



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:45 PM GMT

PDB ID : 3B8T
Title : Crystal structure of Escherichia coli alaine racemase mutant P219A
Authors : Wu, D.; Hu, T.; Zhang, L.; Jiang, H.; Shen, X.
Deposited on : 2007-11-02
Resolution : 3.00 Å(reported)

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

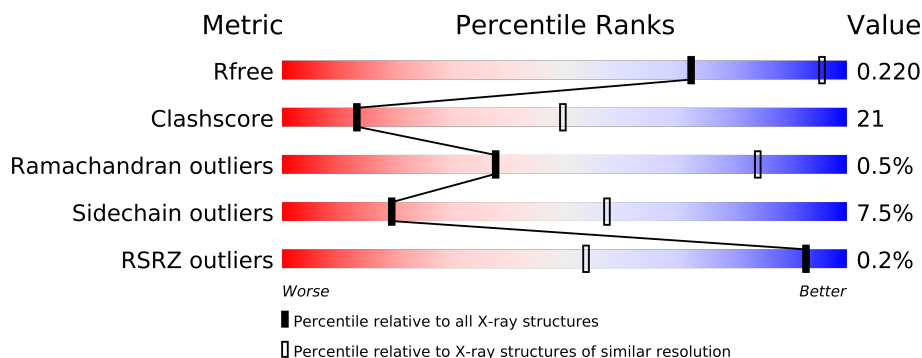
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	379	
1	B	379	
1	C	379	
1	D	379	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	361	-	X
3	PLP	A	1001	-	X
3	PLP	B	1001	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11336 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called Alanine racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2752	1732	498	507	15			
1	B	359	Total	C	N	O	S	0	0	0
			2752	1732	498	507	15			
1	C	350	Total	C	N	O	S	0	0	0
			2682	1692	485	492	13			
1	D	351	Total	C	N	O	S	0	0	0
			2690	1693	487	495	15			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P0A6B4
A	-18	GLY	-	EXPRESSION TAG	UNP P0A6B4
A	-17	SER	-	EXPRESSION TAG	UNP P0A6B4
A	-16	SER	-	EXPRESSION TAG	UNP P0A6B4
A	-15	HIS	-	EXPRESSION TAG	UNP P0A6B4
A	-14	HIS	-	EXPRESSION TAG	UNP P0A6B4
A	-13	HIS	-	EXPRESSION TAG	UNP P0A6B4
A	-12	HIS	-	EXPRESSION TAG	UNP P0A6B4
A	-11	HIS	-	EXPRESSION TAG	UNP P0A6B4
A	-10	HIS	-	EXPRESSION TAG	UNP P0A6B4
A	-9	SER	-	EXPRESSION TAG	UNP P0A6B4
A	-8	SER	-	EXPRESSION TAG	UNP P0A6B4
A	-7	GLY	-	EXPRESSION TAG	UNP P0A6B4
A	-6	LEU	-	EXPRESSION TAG	UNP P0A6B4
A	-5	VAL	-	EXPRESSION TAG	UNP P0A6B4
A	-4	PRO	-	EXPRESSION TAG	UNP P0A6B4
A	-3	ARG	-	EXPRESSION TAG	UNP P0A6B4
A	-2	GLY	-	EXPRESSION TAG	UNP P0A6B4
A	-1	SER	-	EXPRESSION TAG	UNP P0A6B4
A	0	HIS	-	EXPRESSION TAG	UNP P0A6B4
A	219	ALA	PRO	ENGINEERED	UNP P0A6B4

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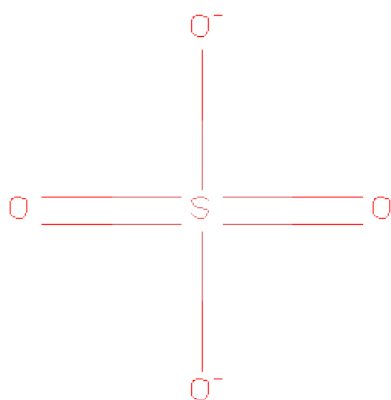
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	EXPRESSION TAG	UNP P0A6B4
B	-18	GLY	-	EXPRESSION TAG	UNP P0A6B4
B	-17	SER	-	EXPRESSION TAG	UNP P0A6B4
B	-16	SER	-	EXPRESSION TAG	UNP P0A6B4
B	-15	HIS	-	EXPRESSION TAG	UNP P0A6B4
B	-14	HIS	-	EXPRESSION TAG	UNP P0A6B4
B	-13	HIS	-	EXPRESSION TAG	UNP P0A6B4
B	-12	HIS	-	EXPRESSION TAG	UNP P0A6B4
B	-11	HIS	-	EXPRESSION TAG	UNP P0A6B4
B	-10	HIS	-	EXPRESSION TAG	UNP P0A6B4
B	-9	SER	-	EXPRESSION TAG	UNP P0A6B4
B	-8	SER	-	EXPRESSION TAG	UNP P0A6B4
B	-7	GLY	-	EXPRESSION TAG	UNP P0A6B4
B	-6	LEU	-	EXPRESSION TAG	UNP P0A6B4
B	-5	VAL	-	EXPRESSION TAG	UNP P0A6B4
B	-4	PRO	-	EXPRESSION TAG	UNP P0A6B4
B	-3	ARG	-	EXPRESSION TAG	UNP P0A6B4
B	-2	GLY	-	EXPRESSION TAG	UNP P0A6B4
B	-1	SER	-	EXPRESSION TAG	UNP P0A6B4
B	0	HIS	-	EXPRESSION TAG	UNP P0A6B4
B	219	ALA	PRO	ENGINEERED	UNP P0A6B4
C	-19	MET	-	EXPRESSION TAG	UNP P0A6B4
C	-18	GLY	-	EXPRESSION TAG	UNP P0A6B4
C	-17	SER	-	EXPRESSION TAG	UNP P0A6B4
C	-16	SER	-	EXPRESSION TAG	UNP P0A6B4
C	-15	HIS	-	EXPRESSION TAG	UNP P0A6B4
C	-14	HIS	-	EXPRESSION TAG	UNP P0A6B4
C	-13	HIS	-	EXPRESSION TAG	UNP P0A6B4
C	-12	HIS	-	EXPRESSION TAG	UNP P0A6B4
C	-11	HIS	-	EXPRESSION TAG	UNP P0A6B4
C	-10	HIS	-	EXPRESSION TAG	UNP P0A6B4
C	-9	SER	-	EXPRESSION TAG	UNP P0A6B4
C	-8	SER	-	EXPRESSION TAG	UNP P0A6B4
C	-7	GLY	-	EXPRESSION TAG	UNP P0A6B4
C	-6	LEU	-	EXPRESSION TAG	UNP P0A6B4
C	-5	VAL	-	EXPRESSION TAG	UNP P0A6B4
C	-4	PRO	-	EXPRESSION TAG	UNP P0A6B4
C	-3	ARG	-	EXPRESSION TAG	UNP P0A6B4
C	-2	GLY	-	EXPRESSION TAG	UNP P0A6B4
C	-1	SER	-	EXPRESSION TAG	UNP P0A6B4
C	0	HIS	-	EXPRESSION TAG	UNP P0A6B4
C	219	ALA	PRO	ENGINEERED	UNP P0A6B4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	EXPRESSION TAG	UNP P0A6B4
D	-18	GLY	-	EXPRESSION TAG	UNP P0A6B4
D	-17	SER	-	EXPRESSION TAG	UNP P0A6B4
D	-16	SER	-	EXPRESSION TAG	UNP P0A6B4
D	-15	HIS	-	EXPRESSION TAG	UNP P0A6B4
D	-14	HIS	-	EXPRESSION TAG	UNP P0A6B4
D	-13	HIS	-	EXPRESSION TAG	UNP P0A6B4
D	-12	HIS	-	EXPRESSION TAG	UNP P0A6B4
D	-11	HIS	-	EXPRESSION TAG	UNP P0A6B4
D	-10	HIS	-	EXPRESSION TAG	UNP P0A6B4
D	-9	SER	-	EXPRESSION TAG	UNP P0A6B4
D	-8	SER	-	EXPRESSION TAG	UNP P0A6B4
D	-7	GLY	-	EXPRESSION TAG	UNP P0A6B4
D	-6	LEU	-	EXPRESSION TAG	UNP P0A6B4
D	-5	VAL	-	EXPRESSION TAG	UNP P0A6B4
D	-4	PRO	-	EXPRESSION TAG	UNP P0A6B4
D	-3	ARG	-	EXPRESSION TAG	UNP P0A6B4
D	-2	GLY	-	EXPRESSION TAG	UNP P0A6B4
D	-1	SER	-	EXPRESSION TAG	UNP P0A6B4
D	0	HIS	-	EXPRESSION TAG	UNP P0A6B4
D	219	ALA	PRO	ENGINEERED	UNP P0A6B4

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



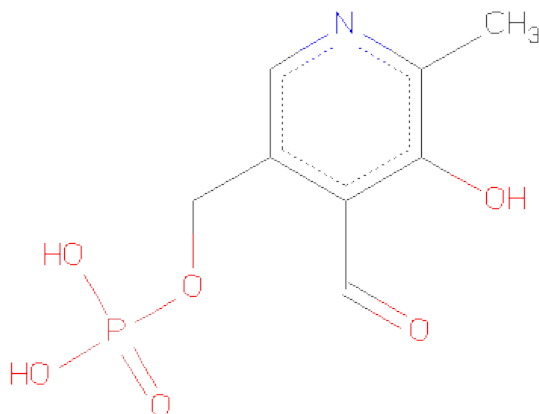
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is water.

