Full wwPDB X-ray Structure Validation Report (i)

Dec 11, 2022 – 01:59 AM EST

PDB ID	:	1DE6
Title	:	L-RHAMNOSE ISOMERASE
Authors	:	Korndorfer, I.P.; Fessner, W.D.; Matthews, B.W.
Deposited on	:	1999-11-13
Resolution	:	2.10 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:

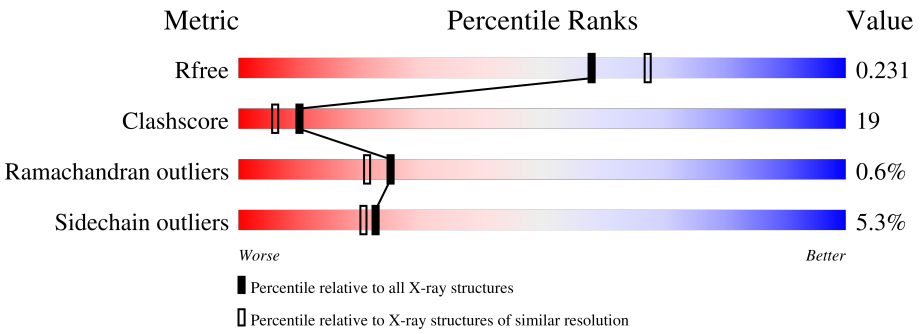
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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%

Mol	Chain	Length	Quality of chain
1	A	426	60% 30% 7% •
1	B	426	55% 34% 8% • •
1	C	426	60% 30% 8% • •
1	D	426	56% 34% 7% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14331 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 L-RHAMNOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	416	3309	2090	587	619	13	0	0	0
1	B	416	3309	2090	587	619	13	0	0	0
1	C	416	3309	2090	587	619	13	0	0	0
1	D	416	3309	2090	587	619	13	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP P32170
A	3	HIS	-	expression tag	UNP P32170
A	4	HIS	-	expression tag	UNP P32170
A	5	HIS	-	expression tag	UNP P32170
A	6	HIS	-	expression tag	UNP P32170
A	7	HIS	-	expression tag	UNP P32170
A	8	HIS	-	expression tag	UNP P32170
B	2	GLY	-	expression tag	UNP P32170
B	3	HIS	-	expression tag	UNP P32170
B	4	HIS	-	expression tag	UNP P32170
B	5	HIS	-	expression tag	UNP P32170
B	6	HIS	-	expression tag	UNP P32170
B	7	HIS	-	expression tag	UNP P32170
B	8	HIS	-	expression tag	UNP P32170
C	2	GLY	-	expression tag	UNP P32170
C	3	HIS	-	expression tag	UNP P32170
C	4	HIS	-	expression tag	UNP P32170
C	5	HIS	-	expression tag	UNP P32170
C	6	HIS	-	expression tag	UNP P32170
C	7	HIS	-	expression tag	UNP P32170
C	8	HIS	-	expression tag	UNP P32170

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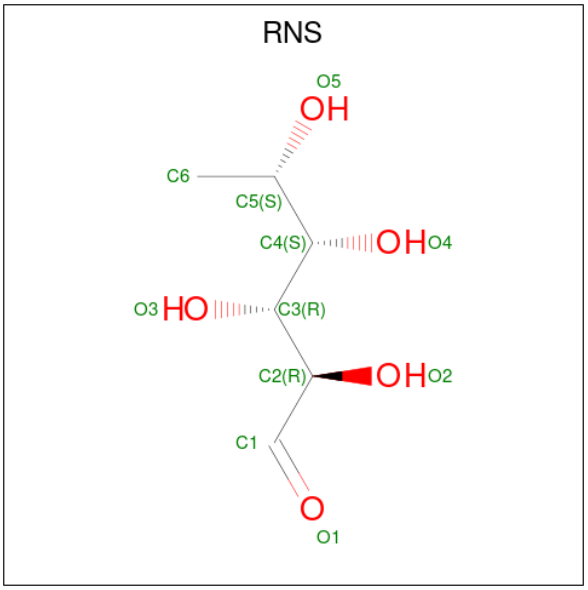
Chain	Residue	Modelled	Actual	Comment	Reference
D	2	GLY	-	expression tag	UNP P32170
D	3	HIS	-	expression tag	UNP P32170
D	4	HIS	-	expression tag	UNP P32170
D	5	HIS	-	expression tag	UNP P32170
D	6	HIS	-	expression tag	UNP P32170
D	7	HIS	-	expression tag	UNP P32170
D	8	HIS	-	expression tag	UNP P32170

