



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:07 PM UTC

PDB ID : 2WC0 / pdb_00002wc0
Title : crystal structure of human insulin degrading enzyme in complex with iodinated insulin
Authors : Manolopoulou, M.; Guo, Q.; Malito, E.; Schilling, A.B.; Tang, W.J.
Deposited on : 2009-03-06
Resolution : 2.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

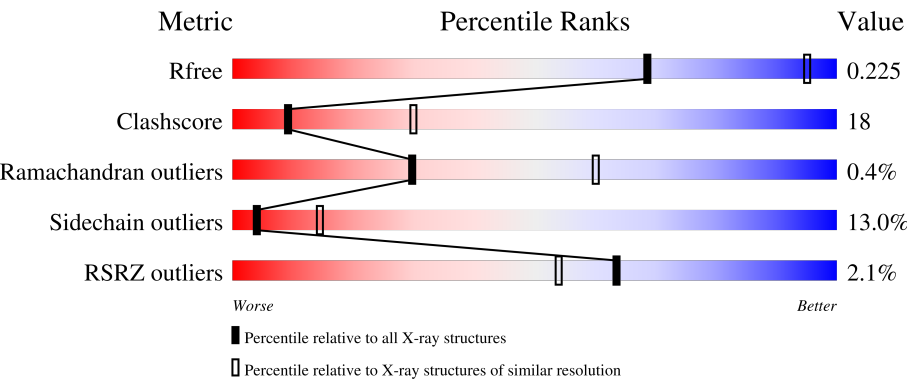
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	990	55% 34% 6% ••
1	B	990	% 54% 33% 9% ••
2	C	21	33% 24% 38% 38%
2	E	21	38% 19% 48% 29% 5%
3	D	30	30% 23% 27% 7% 10% 33%

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Mol	Chain	Length	Quality of chain
3	F	30	30% 27% 20% 10% 10% 33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16597 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 INSULIN-DEGRADING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	953	Total	C	N	O	S	0	0	1
			7781	5013	1307	1439	22			
1	B	955	Total	C	N	O	S	0	0	1
			7790	5019	1308	1441	22			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	LEU	CYS	engineered mutation	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735
A	974	ALA	CYS	engineered mutation	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is a protein called INSULIN A CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	21	Total 155	C 95	N 24	O 32	S 4	0	0	1
2	E	21	Total 155	C 95	N 24	O 32	S 4	0	0	1

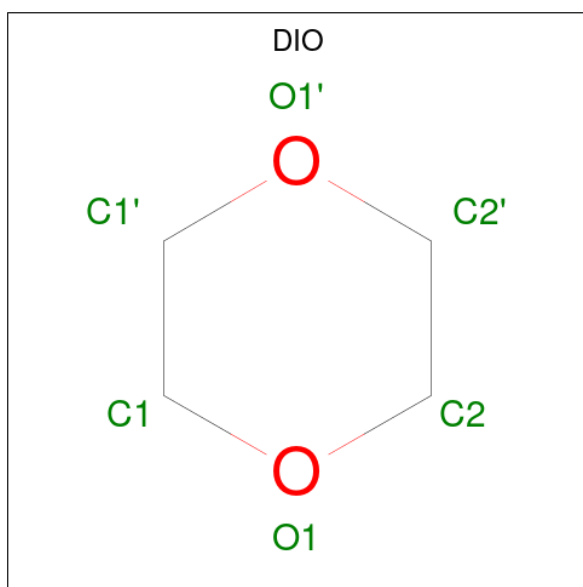
- Molecule 3 is a protein called INSULIN B CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	20	Total 153	C 99	N 26	O 26	S 2	0	0	0
3	F	20	Total 153	C 99	N 26	O 26	S 2	0	0	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: C₄H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	4	2		
5	A	1	Total	C	O	0	0
			6	4	2		
5	A	1	Total	C	O	0	0
			6	4	2		
5	A	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	189	Total	O	0	0
			189	189		
6	B	163	Total	O	0	0
			163	163		
6	C	3	Total	O	0	0
			3	3		
6	D	2	Total	O	0	0
			2	2		

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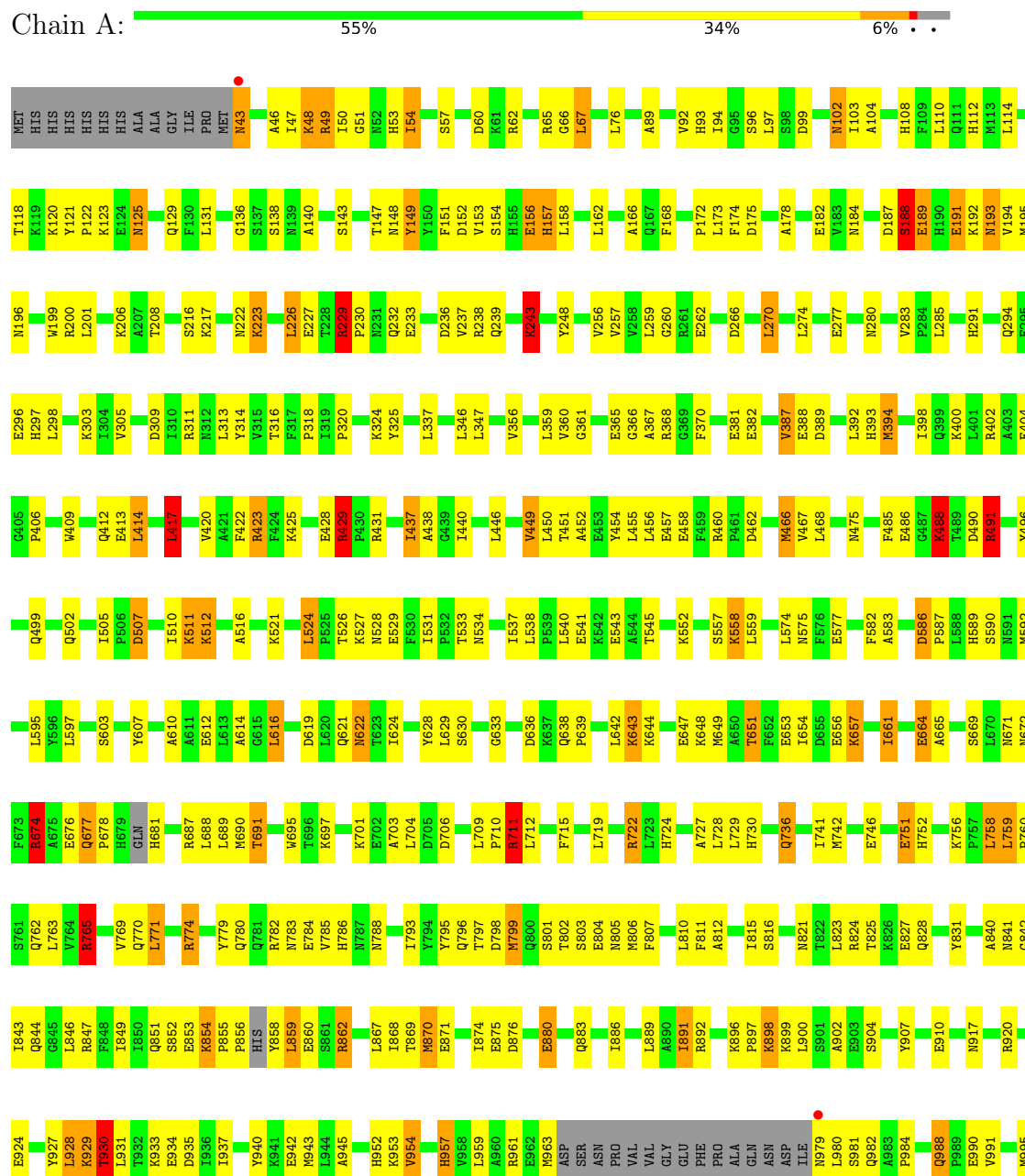
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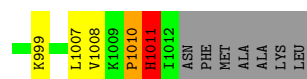
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total	O	0	0
			1	1		
6	F	2	Total	O	0	0
			2	2		

3 Residue-property plots

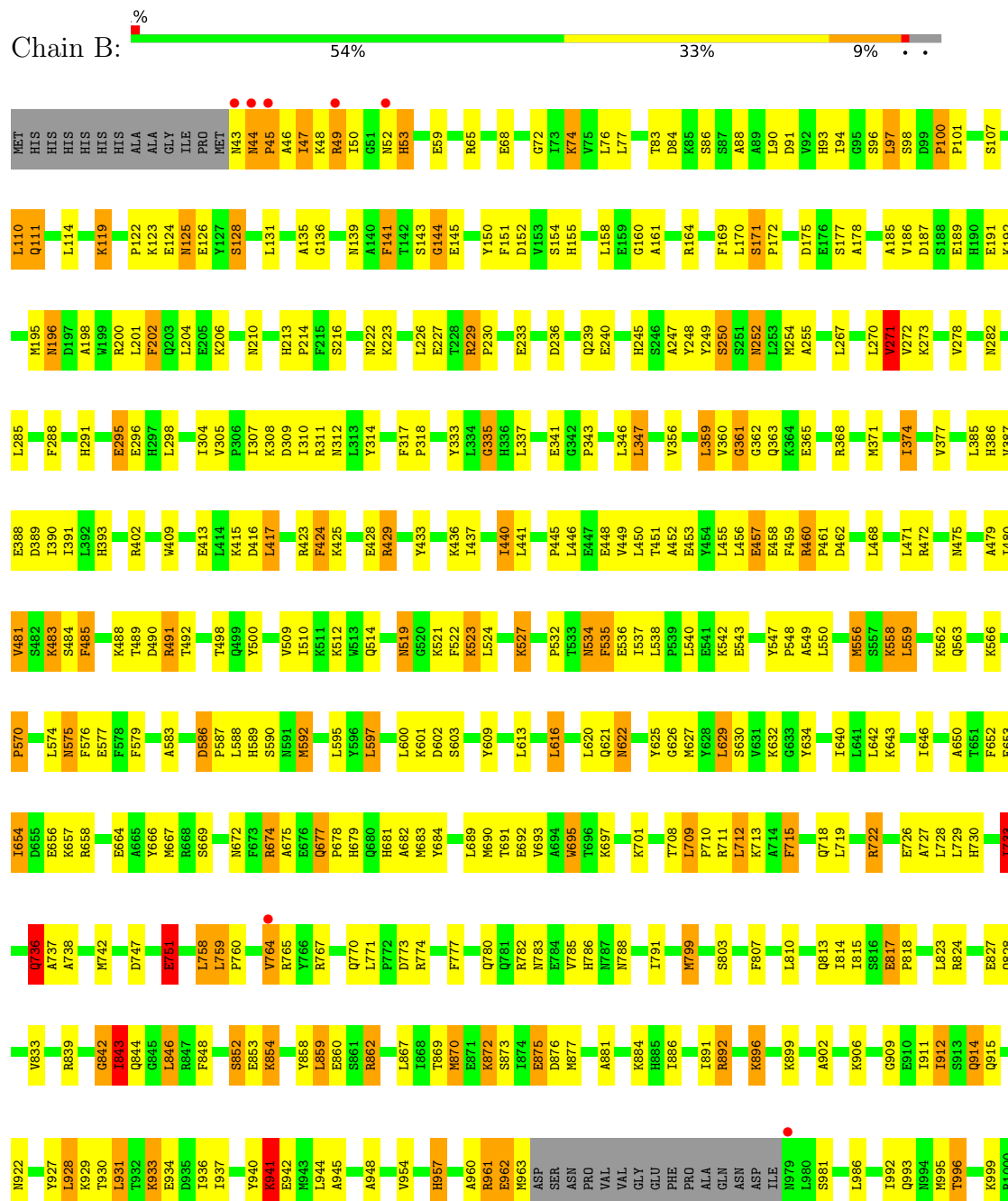
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: INSULIN-DEGRADING ENZYME

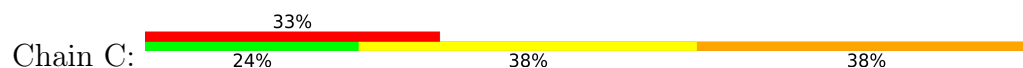


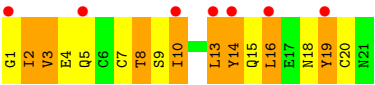


- Molecule 1: INSULIN-DEGRADING ENZYME

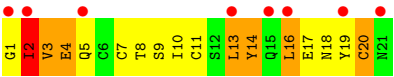
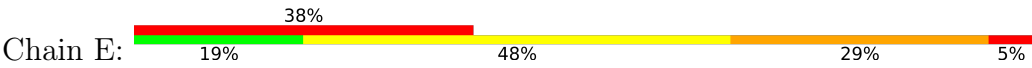