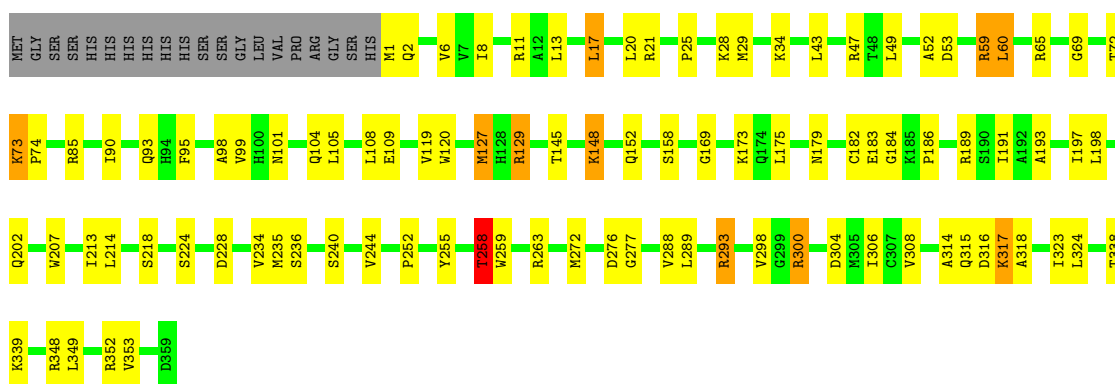
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	96	Total 96	O 96	0	0
4	B	122	Total 122	O 122	0	0
4	C	71	Total 71	O 71	0	0
4	D	76	Total 76	O 76	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

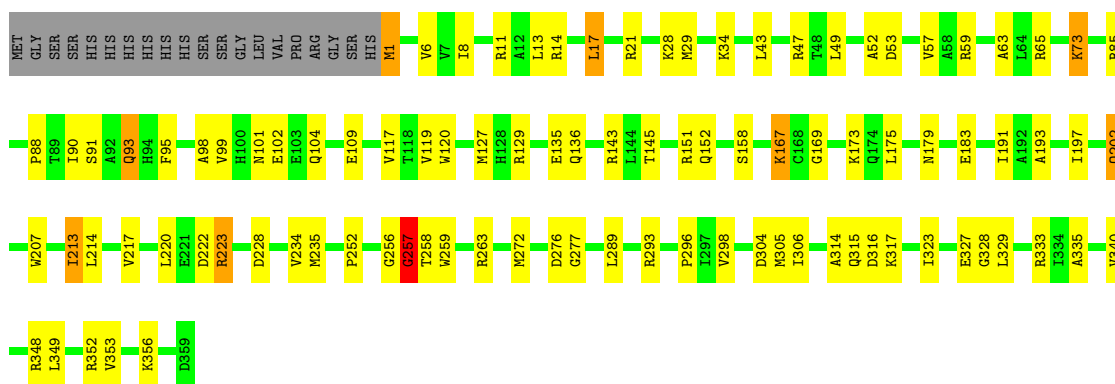
• Molecule 1: Alanine racemase

Chain A:



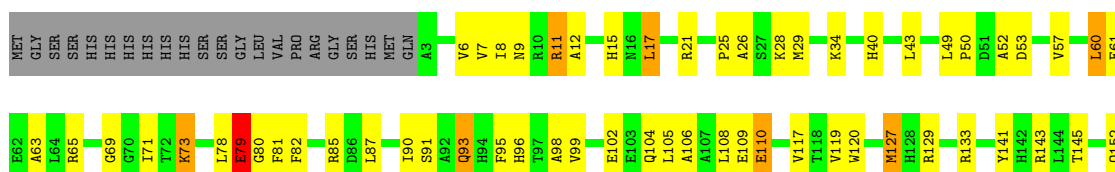
• Molecule 1: Alanine racemase

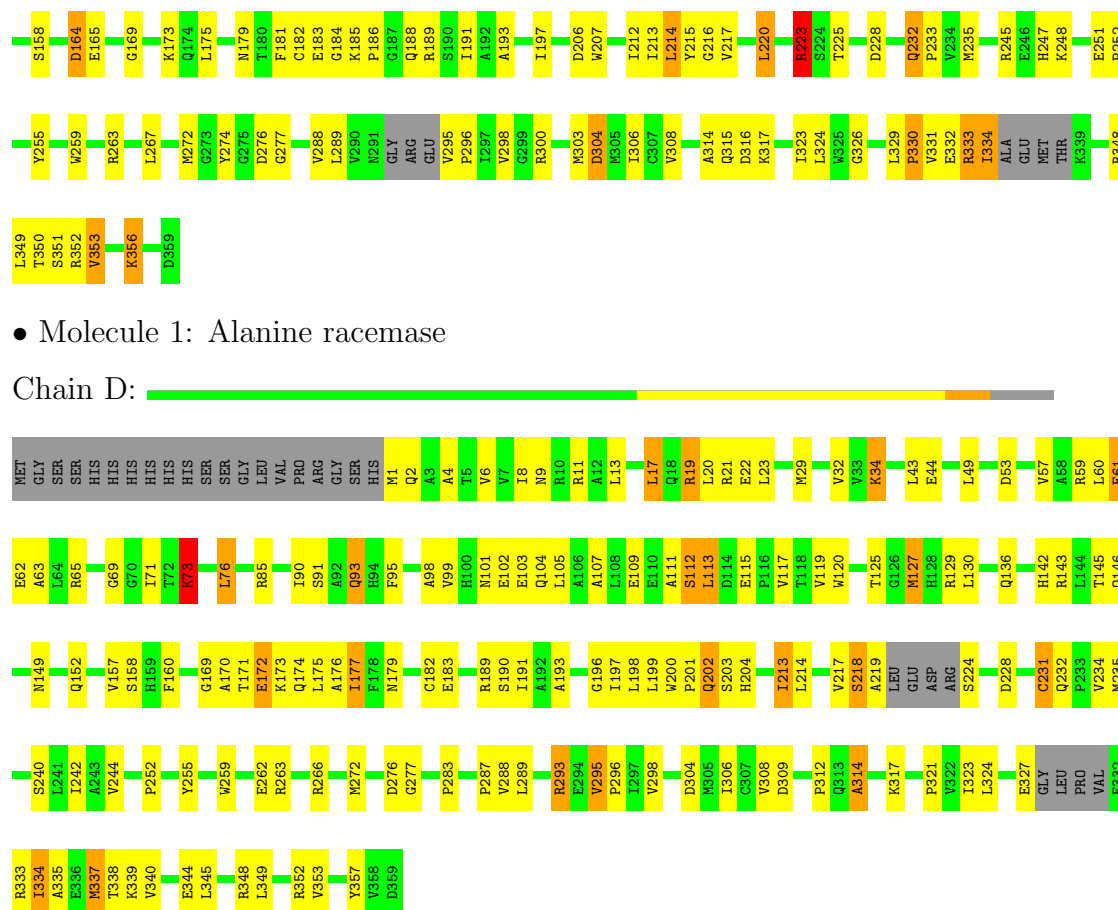
Chain B:



• Molecule 1: Alanine racemase

Chain C:





4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	147.92Å 147.92Å 163.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.00 35.53 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (15.00-3.00) 98.6 (35.53-3.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.226 0.212 , 0.220	Depositor DCC
R_{free} test set	3804 reflections (10.47%)	DCC
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 10.0	EDS
Estimated twinning fraction	0.457 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 40140 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11336	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	0/2796	0.94	12/3795 (0.3%)
1	B	0.61	1/2796 (0.0%)	1.00	15/3795 (0.4%)
1	C	0.56	0/2724	0.90	10/3697 (0.3%)
1	D	0.52	0/2731	0.89	12/3703 (0.3%)
All	All	0.58	1/11047 (0.0%)	0.93	49/14990 (0.3%)

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	B	0	1
1	C	0	3
1	D	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	109	GLU	CD-OE2	-5.69	1.19	1.25