- Molecule 2 is L-RHAMNOSE (three-letter code: RNS) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	11	6	5	0	0
			Total	C	O		
2	B	1	11	6	5	0	0
			Total	C	O		
2	C	1	11	6	5	0	0
			Total	C	O		
2	D	1	11	6	5	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mn 1 1	0	0
4	B	1	Total Mn 1 1	0	0
4	C	1	Total Mn 1 1	0	0
4	D	1	Total Mn 1 1	0	0

- Molecule 5 is water.

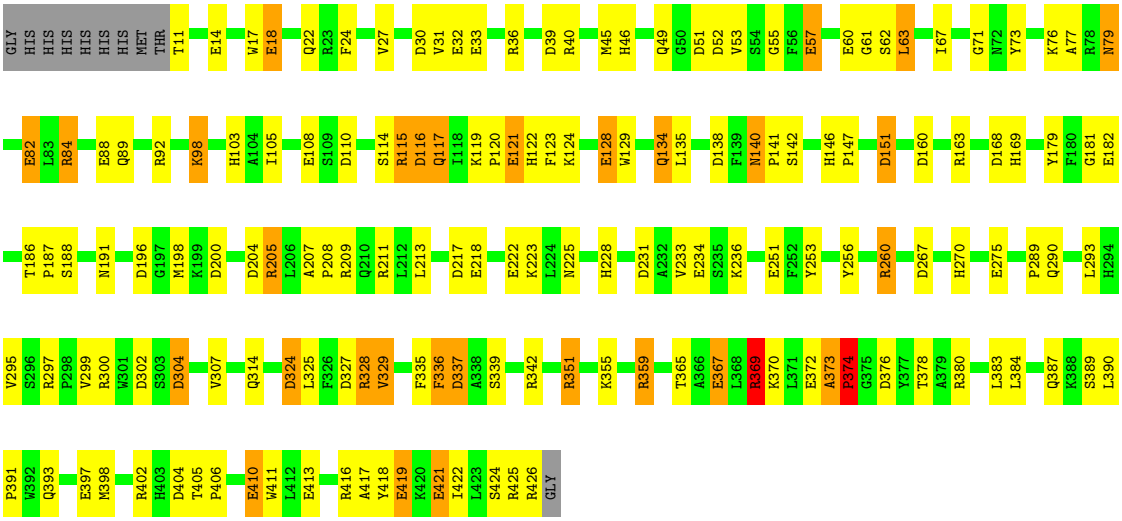
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	250	Total O 250 250	0	0
5	B	286	Total O 286 286	0	0
5	C	263	Total O 263 263	0	0
5	D	244	Total O 244 244	0	0

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. 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. 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.