- Molecule 2: INSULIN A CHAIN

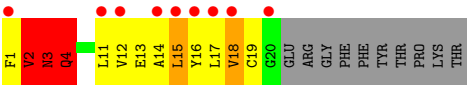




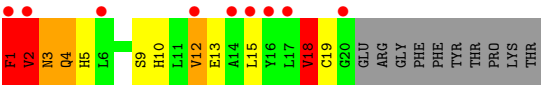
● Molecule 2: INSULIN A CHAIN



● Molecule 3: INSULIN B CHAIN



● Molecule 3: INSULIN B CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	263.17Å 263.17Å 90.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.85 – 2.80 29.85 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.85-2.80) 99.6 (29.85-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.170 , 0.220 0.181 , 0.225	Depositor DCC
R_{free} test set	4422 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16597	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DIO, ZN

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	1.72	80/7973 (1.0%)	1.55	79/10784 (0.7%)
1	B	1.62	54/7985 (0.7%)	1.54	90/10805 (0.8%)
2	C	1.62	1/156 (0.6%)	2.05	7/211 (3.3%)
2	E	1.28	2/156 (1.3%)	1.87	5/211 (2.4%)
3	D	2.09	7/156 (4.5%)	2.28	13/211 (6.2%)
3	F	1.74	1/156 (0.6%)	2.36	7/211 (3.3%)
All	All	1.67	145/16582 (0.9%)	1.57	201/22433 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	D	1	2
All	All	1	3

All (145) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	ALA	CA-CB	-15.28	1.33	1.53
1	B	764	VAL	CA-CB	13.27	1.69	1.54
1	A	305	VAL	CA-CB	8.69	1.62	1.53
1	B	53	HIS	N-CA	-8.44	1.36	1.46
1	B	570	PRO	CA-C	8.32	1.60	1.53
1	A	614	ALA	CA-CB	-7.79	1.41	1.53
3	F	18	VAL	CA-CB	7.75	1.65	1.54
1	A	1008	VAL	CA-CB	7.71	1.63	1.54
1	B	271	VAL	CA-CB	7.61	1.63	1.54
1	B	992	ILE	C-O	-7.55	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	ASN	C-O	-7.54	1.14	1.24
1	A	502	GLN	C-O	-7.52	1.15	1.24
1	B	385	LEU	C-O	-7.26	1.14	1.24
1	A	703	ALA	CA-CB	-7.18	1.41	1.53
1	A	406	PRO	C-O	-7.17	1.15	1.23
1	A	769	VAL	CA-CB	-7.13	1.47	1.54
1	A	880	GLU	N-CA	-6.97	1.38	1.46
1	A	1011	HIS	C-N	-6.92	1.23	1.33
1	B	361	GLY	C-O	6.77	1.34	1.23
3	D	3	ASN	CA-C	6.72	1.62	1.53
3	D	3	ASN	N-CA	-6.71	1.37	1.45
1	B	854	LYS	CA-C	6.69	1.60	1.53
1	B	654	ILE	C-O	-6.69	1.16	1.24
3	D	12	VAL	CA-CB	6.66	1.61	1.54
1	A	243	LYS	CG-CD	6.61	1.72	1.52
1	B	695	TRP	C-O	-6.54	1.16	1.24
1	A	543	GLU	CA-C	6.54	1.61	1.52
1	B	814	ILE	CA-CB	-6.48	1.46	1.54
1	A	438	ALA	CA-CB	-6.47	1.43	1.53
1	B	1011	HIS	C-N	-6.47	1.24	1.33
1	A	811	PHE	N-CA	-6.34	1.38	1.46
1	A	208	THR	N-CA	-6.31	1.38	1.46
1	B	450	LEU	C-O	-6.31	1.15	1.24
1	B	312	ASN	CA-C	-6.29	1.45	1.52
1	A	191	GLU	C-O	-6.29	1.16	1.24
1	A	991	VAL	C-O	-6.29	1.17	1.23
1	A	590	SER	N-CA	-6.25	1.39	1.46
1	B	718	GLN	CA-CB	6.24	1.63	1.53
1	A	387	VAL	CA-CB	-6.22	1.46	1.54
1	A	665	ALA	CA-CB	-6.22	1.43	1.53
3	D	18	VAL	CA-CB	6.22	1.62	1.54
1	A	121	TYR	CA-CB	-6.16	1.45	1.53
1	B	527	LYS	C-O	-6.15	1.16	1.23
1	B	391	ILE	N-CA	-6.14	1.39	1.46
1	B	542	LYS	N-CA	6.13	1.53	1.46
1	A	633	GLY	C-O	6.12	1.30	1.24
1	A	414	LEU	CA-C	6.08	1.60	1.52
1	B	492	THR	C-O	-6.07	1.17	1.23
1	A	516	ALA	CA-CB	-6.07	1.44	1.53
1	A	537	ILE	C-O	-6.04	1.15	1.23
1	B	305	VAL	CA-CB	6.04	1.60	1.53
1	B	1006	PRO	N-CA	6.03	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	669	SER	CA-CB	-6.02	1.44	1.53
1	A	46	ALA	CA-CB	-6.01	1.43	1.53
1	A	366	GLY	C-O	-6.01	1.15	1.23
1	A	647	GLU	N-CA	-6.00	1.39	1.46
1	A	583	ALA	CA-CB	-5.99	1.43	1.53
1	B	669	SER	N-CA	-5.97	1.39	1.46
1	A	860	GLU	C-O	5.97	1.31	1.24
2	E	8	THR	CA-CB	5.97	1.62	1.53
1	A	812	ALA	CA-CB	-5.96	1.43	1.53
1	B	843	ILE	C-O	5.95	1.29	1.23
1	A	320	PRO	CA-C	5.94	1.59	1.52
1	A	751	GLU	C-O	-5.93	1.17	1.24
1	A	409	TRP	CA-C	5.92	1.60	1.52
1	B	892	ARG	NE-CZ	5.87	1.39	1.33
2	C	20	CYS	C-N	-5.87	1.25	1.33
1	A	538	LEU	N-CA	5.86	1.52	1.45
1	A	511	LYS	CG-CD	5.86	1.70	1.52
1	A	417	LEU	N-CA	-5.84	1.39	1.46
1	B	304	ILE	N-CA	-5.84	1.39	1.46
1	A	797	THR	C-O	-5.79	1.15	1.25
1	A	825	THR	CA-C	-5.75	1.45	1.52
1	A	854	LYS	CG-CD	5.74	1.69	1.52
1	A	149	TYR	C-O	5.74	1.30	1.24
1	A	123	LYS	N-CA	5.71	1.53	1.46
1	A	999	LYS	C-O	5.71	1.30	1.24
1	B	632	LYS	CG-CD	5.71	1.69	1.52
1	A	157	HIS	N-CA	-5.70	1.39	1.46
1	B	736	GLN	N-CA	-5.68	1.38	1.46
2	E	20	CYS	C-N	-5.64	1.25	1.33
1	B	391	ILE	C-O	5.62	1.30	1.24
1	A	785	VAL	CA-CB	5.61	1.62	1.54
1	A	104	ALA	CA-CB	-5.58	1.44	1.53
1	A	545	THR	N-CA	5.58	1.52	1.45
1	A	619	ASP	N-CA	-5.58	1.39	1.46
3	D	4	GLN	CA-C	5.58	1.61	1.53
1	B	632	LYS	CD-CE	5.58	1.69	1.52
1	A	178	ALA	CA-CB	-5.55	1.44	1.53
1	A	711	ARG	CA-C	5.53	1.59	1.52
1	A	854	LYS	CB-CG	5.51	1.69	1.52
3	D	14	ALA	CA-C	5.50	1.60	1.52
1	A	243	LYS	CB-CG	5.48	1.68	1.52
1	B	377	VAL	C-O	5.48	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	14	ALA	CA-CB	5.47	1.62	1.53
1	B	317	PHE	CA-C	-5.43	1.48	1.52
1	B	675	ALA	CA-CB	-5.43	1.44	1.53
1	B	643	LYS	CA-C	-5.42	1.45	1.52
1	B	603	SER	C-O	-5.41	1.16	1.24
1	A	892	ARG	NE-CZ	5.41	1.39	1.33
1	B	902	ALA	CA-C	5.41	1.59	1.52
1	A	871	GLU	CG-CD	5.40	1.65	1.52
1	A	394	MET	C-O	5.39	1.30	1.24
1	B	941	LYS	CG-CD	5.38	1.68	1.52
1	B	666	TYR	CA-C	5.37	1.59	1.52
1	A	612	GLU	CA-C	5.37	1.59	1.52
1	A	491	ARG	CA-C	-5.36	1.46	1.52
1	A	458	GLU	CB-CG	-5.32	1.36	1.52
1	B	996	THR	C-O	-5.32	1.18	1.24
1	A	907	TYR	C-O	-5.32	1.17	1.24
1	A	543	GLU	N-CA	5.30	1.53	1.46
1	A	669	SER	N-CA	-5.28	1.40	1.46
1	B	543	GLU	CA-C	5.26	1.59	1.52
1	A	48	LYS	C-O	-5.25	1.17	1.24
1	B	646	ILE	C-O	-5.25	1.18	1.24
1	B	144	GLY	N-CA	5.24	1.52	1.45
1	A	398	ILE	CA-CB	-5.22	1.48	1.54
1	B	247	ALA	CA-C	5.22	1.59	1.52
1	A	54	ILE	CA-CB	5.21	1.60	1.54
1	B	550	LEU	C-O	-5.21	1.17	1.23
1	A	862	ARG	CA-C	5.17	1.59	1.52
1	B	314	TYR	CA-C	-5.17	1.46	1.52
1	A	505	ILE	CA-C	5.16	1.58	1.52
1	A	779	TYR	CA-C	-5.15	1.46	1.52
1	B	575	ASN	CA-C	-5.15	1.46	1.52
1	A	1008	VAL	N-CA	5.14	1.52	1.46
1	A	166	ALA	CA-CB	-5.13	1.45	1.53
1	A	188	SER	CA-C	5.13	1.59	1.52
1	A	449	VAL	C-O	-5.11	1.17	1.24
1	A	990	GLU	CA-C	5.11	1.59	1.52
1	B	549	ALA	CA-CB	-5.09	1.44	1.53
1	B	751	GLU	C-O	-5.09	1.17	1.24
1	B	252	ASN	N-CA	5.09	1.52	1.46
1	A	243	LYS	CD-CE	5.07	1.67	1.52
1	A	788	ASN	C-O	-5.06	1.17	1.23
1	B	650	ALA	C-O	-5.06	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	711	ARG	CA-CB	5.05	1.61	1.53
1	A	654	ILE	C-O	-5.05	1.18	1.24
1	B	416	ASP	N-CA	-5.04	1.40	1.46
1	A	189	GLU	CD-OE1	5.04	1.34	1.25
1	A	260	GLY	N-CA	5.04	1.51	1.45
1	B	535	PHE	CA-C	-5.04	1.46	1.52
1	A	664	GLU	N-CA	-5.03	1.40	1.46
1	B	542	LYS	CA-CB	5.03	1.61	1.53
1	B	892	ARG	N-CA	5.00	1.52	1.46

