



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:20 PM UTC

PDB ID : 2ZBB / pdb_00002zbb
Title : P43 crystal of DctBp
Authors : Zhou, Y.F.; Nan, B.Y.; Liu, X.; Nan, J.; Liang, Y.H.; Panjikar, S.; Ma, Q.J.;
Wang, Y.P.; Su, X.-D.
Deposited on : 2007-10-18
Resolution : 2.50 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

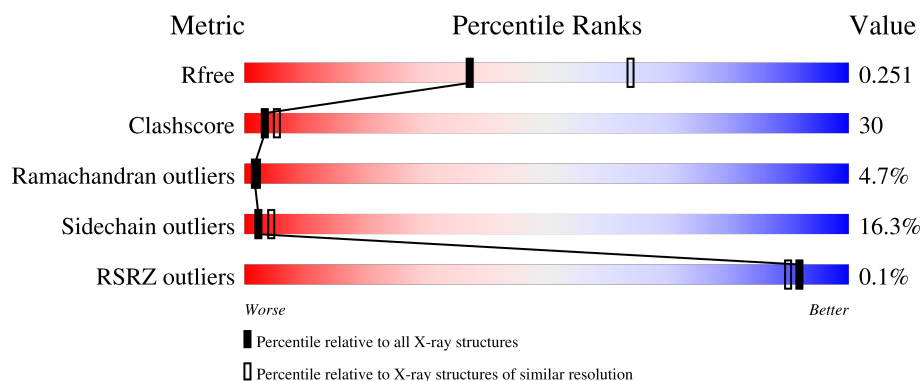
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 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	305	45% 28% 9% • 16%
1	B	305	42% 21% 14% 6% 16%
1	C	305	44% 30% 8% • 16%
1	D	305	48% 24% 9% • 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7852 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 C4-dicarboxylate transport sensor protein dctB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1952	1236	350	362	4			
1	B	255	Total	C	N	O	S	0	0	0
			1952	1236	350	362	4			
1	C	255	Total	C	N	O	S	0	0	0
			1952	1236	350	362	4			
1	D	255	Total	C	N	O	S	0	0	0
			1952	1236	350	362	4			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	expression tag	UNP P13633
A	9	GLY	-	expression tag	UNP P13633
A	10	SER	-	expression tag	UNP P13633
A	11	SER	-	expression tag	UNP P13633
A	12	HIS	-	expression tag	UNP P13633
A	13	HIS	-	expression tag	UNP P13633
A	14	HIS	-	expression tag	UNP P13633
A	15	HIS	-	expression tag	UNP P13633
A	16	HIS	-	expression tag	UNP P13633
A	17	HIS	-	expression tag	UNP P13633
A	18	SER	-	expression tag	UNP P13633
A	19	SER	-	expression tag	UNP P13633
A	20	GLY	-	expression tag	UNP P13633
A	21	LEU	-	expression tag	UNP P13633
A	22	VAL	-	expression tag	UNP P13633
A	23	PRO	-	expression tag	UNP P13633
A	24	ARG	-	expression tag	UNP P13633
A	25	GLY	-	expression tag	UNP P13633
A	26	SER	-	expression tag	UNP P13633
A	27	HIS	-	expression tag	UNP P13633
A	28	MET	-	expression tag	UNP P13633

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Chain	Residue	Modelled	Actual	Comment	Reference
A	29	ALA	-	expression tag	UNP P13633
A	30	SER	-	expression tag	UNP P13633
A	31	MET	-	expression tag	UNP P13633
A	32	THR	-	expression tag	UNP P13633
A	33	GLY	-	expression tag	UNP P13633
A	34	GLY	-	expression tag	UNP P13633
A	35	GLU	-	expression tag	UNP P13633
A	36	GLU	-	expression tag	UNP P13633
A	37	MET	-	expression tag	UNP P13633
A	38	GLY	-	expression tag	UNP P13633
A	39	ARG	-	expression tag	UNP P13633
A	40	GLY	-	expression tag	UNP P13633
A	41	SER	-	expression tag	UNP P13633
A	309	ASN	LYS	SEE REMARK 999	UNP P13633
B	8	MET	-	expression tag	UNP P13633
B	9	GLY	-	expression tag	UNP P13633
B	10	SER	-	expression tag	UNP P13633
B	11	SER	-	expression tag	UNP P13633
B	12	HIS	-	expression tag	UNP P13633
B	13	HIS	-	expression tag	UNP P13633
B	14	HIS	-	expression tag	UNP P13633
B	15	HIS	-	expression tag	UNP P13633
B	16	HIS	-	expression tag	UNP P13633
B	17	HIS	-	expression tag	UNP P13633
B	18	SER	-	expression tag	UNP P13633
B	19	SER	-	expression tag	UNP P13633
B	20	GLY	-	expression tag	UNP P13633
B	21	LEU	-	expression tag	UNP P13633
B	22	VAL	-	expression tag	UNP P13633
B	23	PRO	-	expression tag	UNP P13633
B	24	ARG	-	expression tag	UNP P13633
B	25	GLY	-	expression tag	UNP P13633
B	26	SER	-	expression tag	UNP P13633
B	27	HIS	-	expression tag	UNP P13633
B	28	MET	-	expression tag	UNP P13633
B	29	ALA	-	expression tag	UNP P13633
B	30	SER	-	expression tag	UNP P13633
B	31	MET	-	expression tag	UNP P13633
B	32	THR	-	expression tag	UNP P13633
B	33	GLY	-	expression tag	UNP P13633
B	34	GLY	-	expression tag	UNP P13633
B	35	GLU	-	expression tag	UNP P13633

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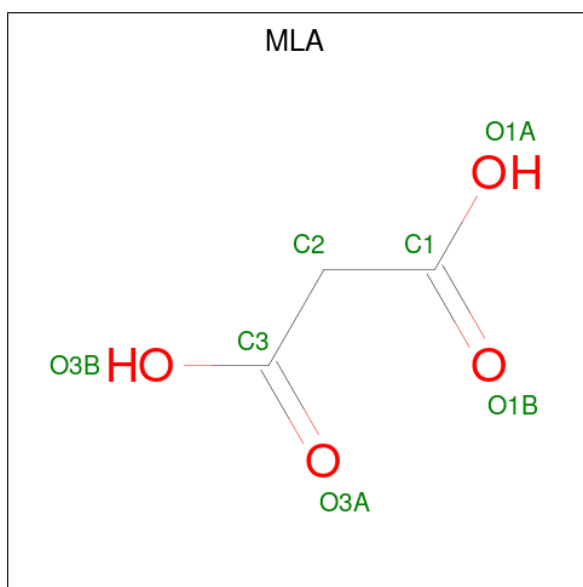
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B	36	GLU	-	expression tag	UNP P13633
B	37	MET	-	expression tag	UNP P13633
B	38	GLY	-	expression tag	UNP P13633
B	39	ARG	-	expression tag	UNP P13633
B	40	GLY	-	expression tag	UNP P13633
B	41	SER	-	expression tag	UNP P13633
B	309	ASN	LYS	SEE REMARK 999	UNP P13633
C	8	MET	-	expression tag	UNP P13633
C	9	GLY	-	expression tag	UNP P13633
C	10	SER	-	expression tag	UNP P13633
C	11	SER	-	expression tag	UNP P13633
C	12	HIS	-	expression tag	UNP P13633
C	13	HIS	-	expression tag	UNP P13633
C	14	HIS	-	expression tag	UNP P13633
C	15	HIS	-	expression tag	UNP P13633
C	16	HIS	-	expression tag	UNP P13633
C	17	HIS	-	expression tag	UNP P13633
C	18	SER	-	expression tag	UNP P13633
C	19	SER	-	expression tag	UNP P13633
C	20	GLY	-	expression tag	UNP P13633
C	21	LEU	-	expression tag	UNP P13633
C	22	VAL	-	expression tag	UNP P13633
C	23	PRO	-	expression tag	UNP P13633
C	24	ARG	-	expression tag	UNP P13633
C	25	GLY	-	expression tag	UNP P13633
C	26	SER	-	expression tag	UNP P13633
C	27	HIS	-	expression tag	UNP P13633
C	28	MET	-	expression tag	UNP P13633
C	29	ALA	-	expression tag	UNP P13633
C	30	SER	-	expression tag	UNP P13633
C	31	MET	-	expression tag	UNP P13633
C	32	THR	-	expression tag	UNP P13633
C	33	GLY	-	expression tag	UNP P13633
C	34	GLY	-	expression tag	UNP P13633
C	35	GLU	-	expression tag	UNP P13633
C	36	GLU	-	expression tag	UNP P13633
C	37	MET	-	expression tag	UNP P13633
C	38	GLY	-	expression tag	UNP P13633
C	39	ARG	-	expression tag	UNP P13633
C	40	GLY	-	expression tag	UNP P13633
C	41	SER	-	expression tag	UNP P13633
C	309	ASN	LYS	SEE REMARK 999	UNP P13633

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Chain	Residue	Modelled	Actual	Comment	Reference
D	8	MET	-	expression tag	UNP P13633
D	9	GLY	-	expression tag	UNP P13633
D	10	SER	-	expression tag	UNP P13633
D	11	SER	-	expression tag	UNP P13633
D	12	HIS	-	expression tag	UNP P13633
D	13	HIS	-	expression tag	UNP P13633
D	14	HIS	-	expression tag	UNP P13633
D	15	HIS	-	expression tag	UNP P13633
D	16	HIS	-	expression tag	UNP P13633
D	17	HIS	-	expression tag	UNP P13633
D	18	SER	-	expression tag	UNP P13633
D	19	SER	-	expression tag	UNP P13633
D	20	GLY	-	expression tag	UNP P13633
D	21	LEU	-	expression tag	UNP P13633
D	22	VAL	-	expression tag	UNP P13633
D	23	PRO	-	expression tag	UNP P13633
D	24	ARG	-	expression tag	UNP P13633
D	25	GLY	-	expression tag	UNP P13633
D	26	SER	-	expression tag	UNP P13633
D	27	HIS	-	expression tag	UNP P13633
D	28	MET	-	expression tag	UNP P13633
D	29	ALA	-	expression tag	UNP P13633
D	30	SER	-	expression tag	UNP P13633
D	31	MET	-	expression tag	UNP P13633
D	32	THR	-	expression tag	UNP P13633
D	33	GLY	-	expression tag	UNP P13633
D	34	GLY	-	expression tag	UNP P13633
D	35	GLU	-	expression tag	UNP P13633
D	36	GLU	-	expression tag	UNP P13633
D	37	MET	-	expression tag	UNP P13633
D	38	GLY	-	expression tag	UNP P13633
D	39	ARG	-	expression tag	UNP P13633
D	40	GLY	-	expression tag	UNP P13633
D	41	SER	-	expression tag	UNP P13633
D	309	ASN	LYS	SEE REMARK 999	UNP P13633