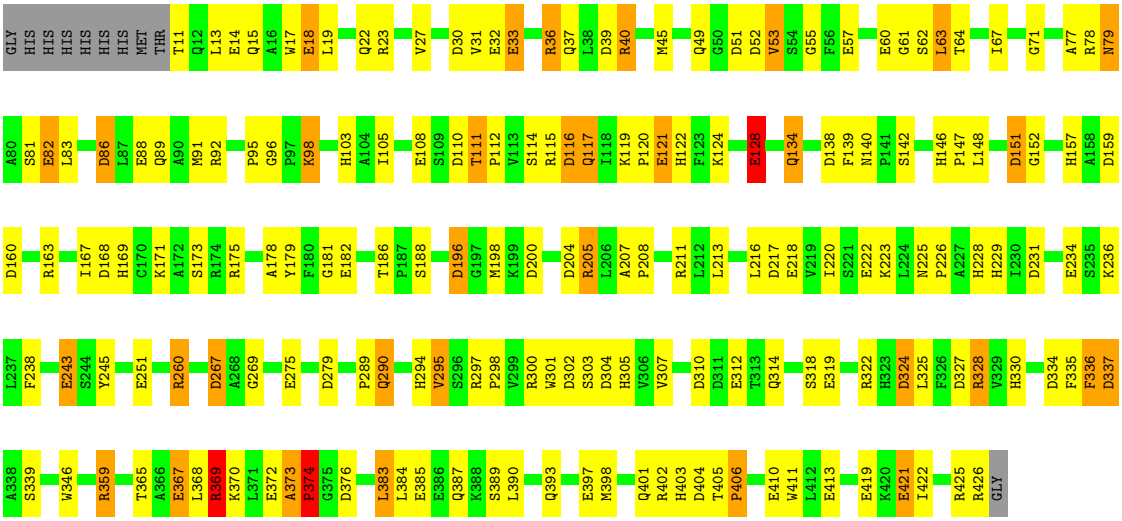
- Molecule 1: L-RHAMNOSE ISOMERASE

Chain A:



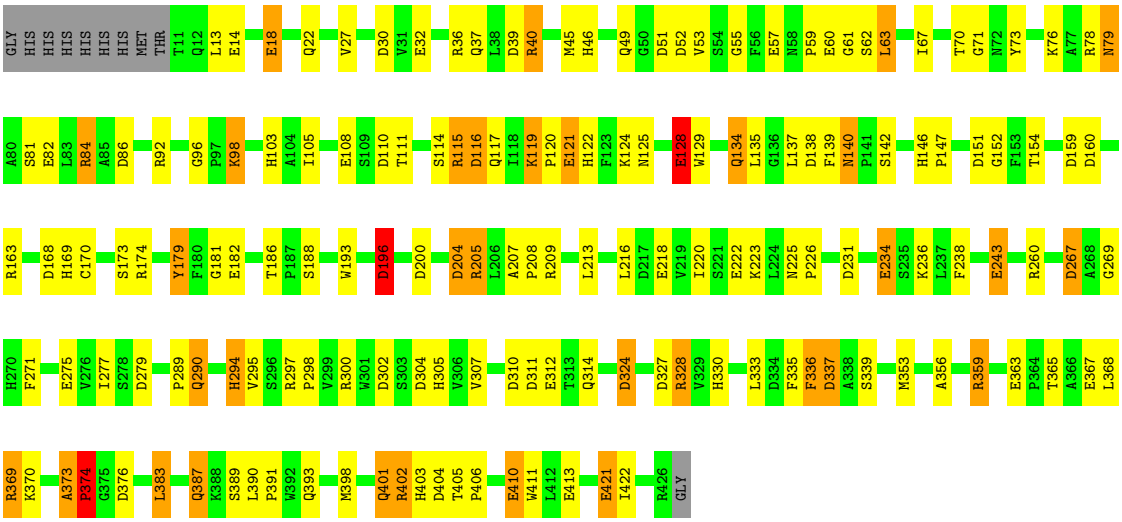
- Molecule 1: L-RHAMNOSE ISOMERASE

Chain B:



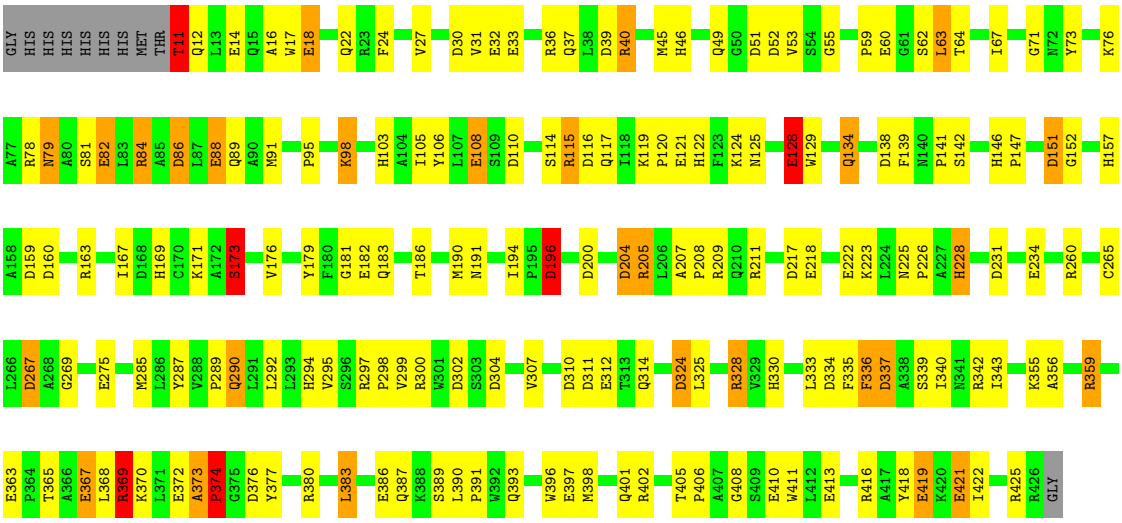
- Molecule 1: L-RHAMNOSE ISOMERASE

Chain C:



- Molecule 1: L-RHAMNOSE ISOMERASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	169.18Å 162.44Å 77.73Å 90.00° 109.89° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 28.81 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.0 (30.00-2.10) 92.3 (28.81-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.10Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.244 , 0.244 0.172 , 0.231	Depositor DCC
R_{free} test set	5391 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 101.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14331	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: ZN, RNS, MN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.28	28/3389 (0.8%)	1.73	73/4602 (1.6%)
1	B	1.30	29/3389 (0.9%)	1.79	74/4602 (1.6%)
1	C	1.25	20/3389 (0.6%)	1.82	81/4602 (1.8%)
1	D	1.26	24/3389 (0.7%)	1.76	73/4602 (1.6%)
All	All	1.27	101/13556 (0.7%)	1.78	301/18408 (1.6%)