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ARG	NE-CZ-NH1	-19.71	110.44	120.30
1	B	85	ARG	NE-CZ-NH1	-19.42	110.59	120.30
1	B	85	ARG	NE-CZ-NH2	18.83	129.71	120.30
1	A	129	ARG	NE-CZ-NH2	15.29	127.94	120.30
1	D	65	ARG	NE-CZ-NH2	-14.85	112.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	65	ARG	NE-CZ-NH2	-14.47	113.06	120.30
1	D	65	ARG	NE-CZ-NH1	14.33	127.47	120.30
1	C	65	ARG	NE-CZ-NH1	13.58	127.09	120.30
1	B	223	ARG	NE-CZ-NH1	-12.33	114.14	120.30
1	B	223	ARG	NE-CZ-NH2	12.29	126.44	120.30
1	C	315	GLN	N-CA-CB	-10.89	90.99	110.60
1	B	11	ARG	NE-CZ-NH1	-10.48	115.06	120.30
1	B	315	GLN	N-CA-CB	-10.46	91.77	110.60
1	B	85	ARG	CD-NE-CZ	10.24	137.94	123.60
1	B	11	ARG	NE-CZ-NH2	9.67	125.14	120.30
1	C	314	ALA	CB-CA-C	-9.14	96.39	110.10
1	A	11	ARG	NE-CZ-NH1	-9.01	115.80	120.30
1	A	85	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	D	85	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	D	85	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	B	314	ALA	CB-CA-C	-8.57	97.24	110.10
1	A	59	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	A	11	ARG	NE-CZ-NH2	8.33	124.46	120.30
1	C	85	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	C	85	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	A	85	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	C	65	ARG	CD-NE-CZ	7.57	134.19	123.60
1	D	129	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	B	129	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	C	232	GLN	C-N-CD	-7.29	104.56	120.60
1	B	59	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	D	65	ARG	CD-NE-CZ	7.25	133.74	123.60
1	D	314	ALA	N-CA-C	-7.13	91.75	111.00
1	A	59	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	129	ARG	CD-NE-CZ	6.67	132.94	123.60
1	D	59	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	B	223	ARG	CD-NE-CZ	6.61	132.85	123.60
1	A	315	GLN	N-CA-CB	-6.58	98.77	110.60
1	A	314	ALA	N-CA-C	-6.47	93.53	111.00
1	C	129	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	D	314	ALA	CB-CA-C	5.98	119.07	110.10
1	C	314	ALA	N-CA-C	-5.89	95.10	111.00
1	B	314	ALA	N-CA-C	-5.84	95.24	111.00
1	D	59	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	129	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	129	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	293	ARG	N-CA-C	-5.34	96.57	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	60	LEU	CB-CG-CD2	5.02	119.54	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	257	GLY	Peptide
1	C	60	LEU	Peptide
1	C	79	GLU	Peptide
1	C	80	GLY	Peptide
1	D	112	SER	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2752	0	2756	73	0
1	B	2752	0	2756	66	0
1	C	2682	0	2685	154	0
1	D	2690	0	2690	173	0
2	A	15	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
3	A	15	0	7	0	0
3	B	15	0	7	0	0
3	C	15	0	7	1	0
3	D	15	0	7	2	0
4	A	96	0	0	3	0
4	B	122	0	0	3	0
4	C	71	0	0	17	0
4	D	76	0	0	21	0
All	All	11336	0	10915	449	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 21.