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	VAL	N-CA-CB	-14.82	86.78	111.23
3	F	1	PHE	N-CA-C	-14.40	70.69	111.00
1	B	52	ASN	N-CA-C	13.57	127.57	111.02
2	C	14	TYR	N-CA-C	12.05	123.97	111.07
3	F	19	CYS	N-CA-C	10.92	127.76	112.04
1	B	295	GLU	N-CA-C	10.49	133.14	110.80
2	E	16	LEU	N-CA-C	10.47	122.66	111.03
3	F	2	VAL	CB-CA-C	-10.36	94.30	111.29
1	B	295	GLU	CB-CA-C	-9.81	90.90	110.42
1	A	988	GLN	CA-C-N	-9.63	110.97	120.21
1	A	988	GLN	C-N-CA	-9.63	110.97	120.21
3	D	3	ASN	CA-C-N	9.51	140.98	122.73
3	D	3	ASN	C-N-CA	9.51	140.98	122.73
1	B	189	GLU	N-CA-C	-8.96	101.21	110.97
1	B	49	ARG	CB-CA-C	8.62	131.52	112.82
1	B	53	HIS	N-CA-C	-8.10	94.57	107.93
1	B	202	PHE	N-CA-C	-8.03	102.48	111.07
1	A	49	ARG	CB-CA-C	7.90	125.41	110.56
1	A	582	PHE	N-CA-C	7.84	122.52	113.19
3	D	2	VAL	N-CA-C	7.80	123.36	112.35
2	E	2	ILE	CB-CA-C	7.70	123.92	111.29
1	B	667	MET	CG-SD-CE	7.63	117.69	100.90
2	C	14	TYR	CB-CA-C	-7.61	98.93	110.88
1	A	129	GLN	N-CA-C	7.51	119.47	111.28
1	A	942	GLU	N-CA-C	7.38	119.40	111.36
1	B	733	ILE	CB-CA-C	-7.37	101.56	111.80
1	A	651	THR	N-CA-C	-7.34	102.41	112.03
3	D	3	ASN	N-CA-C	-7.32	99.12	110.17
3	D	3	ASN	CB-CA-C	-7.14	97.32	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	VAL	CB-CA-C	-7.14	101.14	110.84
1	B	239	GLN	N-CA-C	-7.10	103.47	111.07
1	B	643	LYS	N-CA-C	-7.05	103.60	111.28
1	A	876	ASP	N-CA-C	7.03	119.79	111.71
1	B	674	ARG	NE-CZ-NH1	6.97	128.47	121.50
1	B	751	GLU	N-CA-C	6.95	125.61	110.80
1	B	210	ASN	CA-C-N	-6.94	111.64	119.28
1	B	210	ASN	C-N-CA	-6.94	111.64	119.28
3	D	2	VAL	CA-C-N	-6.92	110.39	122.64
3	D	2	VAL	C-N-CA	-6.92	110.39	122.64
1	B	667	MET	N-CA-C	-6.84	103.76	111.14
1	B	460	ARG	NE-CZ-NH1	-6.83	114.67	121.50
1	B	189	GLU	CG-CD-OE2	6.82	134.09	118.40
1	A	437	ILE	CB-CA-C	-6.82	102.94	112.14
1	B	100	PRO	CA-C-N	6.81	126.51	119.56
1	B	100	PRO	C-N-CA	6.81	126.51	119.56
2	C	14	TYR	CA-C-N	6.79	129.68	120.38
2	C	14	TYR	C-N-CA	6.79	129.68	120.38
1	A	870	MET	N-CA-C	6.78	119.53	111.33
3	D	14	ALA	CA-C-N	6.72	133.54	121.92
3	D	14	ALA	C-N-CA	6.72	133.54	121.92
1	B	452	ALA	CA-C-N	-6.68	109.44	121.14
1	B	452	ALA	C-N-CA	-6.68	109.44	121.14
1	A	681	HIS	N-CA-CB	6.64	121.78	110.50
2	E	16	LEU	CB-CA-C	-6.62	100.69	110.95
1	B	654	ILE	N-CA-C	6.61	118.11	109.58
1	B	948	ALA	CA-C-N	-6.56	112.94	119.56
1	B	948	ALA	C-N-CA	-6.56	112.94	119.56
1	B	853	GLU	N-CA-C	-6.55	105.58	113.97
1	A	871	GLU	N-CA-CB	6.53	119.48	110.01
3	D	14	ALA	N-CA-C	6.52	124.70	110.80
1	B	854	LYS	CB-CG-CD	6.45	126.14	111.30
1	A	283	VAL	CB-CA-C	-6.44	103.94	110.89
1	A	524	LEU	CA-C-N	-6.42	114.11	120.98
1	A	524	LEU	C-N-CA	-6.42	114.11	120.98
1	A	681	HIS	CB-CA-C	-6.40	97.94	110.10
1	B	914	GLN	CB-CA-C	-6.33	101.72	111.66
1	B	335	GLY	N-CA-C	-6.32	104.84	112.49
1	A	816	SER	N-CA-C	6.25	117.79	110.97
1	A	674	ARG	N-CA-C	-6.24	104.92	112.54
1	A	507	ASP	N-CA-C	6.24	118.88	111.33
1	B	630	SER	CA-CB-OG	-6.23	98.65	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	GLU	N-CA-C	6.22	118.85	111.33
1	B	715	PHE	N-CA-C	6.21	118.84	111.33
1	A	774	ARG	CA-C-N	-6.20	115.09	122.16
1	A	774	ARG	C-N-CA	-6.20	115.09	122.16
1	A	812	ALA	N-CA-C	-6.19	104.61	111.36
1	A	541	GLU	N-CA-C	6.17	118.74	110.35
1	A	1010	PRO	N-CA-C	-6.17	101.20	111.26
1	A	621	GLN	N-CA-C	6.16	118.44	109.07
1	A	496	TYR	N-CA-C	-6.10	106.81	114.56
3	F	1	PHE	CB-CA-C	6.10	121.69	110.10
2	E	14	TYR	N-CA-C	6.10	117.62	110.97
2	C	16	LEU	N-CA-C	6.09	117.79	111.03
1	B	892	ARG	NE-CZ-NH2	6.04	124.64	119.20
1	A	65	ARG	NE-CZ-NH1	-6.03	115.47	121.50
3	D	14	ALA	CB-CA-C	6.01	122.39	110.42
1	B	107	SER	N-CA-C	5.99	117.89	111.36
2	E	11	CYS	N-CA-C	5.97	119.40	110.14
1	B	374	ILE	N-CA-C	5.96	118.57	108.86
1	B	652	PHE	CA-C-N	-5.95	114.72	123.05
1	B	652	PHE	C-N-CA	-5.95	114.72	123.05
1	B	876	ASP	N-CA-C	-5.92	105.37	113.30
1	A	449	VAL	CB-CA-C	-5.91	103.00	112.16
1	B	337	LEU	N-CA-C	5.88	118.57	111.40
1	A	49	ARG	CA-C-N	5.88	131.17	123.06
1	A	49	ARG	C-N-CA	5.88	131.17	123.06
1	B	271	VAL	N-CA-CB	5.87	118.09	110.57
1	A	420	VAL	N-CA-C	-5.84	106.02	111.45
1	B	186	VAL	N-CA-C	-5.83	105.06	110.53
3	F	12	VAL	N-CA-C	5.80	115.98	110.53
1	A	256	VAL	CB-CA-C	-5.79	101.99	110.62
1	A	930	THR	CA-CB-CG2	5.79	120.33	110.50
1	A	457	GLU	N-CA-C	-5.78	98.49	110.80
1	A	502	GLN	N-CA-C	5.78	118.31	108.90
1	B	839	ARG	NE-CZ-NH1	-5.77	115.73	121.50
1	A	229	ARG	CA-C-N	-5.77	112.93	119.28
1	A	229	ARG	C-N-CA	-5.77	112.93	119.28
1	B	957	HIS	CA-C-N	-5.77	115.26	123.10
1	B	957	HIS	C-N-CA	-5.77	115.26	123.10
2	C	19	TYR	N-CA-C	5.76	119.29	112.72
3	D	2	VAL	CB-CA-C	-5.75	103.55	111.65
1	B	1001	GLY	CA-C-N	-5.74	115.69	123.96
1	B	1001	GLY	C-N-CA	-5.74	115.69	123.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	19	CYS	N-CA-C	5.73	119.65	107.67
1	A	821	ASN	N-CA-C	5.72	118.25	111.33
1	B	962	GLU	N-CA-C	5.71	119.61	107.67
1	A	248	TYR	CA-C-N	-5.70	113.77	122.21
1	A	248	TYR	C-N-CA	-5.70	113.77	122.21
1	B	669	SER	N-CA-CB	-5.66	101.81	110.01
1	A	558	LYS	CB-CA-C	5.65	119.84	110.74
1	A	1010	PRO	CA-C-O	-5.65	115.16	121.32
1	A	305	VAL	CA-C-N	-5.64	114.95	120.98
1	A	305	VAL	C-N-CA	-5.64	114.95	120.98
1	A	65	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	A	697	LYS	N-CA-C	-5.62	105.25	111.71
1	B	954	VAL	CB-CA-C	-5.62	101.70	110.69
1	A	704	LEU	N-CA-C	5.60	119.21	112.38
1	A	902	ALA	N-CA-C	-5.60	105.32	111.82
1	B	471	LEU	N-CA-C	5.58	118.23	108.52
1	B	47	ILE	N-CA-C	5.57	115.28	107.37
1	B	52	ASN	CB-CA-C	-5.56	102.08	110.92
1	B	359	LEU	CA-C-N	-5.55	115.27	122.99
1	B	359	LEU	C-N-CA	-5.55	115.27	122.99
1	B	402	ARG	N-CA-C	-5.55	105.13	111.07
1	B	986	LEU	CA-C-N	5.52	125.83	119.92
1	B	986	LEU	C-N-CA	5.52	125.83	119.92
1	B	305	VAL	CA-C-N	-5.52	115.07	120.98
1	B	305	VAL	C-N-CA	-5.52	115.07	120.98
1	B	537	ILE	CB-CA-C	-5.52	105.27	111.23
3	F	3	ASN	CB-CA-C	5.49	121.93	111.17
1	B	360	VAL	CA-C-N	-5.48	115.67	121.48
1	B	360	VAL	C-N-CA	-5.48	115.67	121.48
1	A	954	VAL	CB-CA-C	-5.43	102.00	110.69
1	A	681	HIS	CA-CB-CG	5.43	119.23	113.80
1	A	533	THR	CA-C-N	-5.40	115.44	123.11
1	A	533	THR	C-N-CA	-5.40	115.44	123.11
1	B	161	ALA	N-CA-C	-5.40	105.04	111.69
1	B	813	GLN	N-CA-C	-5.40	105.31	111.14
1	A	610	ALA	N-CA-C	-5.39	105.40	111.28
2	C	8	THR	CB-CA-C	5.39	119.41	110.90
1	B	666	TYR	N-CA-C	5.38	117.15	111.28
1	A	957	HIS	CA-C-N	-5.38	115.80	123.11
1	A	957	HIS	C-N-CA	-5.38	115.80	123.11
1	A	910	GLU	N-CA-C	-5.37	105.50	111.36
1	A	366	GLY	N-CA-C	-5.37	100.46	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	PHE	N-CA-C	5.37	117.55	109.23
1	A	765	ARG	CB-CA-C	5.36	118.64	109.80
1	B	390	ILE	N-CA-C	-5.33	105.30	110.42
1	A	193	ASN	N-CA-C	5.33	119.50	112.89
1	B	480	ILE	CA-C-N	-5.33	116.17	123.14
1	B	480	ILE	C-N-CA	-5.33	116.17	123.14
1	B	872	LYS	N-CA-C	-5.31	105.58	111.36
1	A	661	ILE	CB-CA-C	-5.28	105.22	111.81
1	B	535	PHE	N-CA-C	-5.26	105.58	112.41
1	A	488	LYS	N-CA-C	5.24	121.96	110.80
1	B	854	LYS	CA-CB-CG	5.24	124.57	114.10
1	A	917	ASN	N-CA-CB	-5.23	104.49	110.35
1	A	122	PRO	CA-C-N	-5.22	113.45	120.82
1	A	122	PRO	C-N-CA	-5.22	113.45	120.82
1	A	456	LEU	N-CA-C	-5.20	102.36	110.42
1	A	175	ASP	N-CA-C	5.18	117.54	110.24
1	B	576	PHE	CB-CA-C	-5.16	100.61	109.65
1	B	842	GLY	N-CA-C	-5.15	107.43	114.64
1	B	833	VAL	CB-CA-C	-5.15	102.85	111.29
1	B	961	ARG	CA-C-N	-5.14	115.32	123.24
1	B	961	ARG	C-N-CA	-5.14	115.32	123.24
1	B	424	PHE	N-CA-C	5.12	118.35	112.57
1	A	897	PRO	CA-C-N	-5.12	113.41	122.26
1	A	897	PRO	C-N-CA	-5.12	113.41	122.26
1	B	343	PRO	CA-C-O	-5.11	115.76	121.23
1	A	429	ARG	CG-CD-NE	-5.11	100.76	112.00
1	B	751	GLU	CB-CA-C	-5.11	100.26	110.42
1	B	448	GLU	N-CA-C	5.11	119.20	112.92
1	B	884	LYS	N-CA-C	-5.09	105.73	111.28
1	A	232	GLN	CA-C-N	-5.09	114.50	122.79
1	A	232	GLN	C-N-CA	-5.09	114.50	122.79
1	B	701	LYS	N-CA-C	5.09	116.82	111.28
1	A	557	SER	N-CA-C	5.07	116.95	108.99
1	A	586	ASP	CB-CG-OD1	5.07	130.05	118.40
1	A	851	GLN	N-CA-C	-5.06	100.65	108.90
1	B	481	VAL	N-CA-C	5.06	115.20	108.11
1	B	83	THR	N-CA-C	5.06	117.57	110.23
1	B	852	SER	N-CA-C	5.06	116.50	108.96
1	B	485	PHE	N-CA-C	-5.04	107.17	113.38
1	A	636	ASP	N-CA-C	5.04	121.53	110.80
1	B	911	ILE	N-CA-C	5.04	115.16	110.42
1	A	586	ASP	N-CA-C	5.02	113.92	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	922	ASN	CA-C-N	-5.02	113.16	120.29
1	B	922	ASN	C-N-CA	-5.02	113.16	120.29
1	A	388	GLU	N-CA-C	5.02	117.13	111.11
1	A	891	ILE	N-CA-C	-5.02	105.50	110.62

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	14	ALA	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1010	PRO	Peptide
3	D	2	VAL	Peptide
3	D	3	ASN	Peptide

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	7781	0	7719	262	0
1	B	7790	0	7719	287	0
2	C	155	0	143	30	0
2	E	155	0	143	40	0
3	D	153	0	149	8	0
3	F	153	0	149	20	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	24	0	32	1	0
5	B	24	0	32	6	0
6	A	189	0	0	44	0
6	B	163	0	0	27	0
6	C	3	0	0	1	0
6	D	2	0	0	0	0
6	E	1	0	0	0	0
6	F	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16597	0	16086	587	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 18.

