



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:00 PM GMT

PDB ID : 2G3N
Title : Crystal structure of the Sulfolobus solfataricus alpha-glucosidase MalA in complex with beta-octyl-glucopyranoside
Authors : Ernst, H.A.; Lo Leggio, L.; Willemoes, M.; Leonard, G.; Blum, P.; Larsen, S.
Deposited on : 2006-02-20
Resolution : 2.55 Å(reported)

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

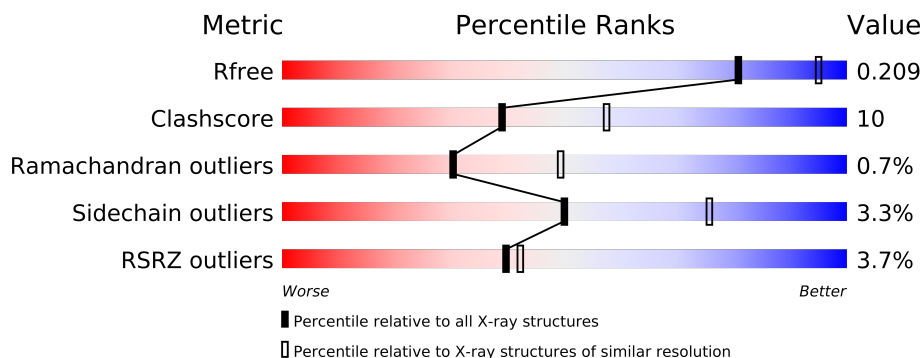
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.55 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	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	693	
1	B	693	
1	C	693	
1	D	693	
1	E	693	
1	F	693	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	BOG	A	2000	-	X
2	BOG	B	2000	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	BOG	C	2000	-	X
2	BOG	D	2000	-	X
2	BOG	E	2000	-	X
2	BOG	F	2000	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34797 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 Alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	691	Total	C	N	O	S	0	1	0
			5683	3703	919	1046	15			
1	B	691	Total	C	N	O	S	0	1	0
			5683	3703	919	1046	15			
1	C	691	Total	C	N	O	S	0	1	0
			5683	3703	919	1046	15			
1	D	691	Total	C	N	O	S	0	1	0
			5683	3703	919	1046	15			
1	E	691	Total	C	N	O	S	0	1	0
			5683	3703	919	1046	15			
1	F	691	Total	C	N	O	S	0	1	0
			5683	3703	919	1046	15			

There are 24 discrepancies between the modelled and reference sequences:

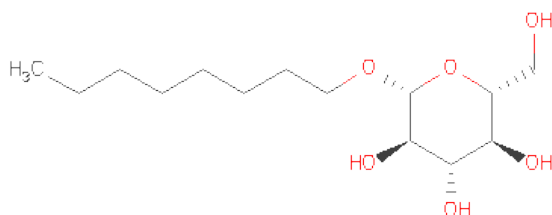
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP O59645
A	2	ARG	-	CLONING ARTIFACT	UNP O59645
A	3	ILE	-	CLONING ARTIFACT	UNP O59645
A	4	LEU	-	CLONING ARTIFACT	UNP O59645
B	1	MET	-	CLONING ARTIFACT	UNP O59645
B	2	ARG	-	CLONING ARTIFACT	UNP O59645
B	3	ILE	-	CLONING ARTIFACT	UNP O59645
B	4	LEU	-	CLONING ARTIFACT	UNP O59645
C	1	MET	-	CLONING ARTIFACT	UNP O59645
C	2	ARG	-	CLONING ARTIFACT	UNP O59645
C	3	ILE	-	CLONING ARTIFACT	UNP O59645
C	4	LEU	-	CLONING ARTIFACT	UNP O59645
D	1	MET	-	CLONING ARTIFACT	UNP O59645
D	2	ARG	-	CLONING ARTIFACT	UNP O59645
D	3	ILE	-	CLONING ARTIFACT	UNP O59645
D	4	LEU	-	CLONING ARTIFACT	UNP O59645
E	1	MET	-	CLONING ARTIFACT	UNP O59645

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2	ARG	-	CLONING ARTIFACT	UNP O59645
E	3	ILE	-	CLONING ARTIFACT	UNP O59645
E	4	LEU	-	CLONING ARTIFACT	UNP O59645
F	1	MET	-	CLONING ARTIFACT	UNP O59645
F	2	ARG	-	CLONING ARTIFACT	UNP O59645
F	3	ILE	-	CLONING ARTIFACT	UNP O59645
F	4	LEU	-	CLONING ARTIFACT	UNP O59645

- Molecule 2 is SUGAR (GLUCOSE) (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 14 8 6	0	0
2	B	1	Total C O 14 8 6	0	0
2	C	1	Total C O 14 8 6	0	0
2	D	1	Total C O 14 8 6	0	0
2	E	1	Total C O 14 8 6	0	0
2	F	1	Total C O 14 8 6	0	0

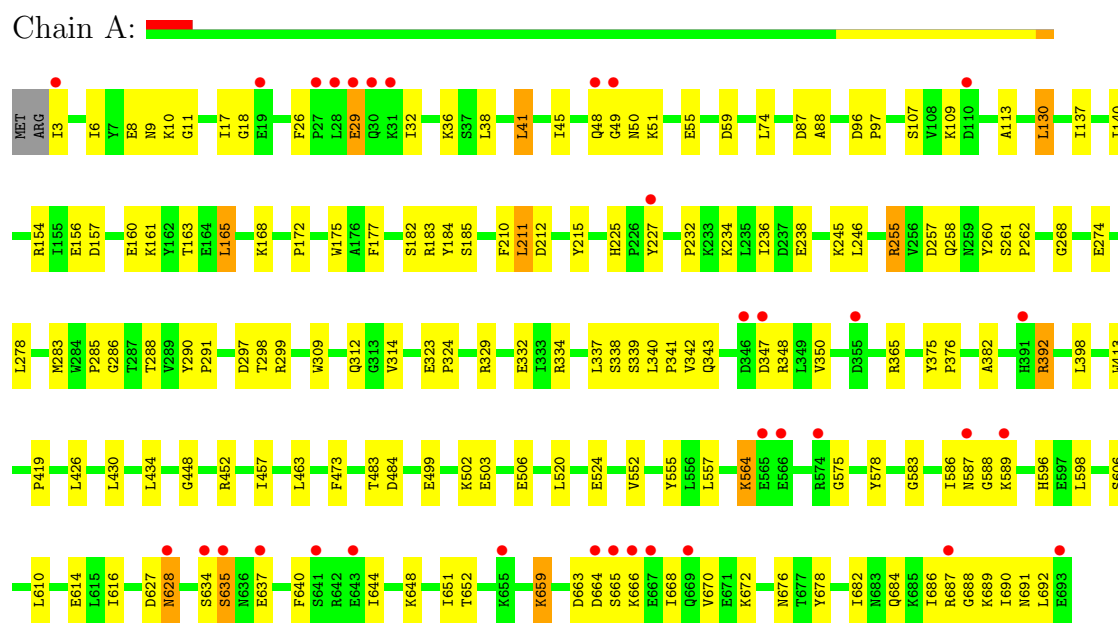
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total 83	O 83	0	0
3	B	74	Total 74	O 74	0	0
3	C	96	Total 96	O 96	0	0
3	D	103	Total 103	O 103	0	0
3	E	127	Total 127	O 127	0	0
3	F	132	Total 132	O 132	0	0

