Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2023 – 06:59 AM EDT

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 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 (i) 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 (i)) were used in the production of this report:

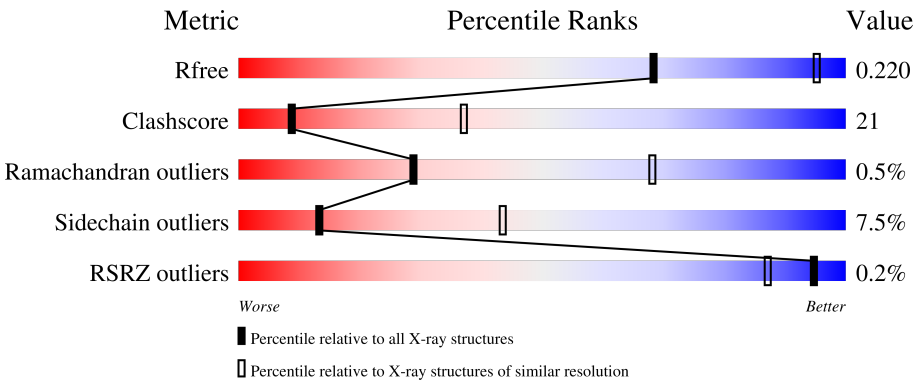
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 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 <=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	379	69% 23% • 5%
1	B	379	69% 23% • 5%
1	C	379	56% 31% • • 8%
1	D	379	.% 53% 34% 5% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PLP	D	1001	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11336 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 Alanine racemase.

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

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 mutation	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 mutation	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 mutation	UNP P0A6B4

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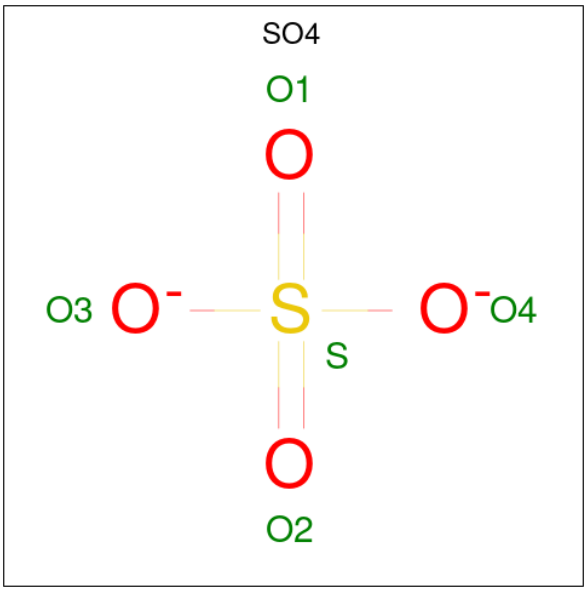
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP P0A6B4
D	-18	GLY	-	expression tag	UNP P0A6B4
D	-17	SER	-	expression tag	UNP P0A6B4
D	-16	SER	-	expression tag	UNP P0A6B4
D	-15	HIS	-	expression tag	UNP P0A6B4
D	-14	HIS	-	expression tag	UNP P0A6B4
D	-13	HIS	-	expression tag	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 mutation	UNP P0A6B4

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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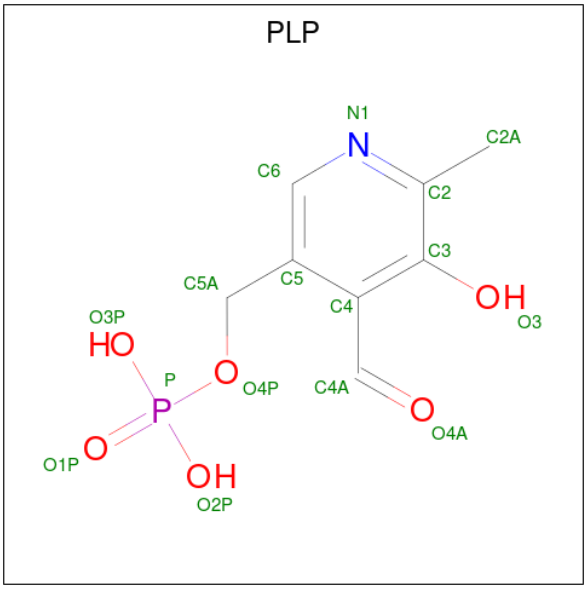
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	A	1	5	4	1		0	0
			Total	O	S			
2	A	1	5	4	1		0	0
			Total	O	S			
2	B	1	5	4	1		0	0
			Total	O	S			
2	B	1	5	4	1		0	0
			Total	O	S			
2	C	1	5	4	1		0	0
			Total	O	S			
2	C	1	5	4	1		0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 4 is water.