All (587) 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:B:597:LEU:HA	6:B:2095:HOH:O	1.17	1.33
1:B:361:GLY:O	2:E:2:ILE:HA	1.29	1.24
6:A:2116:HOH:O	2:C:2:ILE:HG22	1.24	1.24
1:B:736:GLN:HB2	6:B:2123:HOH:O	1.07	1.23
1:A:243:LYS:HG3	6:A:2041:HOH:O	1.38	1.21
1:A:195:MET:HA	6:A:2034:HOH:O	1.39	1.18
1:A:782:ARG:HD3	6:A:2145:HOH:O	1.47	1.14
1:A:359:LEU:O	2:C:1:GLY:HA2	1.52	1.10
1:A:856:PRO:O	1:A:858:TYR:N	1.85	1.10
6:A:2116:HOH:O	2:C:2:ILE:CG2	1.81	1.08
1:A:577:GLU:HG3	6:A:2141:HOH:O	1.55	1.07
2:E:3:VAL:HG12	2:E:7:CYS:SG	1.94	1.06
1:A:431:ARG:HD2	6:A:2022:HOH:O	1.55	1.05
1:B:597:LEU:HD12	6:B:2095:HOH:O	1.53	1.05
1:B:335:GLY:HA3	2:E:2:ILE:CG2	1.86	1.04
1:B:577:GLU:OE2	6:B:2091:HOH:O	1.74	1.03
1:B:44:ASN:O	6:B:2001:HOH:O	1.77	1.01
1:A:361:GLY:N	2:C:1:GLY:O	1.93	1.00
1:A:429:ARG:NH2	2:C:14:TYR:HE1	1.62	0.97
1:A:898:LYS:HE2	6:A:2010:HOH:O	1.63	0.97
1:A:365:GLU:OE2	2:C:9:SER:HB3	1.65	0.96
1:B:335:GLY:CA	2:E:2:ILE:CG2	2.44	0.95
1:B:456:LEU:C	6:B:2070:HOH:O	2.07	0.94
1:B:368:ARG:HD2	6:B:2036:HOH:O	1.65	0.94
1:B:335:GLY:HA3	2:E:2:ILE:HG21	1.45	0.93
1:A:274:LEU:HG	6:A:2046:HOH:O	1.68	0.93
2:C:16:LEU:HG	6:C:2002:HOH:O	1.70	0.90
1:A:782:ARG:CD	6:A:2145:HOH:O	2.08	0.90
2:E:13:LEU:HD13	2:E:17:GLU:CD	1.96	0.90
1:B:363:GLN:O	2:E:3:VAL:HG21	1.72	0.89
1:A:622:ASN:HD22	1:A:622:ASN:H	1.13	0.89
1:B:622:ASN:HD22	1:B:622:ASN:H	1.16	0.89
1:A:243:LYS:CG	6:A:2041:HOH:O	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLU:HG2	6:B:2003:HOH:O	1.74	0.87
1:B:196:ASN:ND2	1:B:198:ALA:H	1.74	0.85
2:E:13:LEU:HD11	2:E:17:GLU:OE2	1.76	0.85
1:B:995:MET:SD	6:B:2129:HOH:O	2.33	0.85
2:E:17:GLU:HG2	3:F:18:VAL:HG13	1.57	0.85
1:B:48:LYS:O	1:B:49:ARG:HB2	1.78	0.82
1:A:622:ASN:H	1:A:622:ASN:ND2	1.78	0.81
1:A:429:ARG:NH2	2:C:14:TYR:CE1	2.48	0.81
3:D:11:LEU:O	3:D:15:LEU:HB2	1.80	0.80
2:E:16:LEU:O	2:E:19:TYR:CD2	2.35	0.79
1:A:99:ASP:O	1:A:217:LYS:NZ	2.16	0.79
1:B:656:GLU:HG3	1:B:709:LEU:HD22	1.62	0.79
1:B:77:LEU:HD21	1:B:271:VAL:HG11	1.63	0.79
1:B:291:HIS:NE2	6:B:2053:HOH:O	2.14	0.78
1:A:309:ASP:H	1:A:672:ASN:HD21	1.31	0.78
1:A:486:GLU:HB2	6:A:2088:HOH:O	1.83	0.78
1:B:456:LEU:O	6:B:2070:HOH:O	2.01	0.78
2:E:16:LEU:O	2:E:19:TYR:HD2	1.64	0.78
1:B:782:ARG:HH21	1:B:963:MET:H	1.29	0.78
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.32	0.77
1:B:579:PHE:HE2	1:B:765:ARG:HH12	1.30	0.77
1:B:335:GLY:CA	2:E:2:ILE:HG21	2.12	0.77
1:A:199:TRP:HH2	3:D:3:ASN:HA	1.51	0.76
1:A:927:TYR:O	1:A:930:THR:HB	1.84	0.76
1:B:196:ASN:C	1:B:196:ASN:HD22	1.92	0.76
1:B:371:MET:O	6:B:2053:HOH:O	2.04	0.76
1:A:722:ARG:HB2	1:A:758:LEU:HD12	1.68	0.76
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.86	0.76
1:B:296:GLU:N	1:B:296:GLU:OE2	2.18	0.75
1:B:335:GLY:CA	2:E:2:ILE:HG23	2.15	0.75
1:B:361:GLY:N	2:E:1:GLY:O	2.20	0.75
1:A:423:ARG:HH11	1:A:423:ARG:CG	2.01	0.74
1:A:875:GLU:HG2	1:B:53:HIS:CE1	2.23	0.74
2:E:13:LEU:CD1	2:E:17:GLU:OE2	2.34	0.74
1:A:783:ASN:ND2	1:A:786:HIS:H	1.85	0.74
1:A:102:ASN:H	1:A:102:ASN:HD22	1.35	0.73
1:B:341:GLU:HG2	1:B:347:LEU:HD12	1.71	0.73
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.71	0.73
1:B:335:GLY:C	2:E:2:ILE:HG23	2.14	0.73
1:B:810:LEU:HD22	1:B:936:ILE:HG13	1.71	0.73
1:A:200:ARG:NH1	6:A:2034:HOH:O	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLN:H	1:A:297:HIS:HD2	1.37	0.72
1:B:49:ARG:O	1:B:50:ILE:HG13	1.89	0.72
1:A:934:GLU:OE1	1:B:53:HIS:HB2	1.90	0.72
1:B:335:GLY:C	2:E:2:ILE:CG2	2.62	0.71
1:B:691:THR:O	1:B:999:LYS:HE3	1.90	0.71
1:A:277:GLU:HG2	6:A:2047:HOH:O	1.89	0.71
1:A:671:ASN:OD1	1:A:701:LYS:HE2	1.91	0.71
2:E:13:LEU:CD1	2:E:17:GLU:CD	2.63	0.71
1:A:431:ARG:CD	6:A:2022:HOH:O	2.23	0.71
1:B:747:ASP:O	1:B:751:GLU:HB2	1.90	0.71
1:A:199:TRP:CH2	3:D:3:ASN:HA	2.26	0.70
1:B:742:MET:HA	1:B:742:MET:HE3	1.74	0.70
1:A:196:ASN:HD22	1:A:199:TRP:H	1.39	0.70
1:B:852:SER:HB3	1:B:859:LEU:HD21	1.72	0.70
1:A:229:ARG:HD2	1:A:233:GLU:OE2	1.93	0.69
1:B:574:LEU:HD22	1:B:729:LEU:HD22	1.75	0.69
1:A:783:ASN:HD22	1:A:786:HIS:H	1.40	0.69
1:A:382:GLU:HB2	6:A:2068:HOH:O	1.93	0.69
1:B:843:ILE:HG22	1:B:844:GLN:H	1.56	0.68
1:B:860:GLU:OE2	1:B:957:HIS:HE1	1.76	0.68
1:B:309:ASP:H	1:B:672:ASN:HD21	1.39	0.68
1:B:843:ILE:HD13	1:B:843:ILE:N	2.08	0.68
1:B:47:ILE:HG22	1:B:49:ARG:O	1.92	0.67
1:A:47:ILE:CG2	1:A:49:ARG:O	2.43	0.67
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.76	0.67
1:A:303:LYS:HD3	1:A:485:PHE:CE2	2.30	0.67
1:A:491:ARG:HG2	1:A:491:ARG:HH11	1.59	0.67
3:F:1:PHE:H3	3:F:1:PHE:HD2	1.43	0.67
1:B:622:ASN:HD22	1:B:622:ASN:N	1.89	0.66
1:B:783:ASN:HD22	1:B:785:VAL:H	1.42	0.66
1:B:621:GLN:HB3	6:B:2102:HOH:O	1.96	0.66
2:C:3:VAL:HG12	2:C:7:CYS:SG	2.35	0.66
1:A:674:ARG:NH1	6:A:2133:HOH:O	2.29	0.66
3:F:2:VAL:HG13	3:F:3:ASN:N	2.10	0.66
1:A:431:ARG:NH1	2:C:14:TYR:HE2	1.94	0.66
1:A:125:ASN:H	1:A:125:ASN:HD22	1.41	0.65
1:B:196:ASN:ND2	1:B:198:ALA:N	2.44	0.65
1:A:491:ARG:HG2	1:A:491:ARG:NH1	2.12	0.65
1:A:512:LYS:NZ	6:A:2094:HOH:O	2.29	0.65
1:B:93:HIS:HD2	1:B:145:GLU:O	1.80	0.65
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:PHE:O	6:A:2078:HOH:O	2.15	0.65
1:A:724:HIS:HA	6:A:2139:HOH:O	1.95	0.65
1:B:68:GLU:CG	6:B:2003:HOH:O	2.38	0.65
1:A:795:TYR:CE2	1:A:953:LYS:HD2	2.31	0.65
1:A:722:ARG:HB2	1:A:758:LEU:CD1	2.27	0.65
1:B:47:ILE:CG2	1:B:49:ARG:O	2.44	0.65
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.33	0.64
1:A:360:VAL:HA	2:C:1:GLY:HA2	1.79	0.64
1:B:713:LYS:HE2	6:B:2107:HOH:O	1.97	0.64
1:A:108:HIS:NE2	1:A:189:GLU:OE1	2.30	0.64
1:A:189:GLU:HG3	1:A:831:TYR:CE1	2.32	0.64
1:B:436:LYS:HE2	6:B:2065:HOH:O	1.96	0.64
1:A:184:ASN:HD21	1:A:223:LYS:HE2	1.62	0.64
1:B:191:GLU:HG3	1:B:788:ASN:HD21	1.63	0.63
1:A:880:GLU:CG	1:B:457:GLU:HG2	2.29	0.63
1:B:125:ASN:HD22	1:B:125:ASN:H	1.46	0.63
1:B:141:PHE:HA	3:F:1:PHE:N	2.14	0.63
1:B:510:ILE:O	1:B:514:GLN:HG3	1.98	0.63
1:B:523:LYS:HD3	1:B:523:LYS:N	2.14	0.62
2:E:3:VAL:CG1	2:E:7:CYS:SG	2.79	0.62
1:A:188:SER:HB3	1:A:831:TYR:HB2	1.80	0.62
1:B:843:ILE:HG22	1:B:844:GLN:N	2.13	0.62
1:A:486:GLU:CB	6:A:2088:HOH:O	2.43	0.62
1:B:309:ASP:H	1:B:672:ASN:ND2	1.97	0.62
1:A:771:LEU:HD21	1:A:954:VAL:CG2	2.30	0.61
1:A:108:HIS:CE1	1:A:189:GLU:OE1	2.53	0.61
1:B:722:ARG:CZ	6:B:2120:HOH:O	2.48	0.61
1:A:360:VAL:HA	2:C:1:GLY:O	1.99	0.61
1:B:318:PRO:HG2	1:B:475:ASN:HD21	1.65	0.61
1:A:423:ARG:HH11	1:A:423:ARG:HG2	1.65	0.61
1:A:431:ARG:NH1	2:C:14:TYR:CE2	2.68	0.61
1:B:429:ARG:HH11	1:B:429:ARG:CG	2.13	0.61
1:B:722:ARG:HB3	1:B:758:LEU:CD1	2.31	0.60
1:B:842:GLY:C	1:B:843:ILE:HD13	2.26	0.60
1:A:616:LEU:HD21	1:A:638:GLN:HG3	1.84	0.60
1:A:852:SER:HB3	1:A:859:LEU:HD21	1.83	0.60
1:A:466:MET:HE2	1:A:467:VAL:HA	1.83	0.60
1:B:451:THR:HB	1:B:455:LEU:HD12	1.83	0.60
1:A:577:GLU:CG	6:A:2141:HOH:O	2.28	0.59
1:A:730:HIS:HD2	1:A:904:SER:OG	1.86	0.59
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:810:LEU:C	1:B:810:LEU:HD23	2.28	0.59
1:B:48:LYS:O	1:B:48:LYS:CG	2.51	0.58
1:B:196:ASN:ND2	1:B:196:ASN:C	2.57	0.58
1:A:724:HIS:CA	6:A:2139:HOH:O	2.49	0.58
1:B:656:GLU:HG3	1:B:709:LEU:CD2	2.31	0.58
1:B:111:GLN:HE22	3:F:1:PHE:N	2.02	0.58
1:B:602:ASP:OD1	1:B:658:ARG:HD2	2.03	0.58
1:B:783:ASN:ND2	1:B:786:HIS:H	2.01	0.58
1:A:309:ASP:H	1:A:672:ASN:ND2	1.97	0.58
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.86	0.58
1:B:335:GLY:C	2:E:2:ILE:HG21	2.27	0.58
1:A:227:GLU:C	1:A:230:PRO:HD2	2.28	0.58
1:A:874:ILE:HG22	1:A:937:ILE:HD11	1.85	0.57
1:B:361:GLY:O	2:E:2:ILE:CA	2.25	0.57
1:A:43:ASN:C	1:A:43:ASN:ND2	2.62	0.57
1:B:227:GLU:C	1:B:230:PRO:HD2	2.29	0.57
1:B:817:GLU:HG3	1:B:818:PRO:HD3	1.86	0.57
1:A:677:GLN:HG3	1:A:678:PRO:HD2	1.87	0.57
1:B:783:ASN:ND2	1:B:785:VAL:H	2.02	0.57
1:A:360:VAL:HA	2:C:1:GLY:C	2.29	0.57
1:A:460:ARG:HD2	1:A:462:ASP:OD2	2.04	0.57
1:B:362:GLY:HA3	2:E:2:ILE:HG22	1.87	0.57
5:B:3013:DIO:H22	6:B:2040:HOH:O	2.05	0.57
3:F:10:HIS:ND1	6:F:2001:HOH:O	2.33	0.57
1:A:162:LEU:HD23	1:A:270:LEU:CD1	2.35	0.57
1:B:692:GLU:HG2	1:B:693:VAL:HG23	1.87	0.57
1:A:423:ARG:CG	1:A:423:ARG:NH1	2.67	0.56
1:A:824:ARG:O	1:A:828:GLN:HA	2.04	0.56
1:B:583:ALA:CB	1:B:626:GLY:HA2	2.35	0.56
1:A:184:ASN:ND2	1:A:223:LYS:HE2	2.20	0.56
1:A:687:ARG:HD2	6:A:2136:HOH:O	2.04	0.56
2:E:17:GLU:HG2	3:F:18:VAL:CG1	2.34	0.56
1:B:782:ARG:NH2	1:B:963:MET:H	2.03	0.56
1:A:294:GLN:H	1:A:297:HIS:CD2	2.22	0.56
1:B:491:ARG:HH11	1:B:491:ARG:CG	2.19	0.56
1:A:574:LEU:HD22	1:A:729:LEU:HD22	1.87	0.55
1:A:688:LEU:HD13	1:A:995:MET:HE1	1.89	0.55
1:B:872:LYS:O	1:B:875:GLU:HB2	2.06	0.55
1:B:722:ARG:HB3	1:B:758:LEU:HD13	1.87	0.55
1:B:479:ALA:HB2	5:B:3013:DIO:H21	1.88	0.55
1:B:679:HIS:O	1:B:683:MET:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:875:GLU:OE1	1:B:875:GLU:HA	2.06	0.55
1:A:722:ARG:CB	1:A:758:LEU:HD12	2.35	0.55
