	0/6/22/26	0/1/1/1
2	GAL	B	4	2	-	0/2/18/22	0/1/1/1
2	SIA	B	5	2	-	0/20/38/38	0/1/1/1
2	SLB	B	6	2	-	0/20/38/38	0/1/1/1
2	SIA	B	7	-	1/1/8/9	0/15/34/38	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5	SIA	C2-C1	-21.21	1.31	1.53
2	B	5	SIA	C2-C1	-20.37	1.32	1.53
2	A	7	SIA	O6-C2	18.28	1.45	1.28
2	B	7	SIA	O6-C2	15.30	1.42	1.28
2	B	5	SIA	O2-C2	6.80	1.48	1.39
2	B	6	SLB	C2-C1	-6.36	1.47	1.53
2	A	5	SIA	O2-C2	5.57	1.47	1.39
2	A	6	SLB	C2-C1	-5.46	1.48	1.53
2	B	2	GAL	C1-C2	-3.59	1.49	1.53
2	A	5	SIA	C3-C2	-2.89	1.47	1.51
2	B	2	GAL	C4-C3	2.79	1.51	1.38
2	A	2	GAL	C4-C3	2.70	1.51	1.38
2	B	5	SIA	C3-C2	-2.65	1.48	1.51
2	B	7	SIA	O1B-C1	-2.62	1.22	1.30
2	B	4	GAL	O2-C2	-2.59	1.38	1.43
2	B	5	SIA	O1B-C1	-2.50	1.20	1.30
2	B	4	GAL	C1-C2	-2.39	1.50	1.53
2	A	6	SLB	O2-C2	2.19	1.42	1.39
2	B	6	SLB	O2-C2	2.16	1.42	1.39
2	A	3	NGA	C2-N2	-2.14	1.43	1.46
2	B	7	SIA	C7-C6	-2.10	1.50	1.52
2	A	6	SLB	O1B-C1	-2.08	1.22	1.30
2	B	6	SLB	O6-C6	-2.05	1.40	1.44
2	A	1	BGC	C1-C2	-2.03	1.49	1.52
2	B	4	GAL	O5-C1	-2.02	1.39	1.43