All (449) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:164:ASP:HB2	1:C:220:LEU:HD21	1.25	1.13
1:D:176:ALA:HB2	4:D:1062:HOH:O	1.47	1.11
1:D:338:THR:HG22	1:D:340:VAL:CG1	1.80	1.11
1:D:113:LEU:HD12	1:D:115:GLU:O	1.51	1.10
1:D:169:GLY:O	1:D:173:LYS:HB2	1.51	1.08
1:A:52:ALA:O	1:A:73:LYS:HE2	1.52	1.06
1:D:160:PHE:CE2	1:D:171:THR:HG23	1.91	1.06
1:D:338:THR:HG22	1:D:340:VAL:HG13	1.10	1.05
1:C:164:ASP:CB	1:C:220:LEU:HD21	1.85	1.05
1:D:170:ALA:O	1:D:174:GLN:HG3	1.56	1.04
1:C:164:ASP:HB2	1:C:220:LEU:CD2	1.88	1.03
1:D:338:THR:CG2	1:D:340:VAL:HG13	1.89	1.02
1:C:353:VAL:HG12	1:C:353:VAL:O	1.55	1.02
1:D:112:SER:O	1:D:113:LEU:HD23	1.62	1.00
1:D:321:PRO:HA	4:D:1025:HOH:O	1.62	0.99
1:C:164:ASP:CB	1:C:220:LEU:CD2	2.41	0.99
1:C:329:LEU:HD12	4:C:1037:HOH:O	1.62	0.98
1:D:19:ARG:HD3	1:D:22:GLU:OE2	1.63	0.97
1:C:215:TYR:HE1	4:C:1024:HOH:O	1.48	0.96
1:D:9:ASN:ND2	1:D:11:ARG:HH21	1.64	0.96
1:D:295:VAL:CG2	1:D:308:VAL:HB	1.96	0.94
1:A:189:ARG:HH11	1:A:189:ARG:HB2	1.33	0.93
1:D:189:ARG:HH11	1:D:189:ARG:HB2	1.34	0.92
1:C:52:ALA:O	1:C:73:LYS:HD3	1.70	0.92
1:D:235:MET:HA	4:D:1039:HOH:O	1.71	0.90
1:D:293:ARG:NH2	1:D:295:VAL:HB	1.87	0.90
1:C:223:ARG:HD3	1:C:223:ARG:O	1.72	0.90
1:D:295:VAL:HG22	1:D:308:VAL:HB	1.51	0.90
1:C:189:ARG:HH11	1:C:189:ARG:HB2	1.37	0.89
1:D:9:ASN:HD21	1:D:11:ARG:NH2	1.69	0.89
1:D:9:ASN:HD21	1:D:11:ARG:HH21	0.89	0.88
1:C:216:GLY:HA3	1:C:232:GLN:O	1.74	0.87
1:D:19:ARG:CD	1:D:22:GLU:OE2	2.23	0.87
1:C:9:ASN:OD1	1:C:11:ARG:HB3	1.76	0.85
4:C:1018:HOH:O	1:D:348:ARG:HB2	1.76	0.85
4:C:1018:HOH:O	1:D:344:GLU:HG3	1.75	0.84
1:C:12:ALA:HA	1:C:232:GLN:OE1	1.77	0.84
1:D:324:LEU:HD11	4:D:1066:HOH:O	1.78	0.84
1:D:125:THR:HG22	1:D:177:ILE:HG22	1.59	0.83
1:C:304:ASP:OD1	1:D:34:LYS:HD2	1.80	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:213:ILE:HG13	1:C:213:ILE:O	1.79	0.81
1:A:189:ARG:HB2	1:A:189:ARG:NH1	1.95	0.80
1:C:106:ALA:O	1:C:110:GLU:HG3	1.80	0.80
1:D:334:ILE:O	1:D:334:ILE:CG2	2.30	0.80
1:D:276:ASP:OD1	1:D:352:ARG:HD3	1.83	0.79
1:D:338:THR:CG2	1:D:340:VAL:CG1	2.53	0.79
1:C:334:ILE:CD1	1:C:334:ILE:N	2.45	0.79
1:C:348:ARG:HD2	1:D:348:ARG:HD2	1.63	0.79
1:C:353:VAL:CG1	1:C:353:VAL:O	2.30	0.79
1:D:189:ARG:NH1	1:D:189:ARG:HB2	1.97	0.79
1:C:164:ASP:CA	1:C:220:LEU:HD21	2.12	0.79
1:D:19:ARG:NH1	1:D:23:LEU:HD21	1.98	0.79
1:D:293:ARG:HH21	1:D:295:VAL:HB	1.44	0.78
1:A:348:ARG:HD2	1:B:348:ARG:HD2	1.64	0.78
1:C:141:TYR:CZ	1:C:185:LYS:HD3	2.19	0.77
1:D:335:ALA:HB2	1:D:345:LEU:CD1	2.15	0.77
1:B:276:ASP:OD1	1:B:352:ARG:HD3	1.85	0.77
1:C:189:ARG:NH1	1:C:189:ARG:HB2	1.99	0.77
1:C:15:HIS:CG	1:C:232:GLN:NE2	2.53	0.77
1:C:334:ILE:O	1:C:334:ILE:HG22	1.83	0.77
1:D:107:ALA:O	1:D:111:ALA:CB	2.33	0.77
1:C:330:PRO:O	1:C:333:ARG:HB2	1.85	0.77
1:D:9:ASN:ND2	1:D:11:ARG:NH2	2.31	0.76
1:A:276:ASP:OD1	1:A:352:ARG:HD3	1.86	0.76
1:C:255:TYR:HB3	4:C:1065:HOH:O	1.86	0.74
1:D:293:ARG:NH2	1:D:295:VAL:CG1	2.50	0.74
1:A:25:PRO:HG3	1:C:184:GLY:O	1.87	0.74
1:D:160:PHE:CZ	1:D:171:THR:HG23	2.23	0.73
1:A:198:LEU:HD11	1:A:213:ILE:HD12	1.70	0.72
1:D:113:LEU:CD1	1:D:115:GLU:O	2.36	0.72
1:C:303:MET:HB3	1:C:304:ASP:OD2	1.88	0.72
1:D:171:THR:O	1:D:173:LYS:N	2.22	0.72
1:A:189:ARG:HH11	1:A:189:ARG:CB	2.02	0.72
1:C:188:GLN:OE1	1:C:206:ASP:HB3	1.90	0.72
1:B:202:GLN:H	1:B:202:GLN:HE21	1.36	0.71
1:D:324:LEU:CD1	4:D:1066:HOH:O	2.34	0.71
1:A:1:MET:HE3	1:A:240:SER:HB2	1.73	0.71
1:D:293:ARG:NH2	1:D:295:VAL:CB	2.52	0.71
1:C:79:GLU:OE1	1:C:82:PHE:HZ	1.72	0.71
1:D:19:ARG:NH1	1:D:23:LEU:CD2	2.55	0.70
1:C:334:ILE:H	1:C:334:ILE:HD13	1.55	0.70
1:C:50:PRO:O	1:C:73:LYS:HE3	1.92	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:189:ARG:HH11	1:D:189:ARG:CB	2.04	0.69
1:C:330:PRO:O	1:C:333:ARG:N	2.26	0.68
1:C:105:LEU:O	1:C:109:GLU:HG3	1.93	0.68
1:C:247:HIS:NE2	1:C:251:GLU:O	2.25	0.68
1:D:235:MET:HG3	4:D:1039:HOH:O	1.93	0.68
1:C:189:ARG:HH11	1:C:189:ARG:CB	2.06	0.68
1:D:335:ALA:HB2	1:D:345:LEU:HD11	1.76	0.68
1:D:8:ILE:HD13	4:D:1039:HOH:O	1.94	0.68
1:B:256:GLY:O	1:B:257:GLY:C	2.30	0.67
1:D:107:ALA:O	1:D:111:ALA:HB3	1.95	0.67
1:A:1:MET:HG2	1:A:2:GLN:H	1.59	0.67
1:A:17:LEU:O	1:A:21:ARG:HG3	1.95	0.67
1:D:171:THR:C	1:D:173:LYS:H	1.97	0.66
1:D:198:LEU:HD11	1:D:213:ILE:HD12	1.77	0.66
1:A:258:THR:HG21	1:A:300:ARG:HB2	1.77	0.66
1:B:17:LEU:O	1:B:21:ARG:HG3	1.96	0.65
1:D:224:SER:HB2	1:D:228:ASP:OD1	1.95	0.65
1:C:17:LEU:O	1:C:21:ARG:HG3	1.96	0.65
1:D:145:THR:HG22	1:D:152:GLN:HE22	1.62	0.65
1:D:338:THR:O	1:D:339:LYS:HB2	1.97	0.65
1:C:145:THR:HG22	1:C:152:GLN:HE22	1.61	0.65
1:C:90:ILE:HG23	1:C:95:PHE:HB2	1.79	0.64
1:D:17:LEU:O	1:D:21:ARG:HG3	1.96	0.64
1:B:1:MET:SD	1:B:356:LYS:HE3	2.37	0.64
1:A:6:VAL:HG23	1:A:353:VAL:HG11	1.78	0.64
1:D:218:SER:OG	1:D:219:ALA:N	2.30	0.64
1:D:171:THR:C	1:D:173:LYS:N	2.51	0.64
1:B:21:ARG:HG2	1:B:29:MET:CE	2.28	0.64
1:A:6:VAL:HG13	1:A:235:MET:HG3	1.79	0.64
1:C:21:ARG:HG2	1:C:29:MET:CE	2.28	0.64
1:D:61:GLU:CG	1:D:62:GLU:N	2.60	0.64
1:C:6:VAL:HG13	1:C:235:MET:HG3	1.79	0.63
1:B:6:VAL:HG13	1:B:235:MET:HG3	1.79	0.63
1:D:262:GLU:HG3	4:D:1063:HOH:O	1.99	0.63
1:C:81:PHE:CZ	1:C:87:LEU:HD21	2.34	0.62
1:D:102:GLU:OE2	1:D:143:ARG:NH2	2.28	0.62
1:A:145:THR:HG22	1:A:152:GLN:HE22	1.64	0.62
1:D:287:PRO:HD2	1:D:337:MET:SD	2.39	0.62
1:D:21:ARG:HG2	1:D:29:MET:CE	2.29	0.62
1:B:90:ILE:HG23	1:B:95:PHE:HB2	1.81	0.62
1:D:334:ILE:O	1:D:334:ILE:HG22	1.99	0.61
1:D:107:ALA:O	1:D:111:ALA:HB2	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:252:PRO:HA	1:A:259:TRP:O	2.00	0.61
1:D:6:VAL:HG13	1:D:235:MET:HG3	1.81	0.61
1:D:125:THR:HG22	1:D:177:ILE:CG2	2.29	0.61
1:D:327:GLU:HB3	4:D:1009:HOH:O	1.99	0.61
1:D:288:VAL:HG11	1:D:308:VAL:HG11	1.83	0.61
1:D:244:VAL:HB	4:D:1002:HOH:O	1.99	0.61
1:D:90:ILE:HG23	1:D:95:PHE:HB2	1.82	0.61
1:B:145:THR:HG22	1:B:152:GLN:HE22	1.65	0.60
1:B:6:VAL:HG23	1:B:353:VAL:HG11	1.83	0.60
1:A:21:ARG:HG2	1:A:29:MET:CE	2.32	0.60
1:A:288:VAL:HG11	1:A:308:VAL:HG11	1.84	0.60
1:D:334:ILE:O	1:D:334:ILE:HG23	2.02	0.60
1:D:6:VAL:HG23	1:D:353:VAL:HG11	1.83	0.59
1:C:334:ILE:HD12	1:C:334:ILE:N	2.16	0.59
1:C:276:ASP:OD1	1:C:352:ARG:HD3	2.02	0.59
1:D:272:MET:O	1:D:306:ILE:HG13	2.02	0.59
1:D:235:MET:CA	4:D:1039:HOH:O	2.40	0.58
1:D:109:GLU:OE2	1:D:143:ARG:HD2	2.03	0.58
1:D:2:GLN:HB3	1:D:240:SER:OG	2.03	0.58
1:A:184:GLY:O	1:C:25:PRO:HG3	2.03	0.58
1:A:90:ILE:HG23	1:A:95:PHE:HB2	1.83	0.58
1:C:164:ASP:HB2	1:C:220:LEU:HD22	1.84	0.58
1:C:15:HIS:ND1	1:C:232:GLN:NE2	2.51	0.58
1:C:193:ALA:O	1:C:197:ILE:HG13	2.04	0.58
1:C:288:VAL:HG11	1:C:308:VAL:HG11	1.83	0.58
1:C:169:GLY:O	1:C:173:LYS:HG3	2.04	0.58
1:B:222:ASP:O	1:B:223:ARG:HG2	2.02	0.58