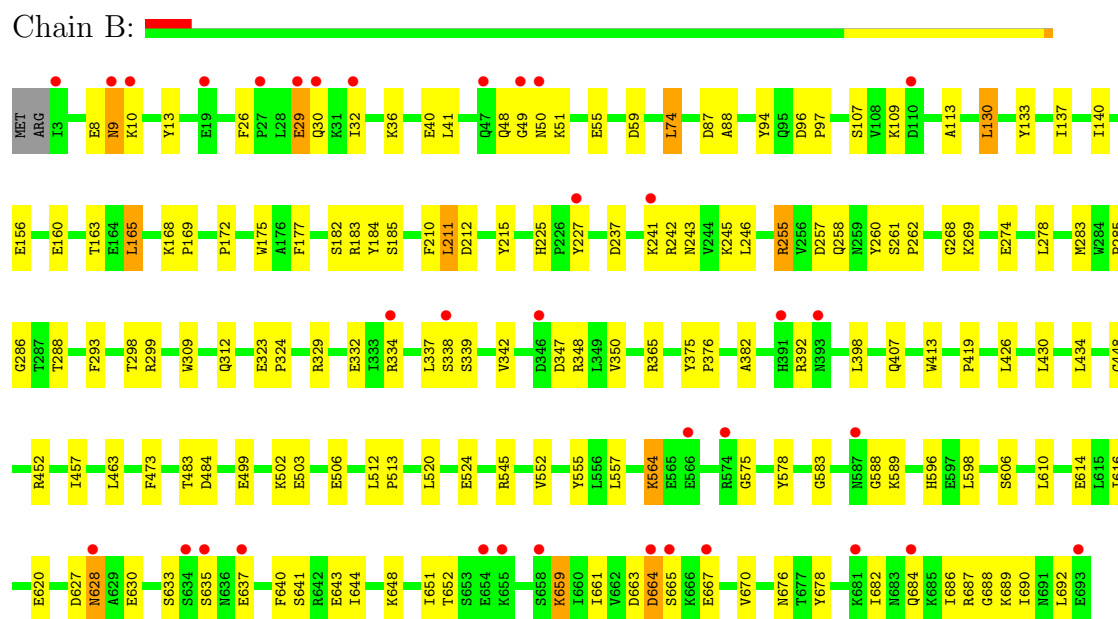
3 Residue-property plots

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: Alpha-glucosidase

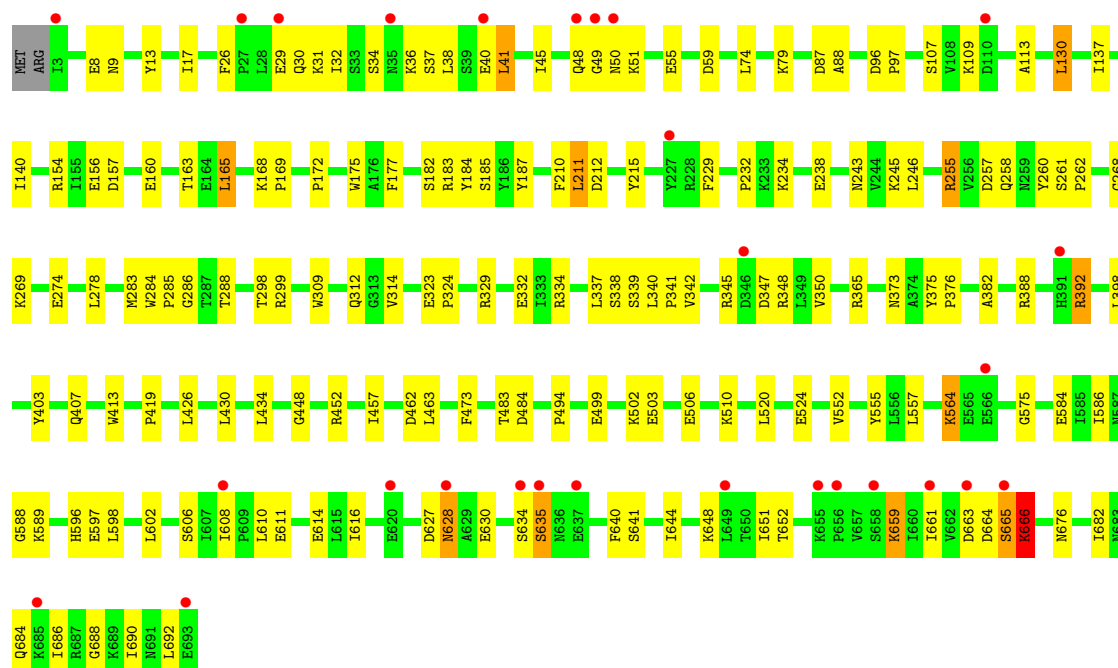


• Molecule 1: Alpha-glucosidase



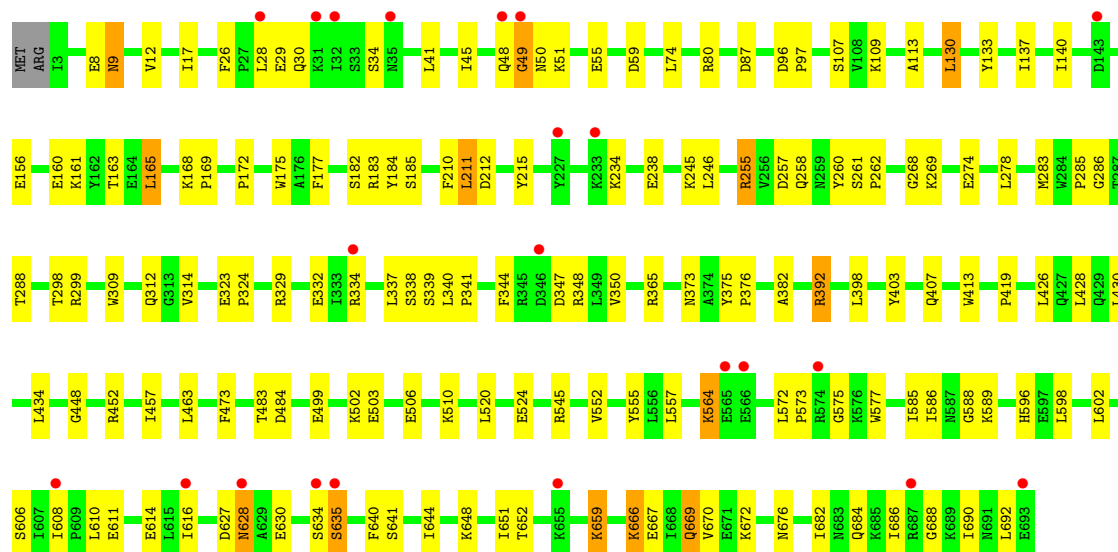
● Molecule 1: Alpha-glucosidase

Chain C:



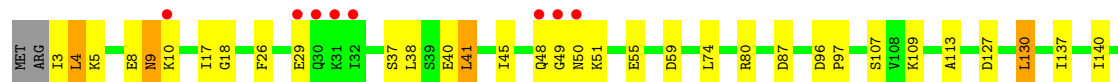
● Molecule 1: Alpha-glucosidase

Chain D:



● Molecule 1: Alpha-glucosidase

Chain E:



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.09Å 174.43Å 144.03Å 90.00° 109.05° 90.00°	Depositor
Resolution (Å)	24.16 – 2.55 24.15 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.3 (24.16-2.55) 96.3 (24.15-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.69 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.191 , 0.213 0.185 , 0.209	Depositor DCC
R_{free} test set	7300 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 37.4	EDS
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 154885 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34797	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: BOG

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	0.38	0/5837	0.62	0/7902
1	B	0.38	0/5837	0.62	0/7902
1	C	0.38	0/5837	0.61	0/7902
1	D	0.38	0/5837	0.62	0/7902
1	E	0.38	0/5837	0.62	0/7902
1	F	0.40	0/5837	0.62	0/7902
All	All	0.38	0/35022	0.62	0/47412

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5683	0	5651	119	0
1	B	5683	0	5651	119	0
1	C	5683	0	5651	127	0
1	D	5683	0	5653	119	0
1	E	5683	0	5651	108	0
1	F	5683	0	5651	121	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
3	A	83	0	0	0	0
3	B	74	0	0	0	0
3	C	96	0	0	3	0
3	D	103	0	0	0	0
3	E	127	0	0	1	0
3	F	132	0	0	2	0
All	All	34797	0	33986	659	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 10.