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5	SIA	O2-C2-O6	-14.23	85.30	109.95
2	B	6	SLB	O6-C2-C3	-10.14	104.23	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5	SIA	O2-C2-C3	-9.97	95.15	109.67
2	A	5	SIA	O6-C2-C3	9.71	115.95	110.22
2	B	5	SIA	O2-C2-C1	-9.57	93.63	109.86
2	B	7	SIA	O6-C2-C3	-8.61	113.66	124.91
2	B	5	SIA	O2-C2-O6	-8.60	95.05	109.95
2	A	7	SIA	O6-C2-C3	-7.85	114.65	124.91
2	B	5	SIA	O6-C2-C3	6.92	114.30	110.22
2	B	5	SIA	C2-O6-C6	-6.35	104.25	113.93
2	B	6	SLB	O2-C2-C1	-6.23	99.29	109.86
2	B	5	SIA	C2-C3-C4	-5.99	99.56	110.75
2	A	5	SIA	C2-C3-C4	-5.72	100.05	110.75
2	B	6	SLB	C4-C5-N5	5.60	122.50	110.12
2	B	5	SIA	O2-C2-C3	-5.55	101.59	109.67
2	B	5	SIA	C3-C2-C1	5.30	122.47	113.58
2	B	6	SLB	O2-C2-O6	4.97	118.56	109.95
2	B	6	SLB	O4-C4-C5	4.73	119.56	110.64
2	A	5	SIA	C2-O6-C6	-4.70	106.78	113.93
2	B	1	BGC	O6-C6-C5	-4.54	105.67	112.42
2	A	6	SLB	C4-C5-N5	4.51	120.08	110.12
2	B	6	SLB	C9-C8-C7	4.45	122.48	112.38
2	A	5	SIA	C3-C2-C1	4.22	120.65	113.58
2	A	5	SIA	O1A-C1-C2	-4.13	117.74	123.48
2	A	6	SLB	O6-C6-C5	4.09	113.41	109.55
2	B	6	SLB	C5-N5-C10	-4.07	112.14	123.02
2	A	5	SIA	O6-C2-C1	4.07	120.83	106.17
2	A	6	SLB	C5-N5-C10	-4.06	112.17	123.02
2	B	6	SLB	O4-C4-C3	-4.06	100.31	109.92
2	A	5	SIA	O6-C6-C5	-4.02	105.75	109.55
2	A	1	BGC	O3-C3-C2	-3.69	102.21	110.18
2	B	7	SIA	O9-C9-C8	-3.69	102.80	111.05
2	B	6	SLB	C6-C5-N5	-3.61	104.68	110.99
2	B	5	SIA	O6-C2-C1	3.60	119.15	106.17
2	B	6	SLB	O2-C2-C3	3.57	114.86	109.67
2	B	6	SLB	O7-C7-C8	3.47	117.50	108.74
2	B	2	GAL	O6-C6-C5	-3.36	107.42	112.42
2	A	6	SLB	O2-C2-C1	-3.32	104.24	109.86
2	B	3	NGA	C8-C7-N2	3.28	122.51	116.11
2	A	6	SLB	C8-C7-C6	-3.21	106.77	112.99
2	B	6	SLB	O6-C6-C5	3.05	112.43	109.55
2	A	6	SLB	C6-C5-N5	-2.97	105.81	110.99
2	A	7	SIA	C8-C7-C6	-2.92	107.33	112.99
2	A	5	SIA	O2-C2-C1	-2.90	104.95	109.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	SIA	C8-C7-C6	-2.89	107.39	112.99
2	A	6	SLB	O8-C8-C9	-2.89	102.46	109.20
2	A	6	SLB	O4-C4-C3	-2.83	103.20	109.92
2	B	5	SIA	C9-C8-C7	2.81	118.74	112.38
2	A	6	SLB	O2-C2-O6	2.79	114.80	109.95
2	A	6	SLB	O6-C2-C3	2.77	111.85	110.22
2	A	6	SLB	C7-C6-C5	-2.68	110.29	114.24
2	B	5	SIA	O7-C7-C6	-2.65	103.73	109.45
2	B	6	SLB	O6-C6-C7	-2.51	103.10	106.34
2	B	3	NGA	O5-C1-C2	2.50	112.14	109.61
2	A	2	GAL	O2-C2-C1	2.45	113.57	109.45
2	A	5	SIA	O6-C6-C7	2.44	109.48	106.34
2	B	6	SLB	C8-C7-C6	-2.43	108.28	112.99
2	A	6	SLB	C11-C10-N5	2.40	120.80	116.11
2	A	6	SLB	C2-O6-C6	2.39	117.57	113.93
2	B	6	SLB	C11-C10-N5	2.38	120.77	116.11
2	B	4	GAL	O5-C5-C4	2.37	113.14	109.30
2	B	1	BGC	O5-C1-C2	-2.36	106.21	109.86
2	A	4	GAL	O2-C2-C1	2.36	113.42	109.45
2	B	7	SIA	O6-C6-C7	2.35	110.10	105.73
2	A	1	BGC	O1-C1-C2	-2.34	102.83	109.47
2	B	7	SIA	C7-C6-C5	-2.32	110.82	114.24
2	A	5	SIA	O4-C4-C5	-2.28	106.35	110.64
2	B	6	SLB	O10-C10-C11	-2.27	117.61	122.04
2	B	7	SIA	O6-C6-C5	-2.23	107.50	110.29
2	B	5	SIA	O9-C9-C8	-2.23	106.07	111.05
2	B	6	SLB	O8-C8-C7	-2.22	103.52	109.05
2	B	1	BGC	O2-C2-C3	-2.20	105.91	109.94
2	B	6	SLB	O9-C9-C8	2.19	115.96	111.05
2	A	1	BGC	O2-C2-C3	-2.15	106.01	109.94
2	A	6	SLB	O4-C4-C5	2.15	114.69	110.64
2	A	3	NGA	O7-C7-C8	-2.14	117.87	122.04
2	A	6	SLB	O1A-C1-C2	-2.13	120.51	123.48
2	B	7	SIA	O7-C7-C8	2.11	114.08	108.74
2	B	1	BGC	O1-C1-C2	2.03	115.22	109.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	7	SIA	C2