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

3 Residue-property plots (i)

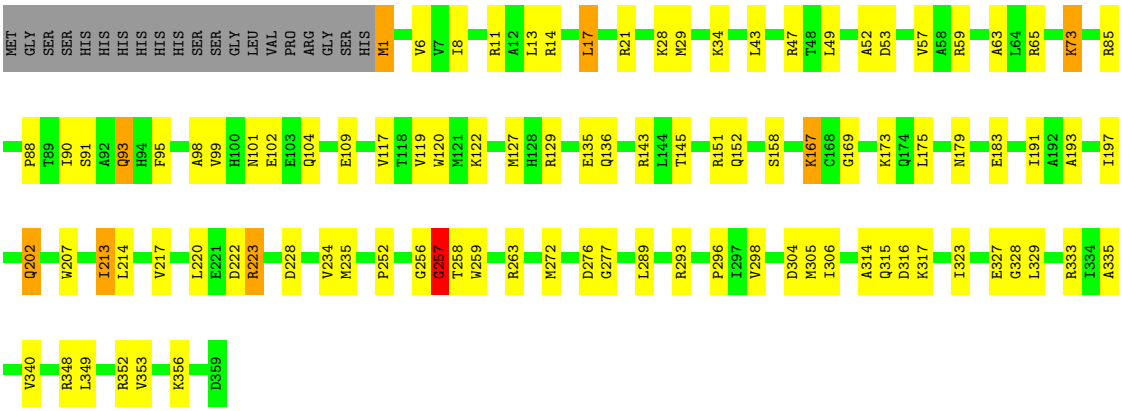
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A:

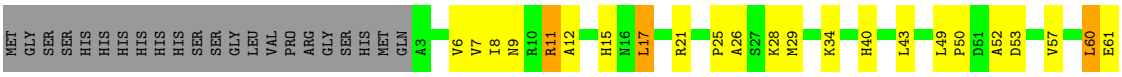
- Molecule 1: Alanine racemase

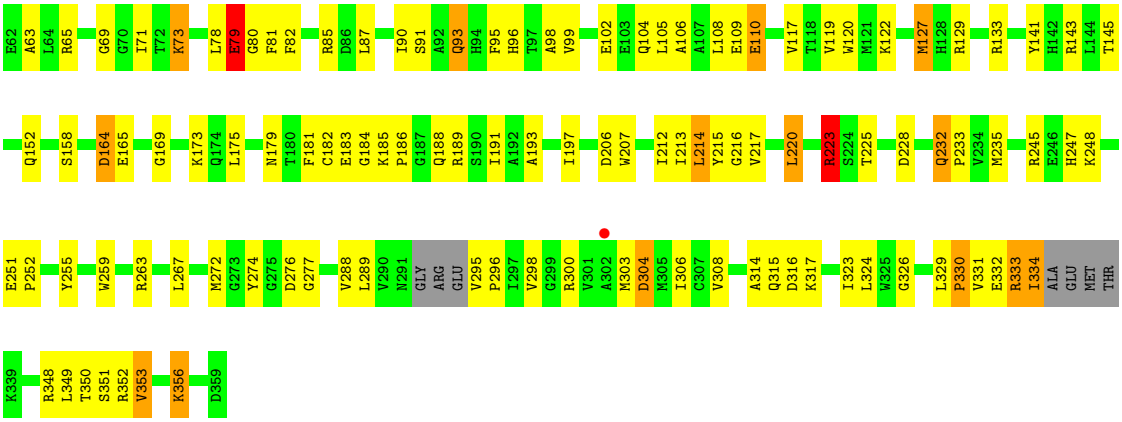
Chain B:



- Molecule 1: Alanine racemase

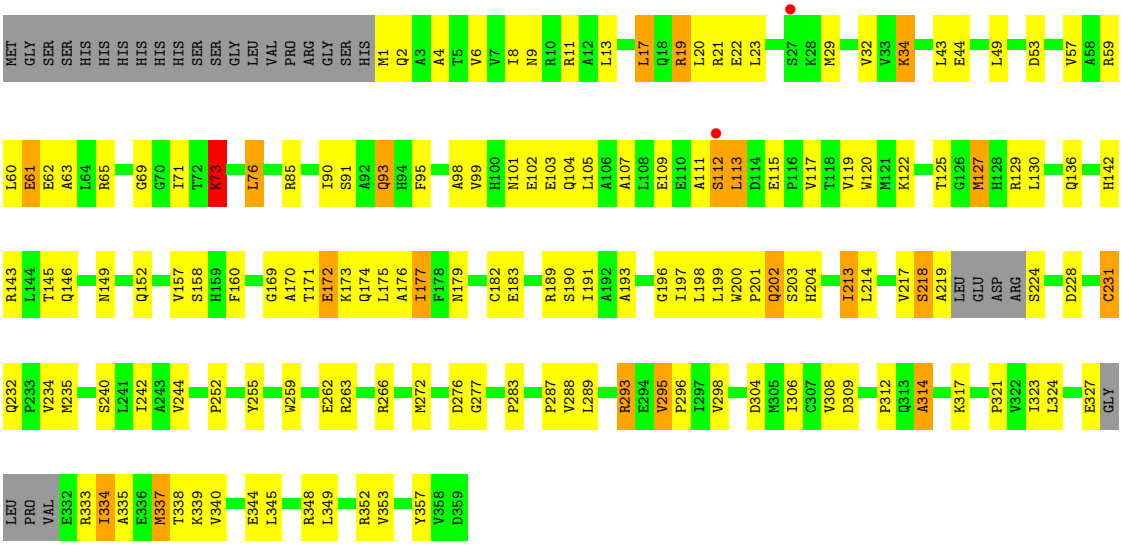
Chain C:





- Molecule 1: Alanine racemase

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (9.48%)	wwPDB-VP
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 4.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.457 for h,-h-k,-l	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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 21.