All (659) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:332:GLU:HG3	1:F:332:GLU:HG3	1.32	1.11
1:B:332:GLU:HG3	1:D:332:GLU:HG3	1.40	1.04
1:F:564:LYS:HE3	1:F:564:LYS:H	1.23	1.04
1:A:564:LYS:H	1:A:564:LYS:HE3	1.24	1.02
1:E:564:LYS:H	1:E:564:LYS:HE3	1.25	1.01
1:D:564:LYS:H	1:D:564:LYS:HE3	1.25	1.00
1:C:564:LYS:H	1:C:564:LYS:HE3	1.23	0.99
1:E:299:ARG:HG3	1:E:382:ALA:HB2	1.44	0.98
1:B:564:LYS:H	1:B:564:LYS:HE3	1.25	0.96
1:A:332:GLU:HG3	1:E:332:GLU:HG3	1.45	0.95
1:C:596:HIS:HD2	1:C:598:LEU:H	1.16	0.93
1:C:278:LEU:HD21	1:F:258:GLN:HG3	1.50	0.93
1:A:36:LYS:HG2	1:A:41:LEU:HD13	1.52	0.89
1:C:666:LYS:HA	1:C:666:LYS:HE3	1.54	0.88
1:C:299:ARG:HG3	1:C:382:ALA:HB2	1.53	0.87
1:D:299:ARG:HG3	1:D:382:ALA:HB2	1.54	0.87
1:F:31:LYS:HG3	1:F:32:ILE:H	1.37	0.87
1:B:258:GLN:HG3	1:D:278:LEU:HD21	1.55	0.86
1:A:596:HIS:HD2	1:A:598:LEU:H	1.24	0.85
1:A:163:THR:HG22	1:A:168:LYS:HD3	1.58	0.85
1:B:163:THR:HG22	1:B:168:LYS:HD3	1.58	0.85
1:C:163:THR:HG22	1:C:168:LYS:HD3	1.59	0.85
1:F:163:THR:HG22	1:F:168:LYS:HD3	1.56	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:4:LEU:HD23	1:F:4:LEU:H	1.42	0.85
1:A:258:GLN:HG3	1:E:278:LEU:HD21	1.56	0.85
1:E:163:THR:HG22	1:E:168:LYS:HD3	1.57	0.84
1:D:163:THR:HG22	1:D:168:LYS:HD3	1.57	0.84
1:C:258:GLN:HG3	1:F:278:LEU:HD21	1.62	0.81
1:B:278:LEU:HD21	1:D:258:GLN:HG3	1.62	0.80
1:B:337:LEU:HD21	1:D:337:LEU:HD21	1.63	0.80
1:A:299:ARG:HG3	1:A:382:ALA:HB2	1.62	0.79
1:E:334:ARG:O	1:E:338:SER:HB3	1.83	0.79
1:D:596:HIS:HD2	1:D:598:LEU:H	1.32	0.77
1:C:564:LYS:N	1:C:564:LYS:HE3	2.00	0.76
1:F:31:LYS:O	1:F:32:ILE:HG12	1.85	0.75
1:F:299:ARG:CG	1:F:382:ALA:HB2	2.17	0.75
1:F:687:ARG:HH11	1:F:687:ARG:HG3	1.50	0.75
1:F:564:LYS:N	1:F:564:LYS:HE3	1.99	0.75
1:B:564:LYS:HE3	1:B:564:LYS:N	2.01	0.74
1:A:278:LEU:HD21	1:E:258:GLN:HG3	1.70	0.74
1:C:258:GLN:HG2	1:F:268:GLY:H	1.52	0.74
1:B:268:GLY:H	1:D:258:GLN:HG2	1.53	0.73
1:A:334:ARG:O	1:A:338:SER:HB3	1.88	0.73
1:D:564:LYS:N	1:D:564:LYS:HE3	2.02	0.73
1:C:36:LYS:HA	1:C:40:GLU:OE1	1.89	0.72
1:A:564:LYS:N	1:A:564:LYS:HE3	2.00	0.72
1:B:258:GLN:CG	1:D:278:LEU:HD21	2.18	0.72
1:D:596:HIS:CD2	1:D:598:LEU:H	2.08	0.72
1:E:564:LYS:N	1:E:564:LYS:HE3	2.01	0.71
1:F:299:ARG:HG3	1:F:382:ALA:HB2	1.71	0.71
1:C:651:ILE:HD13	1:C:692:LEU:HD21	1.72	0.71
1:F:6:ILE:HD11	1:F:38:LEU:HD13	1.72	0.71
1:C:278:LEU:HD21	1:F:258:GLN:CG	2.21	0.71
1:D:651:ILE:HD13	1:D:692:LEU:HD21	1.72	0.71
1:F:614:GLU:HG2	1:F:648:LYS:HB3	1.73	0.70
1:B:299:ARG:HG3	1:B:382:ALA:HB2	1.74	0.70
1:A:596:HIS:CD2	1:A:598:LEU:H	2.10	0.69
1:F:4:LEU:HD23	1:F:4:LEU:N	2.06	0.69
1:A:686:ILE:HD13	1:A:690:ILE:HD11	1.75	0.69
1:C:299:ARG:CG	1:C:382:ALA:HB2	2.22	0.69
1:A:614:GLU:HG2	1:A:648:LYS:HB3	1.75	0.69
1:B:686:ILE:HD13	1:B:690:ILE:HD11	1.74	0.69
1:B:299:ARG:CG	1:B:382:ALA:HB2	2.24	0.68
1:E:596:HIS:HD2	1:E:598:LEU:H	1.42	0.68
1:E:8:GLU:O	1:E:9:ASN:HB2	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:163:THR:CG2	1:F:168:LYS:HD3	2.25	0.67
1:D:614:GLU:HG2	1:D:648:LYS:HB3	1.75	0.67
1:F:686:ILE:HD13	1:F:690:ILE:HD11	1.76	0.67
1:C:234:LYS:O	1:C:238:GLU:HG3	1.94	0.67
1:C:8:GLU:HB2	1:C:34:SER:HB3	1.77	0.67
1:E:285:PRO:HG2	1:E:288:THR:CG2	2.25	0.67
1:C:686:ILE:HD13	1:C:690:ILE:HD11	1.76	0.66
1:D:686:ILE:HD13	1:D:690:ILE:HD11	1.77	0.66
1:B:285:PRO:HG2	1:B:288:THR:CG2	2.26	0.66
1:C:285:PRO:HG2	1:C:288:THR:CG2	2.25	0.66
1:A:9:ASN:HD21	1:A:29:GLU:HB2	1.61	0.66
1:F:31:LYS:HG3	1:F:32:ILE:N	2.11	0.66
1:D:285:PRO:HG2	1:D:288:THR:CG2	2.26	0.65
1:F:87:ASP:O	1:F:348:ARG:HD3	1.96	0.65
1:A:163:THR:CG2	1:A:168:LYS:HD3	2.25	0.65
1:A:285:PRO:HG2	1:A:288:THR:CG2	2.26	0.65
1:E:686:ILE:HD13	1:E:690:ILE:HD11	1.79	0.65
1:B:185:SER:OG	1:B:212:ASP:HB3	1.96	0.65
1:C:614:GLU:HG2	1:C:648:LYS:HB3	1.79	0.65
1:A:185:SER:OG	1:A:212:ASP:HB3	1.97	0.65
1:A:258:GLN:CG	1:E:278:LEU:HD21	2.25	0.65
1:F:334:ARG:O	1:F:338:SER:HB3	1.96	0.65
1:D:87:ASP:O	1:D:348:ARG:HD3	1.94	0.65
1:E:651:ILE:HD13	1:E:692:LEU:HD21	1.79	0.65
1:E:87:ASP:O	1:E:348:ARG:HD3	1.97	0.65
1:D:163:THR:CG2	1:D:168:LYS:HD3	2.26	0.64
1:C:87:ASP:O	1:C:348:ARG:HD3	1.96	0.64
1:D:564:LYS:CE	1:D:564:LYS:H	2.07	0.64
1:C:564:LYS:H	1:C:564:LYS:CE	2.07	0.64
1:E:163:THR:CG2	1:E:168:LYS:HD3	2.26	0.64
1:E:614:GLU:HG2	1:E:648:LYS:HB3	1.78	0.64
1:A:651:ILE:HD13	1:A:692:LEU:HD21	1.80	0.64
1:F:596:HIS:HD2	1:F:598:LEU:H	1.45	0.64
1:F:651:ILE:HD13	1:F:692:LEU:HD21	1.78	0.64
1:A:564:LYS:H	1:A:564:LYS:CE	2.07	0.64
1:C:596:HIS:CD2	1:C:598:LEU:H	2.06	0.64
1:A:87:ASP:O	1:A:348:ARG:HD3	1.98	0.64
1:C:332:GLU:HG3	1:F:332:GLU:CG	2.21	0.64
1:B:87:ASP:O	1:B:348:ARG:HD3	1.98	0.64
1:D:334:ARG:O	1:D:338:SER:HB3	1.97	0.64
1:A:286:GLY:O	1:A:288:THR:HG23	1.98	0.63
1:D:666:LYS:HE3	1:D:666:LYS:HA	1.81	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:163:THR:CG2	1:B:168:LYS:HD3	2.27	0.63
1:D:452:ARG:HD3	1:D:484:ASP:O	1.98	0.63
1:E:286:GLY:O	1:E:288:THR:HG23	1.99	0.63
1:B:286:GLY:O	1:B:288:THR:HG23	1.99	0.63
1:D:627:ASP:O	1:D:628:ASN:HB3	1.97	0.63
1:E:564:LYS:CE	1:E:564:LYS:H	2.09	0.63
1:B:610:LEU:HD11	1:B:616:ILE:HD11	1.80	0.63
1:D:299:ARG:CG	1:D:382:ALA:HB2	2.29	0.63
1:E:4:LEU:HD23	1:E:17:ILE:HD13	1.80	0.63
1:B:334:ARG:O	1:B:338:SER:HB3	1.99	0.63
1:F:285:PRO:HG2	1:F:288:THR:CG2	2.28	0.63
1:E:3:ILE:HB	1:E:18:GLY:HA2	1.80	0.63
1:B:452:ARG:HD3	1:B:484:ASP:O	1.99	0.63
1:C:332:GLU:CG	1:F:332:GLU:HG3	2.20	0.63
1:D:9:ASN:OD1	1:D:30:GLN:HB2	1.98	0.62
1:B:13:TYR:CZ	1:B:36:LYS:HD2	2.34	0.62
1:C:575:GLY:O	1:C:588:GLY:N	2.33	0.62
1:F:286:GLY:O	1:F:288:THR:HG23	1.99	0.62
1:A:686:ILE:CD1	1:A:690:ILE:HD11	2.29	0.62
1:F:627:ASP:O	1:F:628:ASN:HB3	1.99	0.62
1:E:452:ARG:HD3	1:E:484:ASP:O	1.99	0.62
1:F:596:HIS:CD2	1:F:598:LEU:H	2.18	0.62
1:E:185:SER:OG	1:E:212:ASP:HB3	1.99	0.62
1:C:163:THR:CG2	1:C:168:LYS:HD3	2.28	0.62
1:C:258:GLN:HG2	1:F:268:GLY:N	2.14	0.62
1:C:286:GLY:O	1:C:288:THR:HG23	1.98	0.62
1:C:452:ARG:HD3	1:C:484:ASP:O	1.99	0.62
1:D:286:GLY:O	1:D:288:THR:HG23	1.99	0.61
1:E:299:ARG:CG	1:E:382:ALA:HB2	2.24	0.61
1:A:452:ARG:HD3	1:A:484:ASP:O	1.99	0.61
1:B:268:GLY:N	1:D:258:GLN:HG2	2.16	0.61
1:A:627:ASP:O	1:A:628:ASN:HB3	2.01	0.61
1:B:627:ASP:O	1:B:628:ASN:HB3	2.00	0.61
1:B:614:GLU:HG2	1:B:648:LYS:HB3	1.82	0.61
1:C:185:SER:OG	1:C:212:ASP:HB3	2.00	0.61
1:E:575:GLY:O	1:E:588:GLY:N	2.33	0.61
1:D:8:GLU:O	1:D:9:ASN:HB2	2.01	0.61
1:F:620:GLU:HG2	1:F:634:SER:HA	1.83	0.61
1:A:6:ILE:HD11	1:A:38:LEU:CD1	2.31	0.61
1:C:211:LEU:HD22	1:C:246:LEU:HD11	1.83	0.61
1:C:59:ASP:OD2	1:C:109:LYS:HD2	2.01	0.61
1:F:452:ARG:HD3	1:F:484:ASP:O	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:575:GLY:O	1:A:588:GLY:N	2.34	0.60
1:E:211:LEU:HD22	1:E:246:LEU:HD11	1.83	0.60
1:B:575:GLY:O	1:B:588:GLY:N	2.33	0.60
1:E:670:VAL:CG1	1:E:678:TYR:HB3	2.31	0.60
1:D:185:SER:OG	1:D:212:ASP:HB3	2.00	0.60
1:E:620:GLU:HG2	1:E:634:SER:HA	1.83	0.60
1:F:687:ARG:NH1	1:F:687:ARG:HG3	2.16	0.60
1:B:686:ILE:CD1	1:B:690:ILE:HD11	2.30	0.60
1:B:651:ILE:HD13	1:B:692:LEU:HD21	1.83	0.60
1:F:342:VAL:HG22	1:F:343:GLN:H	1.65	0.60
1:B:258:GLN:HG2	1:D:268:GLY:H	1.67	0.60
1:D:575:GLY:O	1:D:588:GLY:N	2.33	0.60
1:B:278:LEU:HD21	1:D:258:GLN:CG	2.30	0.60
1:F:6:ILE:HD11	1:F:38:LEU:CD1	2.32	0.60
1:A:339:SER:CB	1:F:339:SER:HB2	2.32	0.59
1:F:293:PHE:O	1:F:299:ARG:HD3	2.02	0.59
1:E:4:LEU:HD22	1:E:5:LYS:N	2.18	0.59
1:F:575:GLY:O	1:F:588:GLY:N	2.34	0.59
1:F:185:SER:OG	1:F:212:ASP:HB3	2.03	0.59
1:F:323:GLU:N	1:F:324:PRO:HA	2.18	0.59
1:E:627:ASP:O	1:E:628:ASN:HB3	2.02	0.59
1:F:299:ARG:HG2	1:F:382:ALA:HB2	1.85	0.59
1:D:269:LYS:HB3	1:D:298:THR:OG1	2.02	0.59
1:A:211:LEU:HD22	1:A:246:LEU:HD11	1.85	0.59
1:B:59:ASP:OD2	1:B:109:LYS:HD2	2.03	0.59
1:B:323:GLU:N	1:B:324:PRO:HA	2.18	0.59
1:B:225:HIS:CE1	1:B:227:TYR:HB2	2.37	0.58
1:C:269:LYS:HB3	1:C:298:THR:OG1	2.03	0.58
1:A:59:ASP:OD2	1:A:109:LYS:HD2	2.03	0.58
1:E:610:LEU:HD11	1:E:616:ILE:HD11	1.85	0.58
1:C:337:LEU:HD21	1:F:337:LEU:HD21	1.85	0.58
1:C:627:ASP:O	1:C:628:ASN:HB3	2.03	0.58
1:F:340:LEU:HD12	1:F:341:PRO:HD2	1.86	0.58
1:B:211:LEU:HD22	1:B:246:LEU:HD11	1.84	0.58
1:F:578:TYR:CE1	1:F:583:GLY:HA2	2.38	0.58
1:D:610:LEU:HD11	1:D:616:ILE:HD11	1.85	0.58
1:C:686:ILE:CD1	1:C:690:ILE:HD11	2.34	0.57
1:D:59:ASP:OD2	1:D:109:LYS:HD2	2.03	0.57
1:D:261:SER:HB3	1:D:262:PRO:HD3	1.86	0.57
1:E:323:GLU:N	1:E:324:PRO:HA	2.19	0.57
1:E:596:HIS:CD2	1:E:598:LEU:H	2.22	0.57
1:D:323:GLU:N	1:D:324:PRO:HA	2.19	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:36:LYS:HA	1:B:40:GLU:OE1	2.05	0.57
1:E:59:ASP:OD2	1:E:109:LYS:HD2	2.04	0.57
1:D:26:PHE:HB3	1:D:165:LEU:HD22	1.85	0.57
1:F:610:LEU:HD11	1:F:616:ILE:HD11	1.87	0.57
1:B:670:VAL:HG11	1:B:678:TYR:HB3	1.87	0.57
1:C:323:GLU:N	1:C:324:PRO:HA	2.19	0.56
1:F:59:ASP:OD2	1:F:109:LYS:HD2	2.04	0.56
1:F:564:LYS:CE	1:F:564:LYS:N	2.68	0.56
1:B:564:LYS:H	1:B:564:LYS:CE	2.09	0.56
1:B:26:PHE:HB3	1:B:165:LEU:HD22	1.87	0.56
1:F:564:LYS:CE	1:F:564:LYS:H	2.07	0.56
1:D:666:LYS:CE	1:D:667:GLU:H	2.18	0.56
1:C:55:GLU:HG2	1:C:137:ILE:HG12	1.88	0.56
1:A:261:SER:HB3	1:A:262:PRO:HD3	1.87	0.56
1:D:130:LEU:HD22	1:E:483:THR:HG22	1.88	0.56
1:C:258:GLN:CG	1:F:278:LEU:HD21	2.34	0.56
1:F:26:PHE:HB3	1:F:165:LEU:HD22	1.88	0.56
1:B:661:ILE:HG12	1:B:667:GLU:HG3	1.86	0.56
1:C:26:PHE:HB3	1:C:165:LEU:HD22	1.86	0.56
1:F:3:ILE:HG23	1:F:18:GLY:HA2	1.86	0.56
1:D:564:LYS:CE	1:D:564:LYS:N	2.68	0.56
1:E:670:VAL:HG11	1:E:678:TYR:HB3	1.88	0.56
1:C:499:GLU:O	1:C:503:GLU:HG3	2.05	0.56
1:C:610:LEU:HD11	1:C:616:ILE:HD11	1.88	0.56
1:C:334:ARG:O	1:C:338:SER:HB3	2.05	0.56
1:C:340:LEU:C	1:C:342:VAL:H	2.09	0.56
1:E:261:SER:HB3	1:E:262:PRO:HD3	1.87	0.56
1:F:686:ILE:CD1	1:F:690:ILE:HD11	2.35	0.56
1:D:211:LEU:HD22	1:D:246:LEU:HD11	1.87	0.56
1:A:323:GLU:N	1:A:324:PRO:HA	2.20	0.56