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

5 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	$\# Z  > 2$
4	CEQ	A	8[A]	2	5,5,5	2.40	4 (80%)	7,7,7	1.03	1 (14%)
4	CEQ	A	8[B]	2	5,5,5	2.36	4 (80%)	7,7,7	1.00	1 (14%)
3	PO4	B	301	-	4,4,4	0.38	0	6,6,6	0.30	0
4	CEQ	B	8[A]	2	5,5,5	2.35	4 (80%)	7,7,7	0.98	1 (14%)
4	CEQ	B	8[B]	2	5,5,5	2.34	4 (80%)	7,7,7	0.70	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
4	CEQ	A	8[A]	2	-	0/3/3/3	0/0/0/0
4	CEQ	A	8[B]	2	-	0/3/3/3	0/0/0/0
3	PO4	B	301	-	-	0/0/0/0	0/0/0/0
4	CEQ	B	8[A]	2	-	0/3/3/3	0/0/0/0
4	CEQ	B	8[B]	2	-	0/3/3/3	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	8[A]	CEQ	SI1-C5	-3.44	1.78	1.87
4	B	8[B]	CEQ	SI1-C5	-3.33	1.79	1.87
4	A	8[B]	CEQ	SI1-C5	-3.27	1.79	1.87
4	B	8[A]	CEQ	SI1-C5	-3.22	1.79	1.87
4	A	8[A]	CEQ	SI1-C2	-2.51	1.78	1.86
4	A	8[B]	CEQ	SI1-C3	-2.49	1.78	1.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8[A]	CEQ	SI1-C2	-2.42	1.78	1.86
4	A	8[B]	CEQ	SI1-C4	-2.41	1.78	1.86
4	B	8[A]	CEQ	SI1-C4	-2.37	1.79	1.86
4	B	8[B]	CEQ	SI1-C3	-2.37	1.79	1.86
4	B	8[A]	CEQ	SI1-C3	-2.37	1.79	1.86
4	A	8[A]	CEQ	SI1-C3	-2.32	1.79	1.86
4	B	8[B]	CEQ	SI1-C4	-2.32	1.79	1.86
4	A	8[A]	CEQ	SI1-C4	-2.28	1.79	1.86
4	B	8[B]	CEQ	SI1-C2	-2.26	1.79	1.86
4	A	8[B]	CEQ	SI1-C2	-2.23	1.79	1.86

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	8[A]	CEQ	SI1-C5-C6	-2.32	111.18	115.73
4	A	8[A]	CEQ	SI1-C5-C6	-2.19	111.45	115.73
4	A	8[B]	CEQ	SI1-C5-C6	-2.14	111.54	115.73