All (449) 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: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:HB2	1:A:189:ARG:HH11	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:O	1:C:223:ARG:HD3	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
1:C:213:ILE:O	1:C:213:ILE:HG13	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG2	1:D:334:ILE:O	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:O	1:C:353:VAL:CG1	2.30	0.79
1:D:189:ARG:HB2	1:D:189:ARG:NH1	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:A:348:ARG:HD2	1:B:348:ARG:HD2	1.64	0.78
1:D:293:ARG:HH21	1:D:295:VAL:HB	1.44	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:15:HIS:CG	1:C:232:GLN:NE2	2.53	0.77
1:C:189:ARG:HB2	1:C:189:ARG:NH1	1.99	0.77
1:C:334:ILE:HG22	1:C:334:ILE:O	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:A:25:PRO:HG3	1:C:184:GLY:O	1.87	0.74
1:D:293:ARG:NH2	1:D:295:VAL:CG1	2.50	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:C:303:MET:HB3	1:C:304:ASP:OD2	1.88	0.72
1:D:113:LEU:CD1	1:D:115:GLU:O	2.36	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:D:171:THR:O	1:D:173:LYS:N	2.22	0.72
1:B:202:GLN:H	1:B:202:GLN:HE21	1.36	0.71
1:A:1:MET:HE3	1:A:240:SER:HB2	1.73	0.71
1:D:324:LEU:CD1	4:D:1066:HOH:O	2.34	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:HD13	1:C:334:ILE:H	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	Interatomic distance (Å)	Clash overlap (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:C:189:ARG:HH11	1:C:189:ARG:CB	2.06	0.68
1:D:235:MET:HG3	4:D:1039:HOH:O	1.93	0.68
1:D:8:ILE:HD13	4:D:1039:HOH:O	1.94	0.68
1:D:335:ALA:HB2	1:D:345:LEU:HD11	1.76	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:C:17:LEU:O	1:C:21:ARG:HG3	1.96	0.65
1:D:224:SER:HB2	1:D:228:ASP:OD1	1.95	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:A:6:VAL:HG13	1:A:235:MET:HG3	1.79	0.64
1:B:21:ARG:HG2	1:B:29:MET:CE	2.28	0.64
1:D:171:THR:C	1:D:173:LYS:N	2.51	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:21:ARG:HG2	1:D:29:MET:CE	2.29	0.62
1:D:287:PRO:HD2	1:D:337:MET:SD	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PRO:HA	1:A:259:TRP:O	2.00	0.61
1:D:107:ALA:O	1:D:111:ALA:HB2	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:276:ASP:OD1	1:C:352:ARG:HD3	2.02	0.59
1:C:334:ILE:N	1:C:334:ILE:HD12	2.16	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:2:GLN:HB3	1:D:240:SER:OG	2.03	0.58
1:D:109:GLU:OE2	1:D:143:ARG:HD2	2.03	0.58
1:A:90:ILE:HG23	1:A:95:PHE:HB2	1.83	0.58
1:A:184:GLY:O	1:C:25:PRO:HG3	2.03	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:169:GLY:O	1:C:173:LYS:HG3	2.04	0.58
1:C:288:VAL:HG11	1:C:308:VAL:HG11	1.83	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:A:255:TYR:O	1:A:258:THR:HG22	2.04	0.58
1:C:11:ARG:HG2	4:C:1051:HOH:O	2.03	0.58
1:C:164:ASP:CA	1:C:220:LEU:CD2	2.79	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:293:ARG:HH22	1:D:295:VAL:CG1	2.16	0.57
1:D:287:PRO:HG2	1:D:334:ILE:HD12	1.86	0.57
1:D:287:PRO:CD	1:D:337:MET:SD	2.93	0.57
1:C:81:PHE:O	1:C:104:GLN:NE2	2.34	0.57
1:C:330:PRO:HD2	4:C:1037:HOH:O	2.03	0.57
1:C:87:LEU:CD1	1:C:108:LEU:HD23	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ARG:O	1:C:223:ARG:CD	2.48	0.57
1:C:248:LYS:O	1:C:251:GLU:HB2	2.04	0.57
