



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2021 – 06:13 pm GMT

PDB ID : 7NIT
Title : X-ray structure of a multidomain BbgIII from Bifidobacterium bifidum
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Deposited on : 2021-02-14
Resolution : 2.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

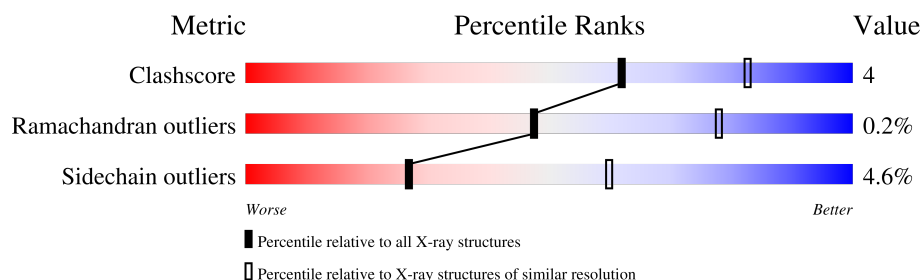
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	1304	
1	B	1304	
1	C	1304	
1	D	1304	
1	E	1304	
1	F	1304	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	2302	-	-	X	-
3	GOL	F	2302	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 55867 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1239	Total	C	N	O	S	0	0	0
			9306	5807	1585	1897	17			
1	B	1235	Total	C	N	O	S	0	0	0
			9246	5768	1574	1888	16			
1	C	1243	Total	C	N	O	S	0	0	0
			9326	5818	1585	1906	17			
1	D	1253	Total	C	N	O	S	0	0	0
			9390	5856	1601	1916	17			
1	E	1235	Total	C	N	O	S	0	0	0
			9195	5733	1567	1879	16			
1	F	1244	Total	C	N	O	S	0	0	0
			9324	5816	1586	1905	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1165	GLU	ASP	conflict	UNP A0A415C3Q2
B	1165	GLU	ASP	conflict	UNP A0A415C3Q2
C	1165	GLU	ASP	conflict	UNP A0A415C3Q2
D	1165	GLU	ASP	conflict	UNP A0A415C3Q2
E	1165	GLU	ASP	conflict	UNP A0A415C3Q2
F	1165	GLU	ASP	conflict	UNP A0A415C3Q2

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	E	1	Total Ca 1 1	0	0
4	F	1	Total Ca 1 1	0	0

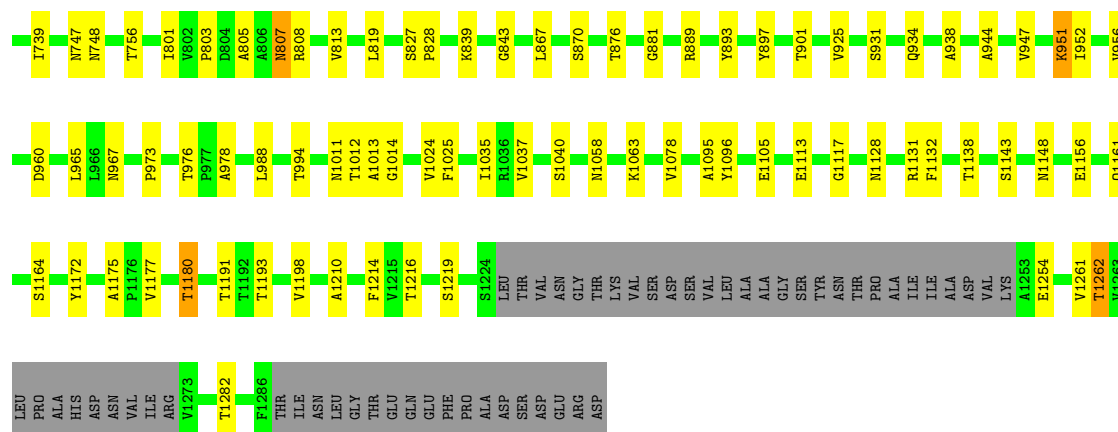
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	B	1	Total O 1 1	0	0
5	C	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0

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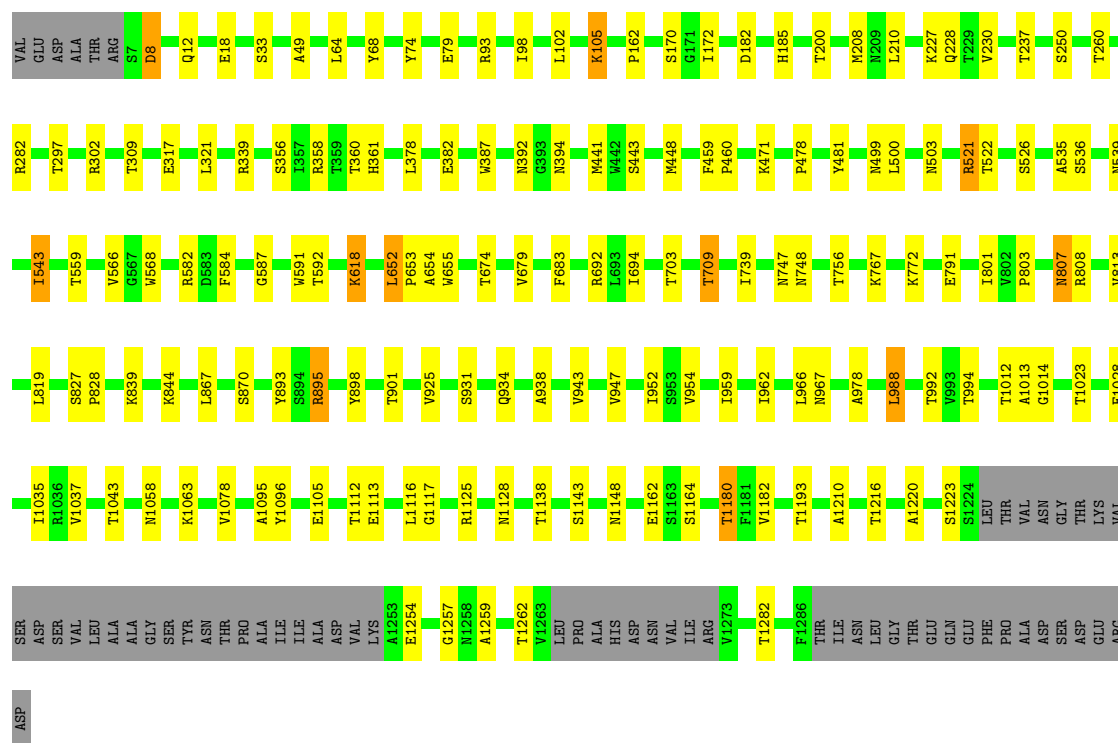
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total	O	0	0
			1	1		
5	F	1	Total	O	0	0
			1	1		