1:A:299:ARG:CG	1:A:382:ALA:HB2	2.35	0.56
1:E:9:ASN:ND2	1:E:10:LYS:HD3	2.21	0.55
1:F:261:SER:HB3	1:F:262:PRO:HD3	1.87	0.55
1:B:640:PHE:CE2	1:B:644:ILE:HD11	2.41	0.55
1:B:499:GLU:O	1:B:503:GLU:HG3	2.06	0.55
1:D:669:GLN:CA	1:D:669:GLN:HE21	2.18	0.55
1:C:261:SER:HB3	1:C:262:PRO:HD3	1.89	0.55
1:E:26:PHE:HB3	1:E:165:LEU:HD22	1.87	0.55
1:A:268:GLY:H	1:E:258:GLN:HG2	1.71	0.55
1:A:285:PRO:HG2	1:A:288:THR:HG21	1.89	0.55
1:A:55:GLU:HG2	1:A:137:ILE:HG12	1.89	0.55
1:A:564:LYS:N	1:A:564:LYS:CE	2.68	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:640:PHE:CE2	1:F:644:ILE:HD11	2.42	0.55
1:B:664:ASP:OD2	1:B:689:LYS:HE2	2.06	0.55
1:F:55:GLU:HG2	1:F:137:ILE:HG12	1.88	0.55
1:E:564:LYS:CE	1:E:564:LYS:N	2.69	0.55
1:A:9:ASN:HD21	1:A:10:LYS:HZ2	1.54	0.55
1:B:670:VAL:CG1	1:B:678:TYR:HB3	2.37	0.55
1:E:487:ASP:OD1	3:E:2054:HOH:O	2.18	0.55
1:F:211:LEU:HD22	1:F:246:LEU:HD11	1.87	0.55
1:C:285:PRO:HG2	1:C:288:THR:HG21	1.88	0.55
1:A:3:ILE:HB	1:A:18:GLY:HA2	1.88	0.55
1:B:261:SER:HB3	1:B:262:PRO:HD3	1.89	0.55
1:D:686:ILE:CD1	1:D:690:ILE:HD11	2.36	0.54
1:E:686:ILE:CD1	1:E:690:ILE:HD11	2.37	0.54
1:D:257:ASP:HB3	1:D:260:TYR:CB	2.37	0.54
1:B:596:HIS:CD2	1:B:598:LEU:H	2.25	0.54
1:E:635:SER:OG	1:E:636:ASN:N	2.41	0.54
1:D:499:GLU:O	1:D:503:GLU:HG3	2.07	0.54
1:C:664:ASP:O	1:C:665:SER:HB3	2.06	0.54
1:A:26:PHE:HB3	1:A:165:LEU:HD22	1.89	0.54
1:E:237:ASP:O	1:E:241:LYS:HG3	2.08	0.54
1:B:13:TYR:OH	1:B:36:LYS:HD2	2.08	0.54
1:D:182:SER:HB2	1:D:210:PHE:HB2	1.90	0.54
1:C:564:LYS:N	1:C:564:LYS:CE	2.68	0.54
1:E:234:LYS:O	1:E:238:GLU:HG3	2.07	0.54
1:B:285:PRO:HG2	1:B:288:THR:HG21	1.90	0.54
1:A:499:GLU:O	1:A:503:GLU:HG3	2.08	0.54
1:E:55:GLU:HG2	1:E:137:ILE:HG12	1.90	0.54
1:E:285:PRO:HG2	1:E:288:THR:HG21	1.89	0.54
1:A:278:LEU:HD21	1:E:258:GLN:CG	2.38	0.53
1:D:586:ILE:N	1:D:586:ILE:HD12	2.23	0.53
1:A:9:ASN:ND2	1:A:29:GLU:HB2	2.23	0.53
1:E:687:ARG:HG2	1:E:687:ARG:HH11	1.73	0.53
1:A:663:ASP:C	1:A:665:SER:H	2.11	0.53
1:F:257:ASP:HB3	1:F:260:TYR:CB	2.39	0.53
1:D:285:PRO:HG2	1:D:288:THR:HG21	1.88	0.53
1:A:640:PHE:CE2	1:A:644:ILE:HD11	2.43	0.53
1:B:578:TYR:CE1	1:B:583:GLY:HA2	2.43	0.53
1:F:285:PRO:HG2	1:F:288:THR:HG21	1.90	0.53
1:D:29:GLU:O	1:D:30:GLN:HG2	2.09	0.53
1:A:483:THR:HG22	1:C:130:LEU:HD22	1.90	0.53
1:A:578:TYR:CE1	1:A:583:GLY:HA2	2.43	0.53
1:A:337:LEU:HD21	1:E:337:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:225:HIS:CE1	1:A:227:TYR:HB2	2.44	0.53
1:C:640:PHE:CE2	1:C:644:ILE:HD11	2.43	0.53
1:B:55:GLU:HG2	1:B:137:ILE:HG12	1.90	0.53
1:C:257:ASP:HB3	1:C:260:TYR:CB	2.39	0.53
1:E:499:GLU:O	1:E:503:GLU:HG3	2.09	0.53
1:A:687:ARG:HH11	1:A:687:ARG:HA	1.73	0.53
1:E:634:SER:O	1:E:635:SER:C	2.46	0.53
1:C:339:SER:O	1:C:340:LEU:HD22	2.09	0.53
1:F:499:GLU:O	1:F:503:GLU:HG3	2.09	0.53
1:A:664:ASP:OD1	1:A:689:LYS:HE2	2.09	0.53
1:E:257:ASP:HB3	1:E:260:TYR:CB	2.39	0.53
1:D:8:GLU:HB2	1:D:34:SER:HB2	1.92	0.52
1:B:564:LYS:N	1:B:564:LYS:CE	2.69	0.52
1:D:234:LYS:O	1:D:238:GLU:HG3	2.09	0.52
1:B:257:ASP:HB3	1:B:260:TYR:CB	2.39	0.52
1:C:175:TRP:CE3	1:C:245:LYS:HG3	2.45	0.52
1:F:419:PRO:HG3	1:F:448:GLY:HA3	1.91	0.52
1:D:652:THR:HA	1:D:676:ASN:O	2.09	0.52
1:A:257:ASP:HB3	1:A:260:TYR:CB	2.40	0.52
1:E:4:LEU:HD22	1:E:5:LYS:H	1.75	0.51
1:A:610:LEU:HD11	1:A:616:ILE:HD11	1.91	0.51
1:C:634:SER:O	1:C:635:SER:C	2.49	0.51
1:D:55:GLU:HG2	1:D:137:ILE:HG12	1.92	0.51
1:C:557:LEU:C	1:C:557:LEU:HD23	2.30	0.51
1:A:557:LEU:HD23	1:A:557:LEU:C	2.32	0.51
1:E:175:TRP:CE3	1:E:245:LYS:HG3	2.46	0.51
1:A:130:LEU:HD22	1:B:483:THR:HG22	1.93	0.50
1:C:182:SER:HB2	1:C:210:PHE:HB2	1.93	0.50
1:A:502:LYS:O	1:A:506:GLU:HG3	2.11	0.50
1:A:154:ARG:HB2	1:A:157:ASP:OD2	2.10	0.50
1:F:182:SER:HB2	1:F:210:PHE:HB2	1.93	0.50
1:A:268:GLY:N	1:E:258:GLN:HG2	2.27	0.50
1:A:182:SER:HB2	1:A:210:PHE:HB2	1.92	0.50
1:B:8:GLU:O	1:B:32:ILE:HB	2.11	0.50
1:E:578:TYR:CE1	1:E:583:GLY:HA2	2.46	0.50
1:A:666:LYS:HD3	1:A:668:ILE:HD11	1.94	0.50
1:F:664:ASP:OD2	1:F:689:LYS:HE2	2.12	0.50
1:C:510:LYS:HA	1:C:611:GLU:CB	2.41	0.50
1:F:557:LEU:C	1:F:557:LEU:HD23	2.32	0.50
1:B:557:LEU:HD23	1:B:557:LEU:C	2.31	0.50
1:F:237:ASP:O	1:F:241:LYS:HG3	2.12	0.50
1:B:502:LYS:O	1:B:506:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:640:PHE:CE2	1:D:644:ILE:HD11	2.46	0.50
1:B:419:PRO:HG3	1:B:448:GLY:HA3	1.93	0.50
1:E:555:TYR:HB3	1:E:606:SER:OG	2.12	0.50
1:E:557:LEU:C	1:E:557:LEU:HD23	2.33	0.50
1:A:659:LYS:HA	1:A:670:VAL:HG23	1.94	0.50
1:D:340:LEU:HD12	1:D:341:PRO:HD2	1.94	0.50
1:F:175:TRP:CE3	1:F:245:LYS:HG3	2.46	0.50
1:F:342:VAL:HG22	1:F:343:GLN:N	2.27	0.49
1:D:257:ASP:HB3	1:D:260:TYR:HB2	1.94	0.49
1:D:175:TRP:CE3	1:D:245:LYS:HG3	2.48	0.49
1:A:11:GLY:HA3	1:A:161:LYS:HE2	1.94	0.49
1:E:182:SER:HB2	1:E:210:PHE:HB2	1.92	0.49
1:D:666:LYS:HE3	1:D:667:GLU:H	1.75	0.49
1:A:419:PRO:HG3	1:A:448:GLY:HA3	1.95	0.49
1:A:652:THR:HA	1:A:676:ASN:O	2.13	0.49
1:A:340:LEU:C	1:A:342:VAL:H	2.15	0.49
1:F:31:LYS:C	1:F:32:ILE:HG23	2.32	0.49
1:E:652:THR:HA	1:E:676:ASN:O	2.13	0.49
1:C:13:TYR:CZ	1:C:36:LYS:HD2	2.48	0.49
1:B:225:HIS:HE1	1:B:227:TYR:HB2	1.77	0.49
1:F:670:VAL:HG22	1:F:680:ALA:HB2	1.95	0.49
1:F:425:LYS:HG3	3:F:2093:HOH:O	2.13	0.49
1:A:9:ASN:OD1	1:A:10:LYS:HG3	2.13	0.48
1:A:225:HIS:HE1	1:A:227:TYR:HB2	1.76	0.48
1:A:175:TRP:CE3	1:A:245:LYS:HG3	2.47	0.48
1:D:557:LEU:HD23	1:D:557:LEU:C	2.33	0.48
1:C:665:SER:OG	1:C:666:LYS:N	2.45	0.48
1:A:9:ASN:ND2	1:A:10:LYS:NZ	2.62	0.48
1:F:257:ASP:HB3	1:F:260:TYR:HB2	1.94	0.48
1:C:462:ASP:HB2	3:C:2091:HOH:O	2.13	0.48
1:B:182:SER:HB2	1:B:210:PHE:HB2	1.95	0.48
1:D:555:TYR:HB3	1:D:606:SER:OG	2.13	0.48
1:F:31:LYS:O	1:F:32:ILE:HG23	2.13	0.48
1:D:183:ARG:O	1:D:185:SER:HA	2.13	0.48
1:F:555:TYR:HB3	1:F:606:SER:OG	2.13	0.48
1:C:154:ARG:HB2	1:C:157:ASP:OD2	2.13	0.48
1:F:31:LYS:CG	1:F:32:ILE:H	2.08	0.48
1:B:285:PRO:HG2	1:B:288:THR:HG22	1.96	0.48
1:B:51:LYS:NZ	1:B:51:LYS:HB2	2.28	0.48
1:A:672:LYS:HD2	1:A:678:TYR:CE1	2.48	0.48
1:F:51:LYS:HB2	1:F:51:LYS:HZ2	1.79	0.48
1:B:652:THR:HA	1:B:676:ASN:O	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:659:LYS:HB3	1:E:659:LYS:NZ	2.28	0.48
1:A:51:LYS:NZ	1:A:51:LYS:HB2	2.28	0.48
1:E:285:PRO:HG2	1:E:288:THR:HG22	1.94	0.48
1:B:175:TRP:CE3	1:B:245:LYS:HG3	2.49	0.48
1:C:156:GLU:O	1:C:160:GLU:HG3	2.13	0.48
1:C:140:ILE:N	1:C:140:ILE:HD12	2.29	0.48
1:E:183:ARG:O	1:E:185:SER:HA	2.14	0.48
1:D:133:TYR:HB3	1:E:187:TYR:O	2.13	0.48
1:E:502:LYS:O	1:E:506:GLU:HG3	2.14	0.48
1:C:285:PRO:HG2	1:C:288:THR:HG22	1.96	0.47
1:B:183:ARG:HG2	1:B:184:TYR:N	2.29	0.47
1:B:257:ASP:HB3	1:B:260:TYR:HB2	1.95	0.47
1:E:347:ASP:O	1:E:350:VAL:HG12	2.14	0.47
1:F:4:LEU:CD2	1:F:4:LEU:N	2.76	0.47
1:C:555:TYR:HB3	1:C:606:SER:OG	2.14	0.47
1:C:666:LYS:HA	1:C:666:LYS:CE	2.36	0.47
1:A:183:ARG:HG2	1:A:184:TYR:N	2.30	0.47
1:C:510:LYS:HA	1:C:611:GLU:HB3	1.97	0.47
1:C:257:ASP:HB3	1:C:260:TYR:HB2	1.96	0.47
1:F:51:LYS:HB2	1:F:51:LYS:NZ	2.30	0.47
1:B:347:ASP:O	1:B:350:VAL:HG12	2.15	0.47
1:A:634:SER:O	1:A:635:SER:C	2.52	0.47
1:C:36:LYS:HD3	1:C:41:LEU:HD13	1.97	0.47
1:A:340:LEU:HD13	1:A:341:PRO:HD2	1.95	0.47
1:C:661:ILE:CG2	1:C:665:SER:H	2.28	0.47
1:B:258:GLN:CD	1:D:278:LEU:HD21	2.35	0.47
1:C:258:GLN:OE1	1:F:270:PHE:N	2.32	0.47
1:F:3:ILE:HG12	1:F:3:ILE:O	2.15	0.47
1:E:257:ASP:HB3	1:E:260:TYR:HB2	1.96	0.47
1:D:502:LYS:O	1:D:506:GLU:HG3	2.14	0.47
1:B:183:ARG:O	1:B:185:SER:HA	2.15	0.47
1:F:419:PRO:HD2	1:F:457:ILE:HG23	1.96	0.47
1:D:682:ILE:HG22	1:D:684:GLN:HG2	1.96	0.47
1:C:652:THR:HA	1:C:676:ASN:O	2.14	0.47
1:D:545:ARG:HB2	1:E:494:PRO:HG3	1.97	0.47
1:C:340:LEU:O	1:C:342:VAL:N	2.47	0.47
1:A:297:ASP:OD1	1:A:298:THR:N	2.47	0.47
1:D:51:LYS:NZ	1:D:51:LYS:HB2	2.29	0.47
1:A:257:ASP:HB3	1:A:260:TYR:HB2	1.97	0.47
1:C:419:PRO:HD2	1:C:457:ILE:HG23	1.97	0.47
1:C:51:LYS:HB2	1:C:51:LYS:NZ	2.30	0.47
1:B:242:ARG:HH11	1:B:242:ARG:HG3	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:96:ASP:OD1	1:C:97:PRO:HA	2.15	0.46
1:F:347:ASP:O	1:F:350:VAL:HG12	2.15	0.46
1:E:156:GLU:O	1:E:160:GLU:HG3	2.15	0.46
1:D:347:ASP:O	1:D:350:VAL:HG12	2.15	0.46
1:A:285:PRO:HG2	1:A:288:THR:HG22	1.97	0.46
1:D:669:GLN:NE2	1:D:669:GLN:HA	2.29	0.46
1:B:156:GLU:O	1:B:160:GLU:HG3	2.15	0.46
1:E:51:LYS:NZ	1:E:51:LYS:HB2	2.28	0.46
1:C:392:ARG:HD3	3:C:2094:HOH:O	2.15	0.46
1:B:94:TYR:CZ	1:C:452:ARG:HG2	2.51	0.46
1:F:502:LYS:O	1:F:506:GLU:HG3	2.16	0.46
1:E:215:TYR:HA	1:E:229:PHE:CE1	2.51	0.46
1:D:419:PRO:HD2	1:D:457:ILE:HG23	1.97	0.46
1:C:502:LYS:O	1:C:506:GLU:HG3	2.14	0.46
1:A:589:LYS:HD2	1:A:589:LYS:HA	1.79	0.46
1:A:332:GLU:HG3	1:E:332:GLU:CG	2.32	0.46
1:C:419:PRO:HG3	1:C:448:GLY:HA3	1.98	0.46
1:D:285:PRO:HG2	1:D:288:THR:HG22	1.96	0.46
1:C:183:ARG:HG2	1:C:184:TYR:N	2.31	0.46
1:B:596:HIS:HD2	1:B:598:LEU:H	1.63	0.46
1:F:652:THR:HA	1:F:676:ASN:O	2.16	0.46
1:A:9:ASN:ND2	1:A:10:LYS:HZ2	2.14	0.46
1:F:183:ARG:HG2	1:F:184:TYR:N	2.31	0.46
1:A:347:ASP:O	1:A:350:VAL:HG12	2.16	0.46
1:B:26:PHE:HB3	1:B:165:LEU:CD2	2.46	0.46
1:A:342:VAL:CG1	1:A:343:GLN:N	2.79	0.46
1:D:659:LYS:HB3	1:D:659:LYS:NZ	2.31	0.46
1:F:586:ILE:HD12	1:F:586:ILE:N	2.30	0.46
1:F:4:LEU:HD12	1:F:38:LEU:HD21	1.98	0.45
1:D:8:GLU:HG2	1:D:9:ASN:N	2.31	0.45
1:A:255:ARG:HG2	1:A:257:ASP:HB2	1.97	0.45
1:E:96:ASP:OD1	1:E:97:PRO:HA	2.16	0.45
1:D:634:SER:O	1:D:635:SER:C	2.54	0.45
1:F:5:LYS:HB2	1:F:5:LYS:NZ	2.30	0.45
1:C:651:ILE:HD13	1:C:692:LEU:CD2	2.44	0.45
1:C:682:ILE:HG22	1:C:684:GLN:HG2	1.98	0.45
1:B:237:ASP:O	1:B:241:LYS:HB2	2.17	0.45
1:D:96:ASP:OD1	1:D:97:PRO:HA	2.16	0.45
1:C:347:ASP:O	1:C:350:VAL:HG12	2.16	0.45
1:D:602:LEU:HD22	1:D:608:ILE:CD1	2.46	0.45
1:F:555:TYR:HB3	1:F:606:SER:CB	2.46	0.45
1:D:156:GLU:O	1:D:160:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:293:PHE:O	1:B:299:ARG:HD3	2.16	0.45