1:B:101:ASN:OD1	1:B:104:GLN:HG3	2.04	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:D:335:ALA:HB2	1:D:345:LEU:HD12	1.86	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:B:272:MET:O	1:B:306:ILE:HG13	2.05	0.56
1:C:274:TYR:HB2	4:C:1018:HOH:O	2.06	0.56
1:C:79:GLU:OE1	1:C:82:PHE:CZ	2.57	0.55
1:D:199:LEU:HG	4:D:1049:HOH:O	2.06	0.55
1:D:266:ARG:NH1	1:D:314:ALA:O	2.39	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:C:182:CYS:HB3	1:C:189:ARG:HD3	1.88	0.54
1:D:235:MET:CG	4:D:1039:HOH:O	2.51	0.54
1:A:182:CYS:HB3	1:A:189:ARG:HD3	1.88	0.54
1:A:193:ALA:O	1:A:197:ILE:HG13	2.08	0.54
1:D:21:ARG:NH2	1:D:53:ASP:OD2	2.40	0.54
1:D:175:LEU:O	1:D:179:ASN:ND2	2.40	0.54
1:C:316:ASP:O	1:C:317:LYS:HG2	2.08	0.54
1:C:331:VAL:HG13	1:C:332:GLU:OE2	2.07	0.54
1:A:73:LYS:HG3	1:A:74:PRO:HD2	1.90	0.54
1:B:52:ALA:O	1:B:73:LYS:HD2	2.08	0.54
1:D:13:LEU:HD13	1:D:234:VAL:HG21	1.89	0.54
1:D:160:PHE:CZ	1:D:171:THR:CG2	2.91	0.54
1:C:87:LEU:HD13	1:C:108:LEU:HD23	1.89	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:D:334:ILE:O	1:D:338:THR:OG1	2.27	0.53
1:A:277:GLY:HA2	1:B:348:ARG:HD3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:164:ASP:O	1:C:220:LEU:HD21	2.07	0.53
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: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:D:19:ARG:HH12	1:D:23:LEU:CD2	2.22	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:A:338:THR:O	1:A:339:LYS:HB2	2.08	0.52
1:D:182:CYS:HB3	1:D:189:ARG:HD3	1.89	0.52
1:D:283:PRO:CD	1:D:337:MET:O	2.57	0.52
1:B:202:GLN:H	1:B:202:GLN:NE2	2.03	0.52
1:B:135:GLU:HG2	1:B:136:GLN:OE1	2.09	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:171:THR:O	1:D:172:GLU:C	2.46	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:D:338:THR:HG22	1:D:340:VAL:HG11	1.85	0.52
1:C:289:LEU:HD13	4:C:1047:HOH:O	2.09	0.52
1:B:252:PRO:HA	1:B:259:TRP:O	2.09	0.52
1:D:19:ARG:NE	1:D:22:GLU:OE2	2.43	0.52
1:B:289:LEU:HD11	1:B:328:GLY:HA3	1.91	0.51
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:C:43:LEU:CD1	1:C:71:ILE:HD13	2.39	0.51
1:D:21:ARG:HG2	1:D:29:MET:HE2	1.90	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:B:135:GLU:CD	1:B:135:GLU:H	2.14	0.51
1:C:81:PHE:HB3	1:C:90:ILE:HD11	1.93	0.51
1:A:21:ARG:NH2	1:A:53:ASP:OD2	2.44	0.51
1:B:276:ASP:OD1	1:B:352:ARG:CD	2.56	0.51
1:C:99:VAL:HG23	1:C:119:VAL:HG13	1.91	0.51
1:D:91:SER:HB2	1:D:113:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:28:LYS:HD2	1:C:207:TRP:CZ2	2.46	0.51
1:C:331:VAL:C	1:C:333:ARG:H	2.13	0.51
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:A:98:ALA:HA	1:A:120:TRP:O	2.11	0.50
1:B:179:ASN:O	1:B:183:GLU:HG3	2.11	0.50
1:C:145:THR:HG22	1:C:152:GLN:NE2	2.24	0.50
1:B:93:GLN:HA	1:B:93:GLN:HE21	1.75	0.50
1:B:169:GLY:O	1:B:173:LYS:HG3	2.11	0.50
1:C:158:SER:O	1:C:191:ILE:HA	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:133:ARG:HB3	4:C:1055:HOH:O	2.12	0.50
1:C:351:SER:C	1:C:353:VAL:H	2.15	0.50
1:A:272:MET:O	1:A:306:ILE:HG13	2.11	0.50
1:C:288:VAL:HG11	1:C:308:VAL:CG1	2.42	0.50
1:D:19:ARG:O	1:D:22:GLU:HB2	2.12	0.50
1:A:73:LYS:HG3	1:A:74:PRO:CD	2.42	0.50
1:D:93:GLN:HE21	1:D:93:GLN:HA	1.77	0.50
1:C:245:ARG:NH1	4:C:1061:HOH:O	2.43	0.49
1:A:169:GLY:O	1:A:173:LYS:HG3	2.12	0.49
1:D:293:ARG:HH22	1:D:295:VAL:HG11	1.77	0.49