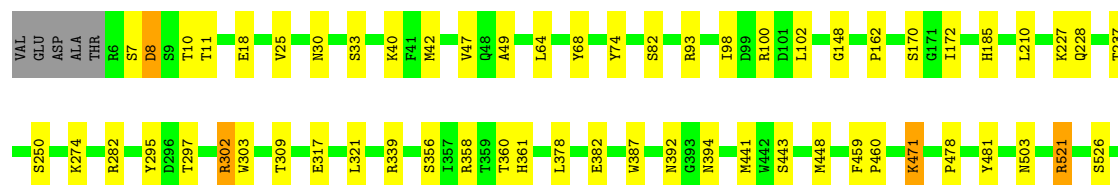
• Molecule 1: Beta-galactosidase

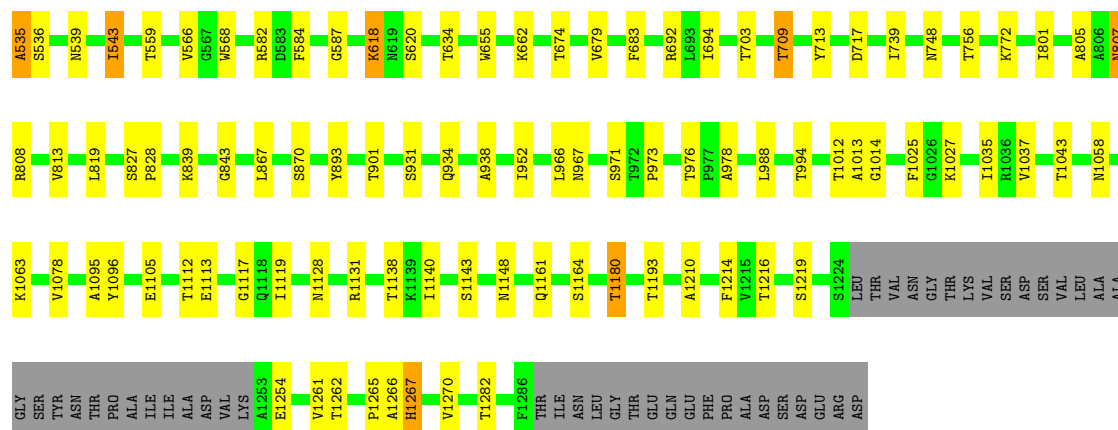
Chain C: 83% 11% 5%



• Molecule 1: Beta-galactosidase

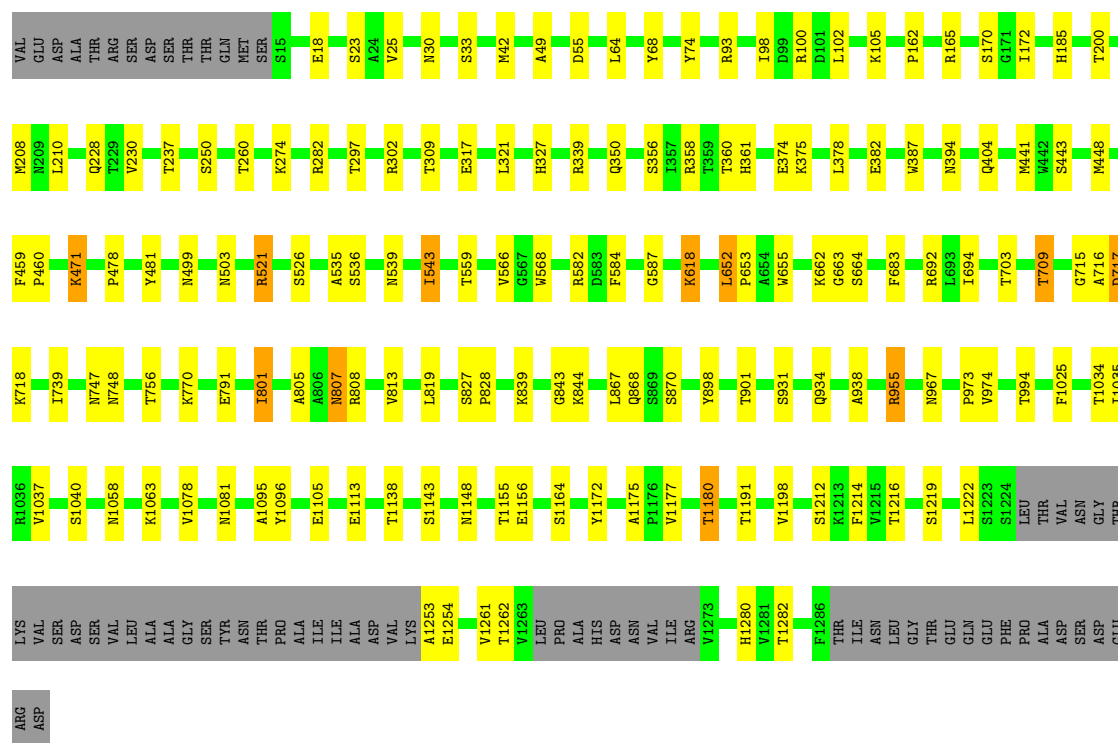
Chain D: 84% 11% 5%





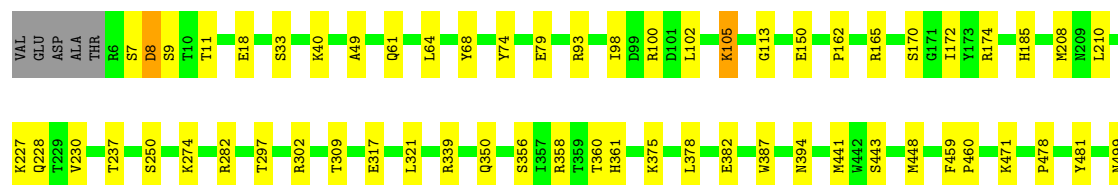
• Molecule 1: Beta-galactosidase

Chain E: 83% 11% • 5%



• Molecule 1: Beta-galactosidase

Chain F: 83% 11% • 5%



ASP	N503	T766	N967
SER		K770	SS971
VAL	R521	L771	L988
LEU		K772	
ALA	S526	E791	T1034
ALA	A535		I1035
GLY	S536	I801	N1058
SER		V802	
TYR	N539	P803	K1063
ASN			
THR	I543	N807	K1072
PRO		R808	
ALA	T559		V1078
ALA	V566	V813	
ILE	G567	L819	A1095
ILE	W568		Y1096
ASP		S827	
VAL	R582	P828	E1105
LYS	D583	K839	E1113
A1253	F584		G1117
E1254	G587	K844	
	W591	E854	R1125
V1261	T592	A855	
T1262			N1128
V1263	K618	L867	T1138
LEU	L852	Q868	
PRO	P653	S869	S1143
ALA	A654	S870	
ALA	W655	A878	N1148
GLY		V879	
THR	V659	P880	E1162
THR	K662	G881	S1163
ILE	G663	T882	S1164
ASN	T674	Y893	T1180
LEU	V679	S894	
GLY		R895	T1193
THR	F683		A1210
GLU	R692	T901	
GLN	L693	S916	T1216
GLU	I694	S931	
PHE		Q934	S1219
PRO	T703		S1224
ALA	T704	A938	LEU
ASP	T709	I952	THR
ASP	I739	R955	VAL
GLU	N748	D960	ASN
GLY			GLY
ARG			THR
ASP			LYS
			VAL
			SER

4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	116.95Å 130.04Å 200.58Å 86.99° 84.83° 83.79°	Depositor
Resolution (Å)	199.58 – 2.89	Depositor
% Data completeness (in resolution range)	96.2 (199.58-2.89)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.214 , 0.247	Depositor
Wilson B-factor (Å ²)	88.8	Xtriage
Anisotropy	0.320	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	55867	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, CA

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	0.36	0/9503	0.71	0/12962
1	B	0.39	0/9443	0.73	0/12889
1	C	0.37	0/9523	0.71	0/12990
1	D	0.36	0/9589	0.71	0/13082
1	E	0.36	0/9390	0.70	0/12825
1	F	0.33	0/9521	0.68	0/12990
All	All	0.36	0/56969	0.70	0/77738