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	GLU	CD-OE2	11.09	1.37	1.25
1	D	108	GLU	CD-OE2	9.36	1.35	1.25
1	B	218	GLU	CD-OE2	9.10	1.35	1.25
1	C	18	GLU	CD-OE2	9.01	1.35	1.25
1	D	397	GLU	CD-OE2	8.96	1.35	1.25
1	B	128	GLU	CD-OE2	8.76	1.35	1.25
1	B	319	GLU	CD-OE2	8.72	1.35	1.25
1	C	32	GLU	CD-OE2	8.63	1.35	1.25
1	D	421	GLU	CD-OE2	8.39	1.34	1.25
1	B	385	GLU	CD-OE2	8.26	1.34	1.25
1	D	367	GLU	CD-OE2	8.19	1.34	1.25
1	A	57	GLU	CD-OE2	8.17	1.34	1.25
1	B	108	GLU	CD-OE2	8.13	1.34	1.25
1	B	82	GLU	CD-OE2	8.09	1.34	1.25
1	D	82	GLU	CD-OE2	8.08	1.34	1.25
1	B	251	GLU	CD-OE2	8.08	1.34	1.25
1	B	18	GLU	CD-OE2	7.95	1.34	1.25
1	D	410	GLU	CD-OE2	7.90	1.34	1.25
1	B	397	GLU	CD-OE2	7.90	1.34	1.25
1	B	312	GLU	CD-OE2	7.74	1.34	1.25
1	B	32	GLU	CD-OE2	7.67	1.34	1.25
1	D	182	GLU	CD-OE2	7.62	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	367	GLU	CD-OE2	7.61	1.34	1.25
1	D	14	GLU	CD-OE2	7.56	1.33	1.25
1	A	421	GLU	CD-OE2	7.56	1.33	1.25
1	A	14	GLU	CD-OE2	7.46	1.33	1.25
1	C	182	GLU	CD-OE2	7.42	1.33	1.25
1	A	88	GLU	CD-OE2	7.40	1.33	1.25
1	B	182	GLU	CD-OE2	7.36	1.33	1.25
1	D	32	GLU	CD-OE2	7.34	1.33	1.25
1	B	88	GLU	CD-OE2	7.33	1.33	1.25
1	C	14	GLU	CD-OE2	7.29	1.33	1.25
1	D	128	GLU	CD-OE2	7.27	1.33	1.25
1	D	419	GLU	CD-OE2	7.12	1.33	1.25
1	C	121	GLU	CD-OE2	7.11	1.33	1.25
1	D	312	GLU	CD-OE2	7.10	1.33	1.25
1	C	363	GLU	CD-OE2	7.09	1.33	1.25
1	B	421	GLU	CD-OE2	7.08	1.33	1.25
1	C	243	GLU	CD-OE2	7.05	1.33	1.25
1	B	275	GLU	CD-OE2	7.03	1.33	1.25
1	A	275	GLU	CD-OE2	6.90	1.33	1.25
1	C	367	GLU	CD-OE2	6.85	1.33	1.25
1	C	234	GLU	CD-OE2	6.80	1.33	1.25
1	A	121	GLU	CD-OE2	6.72	1.33	1.25
1	C	421	GLU	CD-OE2	6.67	1.32	1.25
1	D	18	GLU	CD-OE2	6.60	1.32	1.25
1	A	410	GLU	CD-OE2	6.55	1.32	1.25
1	A	18	GLU	CD-OE2	6.52	1.32	1.25
1	C	128	GLU	CD-OE2	6.51	1.32	1.25
1	C	312	GLU	CD-OE2	6.47	1.32	1.25