1:A:963:MET:C	6:A:2184:HOH:O	2.49	0.55
1:B:459:PHE:CE2	1:B:461:PRO:HG3	2.42	0.55
6:A:2116:HOH:O	2:C:2:ILE:HG21	1.75	0.55
1:B:810:LEU:HD12	1:B:928:LEU:CD2	2.37	0.55
1:A:136:GLY:HA3	1:A:152:ASP:O	2.06	0.55
1:A:815:ILE:HG22	1:A:870:MET:HG3	1.88	0.55
1:B:361:GLY:O	2:E:2:ILE:CG2	2.55	0.55
1:A:423:ARG:HG2	1:A:423:ARG:NH1	2.20	0.54
1:B:45:PRO:HG2	1:B:46:ALA:H	1.72	0.54
1:A:529:GLU:OE2	1:A:529:GLU:HA	2.08	0.54
1:B:110:LEU:HD23	1:B:110:LEU:C	2.32	0.54
2:E:19:TYR:CD2	3:F:15:LEU:HD21	2.42	0.54
3:D:3:ASN:OD1	3:D:3:ASN:C	2.50	0.54
1:B:196:ASN:HD21	1:B:198:ALA:H	1.52	0.54
1:A:807:PHE:HE1	1:A:935:ASP:HB3	1.72	0.54
1:B:298:LEU:HD13	1:B:475:ASN:HD22	1.73	0.54
1:B:597:LEU:HD23	1:B:621:GLN:C	2.33	0.54
1:A:874:ILE:O	1:A:933:LYS:HE3	2.08	0.54
1:B:440:ILE:HD11	1:B:449:VAL:O	2.08	0.54
1:A:114:LEU:HD13	1:A:168:PHE:HB3	1.89	0.53
1:B:311:ARG:HH22	1:B:664:GLU:CD	2.16	0.53
1:B:423:ARG:HD3	1:B:424:PHE:CZ	2.44	0.53
1:B:425:LYS:HD2	1:B:428:GLU:OE2	2.08	0.53
1:B:927:TYR:CE2	1:B:931:LEU:HD11	2.43	0.53
1:A:359:LEU:O	2:C:1:GLY:CA	2.43	0.53
1:A:559:LEU:HD22	1:A:742:MET:HB2	1.90	0.53
3:F:1:PHE:C	3:F:1:PHE:CD2	2.86	0.53
1:A:676:GLU:OE1	1:A:676:GLU:HA	2.09	0.53
1:B:563:GLN:HG3	1:B:733:ILE:O	2.08	0.53
1:B:774:ARG:HG2	1:B:774:ARG:NH1	2.24	0.53
1:A:112:HIS:NE2	1:A:189:GLU:OE1	2.42	0.52
1:A:259:LEU:C	1:A:259:LEU:HD23	2.34	0.52
1:B:457:GLU:N	6:B:2070:HOH:O	2.33	0.52
1:B:860:GLU:OE2	1:B:957:HIS:CE1	2.59	0.52
1:A:360:VAL:HA	2:C:1:GLY:CA	2.38	0.52
1:B:310:ILE:HG13	1:B:310:ILE:O	2.08	0.52
1:B:365:GLU:OE2	2:E:9:SER:HA	2.09	0.52
1:B:196:ASN:HD22	1:B:198:ALA:N	2.07	0.52
1:A:222:ASN:O	1:A:226:LEU:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:LEU:CD2	1:A:995:MET:HG2	2.40	0.52
1:A:880:GLU:HG3	1:B:457:GLU:HG2	1.90	0.52
1:B:620:LEU:HD13	1:B:629:LEU:HG	1.92	0.52
2:C:10:ILE:HG22	3:D:4:GLN:C	2.35	0.52
1:A:346:LEU:HD21	1:A:394:MET:HG2	1.92	0.51
1:B:90:LEU:C	1:B:90:LEU:HD23	2.35	0.51
1:A:147:THR:HG22	1:A:149:TYR:CE1	2.46	0.51
1:B:48:LYS:O	1:B:48:LYS:HG2	2.09	0.51
1:B:229:ARG:HD2	1:B:233:GLU:OE2	2.10	0.51
1:A:824:ARG:O	1:A:828:GLN:N	2.42	0.51
1:B:141:PHE:HA	3:F:1:PHE:O	2.10	0.51
1:B:213:HIS:ND1	1:B:214:PRO:HD2	2.25	0.51
1:B:770:GLN:HA	1:B:1005:PHE:CE1	2.46	0.51
1:A:93:HIS:HE1	1:A:368:ARG:NH2	2.06	0.51
1:B:59:GLU:OE1	1:B:423:ARG:NH1	2.44	0.51
1:B:84:ASP:OD2	1:B:896:LYS:HD3	2.11	0.51
1:B:388:GLU:HB2	5:B:3015:DIO:H11	1.93	0.51
1:B:941:LYS:HD3	1:B:942:GLU:N	2.26	0.50
3:D:17:LEU:HD12	3:D:17:LEU:O	2.11	0.50
1:B:47:ILE:HG22	1:B:49:ARG:H	1.75	0.50
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.59	0.50
1:B:296:GLU:H	1:B:296:GLU:CD	2.16	0.50
2:E:17:GLU:C	2:E:19:TYR:H	2.18	0.50
1:B:72:GLY:HA2	6:B:2003:HOH:O	2.10	0.50
1:B:429:ARG:HH11	1:B:429:ARG:HG2	1.75	0.50
1:B:690:MET:HA	1:B:690:MET:HE2	1.94	0.50
1:B:961:ARG:HD2	6:B:2157:HOH:O	2.10	0.50
1:A:49:ARG:C	1:A:50:ILE:HD12	2.37	0.50
1:B:453:GLU:O	5:B:3014:DIO:H2'1	2.12	0.50
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.21	0.50
1:A:187:ASP:OD1	1:A:222:ASN:HB2	2.12	0.50
1:B:236:ASP:OD1	1:B:236:ASP:C	2.55	0.50
1:B:575:ASN:O	1:B:727:ALA:HA	2.12	0.50
1:A:651:THR:HG22	1:A:752:HIS:HB3	1.93	0.50
1:B:187:ASP:OD1	1:B:222:ASN:HB2	2.11	0.50
2:E:16:LEU:HA	2:E:19:TYR:CE2	2.47	0.50
1:B:359:LEU:O	2:E:1:GLY:N	2.45	0.49
1:B:429:ARG:HD2	2:E:14:TYR:OH	2.12	0.49
1:A:801:SER:O	1:A:802:THR:C	2.56	0.49
1:A:929:LYS:HE2	6:A:2172:HOH:O	2.11	0.49
1:A:431:ARG:NE	6:A:2022:HOH:O	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:LYS:HE3	6:A:2063:HOH:O	2.12	0.49
1:B:191:GLU:CG	1:B:788:ASN:HD21	2.26	0.49
1:A:429:ARG:CZ	2:C:14:TYR:CE1	2.96	0.49
1:A:475:ASN:N	1:A:475:ASN:OD1	2.44	0.49
1:A:784:GLU:O	1:A:961:ARG:HG3	2.12	0.49
1:B:389:ASP:O	1:B:393:HIS:HD2	1.95	0.49
1:B:534:ASN:HD22	1:B:536:GLU:H	1.59	0.49
1:A:140:ALA:HA	1:A:148:ASN:O	2.12	0.49
1:A:511:LYS:HD2	1:A:511:LYS:N	2.27	0.49
1:B:534:ASN:ND2	1:B:536:GLU:H	2.10	0.49
1:B:43:ASN:O	1:B:45:PRO:O	2.30	0.49
1:B:534:ASN:HD22	1:B:534:ASN:C	2.20	0.49
1:A:162:LEU:HD23	1:A:270:LEU:HD11	1.93	0.49
1:A:194:VAL:HG12	1:A:195:MET:HE2	1.94	0.49
1:B:736:GLN:H	1:B:736:GLN:CD	2.20	0.49
1:B:810:LEU:HD22	1:B:936:ILE:CG1	2.42	0.49
1:A:771:LEU:HD21	1:A:954:VAL:HG23	1.94	0.49
1:A:455:LEU:HA	6:A:2084:HOH:O	2.13	0.48
1:A:824:ARG:O	1:A:828:GLN:CA	2.61	0.48
1:A:153:VAL:HG22	1:A:154:SER:N	2.28	0.48
1:A:587:PRO:HD3	1:A:695:TRP:CE2	2.48	0.48
1:B:587:PRO:HD3	1:B:695:TRP:CE2	2.48	0.48
1:B:767:ARG:HG2	1:B:1007:LEU:HD13	1.95	0.48
1:A:795:TYR:HE2	1:A:953:LYS:HD2	1.75	0.48
1:B:135:ALA:HA	1:B:892:ARG:NH2	2.28	0.48
1:B:940:TYR:CE1	1:B:945:ALA:HB2	2.47	0.48
1:A:431:ARG:HH11	2:C:14:TYR:HE2	1.58	0.48
1:B:415:LYS:HG3	6:B:2070:HOH:O	2.12	0.48
1:A:257:VAL:HG21	1:A:437:ILE:HB	1.94	0.48
1:A:526:THR:O	1:A:527:LYS:C	2.57	0.48
1:B:196:ASN:HD22	1:B:198:ALA:H	1.59	0.48
1:B:335:GLY:O	2:E:2:ILE:HG23	2.14	0.48
1:B:815:ILE:HA	1:B:870:MET:HE2	1.96	0.48
1:A:151:PHE:CD1	1:A:151:PHE:C	2.92	0.48
1:B:534:ASN:ND2	1:B:534:ASN:C	2.72	0.48
2:E:13:LEU:HD13	2:E:17:GLU:OE1	2.13	0.48
1:A:324:LYS:HE3	1:A:325:TYR:CZ	2.48	0.48
1:A:657:LYS:O	1:A:661:ILE:HG12	2.14	0.48
1:A:47:ILE:HG22	1:A:49:ARG:O	2.14	0.48
1:B:49:ARG:O	1:B:50:ILE:CG1	2.60	0.48
1:B:597:LEU:CA	6:B:2095:HOH:O	2.05	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:625:TYR:CZ	1:B:765:ARG:HD3	2.48	0.48
1:B:729:LEU:HD12	1:B:738:ALA:HB1	1.96	0.48
1:A:429:ARG:CZ	2:C:14:TYR:HE1	2.24	0.47
1:B:114:LEU:HD22	1:B:172:PRO:HB3	1.96	0.47
1:B:388:GLU:OE1	1:B:509:VAL:HG22	2.13	0.47
1:A:243:LYS:CB	6:A:2041:HOH:O	2.56	0.47
1:B:97:LEU:HB2	1:B:144:GLY:O	2.14	0.47
1:A:108:HIS:CE1	1:A:189:GLU:CD	2.93	0.47
1:B:386:HIS:HD2	1:B:389:ASP:OD2	1.96	0.47
1:A:110:LEU:C	1:A:110:LEU:HD23	2.40	0.47
1:B:170:LEU:HD21	1:B:278:VAL:HG22	1.97	0.47
1:B:202:PHE:CE2	3:F:4:GLN:HB3	2.50	0.47
1:B:483:LYS:C	1:B:485:PHE:H	2.22	0.47
1:A:389:ASP:O	1:A:393:HIS:HD2	1.97	0.47
1:A:422:PHE:O	1:A:423:ARG:C	2.55	0.47
1:A:540:LEU:HA	1:A:540:LEU:HD12	1.59	0.47
1:A:855:PRO:O	1:A:858:TYR:HB3	2.15	0.47
1:B:433:TYR:CE1	1:B:437:ILE:HD11	2.50	0.47
1:A:803:SER:HB2	1:A:927:TYR:OH	2.14	0.47
1:B:267:LEU:O	1:B:271:VAL:HG12	2.14	0.47
1:A:425:LYS:HE3	6:A:2078:HOH:O	2.13	0.47
1:A:842:GLY:C	1:A:843:ILE:HD13	2.40	0.47
1:A:156:GLU:HB2	1:A:157:HIS:CD2	2.50	0.47
1:A:402:ARG:NH1	1:A:468:LEU:O	2.48	0.47
1:B:601:LYS:O	1:B:602:ASP:C	2.55	0.47
1:A:400:LYS:HE3	1:A:404:GLU:HG2	1.97	0.46
1:B:128:SER:HB2	6:B:2010:HOH:O	2.14	0.46
1:A:868:ILE:HD12	1:A:984:PRO:HD3	1.97	0.46
1:A:691:THR:HG23	1:A:841:ASN:HD21	1.81	0.46
1:A:856:PRO:HB2	1:A:957:HIS:CD2	2.51	0.46
1:B:961:ARG:NH1	6:B:2157:HOH:O	2.48	0.46
1:B:491:ARG:HH11	1:B:491:ARG:HG3	1.80	0.46
1:B:588:LEU:HD23	1:B:589:HIS:CD2	2.51	0.46
1:B:622:ASN:N	1:B:622:ASN:ND2	2.58	0.46
1:B:799:MET:HE2	1:B:799:MET:HB2	1.74	0.46
1:A:488:LYS:HB3	1:A:488:LYS:HE3	1.56	0.46
1:A:671:ASN:O	1:A:674:ARG:HB3	2.16	0.46
1:A:815:ILE:CG2	1:A:870:MET:HG3	2.45	0.46
1:B:556:MET:O	1:B:556:MET:HG3	2.16	0.46
1:B:586:ASP:HA	1:B:695:TRP:CZ2	2.50	0.46
1:B:587:PRO:HD3	1:B:695:TRP:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:MET:HE2	1:A:466:MET:C	2.40	0.46
1:A:715:PHE:CZ	1:A:719:LEU:HD22	2.50	0.46
1:A:360:VAL:C	2:C:1:GLY:O	2.58	0.46
2:C:10:ILE:H	2:C:10:ILE:HG12	1.65	0.46
1:A:237:VAL:O	1:A:238:ARG:C	2.58	0.46
1:A:677:GLN:HE21	1:A:786:HIS:CE1	2.33	0.46
1:B:175:ASP:HB3	1:B:178:ALA:HB3	1.96	0.46
1:B:195:MET:HE3	1:B:307:ILE:HG13	1.97	0.46
1:B:417:LEU:HD12	1:B:417:LEU:HA	1.83	0.46
1:B:489:THR:HB	1:B:500:TYR:C	2.41	0.46
2:C:5:GLN:OE1	2:C:5:GLN:HA	2.15	0.46
2:E:19:TYR:CD2	3:F:15:LEU:CD2	2.99	0.46
1:A:48:LYS:O	1:A:49:ARG:HB3	2.14	0.46
1:A:193:ASN:O	1:A:194:VAL:C	2.59	0.46
1:A:360:VAL:CA	2:C:1:GLY:O	2.63	0.46
1:A:689:LEU:HD23	1:A:995:MET:HG2	1.98	0.46
1:A:182:GLU:OE2	1:A:182:GLU:HA	2.16	0.45
1:B:119:LYS:O	1:B:122:PRO:HD3	2.15	0.45
1:B:960:ALA:O	1:B:961:ARG:C	2.59	0.45
1:B:684:TYR:OH	1:B:697:LYS:HG2	2.16	0.45
3:F:2:VAL:O	3:F:2:VAL:HG12	2.03	0.45
1:A:840:ALA:C	1:A:842:GLY:N	2.74	0.45
1:B:462:ASP:OD2	1:B:462:ASP:N	2.47	0.45
1:B:827:GLU:OE1	1:B:862:ARG:HD3	2.16	0.45
1:A:173:LEU:O	1:A:174:PHE:C	2.60	0.45
1:A:709:LEU:HB3	1:A:710:PRO:CD	2.44	0.45
1:B:136:GLY:HA3	1:B:152:ASP:O	2.17	0.45
1:B:363:GLN:HE21	1:B:371:MET:HE1	1.81	0.45
1:A:53:HIS:HE1	6:A:2005:HOH:O	1.99	0.45
1:A:490:ASP:OD1	1:A:491:ARG:HD2	2.17	0.45
1:A:933:LYS:O	1:A:937:ILE:HG12	2.17	0.45
1:B:111:GLN:HE22	3:F:1:PHE:H1	1.64	0.45
1:B:387:VAL:HG12	5:B:3015:DIO:H12	1.98	0.45
1:B:484:SER:O	1:B:488:LYS:HE3	2.16	0.45
1:B:547:TYR:HB3	1:B:548:PRO:CD	2.47	0.45
1:A:706:ASP:OD1	1:A:706:ASP:N	2.48	0.45
1:B:759:LEU:O	1:B:760:PRO:C	2.60	0.45
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.25	0.45
1:A:586:ASP:HA	1:A:695:TRP:CZ2	2.52	0.45
1:B:681:HIS:O	1:B:682:ALA:C	2.56	0.45