- Molecule 2 is MALONIC ACID (CCD ID: MLA) (formula: C₃H₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	3	4		
2	B	1	Total	C	O	0	0
			7	3	4		
2	C	1	Total	C	O	0	0
			7	3	4		
2	D	1	Total	C	O	0	0
			7	3	4		

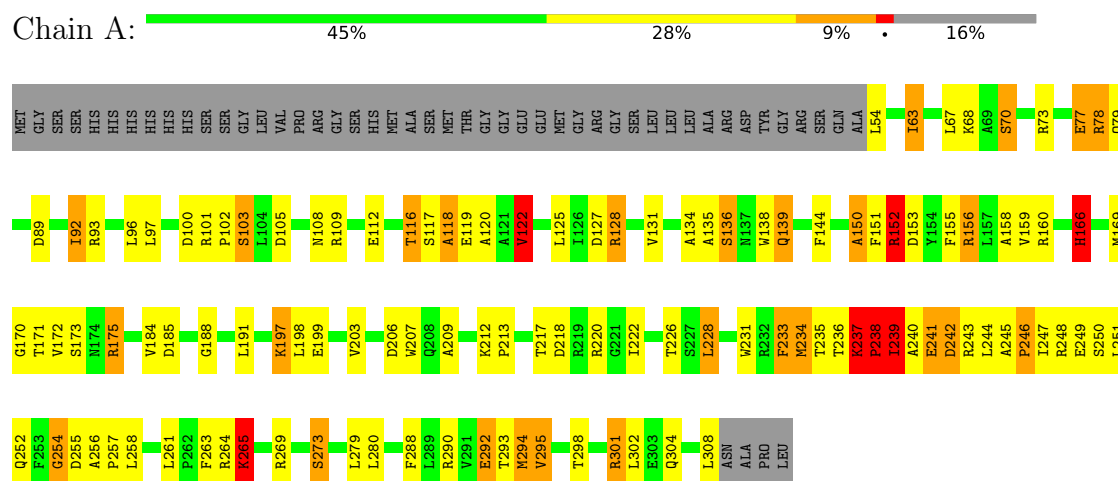
- Molecule 3 is water.

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

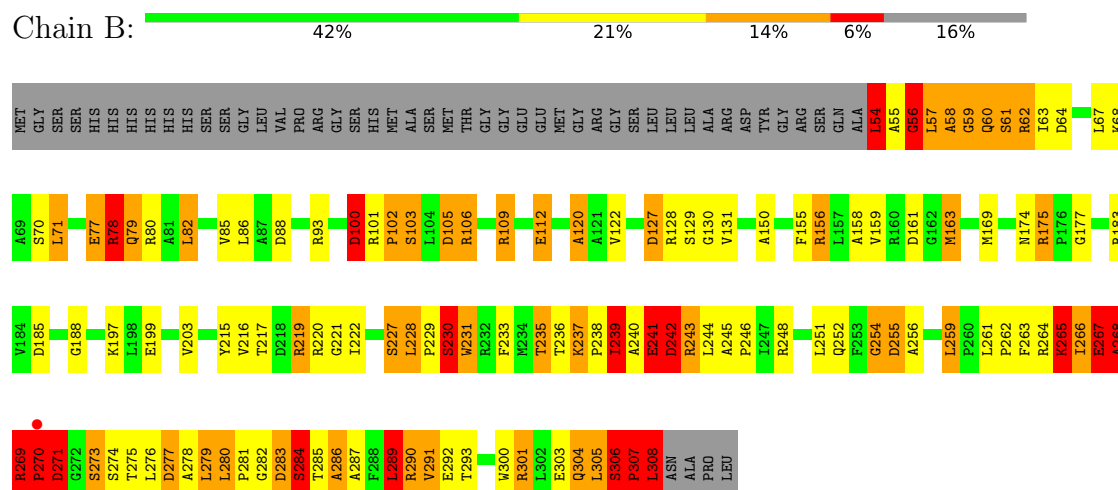
3 Residue-property plots

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: C4-dicarboxylate transport sensor protein dctB

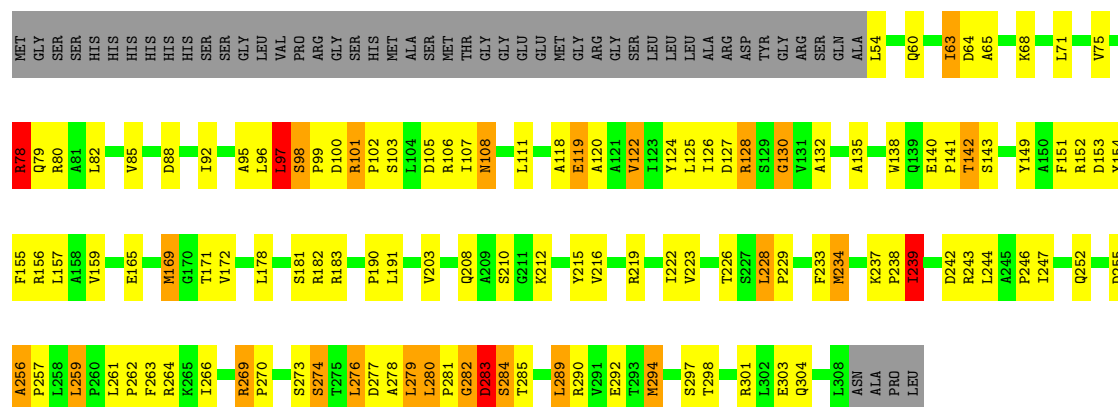


- Molecule 1: C4-dicarboxylate transport sensor protein dctB

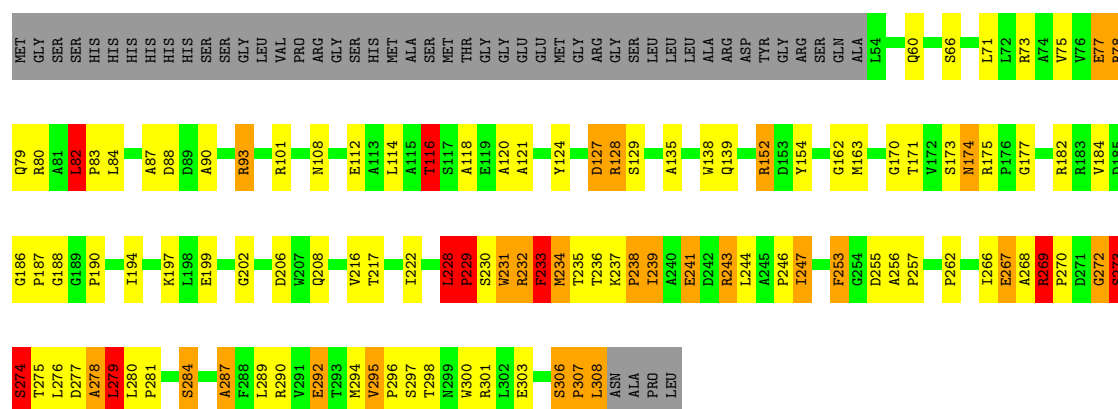


- Molecule 1: C4-dicarboxylate transport sensor protein dctB





• Molecule 1: C4-dicarboxylate transport sensor protein dctB



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	70.36Å 70.36Å 226.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.50) 99.3 (15.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.209 , 0.272 0.225 , 0.251	Depositor DCC
R_{free} test set	1880 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.093 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7852	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: MLA

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	1.16	6/1992 (0.3%)	1.36	21/2710 (0.8%)
1	B	1.96	39/1992 (2.0%)	1.47	40/2710 (1.5%)
1	C	1.68	33/1992 (1.7%)	1.35	20/2710 (0.7%)
1	D	1.18	5/1992 (0.3%)	1.50	24/2710 (0.9%)
All	All	1.53	83/7968 (1.0%)	1.42	105/10840 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	3
1	B	2	14
1	C	2	3
1	D	2	9
All	All	10	29