1	A	367	GLU	CD-OE2	6.45	1.32	1.25
1	D	218	GLU	CD-OE2	6.41	1.32	1.25
1	A	234	GLU	CD-OE2	6.38	1.32	1.25
1	B	359	ARG	CZ-NH1	6.38	1.41	1.33
1	A	419	GLU	CD-OE2	6.37	1.32	1.25
1	A	108	GLU	CD-OE2	6.37	1.32	1.25
1	D	413	GLU	CD-OE2	6.35	1.32	1.25
1	A	413	GLU	CD-OE2	6.33	1.32	1.25
1	B	413	GLU	CD-OE2	6.30	1.32	1.25
1	D	33	GLU	CD-OE2	6.27	1.32	1.25
1	A	251	GLU	CD-OE2	6.26	1.32	1.25
1	A	218	GLU	CD-OE2	6.12	1.32	1.25
1	A	372	GLU	CD-OE2	6.11	1.32	1.25
1	B	372	GLU	CD-OE2	6.09	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	222	GLU	CD-OE2	6.02	1.32	1.25
1	D	359	ARG	CZ-NH1	5.98	1.40	1.33
1	D	60	GLU	CD-OE2	5.97	1.32	1.25
1	B	33	GLU	CD-OE2	5.93	1.32	1.25
1	C	57	GLU	CD-OE2	5.92	1.32	1.25
1	A	60	GLU	CD-OE2	5.92	1.32	1.25
1	B	60	GLU	CD-OE2	5.91	1.32	1.25
1	C	410	GLU	CD-OE2	5.88	1.32	1.25
1	A	182	GLU	CD-OE2	5.87	1.32	1.25
1	B	222	GLU	CD-OE2	5.87	1.32	1.25
1	C	108	GLU	CD-OE1	-5.85	1.19	1.25
1	C	218	GLU	CD-OE2	5.83	1.32	1.25
1	A	128	GLU	CD-OE2	5.81	1.32	1.25
1	B	108	GLU	CD-OE1	-5.80	1.19	1.25
1	D	222	GLU	CD-OE2	5.78	1.32	1.25
1	C	60	GLU	CD-OE2	5.78	1.32	1.25
1	A	397	GLU	CD-OE1	-5.75	1.19	1.25
1	D	275	GLU	CD-OE2	5.73	1.31	1.25
1	C	413	GLU	CD-OE2	5.71	1.31	1.25
1	B	334	ASP	CG-OD2	5.68	1.38	1.25
1	A	33	GLU	CD-OE2	5.47	1.31	1.25
1	C	108	GLU	CD-OE2	5.40	1.31	1.25
1	B	121	GLU	CD-OE2	5.39	1.31	1.25
1	D	363	GLU	CD-OE2	5.37	1.31	1.25
1	A	138	ASP	CG-OD2	5.36	1.37	1.25
1	A	82	GLU	CD-OE2	5.34	1.31	1.25
1	D	372	GLU	CD-OE2	5.32	1.31	1.25
1	A	82	GLU	CD-OE1	-5.28	1.19	1.25
1	A	222	GLU	CD-OE2	5.22	1.31	1.25
1	A	36	ARG	CZ-NH1	5.21	1.39	1.33
1	A	391	PRO	N-CD	5.20	1.55	1.47
1	B	243	GLU	CD-OE2	5.17	1.31	1.25
1	B	243	GLU	CD-OE1	-5.13	1.20	1.25
1	B	14	GLU	CD-OE2	5.12	1.31	1.25
1	B	410	GLU	CD-OE2	5.11	1.31	1.25
1	D	88	GLU	CD-OE2	5.03	1.31	1.25
1	D	386	GLU	CD-OE2	5.03	1.31	1.25