1:D:20:LEU:HD21	1:D:213:ILE:HD13	1.84	0.58
1:A:1:MET:HG2	1:A:2:GLN:N	2.18	0.58
1:C:11:ARG:HG2	4:C:1051:HOH:O	2.03	0.58
1:A:255:TYR:O	1:A:258:THR:HG22	2.04	0.58
1:C:164:ASP:CA	1:C:220:LEU:CD2	2.79	0.57
1:D:293:ARG:HH22	1:D:295:VAL:CG1	2.16	0.57
1:C:141:TYR:CE2	1:C:185:LYS:HD3	2.39	0.57
1:D:201:PRO:HD2	1:D:202:GLN:HE21	1.69	0.57
1:D:287:PRO:CD	1:D:337:MET:SD	2.93	0.57
1:D:287:PRO:HG2	1:D:334:ILE:HD12	1.86	0.57
1:C:330:PRO:HD2	4:C:1037:HOH:O	2.03	0.57
1:C:81:PHE:O	1:C:104:GLN:NE2	2.34	0.57
1:C:223:ARG:CD	1:C:223:ARG:O	2.48	0.57
1:C:248:LYS:O	1:C:251:GLU:HB2	2.04	0.57
1:C:87:LEU:CD1	1:C:108:LEU:HD23	2.35	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:101:ASN:OD1	1:B:104:GLN:HG3	2.04	0.57
1:D:335:ALA:HB2	1:D:345:LEU:HD12	1.86	0.57
1:A:20:LEU:HD21	1:A:213:ILE:HD13	1.86	0.57
1:D:142:HIS:CE1	4:D:1008:HOH:O	2.56	0.57
1:A:52:ALA:O	1:A:73:LYS:CE	2.42	0.56
1:C:188:GLN:OE1	1:C:206:ASP:CB	2.53	0.56
1:C:272:MET:O	1:C:306:ILE:HG13	2.04	0.56
1:D:76:LEU:C	1:D:76:LEU:HD12	2.27	0.56
1:C:274:TYR:HB2	4:C:1018:HOH:O	2.06	0.56
1:B:272:MET:O	1:B:306:ILE:HG13	2.05	0.56
1:C:79:GLU:OE1	1:C:82:PHE:CZ	2.57	0.55
1:D:266:ARG:NH1	1:D:314:ALA:O	2.39	0.55
1:D:199:LEU:HG	4:D:1049:HOH:O	2.06	0.55
1:A:101:ASN:OD1	1:A:104:GLN:HG3	2.06	0.55
1:D:158:SER:O	1:D:191:ILE:HA	2.07	0.55
1:D:101:ASN:OD1	1:D:104:GLN:HG3	2.06	0.55
1:D:198:LEU:HD21	1:D:213:ILE:HD12	1.89	0.55
1:B:21:ARG:HG2	1:B:29:MET:HE2	1.88	0.55
1:B:52:ALA:O	1:B:73:LYS:CD	2.54	0.55
1:C:93:GLN:HE21	1:C:93:GLN:HA	1.72	0.54
1:D:179:ASN:O	1:D:183:GLU:HG3	2.08	0.54
1:D:235:MET:CG	4:D:1039:HOH:O	2.51	0.54
1:C:182:CYS:HB3	1:C:189:ARG:HD3	1.88	0.54
1:A:182:CYS:HB3	1:A:189:ARG:HD3	1.88	0.54
1:D:21:ARG:NH2	1:D:53:ASP:OD2	2.40	0.54
1:A:193:ALA:O	1:A:197:ILE:HG13	2.08	0.54
1:D:175:LEU:O	1:D:179:ASN:ND2	2.40	0.54
1:C:331:VAL:HG13	1:C:332:GLU:OE2	2.07	0.54
1:C:316:ASP:O	1:C:317:LYS:HG2	2.08	0.54
1:D:160:PHE:CZ	1:D:171:THR:CG2	2.91	0.54
1:A:73:LYS:HG3	1:A:74:PRO:HD2	1.90	0.54
1:D:13:LEU:HD13	1:D:234:VAL:HG21	1.89	0.54
1:B:52:ALA:O	1:B:73:LYS:HD2	2.08	0.54
1:C:87:LEU:HD13	1:C:108:LEU:HD23	1.89	0.53
1:D:334:ILE:O	1:D:338:THR:OG1	2.27	0.53
1:A:348:ARG:HD3	1:B:277:GLY:HA2	1.90	0.53
1:C:21:ARG:HG2	1:C:29:MET:HE2	1.89	0.53
1:D:193:ALA:O	1:D:197:ILE:HG13	2.08	0.53
1:C:164:ASP:CB	1:C:220:LEU:HD22	2.34	0.53
1:C:277:GLY:HA2	1:D:348:ARG:HD3	1.90	0.53
1:A:277:GLY:HA2	1:B:348:ARG:HD3	1.89	0.53
1:C:164:ASP:O	1:C:220:LEU:HD21	2.07	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:287:PRO:HG2	1:D:334:ILE:CD1	2.38	0.53
1:B:73:LYS:HG3	4:B:1038:HOH:O	2.08	0.53
1:D:19:ARG:HH12	1:D:23:LEU:CD2	2.22	0.53
1:B:14:ARG:HD2	4:B:1059:HOH:O	2.07	0.53
1:B:193:ALA:O	1:B:197:ILE:HG13	2.09	0.53
1:C:348:ARG:HD3	1:D:277:GLY:HA2	1.90	0.53
1:D:125:THR:CG2	1:D:177:ILE:HG22	2.36	0.53
1:D:283:PRO:CD	1:D:337:MET:O	2.57	0.52
1:D:182:CYS:HB3	1:D:189:ARG:HD3	1.89	0.52
1:A:338:THR:O	1:A:339:LYS:HB2	2.08	0.52
1:B:202:GLN:NE2	1:B:202:GLN:H	2.03	0.52
1:B:135:GLU:HG2	1:B:136:GLN:OE1	2.09	0.52
1:D:171:THR:O	1:D:172:GLU:C	2.46	0.52
1:B:21:ARG:NH2	1:B:53:ASP:OD2	2.43	0.52
1:C:21:ARG:NH2	1:C:53:ASP:OD2	2.43	0.52
1:D:338:THR:HG22	1:D:340:VAL:HG11	1.85	0.52
1:A:198:LEU:HD21	1:A:213:ILE:HD12	1.92	0.52
1:C:188:GLN:HG3	1:C:207:TRP:HE1	1.74	0.52
1:C:289:LEU:HD13	4:C:1047:HOH:O	2.09	0.52
1:D:19:ARG:NE	1:D:22:GLU:OE2	2.43	0.52
1:B:252:PRO:HA	1:B:259:TRP:O	2.09	0.52
1:C:120:TRP:CH2	1:C:188:GLN:HB2	2.46	0.51
1:D:2:GLN:CB	1:D:240:SER:OG	2.58	0.51
1:B:289:LEU:HD11	1:B:328:GLY:HA3	1.91	0.51
1:D:21:ARG:HG2	1:D:29:MET:HE2	1.90	0.51
1:C:43:LEU:CD1	1:C:71:ILE:HD13	2.39	0.51
1:C:50:PRO:HA	1:C:73:LYS:HE2	1.92	0.51
1:C:334:ILE:N	1:C:334:ILE:HD13	2.15	0.51
1:D:252:PRO:HA	1:D:259:TRP:O	2.11	0.51
1:B:213:ILE:HG12	1:B:217:VAL:O	2.10	0.51
1:C:78:LEU:HD22	3:C:1001:PLP:H2A3	1.92	0.51
1:C:252:PRO:HA	1:C:259:TRP:O	2.11	0.51
1:C:81:PHE:HB3	1:C:90:ILE:HD11	1.93	0.51
1:B:135:GLU:CD	1:B:135:GLU:H	2.14	0.51
1:D:91:SER:HB2	1:D:113:LEU:HD13	1.91	0.51
1:B:276:ASP:OD1	1:B:352:ARG:CD	2.56	0.51
1:A:21:ARG:NH2	1:A:53:ASP:OD2	2.44	0.51
1:C:99:VAL:HG23	1:C:119:VAL:HG13	1.91	0.51
1:A:34:LYS:HD2	1:B:304:ASP:OD2	2.11	0.51
1:A:179:ASN:O	1:A:183:GLU:HG3	2.10	0.51
1:C:331:VAL:C	1:C:333:ARG:H	2.13	0.51
1:C:28:LYS:HD2	1:C:207:TRP:CZ2	2.46	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:50:PRO:HA	1:C:73:LYS:CE	2.40	0.50
1:B:28:LYS:HD2	1:B:207:TRP:CZ2	2.46	0.50
1:C:145:THR:HG22	1:C:152:GLN:NE2	2.24	0.50
1:B:179:ASN:O	1:B:183:GLU:HG3	2.11	0.50
1:A:98:ALA:HA	1:A:120:TRP:O	2.11	0.50
1:C:158:SER:O	1:C:191:ILE:HA	2.11	0.50
1:B:93:GLN:HE21	1:B:93:GLN:HA	1.75	0.50
1:B:169:GLY:O	1:B:173:LYS:HG3	2.11	0.50
1:C:289:LEU:HB2	1:C:323:ILE:HB	1.94	0.50
1:B:1:MET:HE1	1:B:356:LYS:HG3	1.94	0.50
1:C:351:SER:C	1:C:353:VAL:H	2.15	0.50
1:C:133:ARG:HB3	4:C:1055:HOH:O	2.12	0.50
1:D:19:ARG:O	1:D:22:GLU:HB2	2.12	0.50
1:C:288:VAL:HG11	1:C:308:VAL:CG1	2.42	0.50
1:A:272:MET:O	1:A:306:ILE:HG13	2.11	0.50
1:A:73:LYS:HG3	1:A:74:PRO:CD	2.42	0.50
1:D:93:GLN:HA	1:D:93:GLN:HE21	1.77	0.50
1:C:245:ARG:NH1	4:C:1061:HOH:O	2.43	0.49
1:D:293:ARG:HH22	1:D:295:VAL:HG11	1.77	0.49
1:A:169:GLY:O	1:A:173:LYS:HG3	2.12	0.49
1:D:296:PRO:HG2	1:D:309:ASP:HB3	1.94	0.49
1:C:212:ILE:HG23	1:C:213:ILE:N	2.27	0.49
1:D:276:ASP:OD1	1:D:352:ARG:CD	2.56	0.49
1:C:334:ILE:CG2	1:C:334:ILE:O	2.55	0.49
1:D:61:GLU:HG2	1:D:62:GLU:N	2.26	0.49
1:A:127:MET:HB3	4:A:1027:HOH:O	2.12	0.49
1:D:289:LEU:HB2	1:D:323:ILE:HB	1.94	0.49
1:C:6:VAL:CG1	1:C:8:ILE:HD11	2.42	0.49
1:C:267:LEU:HD12	4:C:1061:HOH:O	2.13	0.49
1:A:47:ARG:HD2	4:A:1060:HOH:O	2.12	0.49
1:C:179:ASN:O	1:C:183:GLU:HG3	2.13	0.49
1:D:333:ARG:C	1:D:335:ALA:H	2.16	0.49
1:C:350:THR:OG1	1:C:351:SER:N	2.41	0.49
1:D:19:ARG:HD2	1:D:19:ARG:O	2.13	0.49
1:D:338:THR:CG2	1:D:340:VAL:HG11	2.42	0.49
1:A:276:ASP:OD1	1:A:352:ARG:CD	2.57	0.49
1:A:21:ARG:HG2	1:A:29:MET:HE2	1.94	0.49
1:D:43:LEU:CD1	1:D:71:ILE:HD13	2.42	0.49
1:A:6:VAL:CG1	1:A:8:ILE:HD11	2.43	0.49
1:B:17:LEU:HD12	1:B:49:LEU:HD22	1.95	0.49
1:D:340:VAL:CG2	1:D:345:LEU:HG	2.43	0.48
1:C:50:PRO:C	1:C:73:LYS:HE3	2.33	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:198:LEU:HD21	1:A:213:ILE:CD1	2.44	0.48
1:C:98:ALA:HA	1:C:120:TRP:O	2.13	0.48
1:C:133:ARG:NH1	1:C:133:ARG:HG2	2.27	0.48
1:D:200:TRP:HB2	1:D:203:SER:OG	2.13	0.48
1:B:98:ALA:HA	1:B:120:TRP:O	2.12	0.48
1:C:181:PHE:O	1:C:185:LYS:NZ	2.46	0.48
1:A:304:ASP:OD2	1:B:34:LYS:HD2	2.13	0.48
1:D:32:VAL:HG21	3:D:1001:PLP:H5A2	1.94	0.48
1:B:158:SER:O	1:B:191:ILE:HA	2.13	0.48
1:A:158:SER:O	1:A:191:ILE:HA	2.13	0.48
1:C:255:TYR:N	1:D:127:MET:HE3	2.29	0.48