1:A:127:MET:HB3	4:A:1027:HOH:O	2.12	0.49
1:C:212:ILE:HG23	1:C:213:ILE:N	2.27	0.49
1:C:334:ILE:O	1:C:334:ILE:CG2	2.55	0.49
1:D:61:GLU:HG2	1:D:62:GLU:N	2.26	0.49
1:D:276:ASP:OD1	1:D:352:ARG:CD	2.56	0.49
1:D:289:LEU:HB2	1:D:323:ILE:HB	1.94	0.49
1:D:296:PRO:HG2	1:D:309:ASP:HB3	1.94	0.49
1:A:47:ARG:HD2	4:A:1060:HOH:O	2.12	0.49
1:C:6:VAL:CG1	1:C:8:ILE:HD11	2.42	0.49
1:C:179:ASN:O	1:C:183:GLU:HG3	2.13	0.49
1:C:267:LEU:HD12	4:C:1061:HOH:O	2.13	0.49
1:C:350:THR:OG1	1:C:351:SER:N	2.41	0.49
1:D:19:ARG:O	1:D:19:ARG:HD2	2.13	0.49
1:D:333:ARG:C	1:D:335:ALA:H	2.16	0.49
1:A:21:ARG:HG2	1:A:29:MET:HE2	1.94	0.49
1:A:276:ASP:OD1	1:A:352:ARG:CD	2.57	0.49
1:D:43:LEU:CD1	1:D:71:ILE:HD13	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:THR:CG2	1:D:340:VAL:HG11	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:A:198:LEU:HD21	1:A:213:ILE:CD1	2.44	0.48
1:B:98:ALA:HA	1:B:120:TRP:O	2.12	0.48
1:C:50:PRO:C	1:C:73:LYS:HE3	2.33	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:A:304:ASP:OD2	1:B:34:LYS:HD2	2.13	0.48
1:C:181:PHE:O	1:C:185:LYS:NZ	2.46	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:A:28:LYS:HD2	1:A:207:TRP:CZ2	2.48	0.48
1:B:57:VAL:HG21	1:B:63:ALA:HB2	1.96	0.48
1:B:222:ASP:O	1:B:223:ARG:CG	2.62	0.48
1:C:255:TYR:N	1:D:127:MET:HE3	2.29	0.48
1:D:130:LEU:HA	4:D:1044:HOH:O	2.13	0.48
1:B:316:ASP:O	1:B:317:LYS:HG2	2.13	0.48
1:D:312:PRO:CG	4:D:1045:HOH:O	2.62	0.48
1:D:338:THR:HB	1:D:340:VAL:H	1.79	0.48
1:A:13:LEU:HD13	1:A:234:VAL:HG21	1.94	0.47
1:B:6:VAL:CG1	1:B:8:ILE:HD11	2.45	0.47
1:B:13:LEU:HD13	1:B:234:VAL:HG21	1.95	0.47
1:A:288:VAL:HG11	1:A:308:VAL:CG1	2.44	0.47
1:C:17:LEU:HD12	1:C:49:LEU:HD22	1.96	0.47
1:D:4:ALA:HB1	1:D:353:VAL:HG22	1.95	0.47
1:A:293:ARG:NH2	1:A:316:ASP:OD2	2.47	0.47
1:D:295:VAL:HG23	1:D:296:PRO:N	2.30	0.47
1:B:289:LEU:HB2	1:B:323:ILE:HB	1.96	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:C:164:ASP:C	1:C:220:LEU:HD21	2.35	0.47
1:D:111:ALA:O	1:D:149:ASN:ND2	2.48	0.47
1:D:176:ALA:CB	4:D:1062:HOH:O	2.29	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:B:99:VAL:HG23	1:B:119:VAL:HG13	1.97	0.46
1:D:145:THR:HG22	1:D:152:GLN:NE2	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:148:LYS:HD2	1:A:148:LYS:HA	1.66	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:D:198:LEU:HD21	1:D:213:ILE:CD1	2.46	0.46
1:B:8:ILE:HG23	1:B:234:VAL:HG12	1.97	0.46
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: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:A:145:THR:HG22	1:A:152:GLN:NE2	2.29	0.46
1:B:259:TRP:CD2	1:B:298:VAL:HB	2.51	0.46
1:C:259:TRP:CD2	1:C:298:VAL:HB	2.51	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:112:SER:C	1:D:113:LEU:HD23	2.34	0.45
1:D:213:ILE:HG12	1:D:213:ILE:O	2.17	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:201:PRO:HA	1:D:204:HIS:CE1	2.52	0.45
1:D:217:VAL:CG1	1:D:218:SER:N	2.78	0.45
1:B:102:GLU:OE2	1:B:143:ARG:NH2	2.43	0.45
1:D:73:LYS:HA	1:D:73:LYS:HD3	1.38	0.45
1:D:293:ARG:NH2	1:D:295:VAL:HG12	2.30	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: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:D:17:LEU:HD12	1:D:49:LEU:HD22	1.99	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:HA	1:C:93:GLN:NE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:ARG:HG2	1:C:133:ARG:HH11	1.83	0.44