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9306	0	8880	70	0
1	B	9246	0	8784	92	0
1	C	9326	0	8895	93	0
1	D	9390	0	8946	82	0
1	E	9195	0	8696	73	0
1	F	9324	0	8877	74	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	F	5	0	0	0	0
3	A	12	0	16	0	0
3	B	6	0	8	5	0
3	C	6	0	8	0	0
3	D	12	0	16	0	0
3	E	6	0	8	1	0
3	F	6	0	8	9	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	55867	0	53142	474	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (474) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:879:VAL:HB	1:F:882:THR:HG23	1.33	1.06
1:C:1023:THR:HG22	1:C:1028:GLU:HG3	1.52	0.91
1:C:959:ILE:HG21	1:C:962:ILE:HD11	1.59	0.85
1:B:1014:GLY:O	1:B:1037:VAL:HG22	1.79	0.82
1:E:1155:THR:HG22	1:F:704:THR:HA	1.65	0.79
1:C:1014:GLY:O	1:C:1037:VAL:HG22	1.83	0.79
1:D:1014:GLY:O	1:D:1037:VAL:HG22	1.81	0.79
1:C:1023:THR:CG2	1:C:1028:GLU:HG3	2.14	0.77
1:C:959:ILE:HG21	1:C:962:ILE:CD1	2.14	0.77
1:C:1012:THR:O	1:C:1037:VAL:HG21	1.89	0.73
1:D:1012:THR:O	1:D:1037:VAL:HG21	1.88	0.73
1:B:1012:THR:O	1:B:1037:VAL:HG21	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:988:LEU:HD11	1:A:994:THR:CG2	2.19	0.72
1:F:967:ASN:HB2	1:F:1262:THR:HG22	1.72	0.72
1:C:988:LEU:HD22	1:C:992:THR:HB	1.69	0.72
1:D:1131:ARG:HB3	1:E:747:ASN:ND2	2.05	0.71
1:E:358:ARG:HG2	1:E:360:THR:CG2	2.20	0.71
1:A:1131:ARG:HB3	1:B:747:ASN:ND2	2.05	0.71
1:A:1131:ARG:HB3	1:B:747:ASN:HD21	1.55	0.71
1:B:978:ALA:CB	1:B:1035:ILE:HD13	2.21	0.70
1:F:150:GLU:OE2	1:F:895:ARG:NH1	2.24	0.69
1:D:967:ASN:HB2	1:D:1262:THR:HG22	1.73	0.69
1:E:967:ASN:HB2	1:E:1262:THR:HG22	1.75	0.68
1:D:988:LEU:HD11	1:D:994:THR:CG2	2.24	0.68
1:C:967:ASN:HB2	1:C:1262:THR:HG22	1.76	0.68
1:F:683:PHE:HB2	1:F:694:ILE:HD11	1.76	0.68
1:A:967:ASN:HB2	1:A:1262:THR:HG22	1.74	0.67
1:E:358:ARG:HG2	1:E:360:THR:HG22	1.77	0.67
1:C:162:PRO:HG2	1:C:394:ASN:HA	1.77	0.66
1:D:966:LEU:HD12	1:D:1262:THR:HG21	1.77	0.66
1:C:8:ASP:HB2	1:C:12:GLN:O	1.96	0.65
1:C:683:PHE:HB2	1:C:694:ILE:HD11	1.76	0.65
1:A:162:PRO:HG2	1:A:394:ASN:HA	1.78	0.65
1:D:683:PHE:HB2	1:D:694:ILE:HD11	1.78	0.65
1:E:683:PHE:HB2	1:E:694:ILE:HD11	1.78	0.65
1:E:521:ARG:HG3	1:E:521:ARG:HH11	1.62	0.64
1:F:162:PRO:HG2	1:F:394:ASN:HA	1.78	0.64
1:D:1131:ARG:HB3	1:E:747:ASN:HD21	1.60	0.64
1:B:162:PRO:HG2	1:B:394:ASN:HA	1.80	0.64
1:F:591:TRP:CZ2	3:F:2302:GOL:H2	2.34	0.64
1:A:683:PHE:HB2	1:A:694:ILE:HD11	1.79	0.63
1:D:162:PRO:HG2	1:D:394:ASN:HA	1.80	0.63
1:B:521:ARG:HG3	1:B:521:ARG:HH11	1.64	0.63
1:B:988:LEU:HD11	1:B:994:THR:CG2	2.29	0.63
1:E:339:ARG:HH11	1:E:339:ARG:HG2	1.63	0.63
1:C:978:ALA:CB	1:C:1035:ILE:HD13	2.29	0.62
1:C:1125:ARG:NH1	1:C:1162:GLU:OE2	2.33	0.62
1:F:591:TRP:CH2	3:F:2302:GOL:H2	2.35	0.62
1:E:162:PRO:HG2	1:E:394:ASN:HA	1.80	0.62
1:F:591:TRP:CZ2	3:F:2302:GOL:H32	2.35	0.62
1:A:931:SER:HB3	1:A:934:GLN:HG3	1.80	0.62
1:F:8:ASP:HB3	1:F:11:THR:OG1	2.00	0.62
1:B:683:PHE:HB2	1:B:694:ILE:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:967:ASN:HB2	1:B:1262:THR:HG22	1.81	0.61
1:E:55:ASP:CG	1:E:955:ARG:NH1	2.53	0.61
1:C:521:ARG:HG3	1:C:521:ARG:HH11	1.66	0.61
1:C:978:ALA:HB3	1:C:1035:ILE:HD13	1.83	0.61
1:B:339:ARG:HG2	1:B:339:ARG:HH11	1.66	0.61
1:D:978:ALA:CB	1:D:1035:ILE:HD13	2.30	0.61
1:B:1191:THR:O	1:B:1198:VAL:HG21	2.02	0.60
1:E:165:ARG:HH22	3:E:2302:GOL:H32	1.66	0.60
1:C:309:THR:HG23	1:C:521:ARG:NH2	2.17	0.60
1:C:339:ARG:HH11	1:C:339:ARG:HG2	1.67	0.60
1:D:8:ASP:HB3	1:D:11:THR:HB	1.84	0.60
1:E:1191:THR:O	1:E:1198:VAL:HG21	2.01	0.60
1:D:988:LEU:N	1:D:988:LEU:HD12	2.16	0.59
1:D:10:THR:HA	1:D:1025:PHE:HB3	1.84	0.59
1:D:521:ARG:HG3	1:D:521:ARG:HH11	1.67	0.59
1:E:387:TRP:CE2	1:E:448:MET:HG2	2.37	0.59
1:B:807:ASN:HD22	1:B:867:LEU:HD11	1.67	0.59
1:C:988:LEU:HD11	1:C:994:THR:CG2	2.33	0.59
1:E:327:HIS:CD2	1:E:360:THR:O	2.56	0.59
1:B:807:ASN:ND2	1:B:867:LEU:HD11	2.17	0.59
1:B:1011:ASN:HB2	1:C:522:THR:HG23	1.84	0.59
1:C:521:ARG:HH11	1:C:521:ARG:CG	2.16	0.59
1:B:931:SER:HB2	1:B:934:GLN:HG3	1.85	0.58
1:C:925:VAL:HG22	1:C:947:VAL:HG21	1.85	0.58
1:C:1220:ALA:HB3	1:C:1259:ALA:HB2	1.85	0.58
1:D:978:ALA:HB3	1:D:1035:ILE:HD13	1.84	0.58
1:F:931:SER:HB2	1:F:934:GLN:HG3	1.85	0.58
1:F:1125:ARG:NH1	1:F:1162:GLU:OE2	2.35	0.58
1:B:361:HIS:NE2	3:B:2302:GOL:H12	2.19	0.58
1:C:931:SER:HB2	1:C:934:GLN:HG3	1.85	0.58
1:A:988:LEU:HD11	1:A:994:THR:HG22	1.84	0.58
1:D:321:LEU:HB2	1:D:587:GLY:HA3	1.86	0.57
1:E:898:TYR:CE2	1:E:994:THR:HB	2.38	0.57
1:A:339:ARG:HG2	1:A:339:ARG:HH11	1.67	0.57
1:E:521:ARG:HH11	1:E:521:ARG:CG	2.17	0.57
1:A:807:ASN:ND2	1:A:867:LEU:HD11	2.20	0.57
1:B:988:LEU:N	1:B:988:LEU:HD12	2.20	0.57
1:D:339:ARG:HG2	1:D:339:ARG:HH11	1.69	0.57
1:E:931:SER:HB2	1:E:934:GLN:HG3	1.86	0.57
1:A:321:LEU:HB2	1:A:587:GLY:HA3	1.86	0.57
1:B:944:ALA:HB1	1:B:951:LYS:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:THR:HG23	1:D:521:ARG:NH2	2.19	0.57
1:D:931:SER:HB2	1:D:934:GLN:HG3	1.87	0.57
1:E:807:ASN:ND2	1:E:867:LEU:HD11	2.19	0.57
1:B:521:ARG:HH11	1:B:521:ARG:CG	2.17	0.57
1:F:807:ASN:ND2	1:F:867:LEU:HD11	2.20	0.57
1:D:521:ARG:HH11	1:D:521:ARG:CG	2.18	0.57
1:F:1063:LYS:O	1:F:1095:ALA:HB3	2.05	0.57
1:B:309:THR:HG23	1:B:521:ARG:NH2	2.20	0.56
1:B:813:VAL:HG21	1:B:819:LEU:HB2	1.87	0.56
1:C:807:ASN:HD22	1:C:867:LEU:HD11	1.70	0.56
1:E:309:THR:HG23	1:E:521:ARG:NH2	2.21	0.56
1:A:1063:LYS:O	1:A:1095:ALA:HB3	2.06	0.56
1:C:807:ASN:ND2	1:C:867:LEU:HD11	2.19	0.56
1:B:1131:ARG:HB3	1:C:747:ASN:ND2	2.21	0.56
1:E:655:TRP:CZ2	1:E:739:ILE:HD11	2.40	0.56
1:F:879:VAL:HB	1:F:882:THR:CG2	2.22	0.56