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	LEU	C-O	22.79	1.54	1.23
1	B	54	LEU	C-N	20.53	1.59	1.33
1	B	54	LEU	CB-CG	20.45	1.94	1.53
1	B	277	ASP	C-N	17.91	1.58	1.33
1	B	259	LEU	CB-CG	17.29	1.88	1.53
1	C	98	SER	C-N	16.54	1.48	1.33
1	C	98	SER	CA-CB	16.32	1.79	1.53
1	B	59	GLY	C-N	15.13	1.54	1.33
1	C	101	ARG	NE-CZ	14.98	1.49	1.33
1	B	305	LEU	C-O	14.47	1.42	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	54	LEU	CA-CB	14.44	1.82	1.53
1	B	306	SER	CA-CB	13.71	1.75	1.53
1	C	101	ARG	CZ-NH1	13.69	1.51	1.32
1	B	306	SER	CA-C	13.51	1.69	1.52
1	C	99	PRO	N-CD	13.43	1.66	1.47
1	C	140	GLU	N-CA	12.79	1.58	1.46
1	C	95	ALA	C-O	12.58	1.40	1.24
1	C	100	ASP	CG-OD2	11.97	1.48	1.25
1	D	279	LEU	C-O	11.94	1.39	1.24
1	C	141	PRO	N-CD	11.71	1.64	1.47
1	B	54	LEU	CG-CD1	11.51	1.90	1.52
1	B	109	ARG	CZ-NH1	11.44	1.48	1.32
1	A	239	ILE	C-O	11.19	1.37	1.24
1	B	305	LEU	C-N	10.82	1.55	1.33
1	B	60	GLN	C-O	-10.48	1.11	1.23
1	C	97	LEU	C-O	10.45	1.37	1.24
1	D	272	GLY	CA-C	10.12	1.66	1.51
1	B	307	PRO	N-CD	9.84	1.61	1.47
1	B	59	GLY	C-O	9.77	1.35	1.24
1	C	101	ARG	CZ-NH2	9.75	1.46	1.33
1	B	55	ALA	CA-C	9.69	1.66	1.53
1	C	143	SER	CA-CB	9.42	1.69	1.53
1	B	60	GLN	CD-NE2	9.21	1.52	1.33
1	C	100	ASP	CA-CB	9.15	1.69	1.53
1	C	100	ASP	N-CA	8.84	1.57	1.46
1	A	160	ARG	CZ-NH1	8.83	1.45	1.32
1	B	239	ILE	CA-CB	8.73	1.65	1.54
1	C	142	THR	C-N	8.58	1.45	1.33
1	B	277	ASP	C-O	8.56	1.33	1.23
1	C	98	SER	C-O	8.37	1.34	1.24
1	A	239	ILE	C-N	-8.31	1.22	1.33
1	B	307	PRO	C-N	8.11	1.44	1.33
1	B	61	SER	C-O	8.09	1.34	1.24
1	B	239	ILE	C-O	7.63	1.32	1.24
1	C	101	ARG	CD-NE	7.44	1.56	1.46
1	B	278	ALA	C-N	7.08	1.43	1.33
1	B	109	ARG	NE-CZ	7.05	1.40	1.33
1	C	97	LEU	CG-CD1	7.01	1.75	1.52
1	C	130	GLY	C-N	6.89	1.42	1.33
1	B	103	SER	CB-OG	6.76	1.55	1.42
1	B	289	LEU	CB-CG	6.70	1.66	1.53
1	B	57	LEU	C-O	6.70	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	100	ASP	CG-OD2	6.60	1.37	1.25
1	C	98	SER	CB-OG	6.55	1.55	1.42
1	C	100	ASP	C-O	-6.54	1.15	1.23
1	C	95	ALA	C-N	6.50	1.42	1.33
1	C	140	GLU	C-N	6.49	1.42	1.33
1	B	235	THR	C-O	6.25	1.31	1.23
1	B	56	GLY	C-N	6.21	1.42	1.33
1	B	58	ALA	C-N	6.20	1.42	1.34
1	C	99	PRO	CA-CB	5.97	1.61	1.53
1	C	85	VAL	CA-CB	5.95	1.61	1.54
1	C	100	ASP	CG-OD1	5.92	1.36	1.25
1	B	308	LEU	CB-CG	5.90	1.65	1.53
1	C	100	ASP	CB-CG	5.81	1.66	1.52
1	D	287	ALA	CA-CB	5.81	1.62	1.53
1	D	139	GLN	CG-CD	5.77	1.66	1.52
1	B	57	LEU	N-CA	5.66	1.53	1.46
1	A	238	PRO	C-N	-5.59	1.26	1.33
1	C	97	LEU	CG-CD2	5.55	1.70	1.52
1	C	75	VAL	C-O	-5.52	1.17	1.24
1	C	138	TRP	C-O	5.46	1.31	1.24
1	B	256	ALA	C-O	5.46	1.31	1.24
1	B	55	ALA	C-O	5.43	1.31	1.23
1	C	54	LEU	CG-CD2	5.33	1.70	1.52
1	A	184	VAL	CA-C	5.31	1.59	1.52
1	B	304	GLN	CD-NE2	5.24	1.44	1.33
1	D	116	THR	CA-CB	5.20	1.61	1.53
1	C	228	LEU	C-O	-5.12	1.20	1.25
1	B	79	GLN	C-O	-5.11	1.17	1.24
1	A	63	ILE	CA-CB	5.11	1.61	1.54
1	B	307	PRO	CG-CD	5.04	1.67	1.50
1	C	65	ALA	CA-CB	-5.00	1.45	1.53

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	247	ILE	N-CA-C	-25.54	87.41	111.67
1	D	232	ARG	N-CA-C	-18.52	79.51	108.96
1	B	228	LEU	N-CA-C	13.37	133.63	109.44
1	A	118	ALA	N-CA-C	-12.95	92.47	110.35
1	C	101	ARG	NE-CZ-NH2	-12.85	107.64	119.20
1	C	101	ARG	NH1-CZ-NH2	11.08	133.70	119.30
1	A	198	LEU	N-CA-C	-10.44	91.39	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	ARG	N-CA-C	-9.73	102.49	114.75
1	B	231	TRP	N-CA-C	-9.51	102.77	114.75
1	D	269	ARG	CA-C-N	9.51	131.73	119.84
1	D	269	ARG	C-N-CA	9.51	131.73	119.84
1	A	118	ALA	CA-C-N	-9.51	109.18	122.87
1	A	118	ALA	C-N-CA	-9.51	109.18	122.87
1	B	259	LEU	CD1-CG-CD2	8.75	130.05	110.80
1	D	278	ALA	CA-C-N	8.61	137.98	121.54
1	D	278	ALA	C-N-CA	8.61	137.98	121.54
1	A	238	PRO	CA-C-N	8.22	136.77	121.97
1	A	238	PRO	C-N-CA	8.22	136.77	121.97
1	D	231	TRP	N-CA-C	8.20	123.10	113.18
1	B	227	SER	N-CA-C	8.14	122.48	112.23
1	D	233	PHE	N-CA-C	-7.88	94.03	110.80
1	A	239	ILE	CA-C-O	-7.71	111.14	120.78
1	C	98	SER	O-C-N	7.70	130.17	121.32
1	A	254	GLY	N-CA-C	-7.64	98.33	111.47
1	B	289	LEU	CD1-CG-CD2	7.57	127.45	110.80
1	B	306	SER	O-C-N	7.52	129.97	121.32
1	A	197	LYS	N-CA-C	7.37	120.91	108.90
1	B	82	LEU	CA-C-N	-7.24	111.52	119.19
1	B	82	LEU	C-N-CA	-7.24	111.52	119.19
1	B	54	LEU	CA-CB-CG	-7.17	91.19	116.30
1	B	261	LEU	CA-C-N	7.11	128.01	120.12
1	B	261	LEU	C-N-CA	7.11	128.01	120.12
1	C	101	ARG	CD-NE-CZ	-7.06	114.51	124.40
1	B	307	PRO	N-CD-CG	-7.05	92.63	103.20
1	D	273	SER	N-CA-C	6.84	125.37	110.80
1	B	289	LEU	N-CA-CB	6.75	120.10	110.44
1	D	295	VAL	CA-C-N	6.73	126.76	119.90
1	D	295	VAL	C-N-CA	6.73	126.76	119.90
1	D	279	LEU	CA-C-O	-6.68	110.95	120.51
1	A	122	VAL	CB-CA-C	-6.57	102.66	111.80
1	B	54	LEU	CB-CG-CD2	-6.57	90.98	110.70
1	D	234	MET	N-CA-C	6.48	124.61	110.80
1	B	55	ALA	CA-C-O	6.47	128.81	122.01
1	D	82	LEU	CA-C-N	-6.40	111.87	118.85
1	D	82	LEU	C-N-CA	-6.40	111.87	118.85
1	D	229	PRO	N-CA-C	6.37	125.59	112.47
1	B	254	GLY	N-CA-C	6.31	128.14	113.18
1	C	119	GLU	N-CA-CB	6.19	118.08	110.53
1	D	233	PHE	CB-CA-C	-6.19	98.11	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	118	ALA	CA-C-N	-6.17	112.93	122.05
1	C	118	ALA	C-N-CA	-6.17	112.93	122.05
1	B	277	ASP	CA-C-N	-6.09	113.06	122.87
1	B	277	ASP	C-N-CA	-6.09	113.06	122.87
1	C	259	LEU	CA-C-N	-6.07	113.51	119.76
1	C	259	LEU	C-N-CA	-6.07	113.51	119.76
1	D	247	ILE	CB-CA-C	-6.02	104.69	111.80
1	B	61	SER	N-CA-C	-6.00	104.07	111.75
1	C	239	ILE	N-CA-C	5.96	116.69	107.99
1	B	120	ALA	N-CA-C	-5.93	100.03	109.76
1	A	246	PRO	CA-C-N	5.93	127.95	120.72
1	A	246	PRO	C-N-CA	5.93	127.95	120.72
1	A	77	GLU	N-CA-C	5.84	117.72	111.36
1	B	278	ALA	N-CA-C	5.80	119.18	109.95
1	C	141	PRO	N-CA-C	-5.74	104.48	113.78
1	B	101	ARG	NE-CZ-NH2	-5.73	114.04	119.20
1	B	60	GLN	CG-CD-NE2	5.72	124.97	116.40
1	B	60	GLN	O-C-N	5.70	129.99	122.30
1	B	238	PRO	CA-C-N	-5.69	114.90	122.98
1	B	238	PRO	C-N-CA	-5.69	114.90	122.98
1	B	308	LEU	CD1-CG-CD2	5.67	123.27	110.80
1	D	162	GLY	N-CA-C	-5.66	107.16	113.79
1	A	166	HIS	CB-CA-C	5.65	119.55	109.65
1	A	212	LYS	CA-C-N	5.63	125.64	119.89
1	A	212	LYS	C-N-CA	5.63	125.64	119.89
1	A	158	ALA	N-CA-C	-5.61	104.79	111.69
1	B	59	GLY	O-C-N	5.54	129.70	122.71
1	B	255	ASP	N-CA-C	-5.48	99.13	110.80
1	C	228	LEU	CA-C-N	5.44	124.89	119.24
1	C	228	LEU	C-N-CA	5.44	124.89	119.24
1	B	277	ASP	CA-C-O	5.41	126.81	120.20
1	A	233	PHE	N-CA-C	5.41	119.71	113.38
1	B	289	LEU	N-CA-C	-5.36	103.61	110.53
1	C	122	VAL	CB-CA-C	-5.35	102.52	111.29
1	D	268	ALA	N-CA-C	5.34	118.37	110.46
1	D	228	LEU	N-CA-C	-5.34	98.81	108.85
1	D	247	ILE	N-CA-CB	5.31	118.16	110.68
1	B	56	GLY	CA-C-N	-5.28	111.45	121.54
1	B	56	GLY	C-N-CA	-5.28	111.45	121.54
1	B	112	GLU	N-CA-CB	5.27	117.87	110.12
1	A	150	ALA	N-CA-C	5.26	118.49	111.75
1	C	78	ARG	N-CA-CB	5.26	117.78	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	PRO	CA-C-N	5.22	127.23	120.44
1	B	102	PRO	C-N-CA	5.22	127.23	120.44
1	B	242	ASP	N-CA-C	-5.19	106.79	113.02
1	A	295	VAL	CA-C-N	5.17	125.16	119.89
1	A	295	VAL	C-N-CA	5.17	125.16	119.89
1	B	163	MET	CG-SD-CE	-5.16	89.55	100.90
1	C	298	THR	N-CA-C	-5.15	101.64	108.74
1	C	141	PRO	N-CD-CG	-5.11	95.53	103.20
1	D	278	ALA	N-CA-C	5.09	116.71	108.26
1	C	140	GLU	N-CA-CB	5.03	116.00	111.27
1	C	256	ALA	CA-C-N	-5.03	113.37	118.85
1	C	256	ALA	C-N-CA	-5.03	113.37	118.85
1	D	75	VAL	N-CA-C	-5.02	105.53	111.00
1	B	78	ARG	N-CA-C	-5.01	105.81	111.28