1:E:183:ARG:HG2	1:E:184:TYR:N	2.32	0.45
1:D:669:GLN:HE21	1:D:669:GLN:HA	1.80	0.45
1:E:419:PRO:HG3	1:E:448:GLY:HA3	1.97	0.45
1:A:375:TYR:N	1:A:376:PRO:HD2	2.32	0.45
1:F:285:PRO:HG2	1:F:288:THR:HG22	1.98	0.45
1:A:156:GLU:O	1:A:160:GLU:HG3	2.16	0.45
1:D:183:ARG:HG2	1:D:184:TYR:N	2.31	0.45
1:A:88:ALA:O	1:A:348:ARG:HD2	2.17	0.45
1:D:419:PRO:HG3	1:D:448:GLY:HA3	1.98	0.45
1:C:602:LEU:HD22	1:C:608:ILE:CD1	2.47	0.45
1:D:140:ILE:N	1:D:140:ILE:HD12	2.32	0.45
1:B:258:GLN:HG2	1:D:268:GLY:N	2.30	0.45
1:C:510:LYS:HE2	1:C:610:LEU:HD13	1.99	0.45
1:C:183:ARG:O	1:C:185:SER:HA	2.16	0.44
1:E:4:LEU:HD23	1:E:17:ILE:CD1	2.47	0.44
1:F:255:ARG:HG2	1:F:257:ASP:HB2	1.99	0.44
1:F:172:PRO:HG2	1:F:177:PHE:CE1	2.52	0.44
1:E:80[A]:ARG:NH1	1:E:127:ASP:OD2	2.47	0.44
1:A:48:GLN:O	1:A:50:ASN:N	2.50	0.44
1:B:48:GLN:O	1:B:50:ASN:N	2.50	0.44
1:A:183:ARG:O	1:A:185:SER:HA	2.17	0.44
1:B:419:PRO:HD2	1:B:457:ILE:HG23	1.99	0.44
1:F:48:GLN:O	1:F:50:ASN:N	2.50	0.44
1:C:596:HIS:CD2	1:C:597:GLU:N	2.85	0.44
1:B:13:TYR:CE2	1:B:36:LYS:HD2	2.52	0.44
1:D:26:PHE:HB3	1:D:165:LEU:CD2	2.47	0.44
1:E:257:ASP:HB3	1:E:260:TYR:HB3	2.00	0.44
1:F:140:ILE:HD12	1:F:140:ILE:N	2.33	0.44
1:E:419:PRO:HD2	1:E:457:ILE:HG23	1.98	0.44
1:E:640:PHE:CE2	1:E:644:ILE:HD11	2.52	0.44
1:B:630:GLU:HB2	1:B:641:SER:HB3	1.99	0.44
1:B:30:GLN:HA	1:B:30:GLN:HE21	1.82	0.44
1:C:48:GLN:O	1:C:50:ASN:N	2.51	0.44
1:F:156:GLU:O	1:F:160:GLU:HG3	2.16	0.44
1:D:659:LYS:HA	1:D:670:VAL:HG23	2.00	0.44
1:A:309:TRP:O	1:A:312:GLN:HG3	2.17	0.44
1:A:659:LYS:HB3	1:A:659:LYS:NZ	2.33	0.44
1:B:545:ARG:HB2	1:C:494:PRO:HG3	1.98	0.44
1:F:659:LYS:NZ	1:F:659:LYS:HB3	2.32	0.44
1:F:309:TRP:O	1:F:312:GLN:HG3	2.17	0.44
1:A:586:ILE:HG22	1:A:587:ASN:N	2.33	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:589:LYS:HD2	1:C:589:LYS:HA	1.79	0.44
1:E:172:PRO:HG2	1:E:177:PHE:CE1	2.53	0.44
1:D:48:GLN:O	1:D:50:ASN:N	2.51	0.44
1:B:255:ARG:HG2	1:B:257:ASP:HB2	2.00	0.44
1:F:34:SER:OG	1:F:36:LYS:HB2	2.17	0.44
1:B:172:PRO:HG2	1:B:177:PHE:CE1	2.53	0.44
1:A:96:ASP:OD1	1:A:97:PRO:HA	2.18	0.44
1:D:257:ASP:HB3	1:D:260:TYR:HB3	1.98	0.44
1:A:419:PRO:HD2	1:A:457:ILE:HG23	2.00	0.44
1:E:375:TYR:N	1:E:376:PRO:HD2	2.33	0.44
1:B:555:TYR:HB3	1:B:606:SER:OG	2.17	0.44
1:A:172:PRO:HG2	1:A:177:PHE:CE1	2.53	0.44
1:C:665:SER:O	1:C:666:LYS:C	2.56	0.43
1:C:257:ASP:HB3	1:C:260:TYR:HB3	1.99	0.43
1:A:687:ARG:HB3	1:A:687:ARG:NH1	2.33	0.43
1:C:309:TRP:O	1:C:312:GLN:HG3	2.17	0.43
1:C:172:PRO:HG2	1:C:177:PHE:CE1	2.53	0.43
1:B:133:TYR:HB3	1:C:187:TYR:O	2.17	0.43
1:B:375:TYR:N	1:B:376:PRO:HD2	2.32	0.43
1:A:689:LYS:HE3	1:A:691:ASN:OD1	2.17	0.43
1:B:96:ASP:OD1	1:B:97:PRO:HA	2.19	0.43
1:B:610:LEU:HD11	1:B:616:ILE:CD1	2.48	0.43
1:B:589:LYS:HA	1:B:589:LYS:HD2	1.79	0.43
1:D:172:PRO:HG2	1:D:177:PHE:CE1	2.53	0.43
1:D:577:TRP:O	1:D:585:ILE:HA	2.19	0.43
1:D:107:SER:O	1:D:113:ALA:HA	2.19	0.43
1:E:48:GLN:O	1:E:50:ASN:N	2.51	0.43
1:B:663:ASP:C	1:B:665:SER:H	2.22	0.43
1:C:215:TYR:C	1:C:215:TYR:CD1	2.92	0.43
1:E:38:LEU:HD11	1:E:45:ILE:HD12	2.00	0.43
1:E:309:TRP:O	1:E:312:GLN:HG3	2.19	0.43
1:B:682:ILE:HG22	1:B:684:GLN:HG2	2.00	0.43
1:D:130:LEU:CD2	1:E:483:THR:HG22	2.49	0.43
1:A:26:PHE:HB3	1:A:165:LEU:CD2	2.49	0.43
1:D:314:VAL:O	1:D:392:ARG:NH2	2.52	0.43
1:B:269:LYS:HB3	1:B:298:THR:OG1	2.19	0.43
1:B:473:PHE:CG	1:B:552:VAL:HG21	2.53	0.43
1:F:183:ARG:O	1:F:185:SER:HA	2.19	0.43
1:C:314:VAL:O	1:C:392:ARG:NH2	2.52	0.43
1:E:107:SER:O	1:E:113:ALA:HA	2.19	0.43
1:F:373:ASN:O	1:F:403:TYR:HB2	2.18	0.43
1:C:107:SER:O	1:C:113:ALA:HA	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:373:ASN:O	1:D:403:TYR:HB2	2.18	0.43
1:F:4:LEU:HA	1:F:16:VAL:O	2.19	0.43
1:A:258:GLN:CD	1:E:278:LEU:HD21	2.39	0.43
1:A:258:GLN:HG2	1:E:268:GLY:H	1.84	0.43
1:C:37:SER:OG	1:C:40:GLU:HG3	2.19	0.43
1:B:339:SER:HG	1:E:339:SER:CB	2.31	0.43
1:F:466:LYS:NZ	3:F:2049:HOH:O	2.48	0.43
1:B:140:ILE:HD12	1:B:140:ILE:N	2.33	0.43
1:F:375:TYR:N	1:F:376:PRO:HD2	2.33	0.42
1:C:659:LYS:HB3	1:C:659:LYS:NZ	2.34	0.42
1:B:215:TYR:C	1:B:215:TYR:CD1	2.92	0.42
1:C:375:TYR:N	1:C:376:PRO:HD2	2.34	0.42
1:A:257:ASP:HB3	1:A:260:TYR:HB3	2.01	0.42
1:F:670:VAL:CG1	1:F:678:TYR:HB3	2.49	0.42
1:B:520:LEU:O	1:B:524:GLU:HG3	2.18	0.42
1:F:107:SER:O	1:F:113:ALA:HA	2.18	0.42
1:F:661:ILE:HA	1:F:666:LYS:O	2.19	0.42
1:E:130:LEU:HD22	1:F:483:THR:HG22	2.00	0.42
1:C:169:PRO:HA	1:C:407:GLN:O	2.19	0.42
1:B:9:ASN:OD1	1:B:29:GLU:HB2	2.17	0.42
1:D:651:ILE:HD13	1:D:692:LEU:CD2	2.45	0.42
1:E:26:PHE:HB3	1:E:165:LEU:CD2	2.49	0.42
1:B:9:ASN:C	1:B:10:LYS:HG2	2.40	0.42
1:A:107:SER:O	1:A:113:ALA:HA	2.19	0.42
1:D:215:TYR:C	1:D:215:TYR:CD1	2.92	0.42
1:E:428:LEU:HA	1:E:428:LEU:HD12	1.88	0.42
1:D:630:GLU:HB2	1:D:641:SER:HB3	2.00	0.42
1:C:88:ALA:O	1:C:348:ARG:HD2	2.19	0.42
1:D:666:LYS:HE2	1:D:667:GLU:H	1.84	0.42
1:D:375:TYR:N	1:D:376:PRO:HD2	2.33	0.42
1:D:669:GLN:CA	1:D:669:GLN:NE2	2.82	0.42
1:F:257:ASP:HB3	1:F:260:TYR:HB3	2.01	0.42
1:F:428:LEU:HD12	1:F:428:LEU:HA	1.88	0.42
1:A:140:ILE:HD12	1:A:140:ILE:N	2.34	0.42
1:B:659:LYS:NZ	1:B:659:LYS:HB3	2.34	0.42
1:B:643:GLU:OE1	1:B:687:ARG:CZ	2.67	0.42
1:C:26:PHE:HB3	1:C:165:LEU:CD2	2.48	0.42
1:E:215:TYR:CD1	1:E:215:TYR:C	2.92	0.42
1:D:309:TRP:O	1:D:312:GLN:HG3	2.19	0.42
1:D:324:PRO:HB3	1:D:375:TYR:CE2	2.55	0.42
1:C:339:SER:HB2	1:D:339:SER:CB	2.49	0.42
1:D:483:THR:HG22	1:F:130:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:373:ASN:O	1:C:403:TYR:HB2	2.20	0.42
1:D:169:PRO:HA	1:D:407:GLN:O	2.20	0.42
1:C:255:ARG:HG2	1:C:257:ASP:HB2	2.02	0.42
1:A:341:PRO:O	1:C:345:ARG:HG2	2.20	0.42
1:F:659:LYS:HD3	1:F:667:GLU:OE1	2.20	0.42
1:C:584:GLU:CD	1:C:586:ILE:HD11	2.40	0.42
1:D:12:VAL:HG23	1:D:161:LYS:HD3	2.01	0.42
1:B:169:PRO:HA	1:B:407:GLN:O	2.19	0.42
1:A:555:TYR:HB3	1:A:606:SER:OG	2.20	0.42
1:B:74:LEU:HA	1:B:74:LEU:HD12	1.89	0.41
1:F:26:PHE:HB3	1:F:165:LEU:CD2	2.49	0.41
1:E:473:PHE:CG	1:E:552:VAL:HG21	2.55	0.41
1:E:602:LEU:HD22	1:E:608:ILE:CD1	2.49	0.41
1:D:473:PHE:CG	1:D:552:VAL:HG21	2.56	0.41
1:D:344:PHE:HA	1:E:342:VAL:HA	2.03	0.41
1:C:630:GLU:HB2	1:C:641:SER:HB3	2.02	0.41
1:E:274:GLU:O	1:E:365:ARG:NH2	2.54	0.41
1:F:340:LEU:HD12	1:F:340:LEU:HA	1.92	0.41
1:B:107:SER:O	1:B:113:ALA:HA	2.20	0.41
1:E:37:SER:OG	1:E:40:GLU:HG3	2.21	0.41
1:C:229:PHE:O	1:C:232:PRO:HD3	2.19	0.41
1:F:520:LEU:O	1:F:524:GLU:HG3	2.19	0.41
1:D:255:ARG:HG2	1:D:257:ASP:HB2	2.02	0.41
1:A:17:ILE:HD11	1:A:45:ILE:HD13	2.02	0.41
1:C:388:ARG:HD3	3:C:2072:HOH:O	2.20	0.41
1:C:278:LEU:HD21	1:F:258:GLN:CD	2.41	0.41
1:B:640:PHE:HE2	1:B:644:ILE:HD11	1.83	0.41
1:E:663:ASP:O	1:E:664:ASP:HB2	2.21	0.41
1:C:520:LEU:O	1:C:524:GLU:HG3	2.20	0.41
1:C:17:ILE:HD11	1:C:45:ILE:HD13	2.03	0.41
1:E:140:ILE:N	1:E:140:ILE:HD12	2.35	0.41
1:A:651:ILE:HD13	1:A:692:LEU:CD2	2.49	0.41
1:B:637:GLU:OE2	1:B:689:LYS:HD2	2.21	0.41
1:E:255:ARG:HG2	1:E:257:ASP:HB2	2.02	0.41
1:D:572:LEU:HA	1:D:573:PRO:HD3	1.95	0.41
1:B:620:GLU:HA	1:B:633:SER:OG	2.20	0.41
1:A:682:ILE:HG22	1:A:684:GLN:HG2	2.03	0.41
1:D:510:LYS:HA	1:D:611:GLU:CB	2.50	0.41
1:D:8:GLU:O	1:D:9:ASN:CB	2.68	0.41
1:B:324:PRO:HB3	1:B:375:TYR:CE2	2.56	0.41
1:C:510:LYS:HA	1:C:611:GLU:HB2	2.03	0.41
1:B:257:ASP:HB3	1:B:260:TYR:HB3	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:51:LYS:NZ	1:A:51:LYS:CB	2.84	0.41
1:B:172:PRO:HG2	1:B:177:PHE:HE1	1.86	0.41
1:B:274:GLU:O	1:B:365:ARG:NH2	2.54	0.41
1:A:314:VAL:O	1:A:392:ARG:NH2	2.54	0.41
1:B:643:GLU:HA	1:B:686:ILE:O	2.21	0.41
1:F:96:ASP:OD1	1:F:97:PRO:HA	2.20	0.41
1:A:274:GLU:O	1:A:365:ARG:NH2	2.54	0.41
1:A:8:GLU:O	1:A:32:ILE:HB	2.21	0.41
1:D:589:LYS:HA	1:D:589:LYS:HD2	1.78	0.41
1:A:234:LYS:O	1:A:238:GLU:HG3	2.20	0.41
1:C:268:GLY:H	1:F:258:GLN:HG2	1.84	0.41
1:B:299:ARG:HG2	1:B:382:ALA:HB2	1.98	0.41
1:F:689:LYS:HE3	1:F:691:ASN:OD1	2.21	0.41
1:A:342:VAL:CG1	1:B:342:VAL:HG13	2.51	0.41
1:E:51:LYS:CB	1:E:51:LYS:NZ	2.84	0.41
1:F:274:GLU:O	1:F:365:ARG:NH2	2.54	0.41
1:C:79:LYS:HA	1:C:79:LYS:HD2	1.94	0.41
1:E:41:LEU:HD12	1:E:41:LEU:HA	1.91	0.41
1:C:473:PHE:CG	1:C:552:VAL:HG21	2.55	0.41
1:E:651:ILE:HD13	1:E:692:LEU:CD2	2.49	0.40
1:D:17:ILE:HD11	1:D:45:ILE:HD13	2.03	0.40
1:C:663:ASP:O	1:C:664:ASP:HB2	2.20	0.40
1:B:51:LYS:NZ	1:B:51:LYS:CB	2.83	0.40
1:B:10:LYS:HB3	1:B:10:LYS:HE2	1.90	0.40
1:B:512:LEU:HB3	1:B:513:PRO:HD3	2.02	0.40
1:A:290:TYR:HA	1:A:291:PRO:HD3	1.92	0.40
1:D:274:GLU:O	1:D:365:ARG:NH2	2.54	0.40
1:B:309:TRP:O	1:B:312:GLN:HG3	2.19	0.40
1:D:659:LYS:HA	1:D:670:VAL:CG2	2.51	0.40
1:F:630:GLU:HB2	1:F:641:SER:HB3	2.03	0.40
1:A:520:LEU:O	1:A:524:GLU:HG3	2.21	0.40
1:E:512:LEU:HB3	1:E:513:PRO:HD3	2.04	0.40
1:C:284:TRP:HE3	1:C:284:TRP:HA	1.86	0.40
1:C:258:GLN:CG	1:F:268:GLY:H	2.27	0.40
1:B:88:ALA:O	1:B:348:ARG:HD2	2.20	0.40
1:C:324:PRO:HB3	1:C:375:TYR:CE2	2.56	0.40
1:A:637:GLU:OE2	1:A:689:LYS:HD2	2.22	0.40
1:F:572:LEU:HA	1:F:573:PRO:HD3	1.94	0.40
1:C:274:GLU:O	1:C:365:ARG:NH2	2.55	0.40
1:A:215:TYR:CD1	1:A:215:TYR:C	2.93	0.40
1:D:48:GLN:HB3	1:D:49:GLY:H	1.70	0.40
1:B:130:LEU:HD22	1:C:483:THR:HG22	2.04	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:473:PHE:CG	1:A:552:VAL:HG21	2.56	0.40
1:D:520:LEU:O	1:D:524:GLU:HG3	2.22	0.40
1:C:31:LYS:C	1:C:32:ILE:HG13	2.42	0.40
1:D:428:LEU:HD12	1:D:428:LEU:HA	1.88	0.40
1:A:232:PRO:O	1:A:236:ILE:HG13	2.21	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	690/693 (100%)	648 (94%)	38 (6%)	4 (1%)	33	54
1	B	690/693 (100%)	645 (94%)	40 (6%)	5 (1%)	30	49
1	C	690/693 (100%)	647 (94%)	36 (5%)	7 (1%)	22	37
1	D	690/693 (100%)	653 (95%)	33 (5%)	4 (1%)	33	54
1	E	690/693 (100%)	654 (95%)	31 (4%)	5 (1%)	30	49
1	F	690/693 (100%)	652 (94%)	32 (5%)	6 (1%)	25	41
All	All	4140/4158 (100%)	3899 (94%)	210 (5%)	31 (1%)	30	49