1:D:807:ASN:ND2	1:D:867:LEU:HD11	2.20	0.56
1:D:655:TRP:CZ2	1:D:739:ILE:HD11	2.41	0.56
1:E:807:ASN:HD22	1:E:867:LEU:HD11	1.70	0.56
1:F:807:ASN:HD22	1:F:867:LEU:HD11	1.71	0.56
1:B:1131:ARG:HB3	1:C:747:ASN:HD21	1.70	0.55
1:B:1143:SER:HB3	1:B:1148:ASN:O	2.06	0.55
1:C:1063:LYS:O	1:C:1095:ALA:HB3	2.06	0.55
1:F:339:ARG:HG2	1:F:339:ARG:HH11	1.71	0.55
1:B:925:VAL:HG22	1:B:947:VAL:HG21	1.87	0.55
1:B:321:LEU:HB2	1:B:587:GLY:HA3	1.88	0.55
1:C:655:TRP:CZ2	1:C:739:ILE:HD11	2.41	0.55
1:D:1063:LYS:O	1:D:1095:ALA:HB3	2.06	0.55
1:E:1063:LYS:O	1:E:1095:ALA:HB3	2.06	0.55
1:C:925:VAL:HG22	1:C:947:VAL:CG2	2.37	0.55
1:C:1143:SER:HB3	1:C:1148:ASN:O	2.06	0.55
1:F:655:TRP:CZ2	1:F:739:ILE:HD11	2.42	0.55
1:B:655:TRP:CZ2	1:B:739:ILE:HD11	2.42	0.55
1:A:1143:SER:HB3	1:A:1148:ASN:O	2.07	0.54
1:E:49:ALA:O	1:E:93:ARG:NH1	2.39	0.54
1:F:1143:SER:HB3	1:F:1148:ASN:O	2.08	0.54
1:B:1063:LYS:O	1:B:1095:ALA:HB3	2.06	0.54
1:F:49:ALA:O	1:F:93:ARG:NH1	2.39	0.54
1:D:813:VAL:HG21	1:D:819:LEU:HB2	1.89	0.54
1:C:1220:ALA:HB1	1:C:1257:GLY:H	1.73	0.54
1:A:655:TRP:CZ2	1:A:739:ILE:HD11	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:988:LEU:CD1	1:A:994:THR:HG23	2.37	0.54
1:C:988:LEU:HD11	1:C:994:THR:HG22	1.89	0.54
1:C:321:LEU:HB2	1:C:587:GLY:HA3	1.88	0.54
1:E:321:LEU:HB2	1:E:587:GLY:HA3	1.88	0.54
1:D:1143:SER:HB3	1:D:1148:ASN:O	2.08	0.54
1:D:543:ILE:HG22	1:D:559:THR:HA	1.90	0.53
1:E:543:ILE:HG22	1:E:559:THR:HA	1.91	0.53
1:F:321:LEU:HB2	1:F:587:GLY:HA3	1.89	0.53
1:A:807:ASN:HD22	1:A:867:LEU:HD11	1.72	0.53
1:B:49:ALA:O	1:B:93:ARG:NH1	2.38	0.53
1:B:925:VAL:HG22	1:B:947:VAL:CG2	2.39	0.53
1:F:18:GLU:OE2	1:F:40:LYS:NZ	2.39	0.53
1:F:309:THR:HG23	1:F:521:ARG:NH2	2.24	0.53
1:F:813:VAL:HG21	1:F:819:LEU:HB2	1.89	0.53
1:B:978:ALA:HB3	1:B:1035:ILE:HD13	1.90	0.53
1:C:49:ALA:O	1:C:93:ARG:NH1	2.40	0.53
1:B:1013:ALA:HA	1:B:1037:VAL:HG23	1.91	0.52
1:C:543:ILE:HG22	1:C:559:THR:HA	1.91	0.52
1:D:988:LEU:HD11	1:D:994:THR:HG22	1.91	0.52
1:F:350:GLN:HE22	1:F:375:LYS:HB3	1.75	0.52
1:E:1143:SER:HB3	1:E:1148:ASN:O	2.08	0.52
1:E:55:ASP:CG	1:E:955:ARG:HH12	2.12	0.52
1:C:1013:ALA:HA	1:C:1037:VAL:HG23	1.92	0.52
1:A:543:ILE:HG22	1:A:559:THR:HA	1.92	0.52
1:F:356:SER:HA	1:F:378:LEU:O	2.10	0.52
1:A:813:VAL:HG21	1:A:819:LEU:HB2	1.91	0.51
1:F:591:TRP:CZ2	3:F:2302:GOL:C2	2.92	0.51
1:B:49:ALA:HB1	1:B:93:ARG:HD2	1.92	0.51
1:C:813:VAL:HG21	1:C:819:LEU:HB2	1.92	0.51
1:B:165:ARG:HH22	3:B:2302:GOL:C1	2.23	0.51
1:B:973:PRO:HB3	1:B:1214:PHE:CZ	2.44	0.51
1:D:535:ALA:O	1:D:536:SER:OG	2.29	0.51
1:B:1025:PHE:HD1	1:B:1025:PHE:O	1.93	0.51
1:D:295:TYR:CE2	1:D:297:THR:HG23	2.46	0.51
1:D:807:ASN:HD22	1:D:867:LEU:HD11	1.74	0.51
1:E:49:ALA:HB1	1:E:93:ARG:HD2	1.92	0.51
1:F:543:ILE:HG22	1:F:559:THR:HA	1.92	0.51
1:A:988:LEU:HD12	1:A:988:LEU:N	2.27	0.50
1:B:543:ILE:HG22	1:B:559:THR:HA	1.92	0.50
1:B:566:VAL:HG21	1:B:568:TRP:CE2	2.46	0.50
1:A:49:ALA:O	1:A:93:ARG:NH1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:350:GLN:HE22	1:E:375:LYS:HB3	1.76	0.50
1:D:49:ALA:O	1:D:93:ARG:NH1	2.40	0.50
1:E:813:VAL:HG21	1:E:819:LEU:HB2	1.93	0.50
1:A:295:TYR:CE2	1:A:297:THR:HG23	2.46	0.50
1:B:356:SER:HA	1:B:378:LEU:O	2.12	0.50
1:C:703:THR:OG1	1:C:709:THR:HB	2.12	0.50
1:C:1058:ASN:HB2	1:C:1105:GLU:H	1.77	0.50
1:D:49:ALA:HB1	1:D:93:ARG:HD2	1.94	0.50
1:D:356:SER:HA	1:D:378:LEU:O	2.12	0.50
1:A:566:VAL:HG21	1:A:568:TRP:CE2	2.46	0.50
1:E:973:PRO:HB3	1:E:1214:PHE:CZ	2.46	0.50
1:A:356:SER:HA	1:A:378:LEU:O	2.12	0.49
1:B:1156:GLU:HG3	1:B:1172:TYR:CE2	2.47	0.49
1:F:566:VAL:HG21	1:F:568:TRP:CE2	2.47	0.49
1:C:988:LEU:HD13	1:C:992:THR:O	2.13	0.49
1:B:1058:ASN:HB2	1:B:1105:GLU:H	1.77	0.49
1:C:566:VAL:HG21	1:C:568:TRP:CE2	2.47	0.49
1:F:703:THR:OG1	1:F:709:THR:HB	2.13	0.49
1:B:533:GLU:OE2	3:B:2302:GOL:O1	2.31	0.49
1:C:356:SER:HA	1:C:378:LEU:O	2.12	0.49
1:D:566:VAL:HG21	1:D:568:TRP:CE2	2.47	0.49
1:E:356:SER:HA	1:E:378:LEU:O	2.12	0.49
1:C:901:THR:HG21	1:C:938:ALA:HB2	1.94	0.49
1:B:925:VAL:HG13	1:B:947:VAL:HG23	1.93	0.49
1:A:703:THR:OG1	1:A:709:THR:HB	2.13	0.48
1:D:1013:ALA:HA	1:D:1037:VAL:HG23	1.93	0.48
1:E:441:MET:HG2	1:E:478:PRO:HG2	1.96	0.48
1:A:901:THR:HG21	1:A:938:ALA:HB2	1.96	0.48
1:A:1117:GLY:HA3	1:A:1210:ALA:HB2	1.96	0.48
1:E:1156:GLU:HG3	1:E:1172:TYR:CE2	2.48	0.48
1:C:1014:GLY:N	1:C:1037:VAL:HG23	2.28	0.48
1:D:1266:ALA:O	1:D:1267:HIS:CB	2.61	0.48
1:D:703:THR:OG1	1:D:709:THR:HB	2.13	0.48
1:E:566:VAL:HG21	1:E:568:TRP:CE2	2.48	0.48
1:C:441:MET:HG2	1:C:478:PRO:HG2	1.95	0.48
1:E:360:THR:HA	1:E:361:HIS:HA	1.72	0.48
1:E:703:THR:OG1	1:E:709:THR:HB	2.13	0.48
1:D:1113:GLU:HB2	1:D:1180:THR:HG22	1.94	0.48
1:E:360:THR:HB	1:E:361:HIS:CE1	2.49	0.48
1:C:988:LEU:CD1	1:C:994:THR:HG23	2.44	0.48
1:C:1223:SER:OG	1:C:1254:GLU:O	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:988:LEU:CD1	1:D:994:THR:HG23	2.44	0.48
1:B:441:MET:HG2	1:B:478:PRO:HG2	1.95	0.48
1:E:1025:PHE:O	1:E:1025:PHE:HD1	1.97	0.47
1:C:1023:THR:HG22	1:C:1028:GLU:CG	2.36	0.47
1:D:18:GLU:OE2	1:D:40:LYS:NZ	2.40	0.47
1:D:901:THR:HG21	1:D:938:ALA:HB2	1.96	0.47
1:E:827:SER:N	1:E:828:PRO:CD	2.78	0.47
1:A:827:SER:N	1:A:828:PRO:CD	2.78	0.47
1:B:827:SER:N	1:B:828:PRO:CD	2.77	0.47
1:B:1117:GLY:HA3	1:B:1210:ALA:HB2	1.97	0.47
1:D:827:SER:N	1:D:828:PRO:CD	2.77	0.47
1:A:1058:ASN:HB2	1:A:1105:GLU:H	1.79	0.47
1:C:49:ALA:HB1	1:C:93:ARG:HD2	1.97	0.47
1:B:703:THR:OG1	1:B:709:THR:HB	2.14	0.47
1:D:471:LYS:HE3	1:D:503:ASN:HB3	1.97	0.47
1:C:925:VAL:HG13	1:C:947:VAL:HG23	1.97	0.47
1:C:943:VAL:HB	1:C:954:VAL:CG2	2.45	0.47
1:D:1014:GLY:N	1:D:1037:VAL:HG23	2.30	0.47