1:B:222:ASP:O	1:B:223:ARG:CG	2.62	0.48
1:B:57:VAL:HG21	1:B:63:ALA:HB2	1.96	0.48
1:A:28:LYS:HD2	1:A:207:TRP:CZ2	2.48	0.48
1:D:130:LEU:HA	4:D:1044:HOH:O	2.13	0.48
1:D:338:THR:HB	1:D:340:VAL:H	1.79	0.48
1:D:312:PRO:CG	4:D:1045:HOH:O	2.62	0.48
1:B:316:ASP:O	1:B:317:LYS:HG2	2.13	0.48
1:A:13:LEU:HD13	1:A:234:VAL:HG21	1.94	0.47
1:B:13:LEU:HD13	1:B:234:VAL:HG21	1.95	0.47
1:B:6:VAL:CG1	1:B:8:ILE:HD11	2.45	0.47
1:D:4:ALA:HB1	1:D:353:VAL:HG22	1.95	0.47
1:C:17:LEU:HD12	1:C:49:LEU:HD22	1.96	0.47
1:A:288:VAL:HG11	1:A:308:VAL:CG1	2.44	0.47
1:D:295:VAL:HG23	1:D:296:PRO:N	2.30	0.47
1:A:293:ARG:NH2	1:A:316:ASP:OD2	2.47	0.47
1:C:15:HIS:CG	1:C:232:GLN:HE21	2.32	0.47
1:D:105:LEU:HD23	1:D:143:ARG:NH2	2.30	0.47
1:B:289:LEU:HB2	1:B:323:ILE:HB	1.96	0.47
1:C:164:ASP:C	1:C:220:LEU:HD21	2.35	0.47
1:D:176:ALA:CB	4:D:1062:HOH:O	2.29	0.47
1:D:111:ALA:O	1:D:149:ASN:ND2	2.48	0.47
1:D:193:ALA:HB1	3:D:1001:PLP:O4P	2.13	0.47
1:D:304:ASP:OD1	1:D:352:ARG:NH2	2.39	0.47
1:D:145:THR:HG22	1:D:152:GLN:NE2	2.28	0.46
1:B:99:VAL:HG23	1:B:119:VAL:HG13	1.97	0.46
1:A:317:LYS:O	1:A:318:ALA:C	2.51	0.46
1:D:8:ILE:HG23	1:D:234:VAL:HG12	1.96	0.46
1:A:186:PRO:HB3	1:C:25:PRO:HB2	1.96	0.46
1:D:201:PRO:HA	1:D:204:HIS:NE2	2.30	0.46
1:A:148:LYS:HA	1:A:148:LYS:HD2	1.66	0.46
1:D:198:LEU:HD21	1:D:213:ILE:CD1	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:164:ASP:HB3	1:C:220:LEU:CD2	2.39	0.46
1:D:338:THR:HB	1:D:340:VAL:HG22	1.96	0.46
1:B:8:ILE:HG23	1:B:234:VAL:HG12	1.97	0.46
1:D:288:VAL:HG11	1:D:308:VAL:CG1	2.43	0.46
1:D:295:VAL:HG21	1:D:308:VAL:HB	1.89	0.46
1:C:93:GLN:HE21	1:C:93:GLN:CA	2.28	0.46
1:B:259:TRP:CD2	1:B:298:VAL:HB	2.51	0.46
1:A:145:THR:HG22	1:A:152:GLN:NE2	2.29	0.46
1:D:112:SER:C	1:D:113:LEU:HD23	2.34	0.45
1:C:326:GLY:O	1:C:329:LEU:O	2.34	0.45
1:D:19:ARG:HD3	1:D:19:ARG:HA	1.68	0.45
1:D:213:ILE:O	1:D:213:ILE:HG12	2.17	0.45
1:C:259:TRP:CD2	1:C:298:VAL:HB	2.51	0.45
1:D:201:PRO:HA	1:D:204:HIS:CE1	2.52	0.45
1:A:59:ARG:HD2	4:A:1022:HOH:O	2.15	0.45
1:A:99:VAL:HG23	1:A:119:VAL:HG13	1.98	0.45
1:D:217:VAL:CG1	1:D:218:SER:N	2.78	0.45
1:D:293:ARG:NH2	1:D:295:VAL:HG12	2.30	0.45
1:D:73:LYS:HD3	1:D:73:LYS:HA	1.38	0.45
1:B:102:GLU:OE2	1:B:143:ARG:NH2	2.43	0.45
1:C:225:THR:HB	1:C:332:GLU:OE1	2.16	0.45
1:C:323:ILE:CD1	4:C:1058:HOH:O	2.65	0.45
1:D:17:LEU:HD12	1:D:49:LEU:HD22	1.99	0.45
1:B:145:THR:HG22	1:B:152:GLN:NE2	2.30	0.45
1:B:289:LEU:HG	1:B:329:LEU:HD22	1.98	0.45
1:A:129:ARG:HD3	1:B:305:MET:SD	2.57	0.45
1:D:98:ALA:HA	1:D:120:TRP:O	2.16	0.45
1:C:93:GLN:NE2	1:C:93:GLN:HA	2.32	0.45
1:C:102:GLU:OE2	1:C:143:ARG:NH2	2.45	0.45
1:C:43:LEU:HD12	1:C:71:ILE:HD13	1.98	0.44
1:C:186:PRO:O	4:C:1049:HOH:O	2.21	0.44
1:D:43:LEU:HD12	1:D:71:ILE:HD13	1.99	0.44
1:B:93:GLN:HE21	1:B:93:GLN:CA	2.31	0.44
1:A:259:TRP:CD2	1:A:298:VAL:HB	2.53	0.44
1:C:96:HIS:ND1	4:C:1052:HOH:O	2.35	0.44
1:C:133:ARG:HH11	1:C:133:ARG:HG2	1.83	0.44
1:A:289:LEU:HB2	1:A:323:ILE:HB	2.00	0.44
1:C:351:SER:C	1:C:353:VAL:N	2.69	0.44
1:C:91:SER:HA	1:C:117:VAL:HG12	1.99	0.44
1:C:304:ASP:N	1:C:304:ASP:OD2	2.51	0.44
1:D:2:GLN:NE2	1:D:2:GLN:HA	2.32	0.44
1:B:43:LEU:O	1:B:47:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:127:MET:HE3	1:D:255:TYR:N	2.32	0.44
1:C:81:PHE:HB3	1:C:90:ILE:CD1	2.48	0.44
1:B:88:PRO:HG2	4:B:1061:HOH:O	2.17	0.44
1:D:259:TRP:CD2	1:D:298:VAL:HB	2.53	0.43
1:D:277:GLY:HA3	1:D:349:LEU:HA	2.00	0.43
1:D:99:VAL:HG23	1:D:119:VAL:HG13	2.00	0.43
1:D:112:SER:O	1:D:113:LEU:CD2	2.51	0.43
1:C:212:ILE:HG12	1:C:217:VAL:HB	2.00	0.43
1:D:213:ILE:HD11	1:D:231:CYS:SG	2.58	0.43
1:C:245:ARG:HD2	4:D:1044:HOH:O	2.18	0.43
1:A:1:MET:HE2	1:A:2:GLN:O	2.17	0.43
1:A:93:GLN:HE21	1:A:93:GLN:HA	1.82	0.43
1:B:277:GLY:HA3	1:B:349:LEU:HA	2.01	0.43
1:C:108:LEU:HA	1:C:108:LEU:HD23	1.71	0.43
1:C:40:HIS:CD2	1:C:235:MET:HB2	2.54	0.43
1:A:244:VAL:HG21	1:A:317:LYS:HA	2.00	0.43
1:C:164:ASP:HA	1:C:220:LEU:CD2	2.49	0.43
1:D:91:SER:HA	1:D:117:VAL:HG12	2.00	0.43
1:D:136:GLN:O	4:D:1015:HOH:O	2.21	0.43
1:C:330:PRO:O	1:C:332:GLU:N	2.52	0.43
1:B:1:MET:HE3	1:B:356:LYS:CE	2.48	0.43
1:B:1:MET:CE	1:B:356:LYS:HE3	2.49	0.43
1:C:223:ARG:CG	1:C:223:ARG:O	2.67	0.42
1:A:17:LEU:HD12	1:A:49:LEU:HD22	2.01	0.42
1:A:186:PRO:HA	1:C:26:ALA:HB2	2.01	0.42
1:A:105:LEU:O	1:A:109:GLU:HG3	2.18	0.42
1:D:6:VAL:CG1	1:D:8:ILE:HD11	2.48	0.42
1:A:8:ILE:HG23	1:A:234:VAL:HG12	2.01	0.42
1:C:277:GLY:HA3	1:C:349:LEU:HA	2.01	0.42
1:C:34:LYS:HD2	1:D:304:ASP:OD2	2.20	0.42
1:D:43:LEU:HD11	1:D:69:GLY:HA3	2.01	0.42
1:C:330:PRO:O	1:C:331:VAL:C	2.56	0.42
1:A:324:LEU:HD22	1:A:324:LEU:N	2.35	0.42
1:B:167:LYS:HB2	1:B:167:LYS:HE2	1.41	0.42
1:C:57:VAL:HG21	1:C:63:ALA:HB2	2.02	0.42
1:C:330:PRO:C	1:C:332:GLU:N	2.72	0.42
1:A:1:MET:CE	1:A:240:SER:HB2	2.47	0.42
1:D:217:VAL:HG12	1:D:218:SER:N	2.35	0.41
1:C:216:GLY:CA	1:C:232:GLN:O	2.55	0.41
1:D:19:ARG:HH12	1:D:23:LEU:HD21	1.78	0.41
1:D:157:VAL:HA	1:D:190:SER:O	2.21	0.41
1:D:224:SER:CB	1:D:228:ASP:OD1	2.67	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:43:LEU:HD11	1:A:69:GLY:HA3	2.02	0.41
1:D:242:ILE:HG22	4:D:1073:HOH:O	2.20	0.41
1:A:277:GLY:HA3	1:A:349:LEU:HA	2.03	0.41
1:C:303:MET:CB	1:C:304:ASP:OD2	2.62	0.41
1:B:52:ALA:O	1:B:73:LYS:HD3	2.20	0.41
1:D:196:GLY:HA2	1:D:200:TRP:HD1	1.85	0.41
1:C:289:LEU:HG	1:C:329:LEU:HD22	2.02	0.41
1:C:232:GLN:HA	1:C:233:PRO:HD3	1.65	0.41
1:C:324:LEU:HD22	1:C:324:LEU:N	2.36	0.41
1:C:323:ILE:HD13	4:C:1058:HOH:O	2.20	0.41
1:D:11:ARG:NH1	1:D:232:GLN:OE1	2.54	0.41
1:C:43:LEU:HD11	1:C:69:GLY:HA3	2.01	0.41
1:D:57:VAL:HG21	1:D:63:ALA:HB2	2.03	0.41
1:C:329:LEU:HA	1:C:330:PRO:HD2	1.77	0.41
1:C:188:GLN:HG3	1:C:207:TRP:NE1	2.36	0.41
1:C:329:LEU:HA	4:C:1037:HOH:O	2.20	0.40
1:D:8:ILE:HB	1:D:357:TYR:CD1	2.56	0.40
1:A:43:LEU:O	1:A:47:ARG:HG3	2.21	0.40
1:B:91:SER:HA	1:B:117:VAL:HG12	2.02	0.40
1:B:135:GLU:HG2	1:B:136:GLN:CD	2.41	0.40
1:B:93:GLN:NE2	1:B:93:GLN:HA	2.36	0.40
1:B:252:PRO:HB2	1:B:257:GLY:CA	2.51	0.40
1:C:288:VAL:HG13	1:C:295:VAL:HG23	2.03	0.40
1:C:214:LEU:O	1:C:214:LEU:HD22	2.21	0.40
1:A:218:SER:HB3	1:A:224:SER:O	2.22	0.40
1:C:164:ASP:OD1	1:C:165:GLU:HG3	2.21	0.40
1:C:15:HIS:CD2	1:C:15:HIS:C	2.95	0.40
1:C:43:LEU:HD11	1:C:71:ILE:HD13	2.04	0.40
1:C:7:VAL:HA	1:C:356:LYS:HB3	2.04	0.40
1:D:44:GLU:HG2	4:D:1058:HOH:O	2.20	0.40
1:B:335:ALA:HB1	1:B:340:VAL:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	356/379 (94%)	340 (96%)	15 (4%)	1 (0%)	50	90
1	B	356/379 (94%)	341 (96%)	14 (4%)	1 (0%)	50	90
1	C	343/379 (90%)	320 (93%)	20 (6%)	3 (1%)	25	73
1	D	344/379 (91%)	320 (93%)	22 (6%)	2 (1%)	33	81
All	All	1399/1516 (92%)	1321 (94%)	71 (5%)	7 (0%)	38	84