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	635	SER
1	C	29	GLU
1	C	635	SER
1	C	665	SER
1	D	9	ASN
1	D	635	SER
1	E	9	ASN
1	F	29	GLU
1	F	31	LYS

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Mol	Chain	Res	Type
1	A	49	GLY
1	B	49	GLY
1	C	49	GLY
1	D	49	GLY
1	E	49	GLY
1	E	635	SER
1	F	32	ILE
1	F	49	GLY
1	C	666	LYS
1	C	688	GLY
1	E	29	GLU
1	E	688	GLY
1	F	30	GLN
1	B	688	GLY
1	F	688	GLY
1	A	688	GLY
1	B	29	GLU
1	B	635	SER
1	B	664	ASP
1	C	341	PRO
1	D	688	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	623/624 (100%)	605 (97%)	18 (3%)	55	80
1	B	623/624 (100%)	603 (97%)	20 (3%)	51	77
1	C	623/624 (100%)	600 (96%)	23 (4%)	45	71
1	D	623/624 (100%)	601 (96%)	22 (4%)	48	73
1	E	623/624 (100%)	604 (97%)	19 (3%)	53	79
1	F	623/624 (100%)	603 (97%)	20 (3%)	51	77
All	All	3738/3744 (100%)	3616 (97%)	122 (3%)	50	75