1:A:289:LEU:HB2	1:A:323:ILE:HB	2.00	0.44
1:C:91:SER:HA	1:C:117:VAL:HG12	1.99	0.44
1:C:351:SER:C	1:C:353:VAL:N	2.69	0.44
1:B:43:LEU:O	1:B:47:ARG:HG3	2.17	0.44
1:C:127:MET:HE3	1:D:255:TYR:N	2.32	0.44
1:C:304:ASP:OD2	1:C:304:ASP:N	2.51	0.44
1:D:2:GLN:HA	1:D:2:GLN:NE2	2.32	0.44
1:B:88:PRO:HG2	4:B:1061:HOH:O	2.17	0.44
1:C:81:PHE:HB3	1:C:90:ILE:CD1	2.48	0.44
1:D:259:TRP:CD2	1:D:298:VAL:HB	2.53	0.43
1:D:99:VAL:HG23	1:D:119:VAL:HG13	2.00	0.43
1:D:277:GLY:HA3	1:D:349:LEU:HA	2.00	0.43
1:C:212:ILE:HG12	1:C:217:VAL:HB	2.00	0.43
1:C:245:ARG:HD2	4:D:1044:HOH:O	2.18	0.43
1:D:112:SER:O	1:D:113:LEU:CD2	2.51	0.43
1:D:213:ILE:HD11	1:D:231:CYS:SG	2.58	0.43
1:A:1:MET:HE2	1:A:2:GLN:O	2.17	0.43
1:A:93:GLN:HA	1:A:93:GLN:HE21	1.82	0.43
1:A:244:VAL:HG21	1:A:317:LYS:HA	2.00	0.43
1:B:277:GLY:HA3	1:B:349:LEU:HA	2.01	0.43
1:C:40:HIS:CD2	1:C:235:MET:HB2	2.54	0.43
1:C:108:LEU:HD23	1:C:108:LEU:HA	1.71	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:B:1:MET:HE3	1:B:356:LYS:CE	2.48	0.43
1:C:330:PRO:O	1:C:332:GLU:N	2.52	0.43
1:B:1:MET:CE	1:B:356:LYS:HE3	2.49	0.43
1:A:17:LEU:HD12	1:A:49:LEU:HD22	2.01	0.42
1:A:105:LEU:O	1:A:109:GLU:HG3	2.18	0.42
1:A:186:PRO:HA	1:C:26:ALA:HB2	2.01	0.42
1:C:223:ARG:O	1:C:223:ARG:CG	2.67	0.42
1:A:8:ILE:HG23	1:A:234:VAL:HG12	2.01	0.42
1:D:6:VAL:CG1	1:D:8:ILE:HD11	2.48	0.42
1:C:34:LYS:HD2	1:D:304:ASP:OD2	2.20	0.42
1:C:277:GLY:HA3	1:C:349:LEU:HA	2.01	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:N	1:A:324:LEU:HD22	2.35	0.42
1:B:167:LYS:HE2	1:B:167:LYS:HB2	1.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:VAL:HG21	1:C:63:ALA:HB2	2.02	0.42
1:A:1:MET:CE	1:A:240:SER:HB2	2.47	0.42
1:C:330:PRO:C	1:C:332:GLU:N	2.72	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:A:43:LEU:HD11	1:A:69:GLY:HA3	2.02	0.41
1:D:224:SER:CB	1:D:228:ASP:OD1	2.67	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:B:52:ALA:O	1:B:73:LYS:HD3	2.20	0.41
1:C:303:MET:CB	1:C:304:ASP:OD2	2.62	0.41
1:D:196:GLY:HA2	1:D:200:TRP:HD1	1.85	0.41
1:C:232:GLN:HA	1:C:233:PRO:HD3	1.65	0.41
1:C:289:LEU:HG	1:C:329:LEU:HD22	2.02	0.41
1:C:324:LEU:N	1:C:324:LEU:HD22	2.36	0.41
1:C:43:LEU:HD11	1:C:69:GLY:HA3	2.01	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:D:57:VAL:HG21	1:D:63:ALA:HB2	2.03	0.41
1:C:188:GLN:HG3	1:C:207:TRP:NE1	2.36	0.41
1:C:329:LEU:HA	1:C:330:PRO:HD2	1.77	0.41
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: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:B:93:GLN:HA	1:B:93:GLN:NE2	2.36	0.40
1:B:135:GLU:HG2	1:B:136:GLN:CD	2.41	0.40
1:A:218:SER:HB3	1:A:224:SER:O	2.22	0.40
1:B:252:PRO:HB2	1:B:257:GLY:CA	2.51	0.40
1:C:214:LEU:HD22	1:C:214:LEU:O	2.21	0.40
1:C:288:VAL:HG13	1:C:295:VAL:HG23	2.03	0.40
1:C:164:ASP:OD1	1:C:165:GLU:HG3	2.21	0.40
1:B:335:ALA:HB1	1:B:340:VAL:O	2.20	0.40
1:C:7:VAL:HA	1:C:356:LYS:HB3	2.04	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:D:44:GLU:HG2	4:D:1058:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	356/379 (94%)	340 (96%)	15 (4%)	1 (0%)	41	76
1	B	356/379 (94%)	341 (96%)	14 (4%)	1 (0%)	41	76
1	C	343/379 (90%)	320 (93%)	20 (6%)	3 (1%)	17	55
1	D	344/379 (91%)	320 (93%)	22 (6%)	2 (1%)	25	64
All	All	1399/1516 (92%)	1321 (94%)	71 (5%)	7 (0%)	29	68