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	451/472 (95%)	0.96	52 (11%) 5 9	27, 37, 54, 68	0
1	B	451/472 (95%)	0.71	31 (6%) 17 24	17, 29, 51, 71	0
All	All	902/944 (95%)	0.83	83 (9%) 9 15	17, 34, 54, 71	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	871	VAL	9.8
1	B	867	LEU	7.0
1	B	872	ASP	6.2
1	A	1183	ASN	5.6
1	A	870	TRP	5.4
1	B	1068	ASN	5.0
1	B	865	LYS	4.7
1	B	866	ASN	4.7
1	A	1111	ILE	4.7
1	A	879	VAL	4.4
1	A	871	VAL	4.3
1	A	875	GLU	4.2
1	A	1184	ASN	4.2
1	A	1160	GLY	4.1
1	B	868	ASP	4.1
1	B	873	ASN	4.0
1	B	940	ASP	3.9
1	A	865	LYS	3.9
1	A	1185	GLU	3.8
1	A	1186	ILE	3.8
1	B	943	TYR	3.7
1	B	870	TRP	3.7
1	A	1187	ASP	3.6
1	A	1181	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	902	PHE	3.5
1	B	941	ILE	3.4
1	A	1113	PHE	3.3
1	A	1079	ASN	3.3
1	A	1205	ASN	3.3
1	A	1204	ASN	3.2
1	A	1052	LEU	3.2
1	A	961	VAL	3.1
1	A	874	GLU	3.0
1	B	1183	ASN	3.0
1	A	880	ILE	3.0
1	B	1070	ILE	3.0
1	A	986	SER	2.9
1	B	876	ASP	2.9
1	A	976	ILE	2.9
1	A	939	MET	2.8
1	B	909	TYR	2.8
1	A	918	ILE	2.7
1	A	987	ILE	2.7
1	A	1202	TYR	2.7
1	A	1305	PHE	2.7
1	A	873	ASN	2.7
1	B	981	LYS	2.6
1	A	877	ILE	2.6
1	A	909	TYR	2.6
1	B	1182	PRO	2.6
1	A	1076	ARG	2.5
1	A	866	ASN	2.5
1	B	1185	GLU	2.5
1	A	1063	ALA	2.5
1	A	1189	PHE	2.4
1	A	888	ASN	2.4
1	B	869	CYS	2.4
1	A	1203	ASN	2.4
1	A	1059	THR	2.4
1	A	1077	CYS	2.3
1	B	939	MET	2.3
1	A	911	ASP	2.3
1	A	1236	LEU	2.3
1	B	1063	ALA	2.2
1	A	1062	GLY	2.2
1	A	907	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	951	THR	2.2
1	A	881	LEU	2.2
1	A	1220	ASN	2.2
1	B	983	HIS	2.1
1	A	943	TYR	2.1
1	B	985	LEU	2.1
1	B	944	ASN	2.1
1	A	1061	LEU	2.1
1	B	1187	ASP	2.1
1	A	1092	PHE	2.1
1	A	983	HIS	2.0
1	A	947	PHE	2.0
1	B	946	MET	2.0
1	B	1041	LEU	2.0
1	A	1253	VAL	2.0
1	B	987	ILE	2.0
1	B	875	GLU	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
2	SIA	B	7	20/21	0.23	3.89	44,50,60,63	0
2	BGC	A	1	11/12	0.24	3.70	52,54,61,62	0
2	SIA	A	7	20/21	0.23	3.63	44,56,65,65	0
2	SLB	A	6	21/21	0.19	2.63	47,54,60,65	0
2	SIA	B	5	21/21	0.21	2.26	46,62,68,69	0
2	SIA	A	5	21/21	0.24	2.25	53,63,66,67	0
2	GAL	A	4	11/12	0.21	1.95	46,50,51,55	0
2	SLB	B	6	21/21	0.20	1.81	42,49,54,58	0
2	NGA	A	3	14/15	0.19	1.54	50,51,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NGA	B	3	14/15	0.17	1.24	36,39,42,43	0
2	BGC	B	1	11/12	0.18	1.23	45,51,57,61	0
2	GAL	A	2	10/12	0.15	-0.27	45,47,51,52	0
2	GAL	B	4	11/12	0.14	-0.61	34,37,40,40	0
2	GAL	B	2	10/12	0.14	-7.55	39,44,45,45	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( $\text{\AA}^2$ )	Q<0.9
4	CEQ	B	8[A]	6/6	0.66	40.96	71,75,76,76	6
4	CEQ	A	8[A]	6/6	0.40	15.13	72,76,76,76	6
4	CEQ	A	8[B]	6/6	0.40	11.74	66,68,68,68	6
3	PO4	B	301	5/5	0.11	-1.74	58,60,60,61	0
4	CEQ	B	8[B]	6/6	0.66	-	64,65,65,65	6

## 6.5 Other polymers ⓘ

There are no such residues in this entry.