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	152	ARG	CA
1	A	237	LYS	CA
1	A	246	PRO	CA
1	A	264	ARG	CA
1	B	265	LYS	CA
1	B	269	ARG	CA
1	C	283	ASP	CA
1	C	284	SER	CA
1	D	238	PRO	CA
1	D	241	GLU	CA

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ARG	Peptide
1	A	197	LYS	Peptide
1	A	237	LYS	Peptide
1	B	188	GLY	Peptide
1	B	227	SER	Peptide
1	B	230	SER	Peptide
1	B	237	LYS	Peptide
1	B	241	GLU	Peptide
1	B	242	ASP	Peptide
1	B	265	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	267	GLU	Peptide
1	B	268	ALA	Peptide
1	B	269	ARG	Peptide
1	B	270	PRO	Peptide
1	B	271	ASP	Peptide
1	B	56	GLY	Peptide,Mainchain
1	C	281	PRO	Peptide
1	C	282	GLY	Peptide
1	C	284	SER	Peptide
1	D	229	PRO	Peptide
1	D	231	TRP	Peptide
1	D	232	ARG	Peptide
1	D	233	PHE	Peptide
1	D	246	PRO	Peptide
1	D	269	ARG	Peptide
1	D	273	SER	Peptide
1	D	278	ALA	Peptide
1	D	284	SER	Peptide

5.2 Too-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 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	1952	0	1979	121	0
1	B	1952	0	1979	177	1
1	C	1952	0	1979	102	0
1	D	1952	0	1979	88	1
2	A	7	0	2	0	0
2	B	7	0	2	0	0
2	C	7	0	2	1	0
2	D	7	0	2	1	0
3	A	5	0	0	1	0
3	B	6	0	0	0	0
3	C	1	0	0	0	0
3	D	4	0	0	2	0
All	All	7852	0	7924	478	1

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 30.