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 (i)

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%)	18	51
1	B	285/302 (94%)	265 (93%)	20 (7%)	15	47
1	C	278/302 (92%)	256 (92%)	22 (8%)	12	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	278/302 (92%)	254 (91%)	24 (9%)	10	37
All	All	1126/1208 (93%)	1042 (92%)	84 (8%)	13	43

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	D	231	CYS
1	D	263	ARG
1	D	295	VAL
1	D	317	LYS
1	D	334	ILE
1	D	337	MET

Sometimes 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
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 (i)

There are no RNA molecules in this entry.

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

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	D	122	1	9,11,12	1.75	1 (11%)	5,12,14	3.17	2 (40%)
1	KCX	A	122	1	9,11,12	1.67	2 (22%)	5,12,14	2.84	2 (40%)
1	KCX	B	122	1	9,11,12	1.61	1 (11%)	5,12,14	3.07	2 (40%)
1	KCX	C	122	1	9,11,12	1.60	2 (22%)	5,12,14	3.03	2 (40%)

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	D	122	1	-	0/9/10/12	-
1	KCX	A	122	1	-	0/9/10/12	-
1	KCX	B	122	1	-	0/9/10/12	-
1	KCX	C	122	1	-	0/9/10/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	122	KCX	CE-NZ	4.51	1.56	1.46
1	A	122	KCX	CE-NZ	4.27	1.55	1.46
1	B	122	KCX	CE-NZ	3.96	1.55	1.46
1	C	122	KCX	CE-NZ	3.85	1.55	1.46
1	A	122	KCX	OQ1-CX	2.03	1.25	1.21
1	C	122	KCX	OQ1-CX	2.01	1.25	1.21

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	122	KCX	CD-CE-NZ	5.08	126.74	112.21
1	B	122	KCX	OQ1-CX-NZ	-4.79	117.53	124.96
1	D	122	KCX	OQ1-CX-NZ	-4.78	117.55	124.96
1	B	122	KCX	CD-CE-NZ	4.77	125.84	112.21
1	C	122	KCX	OQ1-CX-NZ	-4.77	117.57	124.96
1	C	122	KCX	CD-CE-NZ	4.68	125.58	112.21
1	A	122	KCX	CD-CE-NZ	4.60	125.36	112.21
1	A	122	KCX	OQ1-CX-NZ	-4.17	118.50	124.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	C	1001	1	15,15,16	2.16	7 (46%)	20,22,23	2.50	10 (50%)
2	SO4	A	362	-	4,4,4	0.34	0	6,6,6	0.49	0
2	SO4	A	361	-	4,4,4	0.60	0	6,6,6	0.54	0
2	SO4	C	360	-	4,4,4	0.36	0	6,6,6	0.15	0
3	PLP	D	1001	1	15,15,16	2.68	7 (46%)	20,22,23	3.17	11 (55%)
2	SO4	A	360	-	4,4,4	0.52	0	6,6,6	0.36	0
3	PLP	A	1001	1	15,15,16	2.11	5 (33%)	20,22,23	2.85	11 (55%)
2	SO4	C	361	-	4,4,4	0.42	0	6,6,6	0.38	0
3	PLP	B	1001	1	15,15,16	2.78	6 (40%)	20,22,23	2.36	10 (50%)
2	SO4	B	360	-	4,4,4	0.63	0	6,6,6	0.47	0
2	SO4	B	361	-	4,4,4	0.65	0	6,6,6	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	A	1001	1	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	C	1001	1	-	0/6/6/8	0/1/1/1
3	PLP	B	1001	1	-	0/6/6/8	0/1/1/1
3	PLP	D	1001	1	-	3/6/6/8	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	7.12	1.48	1.40
3	D	1001	PLP	P-O1P	4.80	1.66	1.50
3	A	1001	PLP	P-O4P	-4.72	1.45	1.60
3	D	1001	PLP	C2-N1	4.39	1.42	1.33
3	C	1001	PLP	P-O1P	4.13	1.63	1.50
3	B	1001	PLP	C2-N1	4.03	1.41	1.33
3	D	1001	PLP	C6-C5	3.93	1.45	1.37
3	D	1001	PLP	C5-C4	3.64	1.44	1.40
3	D	1001	PLP	P-O3P	3.49	1.68	1.54
3	B	1001	PLP	C5-C4	3.44	1.44	1.40
3	B	1001	PLP	P-O4P	-3.23	1.49	1.60
3	C	1001	PLP	C3-C2	3.07	1.44	1.40
3	A	1001	PLP	O3-C3	2.96	1.43	1.37
3	D	1001	PLP	C6-N1	2.90	1.40	1.34
3	B	1001	PLP	O3-C3	2.87	1.43	1.37
3	C	1001	PLP	P-O2P	2.80	1.65	1.54
3	B	1001	PLP	C6-C5	2.71	1.43	1.37
3	A	1001	PLP	C6-C5	2.58	1.43	1.37
3	D	1001	PLP	C3-C2	2.50	1.43	1.40
3	C	1001	PLP	C6-N1	2.49	1.39	1.34
3	A	1001	PLP	C2-N1	2.47	1.38	1.33
3	C	1001	PLP	C2-N1	2.42	1.38	1.33
3	A	1001	PLP	C5A-C5	2.40	1.57	1.50
3	C	1001	PLP	C2A-C2	2.22	1.54	1.50
3	C	1001	PLP	C5-C4	2.04	1.42	1.40