1:E:715:GLY:O	1:E:718:LYS:HB3	2.14	0.47
1:F:49:ALA:HB1	1:F:93:ARG:HD2	1.95	0.47
1:A:49:ALA:HB1	1:A:93:ARG:HD2	1.95	0.47
1:B:64:LEU:HD13	1:B:172:ILE:HG21	1.97	0.47
1:C:827:SER:N	1:C:828:PRO:CD	2.78	0.47
1:D:441:MET:HG2	1:D:478:PRO:HG2	1.97	0.47
1:B:988:LEU:CD1	1:B:994:THR:HG23	2.45	0.47
1:A:64:LEU:HD13	1:A:172:ILE:HG21	1.98	0.46
1:E:1113:GLU:HB2	1:E:1180:THR:HG22	1.97	0.46
1:D:1113:GLU:CB	1:D:1180:THR:HG22	2.46	0.46
1:F:827:SER:N	1:F:828:PRO:CD	2.78	0.46
1:C:1023:THR:CG2	1:C:1028:GLU:CG	2.91	0.46
1:D:1058:ASN:HB2	1:D:1105:GLU:H	1.80	0.46
1:A:74:TYR:CE1	1:A:618:LYS:HG3	2.50	0.46
1:B:951:LYS:HD2	1:B:952:ILE:O	2.16	0.46
1:A:931:SER:HB3	1:A:934:GLN:CG	2.46	0.46
1:A:988:LEU:CD1	1:A:988:LEU:N	2.79	0.46
1:D:210:LEU:HD12	1:D:210:LEU:N	2.30	0.46
1:D:966:LEU:CD1	1:D:1262:THR:HG21	2.44	0.46
1:F:64:LEU:HD13	1:F:172:ILE:HG21	1.97	0.46
1:F:1113:GLU:HB2	1:F:1180:THR:HG22	1.98	0.46
1:B:1014:GLY:N	1:B:1037:VAL:HG23	2.31	0.46
1:F:1058:ASN:HB2	1:F:1105:GLU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:988:LEU:CD1	1:C:988:LEU:N	2.78	0.46
1:D:74:TYR:CE1	1:D:618:LYS:HG3	2.51	0.46
1:F:165:ARG:HH22	3:F:2302:GOL:H11	1.80	0.46
1:C:1014:GLY:H	1:C:1037:VAL:HG23	1.81	0.46
1:F:901:THR:HG21	1:F:938:ALA:HB2	1.97	0.45
1:D:358:ARG:HG2	1:D:360:THR:HG23	1.97	0.45
1:D:988:LEU:N	1:D:988:LEU:CD1	2.79	0.45
1:E:64:LEU:HD13	1:E:172:ILE:HG21	1.98	0.45
1:A:441:MET:HG2	1:A:478:PRO:HG2	1.98	0.45
1:B:208:MET:SD	1:B:230:VAL:HG21	2.55	0.45
1:D:64:LEU:HD13	1:D:172:ILE:HG21	1.98	0.45
1:E:360:THR:HB	1:E:361:HIS:ND1	2.32	0.45
1:E:1254:GLU:HA	1:E:1261:VAL:HG21	1.98	0.45
1:A:210:LEU:N	1:A:210:LEU:HD12	2.32	0.45
1:A:1113:GLU:HB2	1:A:1180:THR:HG22	1.99	0.45
1:E:901:THR:HG21	1:E:938:ALA:HB2	1.99	0.45
1:A:988:LEU:CD1	1:A:994:THR:CG2	2.91	0.45
1:A:1254:GLU:HA	1:A:1261:VAL:HG21	1.97	0.45
1:C:210:LEU:N	1:C:210:LEU:HD12	2.32	0.45
1:A:818:LYS:HE2	1:A:818:LYS:HB3	1.81	0.45
1:B:582:ARG:HB3	1:B:584:PHE:CE1	2.52	0.45
1:B:973:PRO:HG2	1:B:976:THR:HB	1.98	0.45
1:D:1117:GLY:HA3	1:D:1210:ALA:HB2	1.98	0.45
1:F:74:TYR:CE1	1:F:618:LYS:HG3	2.52	0.45
1:A:228:GLN:HA	1:A:282:ARG:O	2.17	0.45
1:B:665:GLY:O	1:B:666:ASN:HB2	2.16	0.45
1:F:854:GLU:OE2	1:F:916:SER:HA	2.16	0.45
1:F:1113:GLU:CB	1:F:1180:THR:HG22	2.47	0.45
1:B:965:LEU:HD21	1:B:1024:VAL:HG21	1.99	0.45
1:C:228:GLN:HA	1:C:282:ARG:O	2.16	0.45
1:D:459:PHE:N	1:D:460:PRO:HD2	2.32	0.45
1:E:791:GLU:OE2	1:E:844:LYS:HE2	2.17	0.45
1:E:1113:GLU:CB	1:E:1180:THR:HG22	2.47	0.45
1:F:591:TRP:CH2	3:F:2302:GOL:C2	2.99	0.45
1:C:988:LEU:N	1:C:988:LEU:HD12	2.31	0.45
1:D:392:ASN:OD1	1:D:1112:THR:HG21	2.17	0.45
1:D:988:LEU:CD1	1:D:988:LEU:H	2.30	0.45
1:C:392:ASN:OD1	1:C:1112:THR:HG21	2.17	0.44
1:D:228:GLN:HA	1:D:282:ARG:O	2.17	0.44
1:E:98:ILE:HG23	1:E:102:LEU:HD12	1.99	0.44
1:F:105:LYS:HA	1:F:105:LYS:HD3	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ARG:HG2	1:A:303:TRP:N	2.33	0.44
1:B:1175:ALA:O	1:B:1177:VAL:HG23	2.17	0.44
1:F:228:GLN:HA	1:F:282:ARG:O	2.17	0.44
1:C:74:TYR:CE1	1:C:618:LYS:HG3	2.52	0.44
1:D:1254:GLU:HA	1:D:1261:VAL:HG21	1.99	0.44
1:B:228:GLN:HA	1:B:282:ARG:O	2.17	0.44
1:C:966:LEU:HD12	1:C:1262:THR:HG21	1.99	0.44
1:D:100:ARG:HG2	1:D:148:GLY:HA3	2.00	0.44
1:D:988:LEU:HD11	1:D:994:THR:HG23	1.99	0.44
1:F:361:HIS:NE2	3:F:2302:GOL:O2	2.50	0.44
1:F:674:THR:HG21	1:F:679:VAL:HG21	1.99	0.44
1:A:1113:GLU:CB	1:A:1180:THR:HG22	2.47	0.44
1:D:893:TYR:OH	1:D:952:ILE:HG23	2.18	0.44
1:F:441:MET:HG2	1:F:478:PRO:HG2	1.99	0.44
1:F:893:TYR:OH	1:F:952:ILE:HG23	2.17	0.44
1:C:471:LYS:HE3	1:C:503:ASN:HB3	2.00	0.44
1:E:74:TYR:CE1	1:E:618:LYS:HG3	2.53	0.44
1:F:855:ALA:HB2	1:F:878:ALA:HB2	1.99	0.44
1:A:387:TRP:CE2	1:A:448:MET:HG2	2.52	0.44
1:A:1131:ARG:HD2	1:B:747:ASN:ND2	2.33	0.44
1:B:74:TYR:CE1	1:B:618:LYS:HG3	2.52	0.44
1:B:808:ARG:HA	1:B:839:LYS:HA	2.00	0.44
1:C:591:TRP:HA	1:C:592:THR:HA	1.78	0.44
1:C:1117:GLY:HA3	1:C:1210:ALA:HB2	1.99	0.44
1:E:582:ARG:HB3	1:E:584:PHE:CE1	2.53	0.44
1:E:228:GLN:HA	1:E:282:ARG:O	2.18	0.44
1:B:521:ARG:CG	1:B:521:ARG:NH1	2.81	0.44
1:A:808:ARG:HA	1:A:839:LYS:HA	2.00	0.43
1:B:1113:GLU:CB	1:B:1180:THR:HG22	2.48	0.43
1:D:360:THR:HA	1:D:361:HIS:HA	1.77	0.43
1:B:358:ARG:HG2	1:B:360:THR:HG23	2.00	0.43
1:C:1113:GLU:CB	1:C:1180:THR:HG22	2.48	0.43
1:F:459:PHE:N	1:F:460:PRO:HD2	2.33	0.43
1:B:165:ARG:HH22	3:B:2302:GOL:H12	1.82	0.43
1:B:210:LEU:HD12	1:B:210:LEU:N	2.33	0.43
1:B:350:GLN:HE22	1:B:375:LYS:HB3	1.83	0.43
1:D:973:PRO:HB3	1:D:1214:PHE:CZ	2.53	0.43
1:E:459:PHE:N	1:E:460:PRO:HD2	2.33	0.43
1:E:1222:LEU:HD22	1:E:1253:ALA:HB1	2.01	0.43
1:A:988:LEU:HD22	1:A:992:THR:HB	2.00	0.43
1:B:382:GLU:HA	1:B:443:SER:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:959:ILE:HG21	1:C:962:ILE:HD13	1.98	0.43
1:A:387:TRP:CZ2	1:A:448:MET:HG2	2.53	0.43
1:C:358:ARG:HG2	1:C:360:THR:HG23	2.00	0.43
1:C:360:THR:HA	1:C:361:HIS:HA	1.77	0.43
1:D:805:ALA:HB3	1:D:843:GLY:HA2	2.00	0.43
1:B:901:THR:HG21	1:B:938:ALA:HB2	2.00	0.43
1:C:98:ILE:HG23	1:C:102:LEU:HD12	2.00	0.43
1:D:582:ARG:HB3	1:D:584:PHE:CE1	2.54	0.43
1:D:713:TYR:OH	1:D:717:ASP:OD1	2.21	0.43
1:D:973:PRO:HG2	1:D:976:THR:HB	2.00	0.43
1:E:382:GLU:HA	1:E:443:SER:HB3	2.01	0.43
1:F:360:THR:HA	1:F:361:HIS:HA	1.79	0.43
1:A:471:LYS:HE3	1:A:503:ASN:HB3	2.00	0.43
1:A:805:ALA:HB3	1:A:843:GLY:HA2	2.01	0.43
1:B:98:ILE:HG23	1:B:102:LEU:HD12	2.01	0.43
1:D:382:GLU:HA	1:D:443:SER:HB3	2.01	0.43
1:F:591:TRP:CZ2	3:F:2302:GOL:C3	3.00	0.43
1:E:808:ARG:HA	1:E:839:LYS:HA	1.99	0.43
1:F:654:ALA:HB1	1:F:803:PRO:HG3	2.00	0.43