1:A:389:ASP:O	1:A:393:HIS:CD2	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ASP:OD1	1:A:589:HIS:HD2	2.00	0.45
1:B:44:ASN:HA	1:B:45:PRO:HA	1.72	0.45
1:B:519:ASN:C	1:B:521:LYS:H	2.25	0.45
1:B:773:ASP:O	1:B:774:ARG:HB2	2.17	0.45
1:B:877:MET:HG2	1:B:881:ALA:HB3	1.98	0.45
1:A:262:GLU:OE2	1:A:262:GLU:N	2.49	0.45
1:A:649:MET:HE3	1:A:649:MET:HB2	1.63	0.45
1:A:722:ARG:C	1:A:758:LEU:HD13	2.42	0.45
1:B:558:LYS:HB3	1:B:726:GLU:HG3	1.99	0.45
1:B:657:LYS:HE2	1:B:657:LYS:HB3	1.60	0.45
1:A:799:MET:HE3	1:A:799:MET:HB3	1.81	0.44
1:B:202:PHE:CD2	3:F:4:GLN:HB3	2.52	0.44
1:A:67:LEU:HD23	1:A:67:LEU:N	2.33	0.44
1:B:519:ASN:C	1:B:519:ASN:OD1	2.60	0.44
1:B:160:GLY:O	1:B:164:ARG:HD2	2.17	0.44
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.50	0.44
1:A:94:ILE:HD12	1:A:94:ILE:HG23	1.55	0.44
1:A:425:LYS:HD3	1:A:454:TYR:OH	2.16	0.44
1:A:529:GLU:CB	5:A:3014:DIO:H12	2.47	0.44
1:A:943:MET:HE3	1:A:943:MET:HB3	1.78	0.44
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.53	0.44
1:B:877:MET:O	1:B:933:LYS:CE	2.66	0.44
1:A:131:LEU:CD1	1:A:138:SER:HB2	2.47	0.44
1:A:422:PHE:CZ	1:A:451:THR:HG22	2.52	0.44
1:A:534:ASN:OD1	1:A:534:ASN:C	2.60	0.44
1:A:798:ASP:HB3	1:A:804:GLU:HG2	2.00	0.44
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.71	0.44
1:A:359:LEU:C	1:A:359:LEU:HD23	2.43	0.44
1:A:979:ASN:CG	1:A:980:LEU:H	2.25	0.44
1:B:43:ASN:OD1	6:B:2001:HOH:O	2.21	0.44
1:B:483:LYS:C	1:B:485:PHE:N	2.74	0.44
1:A:206:LYS:HB3	1:A:216:SER:HA	1.99	0.44
1:A:587:PRO:HD3	1:A:695:TRP:CD2	2.53	0.44
1:A:868:ILE:O	1:A:869:THR:C	2.60	0.44
1:B:169:PHE:O	1:B:170:LEU:HD23	2.18	0.44
1:B:535:PHE:HB3	1:B:570:PRO:HG3	1.99	0.44
3:F:2:VAL:CG1	3:F:3:ASN:N	2.56	0.44
1:A:143:SER:HB2	2:C:10:ILE:HD12	2.00	0.44
1:B:74:LYS:O	1:B:255:ALA:HA	2.17	0.44
1:B:96:SER:C	1:B:98:SER:H	2.26	0.44
1:A:120:LYS:HE3	1:B:409:TRP:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LEU:HD23	5:B:3013:DIO:H1'1	2.00	0.44
1:B:588:LEU:HD23	1:B:589:HIS:HD2	1.81	0.44
1:A:806:MET:CE	1:A:928:LEU:HG	2.48	0.43
1:B:559:LEU:HD22	1:B:742:MET:HB2	2.00	0.43
1:B:562:LYS:HD3	1:B:730:HIS:CE1	2.53	0.43
1:A:50:ILE:HD12	1:A:50:ILE:N	2.33	0.43
1:B:200:ARG:NH2	1:B:498:THR:HA	2.33	0.43
2:E:10:ILE:HD11	3:F:5:HIS:CE1	2.53	0.43
1:A:722:ARG:NH1	6:A:2138:HOH:O	2.51	0.43
1:B:708:THR:O	1:B:709:LEU:C	2.60	0.43
1:B:818:PRO:HG2	1:B:870:MET:HE1	2.00	0.43
1:B:858:TYR:CZ	1:B:862:ARG:HD2	2.54	0.43
1:B:927:TYR:O	1:B:930:THR:HB	2.19	0.43
1:A:298:LEU:HD13	1:A:475:ASN:HB3	2.00	0.43
1:B:483:LYS:O	1:B:485:PHE:N	2.51	0.43
2:E:14:TYR:O	2:E:18:ASN:HB2	2.18	0.43
1:A:313:LEU:HD22	1:A:387:VAL:HG13	2.00	0.43
1:B:288:PHE:CD2	1:B:288:PHE:N	2.86	0.43
1:B:519:ASN:O	1:B:521:LYS:N	2.51	0.43
1:B:597:LEU:HD23	1:B:622:ASN:N	2.34	0.43
1:A:291:HIS:CE1	1:A:318:PRO:HB3	2.53	0.43
1:A:963:MET:CA	6:A:2184:HOH:O	2.66	0.43
1:B:86:SER:OG	1:B:155:HIS:HA	2.18	0.43
1:B:532:PRO:HG3	1:B:634:TYR:CD2	2.54	0.43
1:B:272:VAL:O	1:B:273:LYS:C	2.60	0.43
1:B:777:PHE:CD1	1:B:777:PHE:N	2.86	0.43
2:C:4:GLU:O	2:C:8:THR:HG22	2.19	0.43
1:A:381:GLU:OE2	1:A:664:GLU:HG3	2.19	0.43
1:A:898:LYS:CE	6:A:2010:HOH:O	2.41	0.43
1:A:672:ASN:HD22	1:A:672:ASN:HA	1.54	0.43
1:A:796:GLN:HB3	1:A:952:HIS:HB2	2.01	0.43
1:A:899:LYS:O	1:A:900:LEU:C	2.62	0.43
1:B:125:ASN:HD22	1:B:125:ASN:N	2.16	0.43
2:E:17:GLU:C	2:E:19:TYR:N	2.77	0.43
1:A:89:ALA:HA	1:A:149:TYR:O	2.19	0.43
1:B:94:ILE:HD13	1:B:94:ILE:HA	1.79	0.43
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.53	0.43
1:B:733:ILE:HG22	1:B:737:ALA:HB3	1.99	0.43
1:A:47:ILE:HG22	1:A:49:ARG:H	1.83	0.42
1:B:90:LEU:HD23	1:B:91:ASP:N	2.34	0.42
1:B:96:SER:C	1:B:98:SER:N	2.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:PRO:O	1:B:446:LEU:C	2.62	0.42
1:B:307:ILE:O	1:B:483:LYS:NZ	2.51	0.42
1:A:296:GLU:OE1	6:A:2052:HOH:O	2.22	0.42
1:A:622:ASN:ND2	1:A:622:ASN:N	2.54	0.42
1:A:49:ARG:O	1:A:50:ILE:HD12	2.19	0.42
1:A:724:HIS:HB2	6:A:2139:HOH:O	2.19	0.42
1:A:759:LEU:O	1:A:760:PRO:C	2.62	0.42
1:B:123:LYS:HE2	1:B:125:ASN:HD21	1.85	0.42
1:B:151:PHE:CD1	1:B:151:PHE:C	2.97	0.42
1:B:94:ILE:HG13	1:B:248:TYR:HB3	2.02	0.42
1:B:490:ASP:OD2	1:B:490:ASP:N	2.52	0.42
1:B:824:ARG:O	1:B:828:GLN:HA	2.19	0.42
1:A:66:GLY:O	1:A:67:LEU:HB3	2.19	0.42
1:B:872:LYS:O	1:B:875:GLU:CB	2.67	0.42
3:D:2:VAL:HG12	3:D:2:VAL:O	2.20	0.42
1:A:842:GLY:O	1:A:843:ILE:HD13	2.20	0.42
1:A:880:GLU:HG2	1:B:457:GLU:HG2	2.00	0.42
1:B:229:ARG:HD3	1:B:233:GLU:HG3	2.01	0.42
1:B:519:ASN:C	1:B:521:LYS:N	2.78	0.42
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.53	0.42
1:A:499:GLN:HA	1:A:499:GLN:OE1	2.20	0.42
1:A:722:ARG:HA	1:A:756:LYS:O	2.20	0.42
1:A:760:PRO:HA	1:A:763:LEU:HD12	2.00	0.42
1:A:782:ARG:HD2	6:A:2145:HOH:O	1.94	0.42
1:B:206:LYS:HB3	1:B:216:SER:HA	2.01	0.42
1:B:267:LEU:HD23	1:B:267:LEU:HA	1.76	0.42
1:B:361:GLY:HA2	1:B:374:ILE:O	2.20	0.42
1:B:774:ARG:HG2	1:B:774:ARG:HH11	1.84	0.42
1:B:909:GLY:HA2	1:B:912:ILE:HD13	2.01	0.42
1:A:60:ASP:OD1	1:A:62:ARG:HB2	2.19	0.42
1:A:528:ASN:OD1	1:A:528:ASN:C	2.63	0.42
1:B:654:ILE:HD13	1:B:712:LEU:HD13	2.01	0.42
1:B:124:GLU:OE2	1:B:178:ALA:HB2	2.20	0.41
1:B:139:ASN:HB3	1:B:150:TYR:CE1	2.55	0.41
1:A:236:ASP:OD2	1:A:239:GLN:HG2	2.21	0.41
1:A:643:LYS:NZ	6:A:2127:HOH:O	2.54	0.41
1:B:592:MET:HE3	1:B:715:PHE:CD1	2.56	0.41
1:B:592:MET:HE3	1:B:715:PHE:CG	2.55	0.41
1:A:451:THR:O	1:A:452:ALA:C	2.62	0.41
1:A:940:TYR:CE1	1:A:945:ALA:HB2	2.54	0.41
1:B:185:ALA:HB2	1:B:828:GLN:HE22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:SER:OG	1:B:252:ASN:OD1	2.37	0.41
1:B:457:GLU:HA	6:B:2070:HOH:O	2.19	0.41
1:B:616:LEU:HA	1:B:616:LEU:HD23	1.80	0.41
1:B:672:ASN:HD22	1:B:672:ASN:HA	1.55	0.41
1:B:677:GLN:HG3	1:B:678:PRO:HD2	2.03	0.41
1:B:689:LEU:CD2	1:B:995:MET:HG2	2.50	0.41
1:B:803:SER:O	1:B:807:PHE:CD1	2.73	0.41
1:B:817:GLU:N	1:B:818:PRO:CD	2.84	0.41
1:B:846:LEU:HD13	1:B:848:PHE:CE1	2.55	0.41
3:F:9:SER:HA	3:F:12:VAL:HG23	2.03	0.41
1:A:413:GLU:HG2	1:A:531:ILE:CD1	2.50	0.41
1:A:711:ARG:CG	1:A:711:ARG:HH21	2.34	0.41
1:A:765:ARG:HA	1:A:765:ARG:HD2	1.68	0.41
1:B:308:LYS:NZ	3:F:13:GLU:HG3	2.36	0.41
1:B:817:GLU:N	1:B:818:PRO:HD2	2.35	0.41
1:A:793:ILE:O	1:A:847:ARG:HA	2.21	0.41
1:B:361:GLY:O	2:E:2:ILE:HG22	2.21	0.41
1:A:262:GLU:HB3	1:A:266:ASP:HB2	2.03	0.41
1:A:920:ARG:O	1:A:924:GLU:HG3	2.21	0.41
1:B:540:LEU:HD12	1:B:540:LEU:HA	1.78	0.41
1:A:102:ASN:H	1:A:102:ASN:ND2	2.11	0.41
1:A:780:GLN:NE2	1:A:959:LEU:HD11	2.35	0.41
1:B:123:LYS:HB3	1:B:126:GLU:HB2	2.01	0.41
1:B:250:SER:O	1:B:254:MET:HG3	2.21	0.41
1:A:313:LEU:HD12	1:A:314:TYR:N	2.36	0.41
1:A:552:LYS:NZ	1:A:746:GLU:OE1	2.34	0.41
1:A:616:LEU:HD23	1:A:616:LEU:HA	1.81	0.41
1:A:736:GLN:H	1:A:736:GLN:HG3	1.69	0.41
1:A:840:ALA:O	1:A:842:GLY:N	2.54	0.41
1:B:413:GLU:OE2	1:B:527:LYS:HD2	2.21	0.41
1:B:609:TYR:CE2	1:B:613:LEU:HD11	2.55	0.41
1:B:827:GLU:CD	1:B:862:ARG:HH11	2.29	0.41
1:B:1008:VAL:HG13	1:B:1009:LYS:N	2.36	0.41
2:E:13:LEU:O	2:E:17:GLU:HG3	2.20	0.41
1:A:575:ASN:O	1:A:727:ALA:HA	2.21	0.41
2:C:15:GLN:O	2:C:18:ASN:HB3	2.20	0.41
2:E:19:TYR:HD2	3:F:15:LEU:CD2	2.34	0.41
1:A:429:ARG:HH21	2:C:14:TYR:HE1	1.56	0.40
1:A:592:MET:HB3	1:A:715:PHE:CD2	2.56	0.40
1:B:171:SER:N	1:B:172:PRO:CD	2.83	0.40
1:B:460:ARG:NH1	1:B:462:ASP:OD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:ARG:HG2	1:B:472:ARG:HH11	1.86	0.40
1:A:417:LEU:HD12	1:A:417:LEU:HA	1.84	0.40
1:A:896:LYS:HB2	1:A:896:LYS:HE2	1.90	0.40
1:A:49:ARG:NH1	6:A:2001:HOH:O	2.54	0.40
1:A:428:GLU:H	1:A:428:GLU:CD	2.29	0.40
1:A:628:TYR:OH	1:A:630:SER:HB2	2.21	0.40
1:A:862:ARG:NH2	1:A:981:SER:O	2.54	0.40
1:A:924:GLU:OE2	6:A:2179:HOH:O	2.22	0.40
1:B:245:HIS:O	1:B:249:TYR:HB2	2.22	0.40
2:E:4:GLU:O	2:E:7:CYS:HB3	2.21	0.40
1:A:118:THR:HG22	1:A:172:PRO:HA	2.03	0.40
1:A:527:LYS:CD	6:A:2097:HOH:O	2.69	0.40
1:A:724:HIS:CB	6:A:2139:HOH:O	2.69	0.40
1:B:191:GLU:HG3	1:B:788:ASN:ND2	2.32	0.40
1:B:538:LEU:H	1:B:538:LEU:HG	1.73	0.40
1:A:50:ILE:HG22	1:A:51:GLY:O	2.21	0.40
1:A:689:LEU:C	1:A:690:MET:HE2	2.47	0.40
1:B:100:PRO:HA	1:B:101:PRO:HD3	1.89	0.40
1:B:363:GLN:HB2	1:B:371:MET:CE	2.52	0.40
1:B:915:GLN:O	1:B:1011:HIS:HB3	2.22	0.40
2:C:13:LEU:N	3:D:1:PHE:CE2	2.90	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	945/990 (96%)	882 (93%)	60 (6%)	3 (0%)	36	66
1	B	951/990 (96%)	896 (94%)	51 (5%)	4 (0%)	30	60
2	C	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
2	E	19/21 (90%)	15 (79%)	4 (21%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	18/30 (60%)	16 (89%)	2 (11%)	0	100	100
3	F	18/30 (60%)	17 (94%)	1 (6%)	0	100	100
All	All	1970/2082 (95%)	1843 (94%)	120 (6%)	7 (0%)	30	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	45	PRO
1	A	1011	HIS
1	B	295	GLU
1	B	751	GLU
1	A	488	LYS
1	B	869	THR
1	A	103	ILE