All (478) 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:306:SER:CA	1:B:306:SER:CB	1.75	1.61
1:C:97:LEU:CG	1:C:97:LEU:CD1	1.75	1.61
1:C:98:SER:CA	1:C:98:SER:CB	1.79	1.60
1:B:54:LEU:CB	1:B:54:LEU:CA	1.82	1.54
1:B:230:SER:HB3	1:B:231:TRP:CD1	1.45	1.50
1:B:259:LEU:CB	1:B:259:LEU:CG	1.88	1.48
1:B:54:LEU:CG	1:B:54:LEU:CD1	1.90	1.48
1:B:54:LEU:CB	1:B:54:LEU:CG	1.94	1.46
1:B:230:SER:CB	1:B:231:TRP:HD1	1.35	1.35
1:D:235:THR:HG21	1:D:239:ILE:CD1	1.59	1.33
1:C:283:ASP:HA	1:C:284:SER:CB	1.52	1.33
1:D:235:THR:CG2	1:D:239:ILE:HD11	1.67	1.24
1:A:152:ARG:O	1:A:156:ARG:HD3	1.33	1.22
1:D:267:GLU:O	1:D:275:THR:HG22	1.34	1.21
1:A:238:PRO:O	1:A:239:ILE:HG23	1.41	1.21
1:C:283:ASP:CA	1:C:284:SER:HB2	1.63	1.20
1:B:266:ILE:CD1	1:B:267:GLU:H	1.52	1.20
1:B:228:LEU:HD22	1:B:280:LEU:CD2	1.73	1.19
1:C:279:LEU:N	1:C:279:LEU:HD12	1.57	1.17
1:B:268:ALA:CA	1:B:269:ARG:HG3	1.75	1.16
1:D:262:PRO:CB	1:D:279:LEU:HD12	1.75	1.16
1:A:264:ARG:CG	1:A:265:LYS:H	1.55	1.14
1:B:276:LEU:HD12	1:B:290:ARG:HB2	1.19	1.14
1:A:301:ARG:HH11	1:A:301:ARG:CB	1.62	1.13
1:B:276:LEU:CD1	1:B:290:ARG:HB2	1.80	1.11
1:B:228:LEU:HD22	1:B:280:LEU:HD22	1.17	1.09
1:A:100:ASP:OD2	1:A:103:SER:HB2	1.51	1.08
1:A:264:ARG:HG3	1:A:265:LYS:N	1.63	1.07
1:B:219:ARG:HG3	1:B:219:ARG:HH11	0.97	1.07
1:B:266:ILE:HD12	1:B:267:GLU:H	0.98	1.07
1:B:266:ILE:HD12	1:B:267:GLU:N	1.70	1.07
1:B:262:PRO:HB3	1:B:279:LEU:HD12	1.37	1.06
1:D:243:ARG:HH11	1:D:243:ARG:HG2	0.91	1.06
1:C:269:ARG:HB2	1:C:273:SER:OG	1.54	1.06
1:B:268:ALA:CB	1:B:269:ARG:HG3	1.87	1.04
1:B:262:PRO:CB	1:B:279:LEU:HD12	1.88	1.03
1:B:265:LYS:C	1:B:266:ILE:HG23	1.84	1.02
1:B:231:TRP:CZ3	1:B:263:PHE:HE2	1.76	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ALA:HA	1:B:269:ARG:HG3	1.33	1.02
1:C:234:MET:HE1	1:C:257:PRO:HB2	1.41	1.01
1:D:262:PRO:HB2	1:D:279:LEU:CD1	1.89	1.01
1:B:282:GLY:O	1:B:283:ASP:CG	2.03	1.01
1:C:279:LEU:HD12	1:C:279:LEU:H	1.12	1.00
1:D:243:ARG:HH11	1:D:243:ARG:CG	1.72	0.99
1:A:68:LYS:HE2	1:A:304:GLN:HE21	1.23	0.98
1:C:264:ARG:HD2	1:C:277:ASP:HB2	1.44	0.98
1:B:219:ARG:HG3	1:B:219:ARG:NH1	1.76	0.97
1:A:236:THR:O	1:A:237:LYS:HB2	1.65	0.96
1:A:228:LEU:HD13	1:A:231:TRP:CE3	2.00	0.96
1:B:102:PRO:O	1:B:106:ARG:HG3	1.65	0.96
1:B:228:LEU:CD2	1:B:280:LEU:HD22	1.93	0.96
1:A:152:ARG:O	1:A:156:ARG:CD	2.14	0.95
1:A:151:PHE:CZ	1:A:152:ARG:CZ	2.50	0.95
1:A:264:ARG:HG3	1:A:265:LYS:H	0.78	0.94
1:C:154:TYR:OH	2:C:3:MLA:O3B	1.85	0.94
1:B:231:TRP:HZ3	1:B:263:PHE:HE2	1.02	0.93
1:D:243:ARG:HG2	1:D:243:ARG:NH1	1.57	0.93
1:A:301:ARG:HH11	1:A:301:ARG:HB2	1.31	0.93
1:B:231:TRP:CZ3	1:B:263:PHE:CE2	2.59	0.91
1:B:230:SER:CB	1:B:231:TRP:CD1	2.24	0.91
1:B:266:ILE:CG1	1:B:267:GLU:H	1.78	0.90
1:B:282:GLY:O	1:B:283:ASP:OD1	1.91	0.88
1:B:265:LYS:H	1:B:266:ILE:CG2	1.86	0.88
1:D:292:GLU:HG3	1:D:303:GLU:HG2	1.56	0.88
1:A:188:GLY:HA2	1:D:175:ARG:NH1	1.89	0.86
1:A:263:PHE:O	1:A:264:ARG:HB2	1.75	0.86
1:A:301:ARG:NH1	1:A:301:ARG:HB3	1.91	0.86
1:A:139:GLN:H	1:A:139:GLN:CD	1.83	0.86
1:B:269:ARG:HB2	1:B:270:PRO:O	1.75	0.86
1:C:279:LEU:N	1:C:279:LEU:CD1	2.33	0.86
1:B:156:ARG:HG3	1:B:156:ARG:HH11	1.37	0.85
1:B:268:ALA:HB1	1:B:269:ARG:HG3	1.58	0.85
1:B:54:LEU:CB	1:B:54:LEU:CD2	2.54	0.85
1:D:262:PRO:HB2	1:D:279:LEU:HD12	0.93	0.85
1:A:301:ARG:HH11	1:A:301:ARG:HB3	1.38	0.85
1:A:301:ARG:CB	1:A:301:ARG:NH1	2.39	0.85
1:A:228:LEU:HD13	1:A:231:TRP:CZ3	2.12	0.84
1:A:151:PHE:CZ	1:A:152:ARG:NH1	2.45	0.84
1:C:283:ASP:CA	1:C:284:SER:CB	2.30	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:TYR:OH	2:D:4:MLA:O1A	1.96	0.83
1:B:230:SER:HB3	1:B:231:TRP:HD1	0.67	0.83
1:B:265:LYS:H	1:B:266:ILE:HG23	1.44	0.83
1:C:234:MET:HE2	1:C:259:LEU:H	1.43	0.82
1:B:262:PRO:HB3	1:B:279:LEU:CD1	2.08	0.82
1:C:269:ARG:CB	1:C:273:SER:OG	2.27	0.82
1:C:279:LEU:H	1:C:279:LEU:CD1	1.92	0.82
1:B:231:TRP:HZ3	1:B:263:PHE:CE2	1.93	0.81
1:A:263:PHE:O	1:A:264:ARG:CB	2.28	0.81
1:A:237:LYS:O	1:A:237:LYS:HG2	1.79	0.80
1:A:248:ARG:HB3	1:A:254:GLY:HA2	1.63	0.80
1:C:264:ARG:O	1:C:266:ILE:HG23	1.81	0.80
1:A:173:SER:HB2	1:A:175:ARG:HG3	1.64	0.80
1:A:235:THR:HG21	1:A:239:ILE:HD13	1.62	0.80
1:B:276:LEU:CD1	1:B:290:ARG:CB	2.60	0.79
1:A:138:TRP:CD1	1:A:139:GLN:NE2	2.50	0.79
1:D:228:LEU:HG	1:D:281:PRO:HG2	1.64	0.79
1:B:54:LEU:N	1:B:54:LEU:HD12	1.97	0.79
1:B:264:ARG:O	1:B:265:LYS:HG3	1.83	0.79
1:B:264:ARG:C	1:B:265:LYS:HG3	2.06	0.79
1:A:151:PHE:CE2	1:A:152:ARG:NH1	2.50	0.79
1:A:169:MET:HE1	1:A:233:PHE:CE2	2.18	0.78
1:A:175:ARG:HH11	1:A:199:GLU:CD	1.92	0.78
1:B:61:SER:HB3	1:B:291:VAL:CG2	2.13	0.78
1:C:97:LEU:CD1	1:C:97:LEU:CB	2.62	0.78
1:B:268:ALA:HB1	1:B:269:ARG:HD3	1.66	0.77
1:D:253:PHE:HD1	1:D:256:ALA:HB2	1.47	0.77
1:B:219:ARG:HH11	1:B:219:ARG:CG	1.90	0.77
1:A:241:GLU:O	1:A:244:LEU:HG	1.85	0.76
1:A:245:ALA:HB3	1:A:246:PRO:HD3	1.66	0.76
1:B:268:ALA:HA	1:B:269:ARG:CG	2.14	0.76
1:C:78:ARG:HA	1:D:78:ARG:HB2	1.67	0.76
1:B:262:PRO:HB2	1:B:279:LEU:HD12	1.67	0.75
1:B:266:ILE:CG1	1:B:267:GLU:N	2.45	0.75
1:B:56:GLY:C	1:B:58:ALA:H	1.95	0.75
1:C:78:ARG:HA	1:D:78:ARG:CB	2.17	0.75
1:D:241:GLU:CB	1:D:244:LEU:HD12	2.16	0.75
1:B:266:ILE:CD1	1:B:267:GLU:N	2.38	0.74
1:A:151:PHE:HZ	1:A:152:ARG:CZ	1.99	0.74
1:C:68:LYS:NZ	1:C:304:GLN:HE21	1.86	0.74
1:B:268:ALA:HB1	1:B:269:ARG:CD	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ASP:HB3	1:C:157:LEU:HD12	1.68	0.73
1:B:259:LEU:CB	1:B:259:LEU:CD1	2.67	0.73
1:B:263:PHE:O	1:B:263:PHE:CD1	2.42	0.73
1:D:73:ARG:HD2	1:D:296:PRO:HB2	1.69	0.73
1:D:279:LEU:O	1:D:280:LEU:C	2.32	0.72
1:B:268:ALA:HB1	1:B:269:ARG:CG	2.19	0.72
1:A:175:ARG:NH1	1:A:199:GLU:CD	2.47	0.72
1:D:241:GLU:HB2	1:D:244:LEU:HD12	1.69	0.72
1:C:274:SER:O	1:C:289:LEU:HD22	1.90	0.71
1:B:54:LEU:CA	1:B:54:LEU:CG	2.69	0.71
1:C:269:ARG:HB2	1:C:273:SER:HG	1.55	0.71
1:B:306:SER:CB	1:B:306:SER:N	2.53	0.71
1:B:265:LYS:O	1:B:266:ILE:HG23	1.91	0.71
1:A:108:ASN:HD21	1:A:134:ALA:HA	1.55	0.70
1:B:285:THR:O	1:B:285:THR:HG22	1.92	0.70
1:B:59:GLY:HA2	1:B:62:ARG:NH1	2.06	0.69
1:C:234:MET:CE	1:C:259:LEU:H	2.05	0.69
1:A:238:PRO:O	1:A:239:ILE:CG2	2.32	0.69
1:A:153:ASP:HB2	1:A:166:HIS:CE1	2.28	0.68
1:B:265:LYS:C	1:B:266:ILE:CG2	2.57	0.68
1:B:265:LYS:N	1:B:266:ILE:HG23	2.09	0.68
1:B:228:LEU:HD22	1:B:280:LEU:HD23	1.74	0.68
1:B:276:LEU:HD11	1:B:290:ARG:CB	2.23	0.68
1:A:173:SER:CB	1:A:175:ARG:HG3	2.23	0.68
1:A:68:LYS:CE	1:A:304:GLN:HE21	2.01	0.68
1:B:217:THR:HG21	1:B:236:THR:CG2	2.24	0.68
1:B:217:THR:HG21	1:B:236:THR:HG23	1.75	0.67
1:C:152:ARG:O	1:C:156:ARG:HG2	1.95	0.67
1:B:248:ARG:HB3	1:B:254:GLY:HA2	1.77	0.67
1:A:234:MET:HE1	1:A:257:PRO:HB2	1.76	0.67
1:B:259:LEU:CG	1:B:259:LEU:CA	2.71	0.67
1:C:78:ARG:NH1	1:D:77:GLU:HG2	2.09	0.67
1:A:169:MET:HE1	1:A:233:PHE:HE2	1.57	0.66
1:D:90:ALA:HA	1:D:93:ARG:HG2	1.76	0.66
1:D:253:PHE:CD1	1:D:256:ALA:HB2	2.29	0.66
1:A:152:ARG:NH2	1:A:171:THR:OG1	2.29	0.66
1:B:264:ARG:C	1:B:265:LYS:CG	2.69	0.66
1:C:183:ARG:HD2	1:C:190:PRO:HB3	1.77	0.66