1:F:879:VAL:HG12	1:F:881:GLY:H	1.84	0.43
1:B:893:TYR:OH	1:B:952:ILE:HG23	2.18	0.43
1:E:471:LYS:HE3	1:E:503:ASN:HB3	2.01	0.43
1:F:361:HIS:CD2	3:F:2302:GOL:HO2	2.36	0.43
1:F:387:TRP:CZ2	1:F:448:MET:HG2	2.54	0.43
1:A:358:ARG:HG2	1:A:360:THR:HG23	2.00	0.42
1:B:302:ARG:HG2	1:B:303:TRP:N	2.34	0.42
1:C:64:LEU:HD13	1:C:172:ILE:HG21	2.00	0.42
1:E:1175:ALA:O	1:E:1177:VAL:HG23	2.18	0.42
1:F:382:GLU:HA	1:F:443:SER:HB3	2.01	0.42
1:B:459:PHE:N	1:B:460:PRO:HD2	2.34	0.42
1:C:459:PHE:N	1:C:460:PRO:HD2	2.35	0.42
1:D:302:ARG:HG2	1:D:303:TRP:N	2.33	0.42
1:F:791:GLU:OE2	1:F:844:LYS:HE2	2.18	0.42
1:A:1116:LEU:HD11	1:A:1182:VAL:HG21	2.02	0.42
1:C:105:LYS:HA	1:C:105:LYS:HD3	1.90	0.42
1:C:582:ARG:HB3	1:C:584:PHE:CE1	2.55	0.42
1:F:210:LEU:N	1:F:210:LEU:HD12	2.34	0.42
1:A:893:TYR:OH	1:A:952:ILE:HG23	2.19	0.42
1:D:387:TRP:CE2	1:D:448:MET:HG2	2.54	0.42
1:E:25:VAL:HG12	1:E:102:LEU:HD11	2.02	0.42
1:F:8:ASP:HB3	1:F:11:THR:HG1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:ILE:HG23	1:F:102:LEU:HD12	2.00	0.42
1:F:770:LYS:HD3	1:F:868:GLN:OE1	2.20	0.42
1:A:770:LYS:HD3	1:A:868:GLN:OE1	2.20	0.42
1:A:973:PRO:HG2	1:A:976:THR:HB	2.02	0.42
1:A:988:LEU:HD13	1:A:992:THR:O	2.20	0.42
1:B:897:TYR:O	1:B:956:VAL:HA	2.20	0.42
1:D:808:ARG:HA	1:D:839:LYS:HA	2.00	0.42
1:E:1058:ASN:HB2	1:E:1105:GLU:H	1.85	0.42
1:A:459:PHE:N	1:A:460:PRO:HD2	2.34	0.42
1:A:582:ARG:HB3	1:A:584:PHE:CE1	2.55	0.42
1:C:1113:GLU:HB2	1:C:1180:THR:HG22	2.01	0.42
1:D:387:TRP:CZ2	1:D:448:MET:HG2	2.54	0.42
1:D:674:THR:HG21	1:D:679:VAL:HG21	2.01	0.42
1:E:770:LYS:HD3	1:E:868:GLN:OE1	2.20	0.42
1:E:805:ALA:HB3	1:E:843:GLY:HA2	2.01	0.42
1:F:808:ARG:HA	1:F:839:LYS:HA	2.02	0.42
1:D:68:TYR:CZ	1:D:170:SER:HB3	2.54	0.42
1:E:68:TYR:CZ	1:E:170:SER:HB3	2.55	0.42
1:E:652:LEU:HB2	1:E:653:PRO:HA	2.01	0.42
1:A:382:GLU:HA	1:A:443:SER:HB3	2.01	0.42
1:B:387:TRP:CZ2	1:B:448:MET:HG2	2.54	0.42
1:B:659:VAL:HG11	1:B:803:PRO:HB2	2.00	0.42
1:B:1132:PHE:HB2	1:C:747:ASN:OD1	2.19	0.42
1:E:358:ARG:HG2	1:E:360:THR:HG23	1.98	0.42
1:E:801:ILE:H	1:E:801:ILE:HG12	1.63	0.42
1:E:974:VAL:HG22	1:E:1037:VAL:HG12	2.02	0.42
1:F:659:VAL:HG11	1:F:803:PRO:HB2	2.01	0.42
1:F:1254:GLU:HA	1:F:1261:VAL:HG21	2.02	0.42
1:A:98:ILE:HG23	1:A:102:LEU:HD12	2.00	0.42
1:A:208:MET:SD	1:A:230:VAL:HG21	2.60	0.42
1:B:988:LEU:CD1	1:B:994:THR:CG2	2.97	0.42
1:A:591:TRP:HA	1:A:592:THR:HA	1.78	0.41
1:C:208:MET:SD	1:C:230:VAL:HG21	2.60	0.41
1:C:500:LEU:HD23	1:C:500:LEU:HA	1.94	0.41
1:C:988:LEU:CD1	1:C:994:THR:CG2	2.98	0.41
1:B:25:VAL:HG12	1:B:102:LEU:HD11	2.02	0.41
1:B:471:LYS:HE3	1:B:503:ASN:HB3	2.02	0.41
1:B:1113:GLU:HB2	1:B:1180:THR:HG22	2.01	0.41
1:C:68:TYR:CZ	1:C:170:SER:HB3	2.55	0.41
1:C:521:ARG:CG	1:C:521:ARG:NH1	2.80	0.41
1:C:791:GLU:OE2	1:C:844:LYS:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:MET:SD	1:E:230:VAL:HG21	2.60	0.41
1:E:717:ASP:OD1	1:E:717:ASP:N	2.48	0.41
1:A:392:ASN:OD1	1:A:1112:THR:HG21	2.21	0.41
1:B:387:TRP:CE2	1:B:448:MET:HG2	2.56	0.41
1:C:1128:ASN:O	1:C:1193:THR:HB	2.20	0.41
1:F:358:ARG:HG2	1:F:360:THR:HG23	2.01	0.41
1:D:521:ARG:CG	1:D:521:ARG:NH1	2.82	0.41
1:F:652:LEU:HB2	1:F:653:PRO:HA	2.02	0.41
1:A:68:TYR:CZ	1:A:170:SER:HB3	2.55	0.41
1:C:988:LEU:CD1	1:C:988:LEU:H	2.34	0.41
1:D:25:VAL:HG12	1:D:102:LEU:HD11	2.02	0.41
1:D:988:LEU:HD12	1:D:988:LEU:H	1.84	0.41
1:C:652:LEU:HB2	1:C:653:PRO:HA	2.02	0.41
1:C:1116:LEU:HD11	1:C:1182:VAL:HG21	2.01	0.41
1:E:1040:SER:HB3	1:E:1212:SER:HB3	2.02	0.41
1:F:208:MET:SD	1:F:230:VAL:HG21	2.61	0.41
1:A:973:PRO:HB3	1:A:1214:PHE:CZ	2.56	0.41
1:B:717:ASP:OD1	1:B:717:ASP:N	2.48	0.41
1:B:805:ALA:HB3	1:B:843:GLY:HA2	2.01	0.41
1:B:1254:GLU:HA	1:B:1261:VAL:HG21	2.03	0.41
1:C:808:ARG:HA	1:C:839:LYS:HA	2.01	0.41
1:B:68:TYR:CZ	1:B:170:SER:HB3	2.56	0.41
1:B:447:GLU:OE1	3:B:2302:GOL:O1	2.25	0.41
1:D:98:ILE:HG23	1:D:102:LEU:HD12	2.03	0.41
1:D:1014:GLY:H	1:D:1037:VAL:HG23	1.83	0.41
1:E:716:ALA:C	1:E:718:LYS:H	2.23	0.41
1:F:68:TYR:CZ	1:F:170:SER:HB3	2.56	0.41
1:A:652:LEU:HB2	1:A:653:PRO:HA	2.03	0.41
1:B:1128:ASN:O	1:B:1193:THR:HB	2.21	0.41
1:C:382:GLU:HA	1:C:443:SER:HB3	2.02	0.41
1:E:210:LEU:N	1:E:210:LEU:HD12	2.35	0.41
1:F:1117:GLY:HA3	1:F:1210:ALA:HB2	2.02	0.41
1:F:1128:ASN:O	1:F:1193:THR:HB	2.21	0.41
1:A:360:THR:HA	1:A:361:HIS:HA	1.76	0.41
1:C:654:ALA:HB1	1:C:803:PRO:HG3	2.03	0.41
1:F:471:LYS:HE3	1:F:503:ASN:HB3	2.03	0.41
1:F:582:ARG:HB3	1:F:584:PHE:CE1	2.55	0.41
1:C:674:THR:HG21	1:C:679:VAL:HG21	2.02	0.40
1:D:1128:ASN:O	1:D:1193:THR:HB	2.21	0.40
1:A:972:THR:HG22	1:A:1035:ILE:CD1	2.51	0.40
1:C:387:TRP:CZ2	1:C:448:MET:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:THR:HG22	1:B:561:TYR:CE1	2.57	0.40
1:D:1119:ILE:HD12	1:D:1140:ILE:HD13	2.04	0.40
1:A:1128:ASN:O	1:A:1193:THR:HB	2.21	0.40
1:B:674:THR:HG21	1:B:679:VAL:HG21	2.03	0.40
1:C:893:TYR:OH	1:C:952:ILE:HG23	2.21	0.40
1:F:113:GLY:HA3	1:F:174:ARG:HD2	2.03	0.40
1:F:591:TRP:HA	1:F:592:THR:HA	1.80	0.40
1:A:1002:TRP:CH2	1:A:1033:ALA:HB2	2.57	0.40
1:A:1123:PHE:CZ	1:A:1138:THR:HG21	2.56	0.40
1:B:881:GLY:HA3	1:B:889:ARG:HH21	1.87	0.40
1:C:18:GLU:OE1	1:C:895:ARG:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1233/1304 (95%)	1180 (96%)	52 (4%)	1 (0%)	51	82
1	B	1229/1304 (94%)	1180 (96%)	47 (4%)	2 (0%)	47	78
1	C	1237/1304 (95%)	1186 (96%)	50 (4%)	1 (0%)	51	82
1	D	1249/1304 (96%)	1193 (96%)	53 (4%)	3 (0%)	47	78
1	E	1229/1304 (94%)	1179 (96%)	46 (4%)	4 (0%)	41	71
1	F	1238/1304 (95%)	1186 (96%)	49 (4%)	3 (0%)	47	78
All	All	7415/7824 (95%)	7104 (96%)	297 (4%)	14 (0%)	47	78