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	846/879 (96%)	748 (88%)	98 (12%)	5	18
1	B	846/879 (96%)	736 (87%)	110 (13%)	4	14
2	C	19/20 (95%)	14 (74%)	5 (26%)	0	2
2	E	19/20 (95%)	13 (68%)	6 (32%)	0	1
3	D	17/26 (65%)	11 (65%)	6 (35%)	0	0
3	F	17/26 (65%)	13 (76%)	4 (24%)	1	3
All	All	1764/1850 (95%)	1535 (87%)	229 (13%)	4	14

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	54	ILE
1	A	57	SER

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Mol	Chain	Res	Type
1	A	67	LEU
1	A	76	LEU
1	A	96	SER
1	A	97	LEU
1	A	102	ASN
1	A	125	ASN
1	A	156	GLU
1	A	158	LEU
1	A	188	SER
1	A	191	GLU
1	A	192	LYS
1	A	201	LEU
1	A	223	LYS
1	A	226	LEU
1	A	229	ARG
1	A	243	LYS
1	A	270	LEU
1	A	285	LEU
1	A	316	THR
1	A	337	LEU
1	A	347	LEU
1	A	356	VAL
1	A	392	LEU
1	A	412	GLN
1	A	414	LEU
1	A	417	LEU
1	A	423	ARG
1	A	429	ARG
1	A	440	ILE
1	A	446	LEU
1	A	449	VAL
1	A	450	LEU
1	A	466	MET
1	A	488	LYS
1	A	491	ARG
1	A	507	ASP
1	A	510	ILE
1	A	512	LYS
1	A	524	LEU
1	A	558	LYS
1	A	595	LEU
1	A	597	LEU