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1001	PLP	O3P-P-O4P	6.82	124.87	106.73
3	D	1001	PLP	O2P-P-O4P	-6.17	90.33	106.73
3	A	1001	PLP	O4P-C5A-C5	5.52	119.87	109.35
3	A	1001	PLP	C3-C4-C5	4.88	124.01	118.74
3	A	1001	PLP	C4A-C4-C5	-4.73	116.06	120.94
3	B	1001	PLP	C5A-C5-C6	-4.65	111.72	119.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	PLP	C6-N1-C2	4.51	127.52	119.17
3	A	1001	PLP	C5-C6-N1	-4.31	116.65	123.82
3	D	1001	PLP	C5-C6-N1	-4.26	116.72	123.82
3	D	1001	PLP	C4A-C4-C5	-4.26	116.55	120.94
3	C	1001	PLP	C6-N1-C2	4.23	127.01	119.17
3	C	1001	PLP	C3-C2-N1	-4.10	115.48	120.77
3	D	1001	PLP	C5A-C5-C6	-4.05	112.71	119.37
3	C	1001	PLP	C5A-C5-C6	-3.98	112.83	119.37
3	B	1001	PLP	C4A-C4-C5	-3.96	116.86	120.94
3	C	1001	PLP	C5-C6-N1	-3.71	117.63	123.82
3	C	1001	PLP	C3-C4-C5	3.70	122.74	118.74
3	D	1001	PLP	O4P-C5A-C5	3.53	116.07	109.35
3	B	1001	PLP	C3-C4-C5	3.50	122.52	118.74
3	D	1001	PLP	C6-N1-C2	3.41	125.47	119.17
3	B	1001	PLP	C5-C6-N1	-3.28	118.35	123.82
3	A	1001	PLP	O3-C3-C4	3.25	126.66	118.10
3	C	1001	PLP	C4A-C4-C3	-3.24	115.01	120.50
3	B	1001	PLP	C6-N1-C2	3.16	125.02	119.17
3	C	1001	PLP	O3P-P-O2P	2.94	118.87	107.64
3	B	1001	PLP	O3P-P-O4P	2.91	114.48	106.73
3	D	1001	PLP	C3-C2-N1	-2.87	117.06	120.77
3	C	1001	PLP	O3P-P-O1P	-2.85	99.54	110.68
3	B	1001	PLP	O3-C3-C4	2.77	125.39	118.10
3	A	1001	PLP	C3-C2-N1	-2.75	117.21	120.77
3	D	1001	PLP	C2A-C2-C3	2.61	124.11	120.89
3	B	1001	PLP	C3-C2-N1	-2.47	117.58	120.77
3	A	1001	PLP	O2P-P-O4P	-2.47	100.17	106.73
3	A	1001	PLP	C5A-C5-C6	-2.43	115.37	119.37
3	D	1001	PLP	O3-C3-C4	2.42	124.48	118.10
3	C	1001	PLP	C2A-C2-N1	2.31	122.19	117.67
3	A	1001	PLP	C2A-C2-N1	2.21	121.99	117.67
3	B	1001	PLP	O4P-C5A-C5	2.12	113.39	109.35
3	D	1001	PLP	O3-C3-C2	-2.12	112.88	117.49
3	C	1001	PLP	O4P-P-O1P	2.05	112.24	106.47
3	B	1001	PLP	C4A-C4-C3	-2.04	117.04	120.50
3	A	1001	PLP	C4-C3-C2	-2.02	117.09	120.07

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1001	PLP	C5A-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
3	D	1001	PLP	C5A-O4P-P-O1P
3	D	1001	PLP	C5A-O4P-P-O3P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	PLP	1	0
3	D	1001	PLP	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	358/379 (94%)	-0.64	0	100	100	2, 12, 27, 46	0
1	B	358/379 (94%)	-0.60	0	100	100	2, 13, 26, 43	0
1	C	349/379 (92%)	-0.27	1 (0%)	94	84	13, 31, 42, 51	0
1	D	350/379 (92%)	-0.16	2 (0%)	89	72	15, 33, 47, 54	0
All	All	1415/1516 (93%)	-0.42	3 (0%)	95	87	2, 23, 42, 54	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	27	SER	2.6
1	D	112	SER	2.2
1	C	302	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	KCX	D	122	12/13	0.88	0.23	32,35,40,41	0
1	KCX	B	122	12/13	0.92	0.21	1,11,14,15	0
1	KCX	A	122	12/13	0.93	0.18	1,16,17,17	0
1	KCX	C	122	12/13	0.96	0.15	8,18,23,24	0

6.3 Carbohydrates (i)

There are no monosaccharides 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
3	PLP	D	1001	15/16	0.89	0.27	42,46,49,49	0
2	SO4	B	361	5/5	0.90	0.21	78,78,79,79	0
2	SO4	A	361	5/5	0.93	0.28	73,73,74,75	0
2	SO4	A	362	5/5	0.93	0.26	36,37,39,43	0
3	PLP	B	1001	15/16	0.94	0.24	19,25,28,31	0
3	PLP	A	1001	15/16	0.94	0.25	12,22,24,26	0
2	SO4	C	360	5/5	0.95	0.19	41,41,42,43	0
3	PLP	C	1001	15/16	0.95	0.26	37,39,40,41	0
2	SO4	A	360	5/5	0.95	0.16	56,57,58,59	0
2	SO4	C	361	5/5	0.96	0.09	75,75,75,75	0
2	SO4	B	360	5/5	0.97	0.11	39,39,40,41	0

6.5 Other polymers (i)

There are no such residues in this entry.