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1267	HIS

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Mol	Chain	Res	Type
1	F	9	SER
1	B	663	GLY
1	D	1270	VAL
1	E	663	GLY
1	A	535	ALA
1	B	535	ALA
1	C	535	ALA
1	D	535	ALA
1	E	535	ALA
1	E	1081	ASN
1	F	535	ALA
1	E	664	SER
1	F	663	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	982/1056 (93%)	938 (96%)	44 (4%)	27	61
1	B	972/1056 (92%)	927 (95%)	45 (5%)	27	60
1	C	986/1056 (93%)	943 (96%)	43 (4%)	28	61
1	D	989/1056 (94%)	944 (95%)	45 (5%)	27	60
1	E	960/1056 (91%)	911 (95%)	49 (5%)	24	56
1	F	983/1056 (93%)	936 (95%)	47 (5%)	25	58
All	All	5872/6336 (93%)	5599 (95%)	273 (5%)	27	60

All (273) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	33	SER
1	A	79	GLU
1	A	100	ARG
1	A	182	ASP

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Mol	Chain	Res	Type
1	A	185	HIS
1	A	200	THR
1	A	227	LYS
1	A	237	THR
1	A	250	SER
1	A	274	LYS
1	A	302	ARG
1	A	317	GLU
1	A	471	LYS
1	A	481	TYR
1	A	499	ASN
1	A	526	SER
1	A	536	SER
1	A	539	ASN
1	A	543	ILE
1	A	618	LYS
1	A	652	LEU
1	A	692	ARG
1	A	709	THR
1	A	748	ASN
1	A	756	THR
1	A	763	THR
1	A	772	LYS
1	A	801	ILE
1	A	807	ASN
1	A	870	SER
1	A	895	ARG
1	A	971	SER
1	A	1034	THR
1	A	1035	ILE
1	A	1043	THR
1	A	1078	VAL
1	A	1096	TYR
1	A	1138	THR
1	A	1164	SER
1	A	1180	THR
1	A	1216	THR
1	A	1219	SER
1	A	1282	THR
1	B	30	ASN
1	B	33	SER
1	B	42	MET