1:D:77:GLU:HG3	3:D:316:HOH:O	1.96	0.65
1:A:294:MET:HE1	1:A:301:ARG:HH12	1.61	0.65
1:B:242:ASP:OD1	1:B:242:ASP:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:THR:O	1:A:237:LYS:CB	2.43	0.64
1:A:264:ARG:CG	1:A:265:LYS:N	2.30	0.64
1:B:230:SER:HG	1:B:231:TRP:CD1	2.15	0.64
1:A:151:PHE:HZ	1:A:152:ARG:NH2	1.95	0.64
1:C:169:MET:HE1	1:C:233:PHE:CE2	2.32	0.64
1:C:234:MET:HE3	1:C:234:MET:HA	1.79	0.64
1:A:78:ARG:HG2	3:A:314:HOH:O	1.97	0.64
1:C:292:GLU:HG2	1:C:303:GLU:HG2	1.80	0.64
1:B:229:PRO:O	1:B:231:TRP:N	2.31	0.64
1:C:269:ARG:HG2	1:C:270:PRO:HD2	1.79	0.64
1:C:233:PHE:HB2	1:C:257:PRO:HD2	1.80	0.63
1:D:235:THR:HG21	1:D:239:ILE:HD11	0.75	0.63
1:D:77:GLU:CG	3:D:316:HOH:O	2.47	0.63
1:A:245:ALA:CB	1:A:246:PRO:HD3	2.29	0.63
1:A:269:ARG:HD3	1:A:273:SER:OG	1.99	0.63
1:B:61:SER:HB3	1:B:291:VAL:HG21	1.81	0.63
1:B:61:SER:HB3	1:B:291:VAL:HG22	1.80	0.62
1:B:217:THR:OG1	1:B:301:ARG:HG2	1.99	0.62
1:B:230:SER:OG	1:B:231:TRP:CD1	2.51	0.62
1:C:169:MET:HE1	1:C:233:PHE:CZ	2.34	0.62
1:D:292:GLU:CG	1:D:303:GLU:HG2	2.26	0.62
1:B:265:LYS:N	1:B:266:ILE:CG2	2.60	0.62
1:C:234:MET:HE2	1:C:259:LEU:N	2.14	0.62
1:A:280:LEU:HD13	1:A:288:PHE:CZ	2.35	0.62
1:B:263:PHE:O	1:B:263:PHE:HD1	1.81	0.62
1:B:259:LEU:CB	1:B:259:LEU:CD2	2.73	0.61
1:A:70:SER:OG	1:A:73:ARG:NH2	2.33	0.61
1:D:73:ARG:CD	1:D:296:PRO:HB2	2.30	0.61
1:B:276:LEU:HD11	1:B:290:ARG:HB2	1.75	0.61
1:A:138:TRP:CD1	1:A:139:GLN:HE22	2.16	0.61
1:B:231:TRP:CH2	1:B:263:PHE:CD2	2.88	0.61
1:C:92:ILE:HD13	1:C:107:ILE:HD12	1.82	0.61
1:B:266:ILE:HD12	1:B:267:GLU:CA	2.32	0.60
1:C:169:MET:O	1:C:252:GLN:NE2	2.35	0.60
1:A:188:GLY:HA2	1:D:175:ARG:CZ	2.31	0.60
1:B:54:LEU:CB	1:B:54:LEU:C	2.73	0.60
1:B:262:PRO:CB	1:B:279:LEU:CD1	2.73	0.60
1:A:254:GLY:O	1:A:256:ALA:N	2.35	0.60
1:B:266:ILE:O	1:B:275:THR:HG22	2.03	0.59
1:B:231:TRP:CH2	1:B:263:PHE:CE2	2.90	0.59
1:D:170:GLY:O	1:D:174:ASN:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:GLU:HB3	1:D:244:LEU:CD1	2.33	0.59
1:A:78:ARG:HA	1:B:78:ARG:HB2	1.84	0.59
1:A:105:ASP:HB3	1:A:109:ARG:NH2	2.17	0.59
1:A:151:PHE:O	1:A:152:ARG:O	2.20	0.58
1:B:105:ASP:HB3	1:B:109:ARG:HH22	1.69	0.58
1:D:253:PHE:HD1	1:D:256:ALA:CB	2.15	0.58
1:A:152:ARG:HD3	1:A:252:GLN:CD	2.29	0.58
1:A:151:PHE:C	1:A:152:ARG:O	2.47	0.58
1:C:283:ASP:HA	1:C:284:SER:HB2	0.69	0.58
1:C:105:ASP:HA	1:C:108:ASN:HB2	1.86	0.58
1:A:175:ARG:NH1	1:A:199:GLU:OE1	2.37	0.58
1:A:155:PHE:O	1:A:159:VAL:HG23	2.04	0.57
1:B:216:VAL:HG13	1:B:300:TRP:HB3	1.85	0.57
1:B:306:SER:CB	1:B:306:SER:C	2.76	0.57
1:C:68:LYS:HZ2	1:C:304:GLN:HE21	1.52	0.57
1:C:126:ILE:HA	1:C:132:ALA:HA	1.86	0.57
1:B:56:GLY:C	1:B:58:ALA:N	2.62	0.57
1:B:82:LEU:O	1:B:86:LEU:HG	2.04	0.57
1:B:265:LYS:H	1:B:266:ILE:HG22	1.65	0.57
1:B:276:LEU:HD11	1:B:290:ARG:CG	2.35	0.57
1:C:68:LYS:HZ3	1:C:304:GLN:HE21	1.53	0.56
1:D:152:ARG:HG3	1:D:154:TYR:CE2	2.41	0.56
1:B:228:LEU:O	1:B:231:TRP:HB2	2.05	0.56
1:C:98:SER:CB	1:C:98:SER:C	2.75	0.56
1:C:243:ARG:O	1:C:247:ILE:HG13	2.06	0.56
1:D:82:LEU:HB2	1:D:83:PRO:HD3	1.88	0.56
1:B:68:LYS:NZ	1:B:304:GLN:HE21	2.04	0.56
1:B:231:TRP:HH2	1:B:263:PHE:CD2	2.24	0.56
1:A:93:ARG:NH1	1:A:185:ASP:O	2.38	0.55
1:A:243:ARG:O	1:A:247:ILE:HG13	2.06	0.55
1:D:108:ASN:ND2	1:D:135:ALA:H	2.04	0.55
1:A:112:GLU:O	1:A:116:THR:HG23	2.06	0.55
1:A:261:LEU:HD13	1:A:263:PHE:CE1	2.41	0.55
1:B:156:ARG:HH11	1:B:156:ARG:CG	2.13	0.55
1:B:169:MET:HE1	1:B:233:PHE:CZ	2.42	0.55
1:B:54:LEU:CD1	1:B:54:LEU:CD2	2.84	0.55
1:B:231:TRP:HH2	1:B:263:PHE:HD2	1.55	0.55
1:C:101:ARG:HG2	1:C:105:ASP:OD1	2.06	0.55
1:A:218:ASP:OD2	1:A:220:ARG:NH2	2.34	0.55
1:B:105:ASP:OD1	1:B:105:ASP:N	2.36	0.55
1:B:239:ILE:HD11	1:B:244:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:VAL:HG13	1:C:301:ARG:O	2.07	0.54
1:C:294:MET:HE1	1:C:301:ARG:CZ	2.36	0.54
1:B:155:PHE:O	1:B:158:ALA:HB3	2.06	0.54
1:C:108:ASN:HD21	1:C:135:ALA:H	1.55	0.54
1:A:138:TRP:NE1	1:A:139:GLN:HE21	2.05	0.54
1:C:101:ARG:HB3	1:C:102:PRO:HD3	1.90	0.54
1:C:165:GLU:HG2	1:C:178:LEU:HD11	1.90	0.54
1:B:240:ALA:O	1:B:241:GLU:C	2.51	0.54
1:D:80:ARG:O	1:D:83:PRO:HD2	2.07	0.54
1:B:105:ASP:HB3	1:B:109:ARG:NH2	2.23	0.54
1:B:273:SER:O	1:B:274:SER:HB3	2.08	0.54
1:B:301:ARG:NH1	1:B:301:ARG:HB2	2.23	0.53
1:D:127:ASP:HB3	1:D:129:SER:H	1.72	0.53
1:B:283:ASP:O	1:B:285:THR:N	2.42	0.53
1:B:265:LYS:CA	1:B:266:ILE:HG23	2.37	0.53
1:A:78:ARG:NH1	1:B:77:GLU:HG2	2.24	0.53
1:B:268:ALA:CA	1:B:269:ARG:CG	2.69	0.53
1:B:54:LEU:CD1	1:B:54:LEU:N	2.71	0.53
1:B:68:LYS:HZ2	1:B:304:GLN:NE2	2.07	0.53
1:C:264:ARG:HD2	1:C:277:ASP:CB	2.30	0.53
1:B:77:GLU:OE2	1:B:80:ARG:HD2	2.09	0.53
1:B:175:ARG:NH1	1:B:199:GLU:OE1	2.42	0.53
1:A:213:PRO:HB3	1:A:228:LEU:HD11	1.91	0.52
1:A:228:LEU:CD1	1:A:231:TRP:CZ3	2.89	0.52
1:B:259:LEU:HD23	1:B:259:LEU:HA	1.91	0.52
1:C:79:GLN:NE2	1:C:120:ALA:HB2	2.24	0.52
1:A:96:LEU:HD11	1:A:125:LEU:HD11	1.92	0.52
1:D:241:GLU:CB	1:D:244:LEU:CD1	2.85	0.52
1:A:108:ASN:HB3	1:A:138:TRP:CD1	2.44	0.52
1:C:234:MET:HG3	1:C:259:LEU:O	2.10	0.52
1:B:68:LYS:NZ	1:B:304:GLN:NE2	2.58	0.52
1:B:266:ILE:HG13	1:B:267:GLU:N	2.23	0.52
1:B:276:LEU:HD11	1:B:290:ARG:HE	1.74	0.52
1:D:152:ARG:CG	1:D:154:TYR:CE2	2.92	0.51
1:D:217:THR:HA	1:D:222:ILE:O	2.11	0.51
1:B:220:ARG:HB2	1:B:222:ILE:HD12	1.92	0.51
1:B:63:ILE:C	1:B:63:ILE:HD12	2.36	0.51
1:B:106:ARG:HH11	1:B:106:ARG:HB3	1.76	0.51
1:C:63:ILE:HG12	1:C:64:ASP:N	2.25	0.51
1:C:68:LYS:NZ	1:C:304:GLN:NE2	2.56	0.51
1:C:278:ALA:C	1:C:279:LEU:HD12	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:SER:O	1:C:289:LEU:CD2	2.57	0.51
1:D:186:GLY:O	1:D:188:GLY:N	2.41	0.51
1:D:279:LEU:O	1:D:280:LEU:O	2.28	0.51
1:A:246:PRO:O	1:A:250:SER:N	2.37	0.51
1:C:126:ILE:HG21	1:C:130:GLY:HA2	1.92	0.51
1:C:156:ARG:HG3	1:C:156:ARG:HH11	1.76	0.51
1:C:237:LYS:HB2	1:C:238:PRO:HD2	1.93	0.50
1:B:269:ARG:HH21	1:B:270:PRO:HA	1.75	0.50
1:D:84:LEU:HA	1:D:182:ARG:HD2	1.93	0.50
1:A:240:ALA:O	1:A:241:GLU:C	2.55	0.50
1:A:280:LEU:HD13	1:A:288:PHE:HZ	1.76	0.50
1:B:231:TRP:CH2	1:B:263:PHE:HD2	2.29	0.50
1:B:277:ASP:OD1	1:B:287:ALA:HA	2.11	0.50
1:C:126:ILE:CG2	1:C:130:GLY:HA2	2.41	0.50
1:C:234:MET:HE2	1:C:259:LEU:HB2	1.93	0.50
1:C:101:ARG:O	1:C:105:ASP:OD1	2.30	0.50
1:C:266:ILE:HG13	1:C:266:ILE:O	2.12	0.50
1:A:79:GLN:NE2	1:A:120:ALA:HB2	2.26	0.50
1:B:169:MET:HE1	1:B:233:PHE:HZ	1.77	0.50
1:A:217:THR:HA	1:A:222:ILE:O	2.12	0.50
1:C:234:MET:CE	1:C:234:MET:HA	2.41	0.50
1:C:290:ARG:HA	1:C:304:GLN:O	2.11	0.50
1:A:188:GLY:HA2	1:D:175:ARG:HH12	1.76	0.50
1:C:68:LYS:HZ2	1:C:304:GLN:NE2	2.10	0.49
1:C:79:GLN:HA	1:C:79:GLN:OE1	2.11	0.49
1:C:80:ARG:NH2	1:C:165:GLU:OE2	2.38	0.49
1:C:128:ARG:HB3	1:C:191:LEU:O	2.12	0.49
1:D:79:GLN:NE2	1:D:120:ALA:HB2	2.28	0.49
1:C:78:ARG:HA	1:D:78:ARG:HB3	1.92	0.49
1:C:280:LEU:O	1:C:282:GLY:HA2	2.12	0.49
1:A:117:SER:C	1:A:118:ALA:O	2.47	0.49
1:B:292:GLU:HG3	1:B:301:ARG:HD3	1.93	0.49
1:D:269:ARG:HD3	1:D:272:GLY:HA2	1.93	0.49
1:D:292:GLU:HG2	1:D:301:ARG:HD3	1.94	0.49
1:D:108:ASN:HD22	1:D:135:ALA:H	1.59	0.49