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Mol	Chain	Res	Type
1	A	603	SER
1	A	607	TYR
1	A	616	LEU
1	A	622	ASN
1	A	624	ILE
1	A	629	LEU
1	A	639	PRO
1	A	642	LEU
1	A	643	LYS
1	A	644	LYS
1	A	648	LYS
1	A	653	GLU
1	A	656	GLU
1	A	657	LYS
1	A	674	ARG
1	A	677	GLN
1	A	691	THR
1	A	711	ARG
1	A	712	LEU
1	A	722	ARG
1	A	728	LEU
1	A	736	GLN
1	A	741	ILE
1	A	751	GLU
1	A	758	LEU
1	A	759	LEU
1	A	762	GLN
1	A	765	ARG
1	A	770	GLN
1	A	771	LEU
1	A	774	ARG
1	A	799	MET
1	A	810	LEU
1	A	823	LEU
1	A	846	LEU
1	A	849	ILE
1	A	853	GLU
1	A	854	LYS
1	A	859	LEU
1	A	867	LEU
1	A	883	GLN
1	A	886	ILE

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Mol	Chain	Res	Type
1	A	889	LEU
1	A	891	ILE
1	A	898	LYS
1	A	928	LEU
1	A	929	LYS
1	A	930	THR
1	A	931	LEU
1	A	982	GLN
1	A	988	GLN
1	A	1007	LEU
1	A	1011	HIS
1	B	44	ASN
1	B	65	ARG
1	B	74	LYS
1	B	76	LEU
1	B	97	LEU
1	B	110	LEU
1	B	111	GLN
1	B	119	LYS
1	B	125	ASN
1	B	128	SER
1	B	131	LEU
1	B	143	SER
1	B	154	SER
1	B	158	LEU
1	B	171	SER
1	B	177	SER
1	B	192	LYS
1	B	196	ASN
1	B	201	LEU
1	B	223	LYS
1	B	226	LEU
1	B	229	ARG
1	B	250	SER
1	B	270	LEU
1	B	271	VAL
1	B	282	ASN
1	B	285	LEU
1	B	333	TYR
1	B	347	LEU
1	B	356	VAL
1	B	417	LEU

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Mol	Chain	Res	Type
1	B	429	ARG
1	B	440	ILE
1	B	457	GLU
1	B	458	GLU
1	B	468	LEU
1	B	481	VAL
1	B	483	LYS
1	B	491	ARG
1	B	512	LYS
1	B	519	ASN
1	B	523	LYS
1	B	524	LEU
1	B	534	ASN
1	B	556	MET
1	B	558	LYS
1	B	559	LEU
1	B	566	LYS
1	B	586	ASP
1	B	590	SER
1	B	592	MET
1	B	595	LEU
1	B	597	LEU
1	B	600	LEU
1	B	616	LEU
1	B	622	ASN
1	B	627	MET
1	B	629	LEU
1	B	640	ILE
1	B	642	LEU
1	B	653	GLU
1	B	674	ARG
1	B	677	GLN
1	B	709	LEU
1	B	712	LEU
1	B	719	LEU
1	B	722	ARG
1	B	728	LEU
1	B	733	ILE
1	B	736	GLN
1	B	751	GLU
1	B	758	LEU
1	B	759	LEU

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Mol	Chain	Res	Type
1	B	764	VAL
1	B	771	LEU
1	B	780	GLN
1	B	791	ILE
1	B	799	MET
1	B	817	GLU
1	B	823	LEU
1	B	843	ILE
1	B	846	LEU
1	B	854	LYS
1	B	859	LEU
1	B	862	ARG
1	B	867	LEU
1	B	870	MET
1	B	873	SER
1	B	875	GLU
1	B	886	ILE
1	B	891	ILE
1	B	896	LYS
1	B	899	LYS
1	B	906	LYS
1	B	912	ILE
1	B	914	GLN
1	B	928	LEU
1	B	929	LYS
1	B	931	LEU
1	B	933	LYS
1	B	934	GLU
1	B	937	ILE
1	B	941	LYS
1	B	944	LEU
1	B	962	GLU
1	B	981	SER
1	B	993	GLN
1	B	996	THR
1	B	1007	LEU
1	B	1008	VAL
2	C	2	ILE
2	C	3	VAL
2	C	10	ILE
2	C	13	LEU
2	C	19	TYR

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Mol	Chain	Res	Type
3	D	2	VAL
3	D	4	GLN
3	D	13	GLU
3	D	15	LEU
3	D	16	TYR
3	D	18	VAL
2	E	2	ILE
2	E	3	VAL
2	E	4	GLU
2	E	5	GLN
2	E	13	LEU
2	E	20	CYS
3	F	1	PHE
3	F	2	VAL
3	F	4	GLN
3	F	18	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	53	HIS
1	A	93	HIS
1	A	102	ASN
1	A	125	ASN
1	A	129	GLN
1	A	148	ASN
1	A	157	HIS
1	A	184	ASN
1	A	196	ASN
1	A	231	ASN
1	A	232	GLN
1	A	294	GLN
1	A	297	HIS
1	A	300	GLN
1	A	329	ASN
1	A	393	HIS
1	A	407	GLN
1	A	412	GLN
1	A	502	GLN
1	A	515	ASN
1	A	575	ASN

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Mol	Chain	Res	Type
1	A	589	HIS
1	A	622	ASN
1	A	672	ASN
1	A	677	GLN
1	A	681	HIS
1	A	718	GLN
1	A	730	HIS
1	A	770	GLN
1	A	780	GLN
1	A	783	ASN
1	A	788	ASN
1	A	805	ASN
1	A	828	GLN
1	A	841	ASN
1	A	883	GLN
1	A	922	ASN
1	A	957	HIS
1	A	979	ASN
1	A	988	GLN
1	B	52	ASN
1	B	53	HIS
1	B	93	HIS
1	B	111	GLN
1	B	125	ASN
1	B	184	ASN
1	B	190	HIS
1	B	196	ASN
1	B	231	ASN
1	B	239	GLN
1	B	294	GLN
1	B	363	GLN
1	B	386	HIS
1	B	393	HIS
1	B	475	ASN
1	B	502	GLN
1	B	534	ASN
1	B	589	HIS
1	B	622	ASN
1	B	672	ASN
1	B	730	HIS
1	B	783	ASN
1	B	788	ASN

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Mol	Chain	Res	Type
1	B	805	ASN
1	B	828	GLN
1	B	914	GLN
1	B	957	HIS
2	C	18	ASN
3	D	4	GLN
3	D	5	HIS
2	E	18	ASN
3	F	5	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	DIO	B	3013	-	6,6,6	0.66	0	6,6,6	0.97	1 (16%)
5	DIO	A	3016	-	6,6,6	0.46	0	6,6,6	1.02	0
5	DIO	A	3015	-	6,6,6	0.63	0	6,6,6	1.30	1 (16%)
5	DIO	A	3014	-	6,6,6	0.66	0	6,6,6	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DIO	B	3016	-	6,6,6	0.61	0	6,6,6	1.28	1 (16%)
5	DIO	B	3014	-	6,6,6	0.87	0	6,6,6	1.60	2 (33%)
5	DIO	B	3015	-	6,6,6	0.64	0	6,6,6	1.73	1 (16%)
5	DIO	A	3013	-	6,6,6	0.55	0	6,6,6	1.33	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DIO	B	3013	-	-	-	0/1/1/1
5	DIO	A	3016	-	-	-	0/1/1/1
5	DIO	A	3015	-	-	-	0/1/1/1
5	DIO	A	3014	-	-	-	0/1/1/1
5	DIO	B	3016	-	-	-	0/1/1/1
5	DIO	B	3014	-	-	-	0/1/1/1
5	DIO	B	3015	-	-	-	0/1/1/1
5	DIO	A	3013	-	-	-	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3015	DIO	C2'-O1'-C1'	2.97	119.48	109.88
5	B	3014	DIO	C2'-O1'-C1'	2.84	119.06	109.88
5	B	3014	DIO	C2-O1-C1	2.53	118.05	109.88
5	A	3015	DIO	C2'-O1'-C1'	2.45	117.79	109.88
5	A	3013	DIO	C2'-O1'-C1'	2.39	117.60	109.88
5	B	3013	DIO	C2'-O1'-C1'	2.13	116.77	109.88
5	B	3016	DIO	C2'-O1'-C1'	2.04	116.46	109.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	3013	DIO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3014	DIO	1	0
5	B	3014	DIO	1	0
5	B	3015	DIO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	953/990 (96%)	-0.87	2 (0%) 91 88	22, 35, 51, 70	0
1	B	955/990 (96%)	-0.71	7 (0%) 84 77	24, 41, 57, 76	0
2	C	21/21 (100%)	1.56	7 (33%) 1 1	34, 53, 56, 57	0
2	E	21/21 (100%)	1.97	8 (38%) 1 0	33, 46, 65, 67	0
3	D	20/30 (66%)	2.33	9 (45%) 0 0	33, 62, 73, 75	0
3	F	20/30 (66%)	1.98	9 (45%) 0 0	43, 54, 58, 59	0
All	All	1990/2082 (95%)	-0.68	42 (2%) 63 54	22, 38, 56, 76	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	14	ALA	6.0
3	D	18	VAL	5.1
2	E	2	ILE	4.9
2	E	16	LEU	4.6
3	F	1	PHE	4.5
3	D	20	GLY	4.2
3	D	16	TYR	3.8
2	E	19	TYR	3.6
3	F	20	GLY	3.5
2	E	1	GLY	3.4
3	F	12	VAL	3.3
2	C	1	GLY	3.3
2	C	19	TYR	3.2
1	B	45	PRO	3.2
3	D	17	LEU	3.2
1	B	44	ASN	3.2
3	D	12	VAL	3.2
2	C	10	ILE	3.1
3	D	15	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	6	LEU	3.0
3	F	15	LEU	2.8
2	E	21	ASN	2.6
2	C	13	LEU	2.6
3	F	16	TYR	2.5
2	C	5	GLN	2.5
1	B	49	ARG	2.5
1	B	43	ASN	2.5
2	C	16	LEU	2.4
1	B	979	ASN	2.3
2	E	15	GLN	2.3
3	F	14	ALA	2.3
3	D	11	LEU	2.3
1	A	43	ASN	2.2
1	B	764	VAL	2.2
2	E	13	LEU	2.2
2	E	5	GLN	2.2
3	F	17	LEU	2.1
1	A	979	ASN	2.1
2	C	14	TYR	2.1
1	B	52	ASN	2.1
3	D	1	PHE	2.0
3	F	2	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DIO	B	3016	6/6	0.89	0.18	81,83,84,85	0
5	DIO	B	3015	6/6	0.93	0.16	68,73,74,74	0
5	DIO	B	3014	6/6	0.93	0.17	64,66,67,67	0
5	DIO	A	3016	6/6	0.94	0.15	71,72,74,74	0
5	DIO	A	3015	6/6	0.94	0.17	69,70,70,71	0
5	DIO	A	3013	6/6	0.95	0.11	61,63,65,66	0
5	DIO	A	3014	6/6	0.96	0.12	54,57,59,60	0
5	DIO	B	3013	6/6	0.97	0.09	50,53,54,55	0
4	ZN	A	3012	1/1	0.99	0.39	2,2,2,2	0
4	ZN	B	3012	1/1	0.99	0.41	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.