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Mol	Chain	Res	Type
1	B	185	HIS
1	B	200	THR
1	B	227	LYS
1	B	237	THR
1	B	260	THR
1	B	274	LYS
1	B	297	THR
1	B	302	ARG
1	B	317	GLU
1	B	374	GLU
1	B	404	GLN
1	B	481	TYR
1	B	499	ASN
1	B	521	ARG
1	B	526	SER
1	B	536	SER
1	B	539	ASN
1	B	543	ILE
1	B	618	LYS
1	B	652	LEU
1	B	662	LYS
1	B	692	ARG
1	B	709	THR
1	B	748	ASN
1	B	756	THR
1	B	801	ILE
1	B	807	ASN
1	B	870	SER
1	B	876	THR
1	B	951	LYS
1	B	960	ASP
1	B	1040	SER
1	B	1078	VAL
1	B	1096	TYR
1	B	1138	THR
1	B	1161	GLN
1	B	1164	SER
1	B	1180	THR
1	B	1216	THR
1	B	1219	SER
1	B	1262	THR
1	B	1282	THR

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Mol	Chain	Res	Type
1	C	8	ASP
1	C	33	SER
1	C	79	GLU
1	C	105	LYS
1	C	182	ASP
1	C	185	HIS
1	C	200	THR
1	C	227	LYS
1	C	237	THR
1	C	250	SER
1	C	260	THR
1	C	297	THR
1	C	302	ARG
1	C	317	GLU
1	C	481	TYR
1	C	499	ASN
1	C	521	ARG
1	C	526	SER
1	C	536	SER
1	C	539	ASN
1	C	543	ILE
1	C	618	LYS
1	C	652	LEU
1	C	692	ARG
1	C	709	THR
1	C	748	ASN
1	C	756	THR
1	C	767	LYS
1	C	772	LYS
1	C	801	ILE
1	C	807	ASN
1	C	870	SER
1	C	895	ARG
1	C	898	TYR
1	C	988	LEU
1	C	1043	THR
1	C	1078	VAL
1	C	1096	TYR
1	C	1138	THR
1	C	1164	SER
1	C	1180	THR
1	C	1216	THR

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Mol	Chain	Res	Type
1	C	1282	THR
1	D	7	SER
1	D	8	ASP
1	D	30	ASN
1	D	33	SER
1	D	42	MET
1	D	47	VAL
1	D	82	SER
1	D	185	HIS
1	D	227	LYS
1	D	237	THR
1	D	250	SER
1	D	274	LYS
1	D	302	ARG
1	D	317	GLU
1	D	471	LYS
1	D	481	TYR
1	D	521	ARG
1	D	526	SER
1	D	539	ASN
1	D	543	ILE
1	D	618	LYS
1	D	620	SER
1	D	634	THR
1	D	662	LYS
1	D	692	ARG
1	D	709	THR
1	D	748	ASN
1	D	756	THR
1	D	772	LYS
1	D	801	ILE
1	D	807	ASN
1	D	870	SER
1	D	971	SER
1	D	1027	LYS
1	D	1043	THR
1	D	1078	VAL
1	D	1096	TYR
1	D	1138	THR
1	D	1161	GLN
1	D	1164	SER
1	D	1180	THR

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Mol	Chain	Res	Type
1	D	1216	THR
1	D	1219	SER
1	D	1265	PRO
1	D	1282	THR
1	E	18	GLU
1	E	23	SER
1	E	30	ASN
1	E	33	SER
1	E	42	MET
1	E	100	ARG
1	E	105	LYS
1	E	185	HIS
1	E	200	THR
1	E	237	THR
1	E	250	SER
1	E	260	THR
1	E	274	LYS
1	E	297	THR
1	E	302	ARG
1	E	317	GLU
1	E	374	GLU
1	E	404	GLN
1	E	471	LYS
1	E	481	TYR
1	E	499	ASN
1	E	521	ARG
1	E	526	SER
1	E	536	SER
1	E	539	ASN
1	E	543	ILE
1	E	618	LYS
1	E	652	LEU
1	E	662	LYS
1	E	692	ARG
1	E	709	THR
1	E	717	ASP
1	E	748	ASN
1	E	756	THR
1	E	801	ILE
1	E	807	ASN
1	E	870	SER
1	E	955	ARG

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Mol	Chain	Res	Type
1	E	1034	THR
1	E	1035	ILE
1	E	1078	VAL
1	E	1096	TYR
1	E	1138	THR
1	E	1164	SER
1	E	1180	THR
1	E	1216	THR
1	E	1219	SER
1	E	1280	HIS
1	E	1282	THR
1	F	7	SER
1	F	8	ASP
1	F	33	SER
1	F	61	GLN
1	F	79	GLU
1	F	100	ARG
1	F	105	LYS
1	F	185	HIS
1	F	227	LYS
1	F	237	THR
1	F	250	SER
1	F	274	LYS
1	F	297	THR
1	F	302	ARG
1	F	317	GLU
1	F	481	TYR
1	F	499	ASN
1	F	526	SER
1	F	536	SER
1	F	539	ASN
1	F	543	ILE
1	F	618	LYS
1	F	652	LEU
1	F	662	LYS
1	F	692	ARG
1	F	709	THR
1	F	748	ASN
1	F	756	THR
1	F	772	LYS
1	F	801	ILE
1	F	807	ASN

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Mol	Chain	Res	Type
1	F	870	SER
1	F	955	ARG
1	F	960	ASP
1	F	971	SER
1	F	988	LEU
1	F	1034	THR
1	F	1035	ILE
1	F	1072	LYS
1	F	1078	VAL
1	F	1096	TYR
1	F	1138	THR
1	F	1164	SER
1	F	1180	THR
1	F	1216	THR
1	F	1219	SER
1	F	1282	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	896	ASN
1	C	896	ASN
1	E	327	HIS
1	E	711	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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
3	GOL	D	2302	-	5,5,5	0.15	0	5,5,5	0.48	0
3	GOL	E	2302	-	5,5,5	0.23	0	5,5,5	0.38	0
3	GOL	A	2302	-	5,5,5	0.18	0	5,5,5	0.59	0
3	GOL	F	2302	-	5,5,5	0.08	0	5,5,5	0.43	0
3	GOL	A	2303	-	5,5,5	0.20	0	5,5,5	0.61	0
3	GOL	B	2302	-	5,5,5	0.17	0	5,5,5	0.53	0
2	SO4	D	2301	-	4,4,4	0.33	0	6,6,6	0.23	0
3	GOL	C	2302	-	5,5,5	0.16	0	5,5,5	0.46	0
2	SO4	A	2301	-	4,4,4	0.17	0	6,6,6	0.31	0
3	GOL	D	2303	-	5,5,5	0.16	0	5,5,5	0.60	0
2	SO4	F	2301	-	4,4,4	0.32	0	6,6,6	0.07	0
2	SO4	C	2301	-	4,4,4	0.35	0	6,6,6	0.13	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	GOL	D	2302	-	-	0/4/4/4	-
3	GOL	E	2302	-	-	2/4/4/4	-
3	GOL	A	2302	-	-	4/4/4/4	-
3	GOL	F	2302	-	-	0/4/4/4	-
3	GOL	A	2303	-	-	2/4/4/4	-
3	GOL	B	2302	-	-	0/4/4/4	-
3	GOL	C	2302	-	-	2/4/4/4	-
3	GOL	D	2303	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2302	GOL	C1-C2-C3-O3
3	A	2303	GOL	C1-C2-C3-O3
3	A	2303	GOL	O2-C2-C3-O3
3	A	2302	GOL	O1-C1-C2-C3
3	C	2302	GOL	O1-C1-C2-C3
3	A	2302	GOL	O1-C1-C2-O2
3	A	2302	GOL	O2-C2-C3-O3
3	C	2302	GOL	O1-C1-C2-O2
3	E	2302	GOL	C1-C2-C3-O3
3	E	2302	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2302	GOL	1	0
3	F	2302	GOL	9	0
3	B	2302	GOL	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.