1:D:112:GLU:O	1:D:116:THR:HG23	2.12	0.49
1:C:243:ARG:HA	1:C:246:PRO:HG2	1.94	0.49
1:C:183:ARG:HD2	1:C:190:PRO:CB	2.42	0.49
1:D:262:PRO:CB	1:D:279:LEU:CD1	2.68	0.49
1:B:219:ARG:NH1	1:B:219:ARG:CG	2.59	0.48
1:A:138:TRP:CD1	1:A:139:GLN:HE21	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ASP:O	1:B:284:SER:C	2.56	0.48
1:D:186:GLY:C	1:D:188:GLY:H	2.20	0.48
1:C:126:ILE:HG22	1:C:127:ASP:O	2.13	0.48
1:D:79:GLN:HA	1:D:82:LEU:CD2	2.44	0.48
1:D:237:LYS:HA	1:D:238:PRO:HD3	1.41	0.48
1:A:173:SER:HB2	1:A:175:ARG:CG	2.38	0.48
1:B:177:GLY:HA3	1:B:197:LYS:HE2	1.95	0.48
1:C:215:TYR:OH	1:C:303:GLU:OE1	2.19	0.48
1:D:253:PHE:O	1:D:255:ASP:N	2.47	0.48
1:A:234:MET:CE	1:A:257:PRO:HB2	2.43	0.47
1:A:139:GLN:CD	1:A:139:GLN:N	2.59	0.47
1:D:128:ARG:HH21	1:D:190:PRO:HG2	1.79	0.47
1:B:105:ASP:CB	1:B:109:ARG:NH2	2.77	0.47
1:B:264:ARG:HB3	1:B:265:LYS:HG2	1.95	0.47
1:D:121:ALA:HB2	1:D:199:GLU:HG3	1.96	0.47
1:D:306:SER:O	1:D:307:PRO:O	2.31	0.47
1:A:217:THR:OG1	1:A:301:ARG:HG3	2.15	0.47
1:A:108:ASN:HB3	1:A:138:TRP:CG	2.50	0.47
1:A:237:LYS:O	1:A:237:LYS:CG	2.57	0.47
1:C:210:SER:C	1:C:212:LYS:H	2.21	0.47
1:D:294:MET:O	1:D:296:PRO:HD3	2.15	0.47
1:A:68:LYS:HD3	1:A:207:TRP:CD1	2.50	0.47
1:A:302:LEU:C	1:A:302:LEU:HD23	2.40	0.47
1:B:105:ASP:OD2	1:C:297:SER:HB3	2.15	0.47
1:B:130:GLY:HA3	1:B:150:ALA:HB2	1.97	0.47
1:D:287:ALA:HB1	1:D:308:LEU:HD23	1.97	0.46
1:D:173:SER:O	1:D:174:ASN:ND2	2.48	0.46
1:C:283:ASP:CA	1:C:284:SER:HB3	2.37	0.46
1:B:60:GLN:HG3	1:B:64:ASP:OD2	2.16	0.46
1:A:68:LYS:HE2	1:A:304:GLN:NE2	2.08	0.46
1:C:149:TYR:C	1:C:151:PHE:H	2.24	0.46
1:C:107:ILE:O	1:C:111:LEU:HG	2.15	0.46
1:A:127:ASP:HB2	1:A:131:VAL:O	2.16	0.46
1:A:169:MET:CE	1:A:233:PHE:CE2	2.95	0.46
1:D:177:GLY:HA3	1:D:197:LYS:HE2	1.98	0.46
1:B:275:THR:C	1:B:276:LEU:HG	2.41	0.45
1:A:97:LEU:HD23	1:A:191:LEU:HD21	1.99	0.45
1:A:152:ARG:HD3	1:A:252:GLN:NE2	2.32	0.45
1:A:292:GLU:HG2	1:A:293:THR:N	2.31	0.45
1:C:128:ARG:HE	1:C:128:ARG:HB2	1.48	0.45
1:B:240:ALA:O	1:B:242:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:SER:OG	1:B:290:ARG:NE	2.49	0.45
1:C:255:ASP:O	1:C:256:ALA:C	2.60	0.45
1:B:217:THR:HA	1:B:222:ILE:O	2.16	0.45
1:B:301:ARG:HB2	1:B:301:ARG:HH11	1.81	0.45
1:C:262:PRO:O	1:C:263:PHE:HD1	1.99	0.45
1:D:253:PHE:HB3	1:D:256:ALA:HB2	1.98	0.45
1:B:276:LEU:O	1:B:277:ASP:OD1	2.34	0.45
1:B:285:THR:O	1:B:286:ALA:O	2.35	0.45
1:C:79:GLN:HE22	1:C:120:ALA:HB2	1.80	0.45
1:D:217:THR:HG21	1:D:236:THR:HG23	1.99	0.45
1:D:228:LEU:HD21	1:D:281:PRO:HD2	1.99	0.45
1:A:251:LEU:O	1:A:252:GLN:HB2	2.16	0.45
1:B:301:ARG:HD2	1:B:303:GLU:OE2	2.17	0.45
1:D:306:SER:HA	1:D:307:PRO:HD2	1.90	0.45
1:A:151:PHE:CZ	1:A:152:ARG:NH2	2.74	0.45
1:B:216:VAL:CG1	1:B:300:TRP:HB3	2.47	0.45
1:C:284:SER:OG	1:C:285:THR:N	2.50	0.45
1:A:290:ARG:HA	1:A:304:GLN:O	2.17	0.44
1:B:217:THR:HG21	1:B:236:THR:HG21	1.98	0.44
1:B:239:ILE:O	1:B:239:ILE:HG13	2.17	0.44
1:A:170:GLY:O	1:A:171:THR:C	2.60	0.44
1:C:222:ILE:HD11	1:C:247:ILE:HD13	1.99	0.44
1:D:217:THR:HG21	1:D:236:THR:CG2	2.46	0.44
1:A:89:ASP:HB3	1:A:92:ILE:HG13	1.99	0.44
1:B:169:MET:CA	1:B:169:MET:HE2	2.48	0.44
1:D:73:ARG:HH11	1:D:296:PRO:HG2	1.82	0.44
1:A:108:ASN:ND2	1:A:134:ALA:HA	2.29	0.44
1:D:269:ARG:H	1:D:274:SER:H	1.64	0.44
1:B:279:LEU:O	1:B:280:LEU:HB2	2.18	0.44
1:A:100:ASP:OD2	1:A:103:SER:CB	2.44	0.44
1:B:251:LEU:O	1:B:252:GLN:HB2	2.16	0.44
1:D:87:ALA:HA	1:D:184:VAL:HG22	2.00	0.43
1:B:269:ARG:O	1:B:271:ASP:HB2	2.17	0.43
1:B:100:ASP:O	1:B:103:SER:HB2	2.18	0.43
1:C:98:SER:CA	1:C:98:SER:OG	2.59	0.43
1:A:138:TRP:NE1	1:A:139:GLN:NE2	2.65	0.43
1:D:274:SER:HB3	1:D:290:ARG:HB3	1.99	0.43
1:D:295:VAL:O	1:D:298:THR:OG1	2.35	0.43
1:A:73:ARG:HG2	1:A:73:ARG:HH11	1.83	0.43
1:B:228:LEU:HA	1:B:229:PRO:HD3	1.77	0.43
1:C:96:LEU:HD11	1:C:125:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:MET:HE3	1:B:169:MET:HB2	1.89	0.43
1:D:216:VAL:HA	1:D:301:ARG:O	2.18	0.43
1:C:239:ILE:HD11	1:C:244:LEU:CD1	2.49	0.43
1:B:229:PRO:C	1:B:231:TRP:N	2.77	0.43
1:B:127:ASP:HB2	1:B:131:VAL:O	2.19	0.43
1:D:280:LEU:HD12	1:D:280:LEU:HA	1.84	0.43
1:C:228:LEU:HA	1:C:229:PRO:HD2	1.89	0.43
1:A:245:ALA:O	1:A:246:PRO:C	2.62	0.42
1:A:150:ALA:HA	1:A:155:PHE:CD2	2.54	0.42
1:B:59:GLY:HA2	1:B:62:ARG:HH12	1.80	0.42
1:B:266:ILE:O	1:B:267:GLU:O	2.38	0.42
1:C:283:ASP:N	1:C:284:SER:HB3	2.33	0.42
1:D:273:SER:O	1:D:274:SER:HB2	2.18	0.42
1:B:306:SER:HA	1:B:307:PRO:HD2	1.79	0.42
1:C:155:PHE:O	1:C:159:VAL:HG23	2.18	0.42
1:D:138:TRP:H	1:D:138:TRP:CD1	2.37	0.42
1:D:216:VAL:HG13	1:D:300:TRP:HB3	2.01	0.42
1:A:152:ARG:HD3	1:A:252:GLN:OE1	2.20	0.42
1:A:233:PHE:O	1:A:258:LEU:HD23	2.20	0.42
1:A:234:MET:HE1	1:A:257:PRO:CB	2.47	0.42
1:C:108:ASN:ND2	1:C:135:ALA:H	2.15	0.42
1:A:240:ALA:O	1:A:242:ASP:N	2.53	0.42
1:A:249:GLU:O	1:A:250:SER:C	2.63	0.42
1:A:151:PHE:HZ	1:A:152:ARG:NH1	2.06	0.42
1:B:265:LYS:N	1:B:266:ILE:HG22	2.31	0.42
1:B:276:LEU:HD11	1:B:290:ARG:NE	2.34	0.42
1:D:202:GLY:O	1:D:206:ASP:OD1	2.37	0.42
1:A:97:LEU:HD23	1:A:191:LEU:CD2	2.50	0.42
1:A:173:SER:OG	1:A:175:ARG:HG3	2.19	0.42
1:B:271:ASP:HB3	1:B:273:SER:OG	2.19	0.42
1:B:284:SER:C	1:B:285:THR:OG1	2.63	0.42
1:A:92:ILE:O	1:A:93:ARG:C	2.63	0.42
1:B:289:LEU:HD23	1:B:308:LEU:HD11	2.01	0.42
1:D:253:PHE:CD1	1:D:256:ALA:CA	3.03	0.42
1:B:79:GLN:NE2	1:B:120:ALA:HB2	2.35	0.42
1:B:276:LEU:HD11	1:B:290:ARG:HG3	2.01	0.42
1:B:70:SER:O	1:B:71:LEU:C	2.63	0.41
1:B:183:ARG:HE	1:B:185:ASP:CG	2.28	0.41
1:C:156:ARG:HG3	1:C:156:ARG:NH1	2.35	0.41
1:D:79:GLN:HE22	1:D:120:ALA:HB2	1.85	0.41
1:A:101:ARG:HB3	1:A:102:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:TRP:O	1:A:234:MET:HB2	2.19	0.41
1:C:108:ASN:HD22	1:C:108:ASN:HA	1.52	0.41
1:C:234:MET:HE2	1:C:259:LEU:CB	2.51	0.41
1:C:239:ILE:HD11	1:C:244:LEU:HD13	2.02	0.41
1:C:261:LEU:HD13	1:C:263:PHE:CE2	2.55	0.41
1:D:294:MET:HE1	1:D:301:ARG:CZ	2.51	0.41
1:A:135:ALA:O	1:A:136:SER:C	2.63	0.41
1:B:169:MET:CE	1:B:233:PHE:CZ	3.03	0.41
1:C:181:SER:O	1:C:182:ARG:HG3	2.21	0.41
1:C:283:ASP:N	1:C:284:SER:CB	2.82	0.41
1:D:276:LEU:HD12	1:D:277:ASP:N	2.36	0.41
1:D:279:LEU:C	1:D:280:LEU:O	2.60	0.41
1:A:206:ASP:O	1:A:209:ALA:N	2.51	0.41
1:B:156:ARG:HG3	1:B:156:ARG:NH1	2.16	0.41
1:B:215:TYR:OH	1:B:303:GLU:OE1	2.29	0.41
1:D:237:LYS:O	1:D:238:PRO:C	2.63	0.41
1:D:253:PHE:HD1	1:D:256:ALA:CA	2.34	0.41
1:D:276:LEU:HD12	1:D:276:LEU:C	2.46	0.41
1:A:151:PHE:O	1:A:152:ARG:C	2.64	0.41
1:B:68:LYS:HZ2	1:B:304:GLN:HE21	1.68	0.41
1:B:289:LEU:O	1:B:305:LEU:HA	2.21	0.41
1:A:122:VAL:HG21	1:A:144:PHE:CE2	2.56	0.40
1:A:295:VAL:O	1:A:298:THR:OG1	2.30	0.40
1:B:266:ILE:HD12	1:B:267:GLU:HA	2.03	0.40
1:C:215:TYR:HB2	1:C:223:VAL:HG13	2.03	0.40
1:B:245:ALA:N	1:B:246:PRO:HD2	2.36	0.40
1:D:78:ARG:NH1	1:D:118:ALA:HA	2.36	0.40
1:D:121:ALA:CB	1:D:199:GLU:HG3	2.51	0.40
1:C:263:PHE:CD1	1:C:276:LEU:HD13	2.57	0.40
1:B:221:GLY:O	1:B:235:THR:HA	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ASP:OD1	1:D:241:GLU:OE2[3_554]	1.76	0.44