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	74	LEU
1	A	130	LEU
1	A	165	LEU
1	A	211	LEU
1	A	255	ARG
1	A	283	MET
1	A	329	ARG
1	A	392	ARG
1	A	398	LEU
1	A	413	TRP
1	A	426	LEU
1	A	430	LEU
1	A	434	LEU
1	A	463	LEU
1	A	564	LYS
1	A	628	ASN
1	A	659	LYS
1	B	9	ASN
1	B	41	LEU
1	B	74	LEU
1	B	130	LEU
1	B	165	LEU
1	B	211	LEU
1	B	243	ASN
1	B	255	ARG
1	B	283	MET
1	B	329	ARG
1	B	392	ARG
1	B	398	LEU
1	B	413	TRP
1	B	426	LEU
1	B	430	LEU
1	B	434	LEU
1	B	463	LEU
1	B	564	LYS
1	B	628	ASN
1	B	659	LYS
1	C	9	ASN
1	C	30	GLN
1	C	38	LEU
1	C	41	LEU
1	C	74	LEU

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Mol	Chain	Res	Type
1	C	130	LEU
1	C	165	LEU
1	C	211	LEU
1	C	243	ASN
1	C	255	ARG
1	C	283	MET
1	C	329	ARG
1	C	392	ARG
1	C	398	LEU
1	C	413	TRP
1	C	426	LEU
1	C	430	LEU
1	C	434	LEU
1	C	463	LEU
1	C	564	LYS
1	C	628	ASN
1	C	659	LYS
1	C	666	LYS
1	D	28	LEU
1	D	41	LEU
1	D	74	LEU
1	D	130	LEU
1	D	165	LEU
1	D	211	LEU
1	D	255	ARG
1	D	283	MET
1	D	329	ARG
1	D	392	ARG
1	D	398	LEU
1	D	413	TRP
1	D	426	LEU
1	D	430	LEU
1	D	434	LEU
1	D	463	LEU
1	D	564	LYS
1	D	628	ASN
1	D	659	LYS
1	D	666	LYS
1	D	669	GLN
1	D	672	LYS
1	E	4	LEU
1	E	41	LEU