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	61	GLU
1	D	172	GLU
1	A	258	THR
1	C	223	ARG
1	B	257	GLY
1	C	330	PRO
1	D	73	LYS

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	285/302 (94%)	267 (94%)	18 (6%)	25	66
1	B	285/302 (94%)	265 (93%)	20 (7%)	21	62
1	C	278/302 (92%)	256 (92%)	22 (8%)	18	54
1	D	278/302 (92%)	254 (91%)	24 (9%)	15	50
All	All	1126/1208 (93%)	1042 (92%)	84 (8%)	19	57

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	60	LEU
1	A	65	ARG
1	A	72	THR
1	A	73	LYS

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Mol	Chain	Res	Type
1	A	108	LEU
1	A	127	MET
1	A	148	LYS
1	A	175	LEU
1	A	202	GLN
1	A	214	LEU
1	A	228	ASP
1	A	236	SER
1	A	258	THR
1	A	263	ARG
1	A	293	ARG
1	A	300	ARG
1	A	317	LYS
1	B	1	MET
1	B	17	LEU
1	B	65	ARG
1	B	73	LYS
1	B	93	GLN
1	B	127	MET
1	B	151	ARG
1	B	167	LYS
1	B	175	LEU
1	B	202	GLN
1	B	213	ILE
1	B	214	LEU
1	B	220	LEU
1	B	228	ASP
1	B	258	THR
1	B	263	ARG
1	B	293	ARG
1	B	296	PRO
1	B	327	GLU
1	B	333	ARG
1	C	11	ARG
1	C	17	LEU
1	C	60	LEU
1	C	73	LYS
1	C	79	GLU
1	C	93	GLN
1	C	110	GLU
1	C	127	MET
1	C	164	ASP

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Mol	Chain	Res	Type
1	C	175	LEU
1	C	214	LEU
1	C	220	LEU
1	C	223	ARG
1	C	228	ASP
1	C	263	ARG
1	C	296	PRO
1	C	300	ARG
1	C	304	ASP
1	C	333	ARG
1	C	334	ILE
1	C	353	VAL
1	C	356	LYS
1	D	1	MET
1	D	17	LEU
1	D	19	ARG
1	D	34	LYS
1	D	60	LEU
1	D	61	GLU
1	D	73	LYS
1	D	76	LEU
1	D	93	GLN
1	D	103	GLU
1	D	113	LEU
1	D	127	MET
1	D	146	GLN
1	D	177	ILE
1	D	202	GLN
1	D	213	ILE
1	D	214	LEU
1	D	218	SER
1	D	231	CYS
1	D	263	ARG
1	D	295	VAL
1	D	317	LYS
1	D	334	ILE
1	D	337	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN

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Mol	Chain	Res	Type
1	A	96	HIS
1	A	152	GLN
1	B	93	GLN
1	B	152	GLN
1	B	202	GLN
1	C	93	GLN
1	C	152	GLN
1	C	179	ASN
1	C	202	GLN
1	C	232	GLN
1	D	2	GLN
1	D	93	GLN
1	D	152	GLN
1	D	202	GLN
1	D	315	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	KCX	A	122	1	11,11,12	5.54	3 (27%)	10,12,14	2.90	3 (30%)
1	KCX	B	122	1	11,11,12	5.50	4 (36%)	10,12,14	3.08	3 (30%)
1	KCX	C	122	1	11,11,12	5.57	4 (36%)	10,12,14	2.92	3 (30%)
1	KCX	D	122	1	11,11,12	5.55	2 (18%)	10,12,14	3.10	3 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	A	122	1	-	0/8/10/12	0/0/0/0
1	KCX	B	122	1	-	0/8/10/12	0/0/0/0
1	KCX	C	122	1	-	0/8/10/12	0/0/0/0
1	KCX	D	122	1	-	0/8/10/12	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	122	KCX	O-C	17.53	1.23	1.11
1	D	122	KCX	O-C	17.52	1.23	1.11
1	A	122	KCX	O-C	17.50	1.23	1.11
1	B	122	KCX	O-C	17.41	1.23	1.11
1	D	122	KCX	CE-NZ	4.32	1.56	1.46
1	A	122	KCX	CE-NZ	4.10	1.55	1.46
1	B	122	KCX	CE-NZ	3.79	1.55	1.46
1	C	122	KCX	CE-NZ	3.69	1.55	1.46
1	C	122	KCX	CA-C	2.76	1.53	1.48
1	C	122	KCX	CB-CA	2.63	1.55	1.53
1	A	122	KCX	CA-C	2.36	1.52	1.48
1	B	122	KCX	CA-C	2.34	1.52	1.48
1	B	122	KCX	CB-CA	2.22	1.55	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	KCX	C-CA-N	-6.90	106.94	113.83
1	D	122	KCX	C-CA-N	-6.80	107.04	113.83
1	A	122	KCX	C-CA-N	-6.72	107.11	113.83
1	C	122	KCX	C-CA-N	-6.26	107.58	113.83
1	D	122	KCX	CD-CE-NZ	4.82	126.74	112.21
1	B	122	KCX	CD-CE-NZ	4.53	125.84	112.21
1	B	122	KCX	OQ1-CX-NZ	-4.46	117.53	124.94
1	C	122	KCX	CD-CE-NZ	4.44	125.58	112.21
1	D	122	KCX	OQ1-CX-NZ	-4.44	117.55	124.94
1	C	122	KCX	OQ1-CX-NZ	-4.43	117.57	124.94
1	A	122	KCX	CD-CE-NZ	4.37	125.36	112.21
1	A	122	KCX	OQ1-CX-NZ	-3.87	118.50	124.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