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	253/305 (83%)	225 (89%)	17 (7%)	11 (4%)	2	2
1	B	253/305 (83%)	216 (85%)	20 (8%)	17 (7%)	1	1
1	C	253/305 (83%)	226 (89%)	23 (9%)	4 (2%)	7	14
1	D	253/305 (83%)	216 (85%)	21 (8%)	16 (6%)	1	1
All	All	1012/1220 (83%)	883 (87%)	81 (8%)	48 (5%)	2	2

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	ARG
1	A	237	LYS
1	A	238	PRO
1	A	239	ILE
1	A	255	ASP
1	B	230	SER
1	B	255	ASP
1	B	265	LYS
1	B	266	ILE
1	B	268	ALA
1	B	269	ARG
1	B	270	PRO
1	B	279	LEU
1	B	283	ASP
1	C	283	ASP
1	D	230	SER
1	D	233	PHE
1	D	234	MET
1	D	269	ARG
1	D	270	PRO
1	D	273	SER
1	D	274	SER

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Mol	Chain	Res	Type
1	D	279	LEU
1	D	307	PRO
1	A	128	ARG
1	A	241	GLU
1	B	267	GLU
1	B	280	LEU
1	B	281	PRO
1	B	284	SER
1	B	286	ALA
1	A	136	SER
1	B	271	ASP
1	B	307	PRO
1	C	97	LEU
1	C	142	THR
1	A	265	LYS
1	A	273	SER
1	D	127	ASP
1	D	238	PRO
1	B	57	LEU
1	A	92	ILE
1	C	242	ASP
1	D	239	ILE
1	D	257	PRO
1	D	284	SER
1	D	229	PRO
1	D	187	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	204/242 (84%)	175 (86%)	29 (14%)	3	7
1	B	204/242 (84%)	163 (80%)	41 (20%)	1	2
1	C	204/242 (84%)	174 (85%)	30 (15%)	3	6
1	D	204/242 (84%)	171 (84%)	33 (16%)	2	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	816/968 (84%)	683 (84%)	133 (16%)	2 4

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	63	ILE
1	A	67	LEU
1	A	70	SER
1	A	77	GLU
1	A	78	ARG
1	A	103	SER
1	A	116	THR
1	A	119	GLU
1	A	122	VAL
1	A	128	ARG
1	A	139	GLN
1	A	152	ARG
1	A	156	ARG
1	A	166	HIS
1	A	172	VAL
1	A	175	ARG
1	A	203	VAL
1	A	226	THR
1	A	228	LEU
1	A	234	MET
1	A	237	LYS
1	A	242	ASP
1	A	265	LYS
1	A	279	LEU
1	A	292	GLU
1	A	294	MET
1	A	301	ARG
1	A	308	LEU
1	B	54	LEU
1	B	62	ARG
1	B	67	LEU
1	B	71	LEU
1	B	77	GLU
1	B	78	ARG
1	B	85	VAL
1	B	88	ASP

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Mol	Chain	Res	Type
1	B	93	ARG
1	B	100	ASP
1	B	105	ASP
1	B	106	ARG
1	B	112	GLU
1	B	122	VAL
1	B	127	ASP
1	B	128	ARG
1	B	129	SER
1	B	156	ARG
1	B	159	VAL
1	B	163	MET
1	B	174	ASN
1	B	175	ARG
1	B	203	VAL
1	B	219	ARG
1	B	237	LYS
1	B	239	ILE
1	B	241	GLU
1	B	242	ASP
1	B	243	ARG
1	B	267	GLU
1	B	269	ARG
1	B	271	ASP
1	B	273	SER
1	B	284	SER
1	B	289	LEU
1	B	290	ARG
1	B	291	VAL
1	B	293	THR
1	B	301	ARG
1	B	306	SER
1	B	308	LEU
1	C	60	GLN
1	C	63	ILE
1	C	71	LEU
1	C	78	ARG
1	C	82	LEU
1	C	88	ASP
1	C	103	SER
1	C	106	ARG
1	C	108	ASN

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Mol	Chain	Res	Type
1	C	119	GLU
1	C	122	VAL
1	C	124	TYR
1	C	128	ARG
1	C	169	MET
1	C	171	THR
1	C	172	VAL
1	C	203	VAL
1	C	208	GLN
1	C	219	ARG
1	C	226	THR
1	C	234	MET
1	C	239	ILE
1	C	269	ARG
1	C	274	SER
1	C	276	LEU
1	C	279	LEU
1	C	280	LEU
1	C	283	ASP
1	C	289	LEU
1	C	294	MET
1	D	60	GLN
1	D	66	SER
1	D	71	LEU
1	D	77	GLU
1	D	78	ARG
1	D	82	LEU
1	D	88	ASP
1	D	93	ARG
1	D	101	ARG
1	D	114	LEU
1	D	116	THR
1	D	124	TYR
1	D	128	ARG
1	D	152	ARG
1	D	163	MET
1	D	171	THR
1	D	174	ASN
1	D	194	ILE
1	D	208	GLN
1	D	228	LEU
1	D	241	GLU

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Mol	Chain	Res	Type
1	D	243	ARG
1	D	247	ILE
1	D	253	PHE
1	D	266	ILE
1	D	267	GLU
1	D	273	SER
1	D	274	SER
1	D	289	LEU
1	D	292	GLU
1	D	297	SER
1	D	306	SER
1	D	308	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	108	ASN
1	A	166	HIS
1	A	252	GLN
1	A	304	GLN
1	B	79	GLN
1	B	108	ASN
1	B	139	GLN
1	B	299	ASN
1	B	304	GLN
1	C	60	GLN
1	C	108	ASN
1	C	208	GLN
1	C	304	GLN
1	D	60	GLN
1	D	79	GLN
1	D	108	ASN
1	D	174	ASN
1	D	252	GLN
1	D	304	GLN

5.3.3 RNA ⓘ

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](#)

4 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	MLA	D	4	-	6,6,6	1.33	1 (16%)	7,7,7	0.98	0
2	MLA	C	3	-	6,6,6	1.18	0	7,7,7	1.30	0
2	MLA	B	2	-	6,6,6	1.92	1 (16%)	7,7,7	1.39	1 (14%)
2	MLA	A	1	-	6,6,6	1.24	0	7,7,7	1.55	2 (28%)

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	MLA	D	4	-	-	2/4/4/4	-
2	MLA	C	3	-	-	0/4/4/4	-
2	MLA	B	2	-	-	0/4/4/4	-
2	MLA	A	1	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	MLA	C2-C3	3.72	1.56	1.51
2	D	4	MLA	O1A-C1	-2.02	1.24	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	1	MLA	O3A-C3-C2	-2.48	115.06	122.11
2	B	2	MLA	O1B-C1-C2	-2.11	116.10	122.11
2	A	1	MLA	O1B-C1-C2	-2.09	116.16	122.11

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	4	MLA	O1A-C1-C2-C3
2	A	1	MLA	C1-C2-C3-O3B
2	D	4	MLA	O1B-C1-C2-C3
2	A	1	MLA	C1-C2-C3-O3A
2	A	1	MLA	O1B-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4	MLA	1	0
2	C	3	MLA	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	255/305 (83%)	-1.25	0 100 100	20, 45, 55, 63	21 (8%)
1	B	255/305 (83%)	-0.92	1 (0%) 88 86	21, 46, 55, 64	4 (1%)
1	C	255/305 (83%)	-0.98	0 100 100	21, 47, 55, 60	12 (4%)
1	D	255/305 (83%)	-1.20	0 100 100	16, 47, 55, 62	14 (5%)
All	All	1020/1220 (83%)	-1.09	1 (0%) 92 90	16, 46, 55, 64	51 (5%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	270	PRO	2.1

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MLA	A	1	7/7	0.98	0.03	46,48,49,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MLA	B	2	7/7	0.99	0.03	39,41,44,46	0
2	MLA	C	3	7/7	0.99	0.05	38,44,47,48	0
2	MLA	D	4	7/7	0.99	0.03	43,47,51,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.