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Mol	Chain	Res	Type
1	E	74	LEU
1	E	130	LEU
1	E	165	LEU
1	E	211	LEU
1	E	255	ARG
1	E	283	MET
1	E	329	ARG
1	E	392	ARG
1	E	398	LEU
1	E	413	TRP
1	E	426	LEU
1	E	430	LEU
1	E	434	LEU
1	E	463	LEU
1	E	564	LYS
1	E	628	ASN
1	E	659	LYS
1	F	4	LEU
1	F	38	LEU
1	F	41	LEU
1	F	74	LEU
1	F	130	LEU
1	F	165	LEU
1	F	211	LEU
1	F	255	ARG
1	F	283	MET
1	F	329	ARG
1	F	392	ARG
1	F	398	LEU
1	F	413	TRP
1	F	426	LEU
1	F	430	LEU
1	F	434	LEU
1	F	463	LEU
1	F	564	LYS
1	F	628	ASN
1	F	659	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN

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Mol	Chain	Res	Type
1	A	48	GLN
1	A	243	ASN
1	A	596	HIS
1	B	30	GLN
1	B	48	GLN
1	B	243	ASN
1	B	343	GLN
1	B	596	HIS
1	C	9	ASN
1	C	30	GLN
1	C	48	GLN
1	C	243	ASN
1	C	596	HIS
1	D	48	GLN
1	D	596	HIS
1	D	669	GLN
1	E	9	ASN
1	E	30	GLN
1	E	48	GLN
1	E	243	ASN
1	E	596	HIS
1	E	636	ASN
1	F	30	GLN
1	F	48	GLN
1	F	596	HIS
1	F	636	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 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$
2	BOG	A	2000	-	14,14,20	2.78	3 (21%)	18,19,25	0.67	0
2	BOG	B	2000	-	14,14,20	3.21	4 (28%)	18,19,25	0.65	0
2	BOG	C	2000	-	14,14,20	2.71	3 (21%)	18,19,25	0.68	0
2	BOG	D	2000	-	14,14,20	2.75	3 (21%)	18,19,25	0.69	0
2	BOG	E	2000	-	14,14,20	2.82	4 (28%)	18,19,25	0.68	0
2	BOG	F	2000	-	14,14,20	2.89	4 (28%)	18,19,25	0.66	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
2	BOG	A	2000	-	-	0/5/25/31	0/1/1/1
2	BOG	B	2000	-	-	0/5/25/31	0/1/1/1
2	BOG	C	2000	-	-	0/5/25/31	0/1/1/1
2	BOG	D	2000	-	-	0/5/25/31	0/1/1/1
2	BOG	E	2000	-	-	0/5/25/31	0/1/1/1
2	BOG	F	2000	-	-	0/5/25/31	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	BOG	C2'-C1'	-10.73	1.50	1.55
2	F	2000	BOG	C2'-C1'	-9.46	1.51	1.55
2	A	2000	BOG	C2'-C1'	-9.14	1.51	1.55
2	E	2000	BOG	C2'-C1'	-9.11	1.51	1.55
2	D	2000	BOG	C2'-C1'	-8.95	1.51	1.55
2	C	2000	BOG	C2'-C1'	-8.87	1.51	1.55
2	B	2000	BOG	O5-C1	3.04	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2000	BOG	O5-C1	2.94	1.49	1.41
2	F	2000	BOG	O5-C1	2.88	1.49	1.41
2	D	2000	BOG	O5-C1	2.81	1.49	1.41
2	A	2000	BOG	O5-C1	2.77	1.48	1.41
2	C	2000	BOG	O5-C1	2.77	1.48	1.41
2	E	2000	BOG	C4-C5	2.56	1.58	1.53
2	F	2000	BOG	C4-C5	2.53	1.58	1.53
2	B	2000	BOG	C4-C5	2.53	1.58	1.53
2	D	2000	BOG	C4-C5	2.37	1.58	1.53
2	A	2000	BOG	C4-C5	2.19	1.57	1.53
2	E	2000	BOG	O1-C1	2.15	1.44	1.40
2	C	2000	BOG	C4-C5	2.14	1.57	1.53
2	F	2000	BOG	O1-C1	2.06	1.43	1.40
2	B	2000	BOG	O1-C1	2.02	1.43	1.40

There are no bond angle outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	691/693 (99%)	0.10	34 (4%)	28	30	28, 42, 68, 87	0
1	B	691/693 (99%)	0.09	35 (5%)	27	28	30, 42, 69, 89	0
1	C	691/693 (99%)	0.11	28 (4%)	35	38	26, 41, 67, 85	0
1	D	691/693 (99%)	0.06	22 (3%)	45	48	28, 40, 67, 81	0
1	E	691/693 (99%)	0.04	17 (2%)	54	58	27, 39, 64, 84	0
1	F	691/693 (99%)	0.06	19 (2%)	52	55	27, 38, 62, 84	0
All	All	4146/4158 (99%)	0.08	155 (3%)	39	42	26, 40, 66, 89	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	49	GLY	5.4
1	E	49	GLY	5.2
1	B	3	ILE	4.9
1	C	29	GLU	4.6
1	A	31	LYS	4.6
1	B	628	ASN	4.5
1	F	30	GLN	4.4
1	A	49	GLY	4.3
1	D	346	ASP	4.3
1	B	32	ILE	4.2
1	F	32	ILE	4.1
1	A	693	GLU	4.1
1	F	49	GLY	4.0
1	B	29	GLU	4.0
1	A	346	ASP	4.0
1	C	635	SER	3.7
1	D	693	GLU	3.7
1	B	693	GLU	3.7
1	B	50	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	29	GLU	3.7
1	F	29	GLU	3.7
1	A	655	LYS	3.6
1	A	664	ASP	3.6
1	A	30	GLN	3.6
1	C	35	ASN	3.6
1	F	31	LYS	3.6
1	D	687	ARG	3.6
1	B	346	ASP	3.6
1	E	29	GLU	3.5
1	E	30	GLN	3.5
1	A	637	GLU	3.5
1	C	391	HIS	3.4
1	A	28	LEU	3.4
1	B	664	ASP	3.4
1	D	35	ASN	3.4
1	E	346	ASP	3.3
1	A	635	SER	3.3
1	B	637	GLU	3.3
1	C	227	TYR	3.2
1	A	628	ASN	3.2
1	C	661	ILE	3.2
1	F	227	TYR	3.2
1	B	566	GLU	3.1
1	E	48	GLN	3.1
1	C	658	SER	3.1
1	B	635	SER	3.1
1	B	391	HIS	3.1
1	C	637	GLU	3.0
1	E	31	LYS	3.0
1	C	656	PRO	3.0
1	C	3	ILE	3.0
1	C	566	GLU	3.0
1	C	693	GLU	3.0
1	F	50	ASN	2.9
1	C	346	ASP	2.9
1	F	35	ASN	2.9
1	F	574	ARG	2.9
1	A	574	ARG	2.9
1	D	227	TYR	2.9
1	A	48	GLN	2.9
1	C	48	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	666	LYS	2.9
1	C	50	ASN	2.9
1	D	49	GLY	2.8
1	B	241	LYS	2.8
1	A	669	GLN	2.8
1	A	687	ARG	2.8
1	B	654	GLU	2.8
1	E	574	ARG	2.8
1	E	10	LYS	2.8
1	A	634	SER	2.8
1	D	28	LEU	2.8
1	C	655	LYS	2.8
1	A	355	ASP	2.8
1	B	334	ARG	2.8
1	D	574	ARG	2.8
1	A	391	HIS	2.8
1	F	339	SER	2.7
1	B	587	ASN	2.7
1	E	227	TYR	2.7
1	B	681	LYS	2.7
1	C	665	SER	2.7
1	B	574	ARG	2.7
1	C	40	GLU	2.7
1	B	30	GLN	2.7
1	A	566	GLU	2.6
1	B	19	GLU	2.6
1	F	566	GLU	2.6
1	C	663	ASP	2.6
1	B	667	GLU	2.6
1	E	50	ASN	2.6
1	C	649	LEU	2.6
1	A	347	ASP	2.5
1	D	32	ILE	2.5
1	F	355	ASP	2.5
1	C	620	GLU	2.5
1	D	634	SER	2.5
1	F	346	ASP	2.5
1	A	27	PRO	2.5
1	C	27	PRO	2.5
1	B	665	SER	2.5
1	C	685	LYS	2.5
1	A	667	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	110	ASP	2.4
1	C	110	ASP	2.4
1	D	233	LYS	2.4
1	B	9	ASN	2.4
1	B	393	ASN	2.4
1	D	628	ASN	2.4
1	E	566	GLU	2.4
1	B	655	LYS	2.4
1	D	608	ILE	2.3
1	D	31	LYS	2.3
1	C	608	ILE	2.3
1	A	643	GLU	2.3
1	E	693	GLU	2.3
1	D	48	GLN	2.3
1	B	110	ASP	2.3
1	B	49	GLY	2.3
1	B	658	SER	2.3
1	B	27	PRO	2.3
1	C	634	SER	2.3
1	B	338	SER	2.3
1	B	684	GLN	2.2
1	A	587	ASN	2.2
1	A	3	ILE	2.2
1	F	19	GLU	2.2
1	F	655	LYS	2.2
1	A	565	GLU	2.2
1	E	565	GLU	2.2
1	A	589	LYS	2.2
1	F	237	ASP	2.2
1	D	566	GLU	2.2
1	D	655	LYS	2.2
1	D	334	ARG	2.1
1	A	641	SER	2.1
1	B	47	GLN	2.1
1	E	32	ILE	2.1
1	B	634	SER	2.1
1	E	391	HIS	2.1
1	A	227	TYR	2.1
1	B	227	TYR	2.1
1	D	635	SER	2.1
1	B	10	LYS	2.1
1	C	628	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	665	SER	2.1
1	D	616	ILE	2.1
1	E	602	LEU	2.1
1	D	143	ASP	2.1
1	D	565	GLU	2.0
1	F	118	PHE	2.0
1	E	655	LYS	2.0
1	F	27	PRO	2.0
1	A	19	GLU	2.0
1	F	211	LEU	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	BOG	F	2000	14/20	0.25	6.81	62,64,65,65	0
2	BOG	E	2000	14/20	0.24	6.62	62,64,65,66	0
2	BOG	A	2000	14/20	0.26	5.32	60,64,65,66	0
2	BOG	D	2000	14/20	0.31	5.12	62,64,64,65	0
2	BOG	B	2000	14/20	0.23	2.89	64,65,66,66	0
2	BOG	C	2000	14/20	0.23	2.67	63,64,65,65	0

6.5 Other polymers ⓘ

There are no such residues in this entry.