11 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	$\# Z > 2$
3	PLP	A	1001	1	14,15,16	2.10	6 (42%)	20,22,23	2.28	9 (45%)
2	SO4	A	360	-	4,4,4	0.73	0	6,6,6	0.36	0
2	SO4	A	361	-	4,4,4	1.27	0	6,6,6	0.67	0
2	SO4	A	362	-	4,4,4	0.75	0	6,6,6	0.40	0
3	PLP	B	1001	1	14,15,16	3.38	6 (42%)	20,22,23	2.02	8 (40%)
2	SO4	B	360	-	4,4,4	1.35	0	6,6,6	0.41	0
2	SO4	B	361	-	4,4,4	1.40	0	6,6,6	0.67	0
3	PLP	C	1001	1	14,15,16	2.32	6 (42%)	20,22,23	2.22	7 (35%)
2	SO4	C	360	-	4,4,4	0.50	0	6,6,6	0.16	0
2	SO4	C	361	-	4,4,4	0.91	0	6,6,6	0.29	0
3	PLP	D	1001	1	14,15,16	2.70	7 (50%)	20,22,23	2.85	10 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	A	1001	1	-	0/6/6/8	0/1/1/1
2	SO4	A	360	-	-	0/0/0/0	0/0/0/0
2	SO4	A	361	-	-	0/0/0/0	0/0/0/0
2	SO4	A	362	-	-	0/0/0/0	0/0/0/0
3	PLP	B	1001	1	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	B	360	-	-	0/0/0/0	0/0/0/0
2	SO4	B	361	-	-	0/0/0/0	0/0/0/0
3	PLP	C	1001	1	-	0/6/6/8	0/1/1/1
2	SO4	C	360	-	-	0/0/0/0	0/0/0/0
2	SO4	C	361	-	-	0/0/0/0	0/0/0/0
3	PLP	D	1001	1	-	0/6/6/8	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	PLP	C3-C2	10.14	1.48	1.40
3	C	1001	PLP	C3-C2	4.47	1.44	1.40
3	D	1001	PLP	C2-N1	4.44	1.42	1.33
3	D	1001	PLP	P-O1P	4.42	1.66	1.51
3	A	1001	PLP	P-O4P	-4.36	1.45	1.60
3	B	1001	PLP	C2-N1	4.08	1.41	1.33
3	C	1001	PLP	P-O1P	3.77	1.63	1.51
3	D	1001	PLP	P-O3P	3.72	1.68	1.54
3	D	1001	PLP	C3-C2	3.68	1.43	1.40
3	D	1001	PLP	C6-C5	3.55	1.45	1.37
3	D	1001	PLP	C4-C5	3.08	1.44	1.39
3	C	1001	PLP	P-O2P	2.98	1.65	1.54
3	B	1001	PLP	P-O4P	-2.97	1.49	1.60
3	B	1001	PLP	C4-C5	2.95	1.44	1.39
3	A	1001	PLP	O3-C3	2.78	1.43	1.37
3	D	1001	PLP	C6-N1	2.70	1.40	1.34
3	B	1001	PLP	O3-C3	2.70	1.43	1.37
3	A	1001	PLP	C2-N1	2.50	1.38	1.33
3	B	1001	PLP	C6-C5	2.47	1.43	1.37
3	C	1001	PLP	C2-N1	2.46	1.38	1.33
3	A	1001	PLP	C3-C2	2.43	1.42	1.40
3	A	1001	PLP	C6-C5	2.36	1.43	1.37
3	A	1001	PLP	C5A-C5	2.34	1.57	1.51
3	C	1001	PLP	C6-N1	2.32	1.39	1.34
3	C	1001	PLP	C4-C5	2.08	1.42	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1001	PLP	O3P-P-O4P	6.60	124.87	106.65
3	D	1001	PLP	O2P-P-O4P	-5.91	90.33	106.65
3	A	1001	PLP	O4P-C5A-C5	5.22	119.87	109.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	PLP	C5-C6-N1	-4.00	116.65	123.86
3	B	1001	PLP	C5A-C5-C6	-3.99	111.72	119.28
3	D	1001	PLP	C5-C6-N1	-3.96	116.72	123.86
3	A	1001	PLP	C6-N1-C2	3.85	127.52	119.28
3	C	1001	PLP	C3-C2-N1	-3.78	115.48	120.66
3	C	1001	PLP	C6-N1-C2	3.61	127.01	119.28
3	D	1001	PLP	C5A-C5-C6	-3.47	112.71	119.28
3	C	1001	PLP	C5-C6-N1	-3.45	117.63	123.86
3	B	1001	PLP	C5A-C5-C4	3.44	129.41	121.41
3	C	1001	PLP	C5A-C5-C6	-3.41	112.83	119.28
3	C	1001	PLP	C5A-C5-C4	3.39	129.30	121.41
3	D	1001	PLP	O4P-C5A-C5	3.35	116.07	109.26
3	C	1001	PLP	O3P-P-O1P	-3.33	99.54	110.44
3	B	1001	PLP	C5-C6-N1	-3.05	118.35	123.86
3	B	1001	PLP	P-O4P-C5A	3.00	132.03	121.22
3	D	1001	PLP	C6-N1-C2	2.89	125.47	119.28
3	C	1001	PLP	O3P-P-O2P	2.89	118.87	107.61
3	B	1001	PLP	O3P-P-O4P	2.84	114.48	106.65
3	B	1001	PLP	C6-N1-C2	2.68	125.02	119.28
3	D	1001	PLP	C5A-C5-C4	2.66	127.59	121.41
3	D	1001	PLP	O3-C3-C2	-2.65	112.88	117.61
3	D	1001	PLP	C3-C2-N1	-2.63	117.06	120.66
3	D	1001	PLP	C2A-C2-C3	2.54	124.11	121.02
3	A	1001	PLP	C3-C2-N1	-2.52	117.21	120.66
3	A	1001	PLP	O2P-P-O4P	-2.35	100.17	106.65
3	A	1001	PLP	C5A-C5-C4	2.26	126.67	121.41
3	A	1001	PLP	C4-C3-C2	-2.26	117.09	119.67
3	B	1001	PLP	C3-C2-N1	-2.25	117.58	120.66
3	A	1001	PLP	P-O4P-C5A	2.21	129.21	121.22
3	A	1001	PLP	C5A-C5-C6	-2.07	115.37	119.28
3	B	1001	PLP	O4P-C5A-C5	2.03	113.39	109.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	359/379 (94%)	-0.32	0 100 100	2, 12, 27, 46	0
1	B	359/379 (94%)	-0.30	0 100 100	2, 13, 26, 43	0
1	C	350/379 (92%)	-0.11	0 100 100	13, 31, 42, 51	0
1	D	351/379 (92%)	-0.04	0 100 100	15, 33, 47, 54	0
All	All	1419/1516 (93%)	-0.20	0 93 100	2, 23, 42, 54	0

There are no RSRZ outliers to report.

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	KCX	B	122	12/13	0.23	2.61	1,11,14,15	0
1	KCX	D	122	12/13	0.24	1.00	32,35,40,41	0
1	KCX	A	122	12/13	0.20	0.88	1,16,17,17	0
1	KCX	C	122	12/13	0.17	-0.28	8,18,23,24	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	PLP	A	1001	15/16	0.28	4.29	12,22,24,26	0
2	SO4	A	361	5/5	0.27	3.42	73,73,74,75	0
3	PLP	B	1001	15/16	0.27	2.60	19,25,28,31	0
3	PLP	D	1001	15/16	0.30	1.76	42,46,49,49	0
2	SO4	A	362	5/5	0.26	1.70	36,37,39,43	0
3	PLP	C	1001	15/16	0.29	1.26	37,39,40,41	0
2	SO4	B	361	5/5	0.20	-0.00	78,78,79,79	0
2	SO4	C	360	5/5	0.20	-0.39	41,41,42,43	0
2	SO4	C	361	5/5	0.09	-1.62	75,75,75,75	0
2	SO4	A	360	5/5	0.16	-1.82	56,57,58,59	0
2	SO4	B	360	5/5	0.11	-3.26	39,39,40,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.