All (301) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	205	ARG	NE-CZ-NH2	-25.65	107.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	205	ARG	NE-CZ-NH1	20.12	130.36	120.30
1	B	359	ARG	NE-CZ-NH2	-19.60	110.50	120.30
1	D	205	ARG	NE-CZ-NH1	18.95	129.78	120.30
1	C	359	ARG	NE-CZ-NH2	-18.36	111.12	120.30
1	A	205	ARG	NE-CZ-NH1	18.34	129.47	120.30
1	B	205	ARG	NE-CZ-NH1	16.73	128.66	120.30
1	D	359	ARG	NE-CZ-NH2	-15.98	112.31	120.30
1	B	328	ARG	NE-CZ-NH1	15.80	128.20	120.30
1	D	205	ARG	NE-CZ-NH2	-15.75	112.43	120.30
1	B	205	ARG	NE-CZ-NH2	-15.44	112.58	120.30
1	C	373	ALA	C-N-CD	-14.78	88.08	120.60
1	B	373	ALA	C-N-CD	-14.55	88.58	120.60
1	A	359	ARG	NE-CZ-NH2	-13.64	113.48	120.30
1	C	337	ASP	CB-CG-OD2	-13.62	106.04	118.30
1	B	30	ASP	CB-CG-OD2	-13.47	106.18	118.30
1	A	373	ALA	C-N-CD	-13.46	90.99	120.60
1	B	300	ARG	NE-CZ-NH2	-13.25	113.68	120.30
1	A	205	ARG	NE-CZ-NH2	-12.92	113.84	120.30
1	D	373	ALA	C-N-CD	-12.90	92.21	120.60
1	D	328	ARG	NE-CZ-NH2	-12.68	113.96	120.30
1	C	267	ASP	CB-CG-OD2	12.38	129.44	118.30
1	C	30	ASP	CB-CG-OD2	-12.29	107.24	118.30
1	D	209	ARG	NE-CZ-NH1	12.21	126.41	120.30
1	D	209	ARG	NE-CZ-NH2	-12.14	114.23	120.30
1	B	36	ARG	NE-CZ-NH2	-11.92	114.34	120.30
1	C	267	ASP	CB-CG-OD1	-11.90	107.59	118.30
1	D	30	ASP	CB-CG-OD2	-11.85	107.64	118.30
1	B	30	ASP	CB-CG-OD1	11.82	128.94	118.30
1	C	324	ASP	CB-CG-OD2	-11.81	107.67	118.30
1	B	260	ARG	NE-CZ-NH2	-11.70	114.45	120.30
1	D	204	ASP	CB-CG-OD1	11.62	128.76	118.30
1	B	324	ASP	CB-CG-OD2	-11.59	107.87	118.30
1	C	328	ARG	NE-CZ-NH1	11.53	126.06	120.30
1	C	116	ASP	CB-CG-OD2	-11.38	108.06	118.30
1	B	260	ARG	NE-CZ-NH1	11.07	125.83	120.30
1	A	30	ASP	CB-CG-OD1	10.84	128.06	118.30
1	A	380	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	C	359	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	C	337	ASP	CB-CG-OD1	10.57	127.81	118.30
1	D	342	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	A	40	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	C	86	ASP	CB-CG-OD2	-10.44	108.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	328	ARG	NE-CZ-NH2	-10.31	115.14	120.30
1	C	204	ASP	CB-CG-OD1	10.26	127.53	118.30
1	A	260	ARG	NE-CZ-NH2	-10.15	115.22	120.30
1	C	36	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	A	328	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	B	217	ASP	CB-CG-OD1	9.99	127.29	118.30
1	A	204	ASP	CB-CG-OD1	9.83	127.15	118.30
1	C	369	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	C	163	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	A	39	ASP	CB-CG-OD1	9.66	127.00	118.30
1	B	324	ASP	CB-CG-OD1	9.66	127.00	118.30
1	C	84	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	C	374	PRO	CA-N-CD	-9.60	98.06	111.50
1	D	337	ASP	CB-CG-OD2	-9.54	109.71	118.30
1	B	217	ASP	CB-CG-OD2	-9.49	109.76	118.30
1	A	337	ASP	CB-CG-OD2	-9.47	109.77	118.30
1	A	151	ASP	CB-CG-OD2	-9.46	109.79	118.30
1	A	39	ASP	CB-CG-OD2	-9.45	109.80	118.30
1	C	30	ASP	CB-CG-OD1	9.41	126.77	118.30
1	A	376	ASP	CB-CG-OD2	-9.39	109.85	118.30
1	B	369	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	D	328	ARG	NE-CZ-NH1	9.27	124.93	120.30
1	D	116	ASP	CB-CG-OD1	9.21	126.59	118.30
1	C	310	ASP	CB-CG-OD2	-9.18	110.04	118.30
1	A	204	ASP	CB-CG-OD2	-9.16	110.06	118.30
1	D	204	ASP	CB-CG-OD2	-9.11	110.10	118.30
1	A	205	ARG	CD-NE-CZ	9.07	136.29	123.60
1	C	84	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	C	328	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	A	231	ASP	CB-CG-OD1	8.97	126.37	118.30
1	D	36	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	C	310	ASP	CB-CG-OD1	8.88	126.30	118.30
1	B	204	ASP	CB-CG-OD1	8.88	126.30	118.30
1	A	324	ASP	CB-CG-OD2	-8.88	110.31	118.30
1	D	324	ASP	CB-CG-OD2	-8.87	110.31	118.30
1	B	404	ASP	CB-CG-OD2	-8.86	110.33	118.30
1	C	311	ASP	CB-CG-OD2	-8.85	110.33	118.30
1	B	359	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	C	205	ARG	CD-NE-CZ	8.84	135.97	123.60
1	A	374	PRO	CA-N-CD	-8.82	99.15	111.50
1	B	310	ASP	CB-CG-OD1	8.80	126.22	118.30
1	C	196	ASP	CB-CG-OD2	-8.77	110.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	40	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	A	376	ASP	CB-CG-OD1	8.56	126.01	118.30
1	D	359	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	B	404	ASP	CB-CG-OD1	8.54	125.99	118.30
1	C	52	ASP	CB-CG-OD2	-8.54	110.62	118.30
1	B	279	ASP	CB-CG-OD1	8.50	125.95	118.30
1	B	310	ASP	CB-CG-OD2	-8.43	110.72	118.30
1	D	337	ASP	CB-CG-OD1	8.30	125.77	118.30
1	C	86	ASP	CB-CG-OD1	8.24	125.72	118.30
1	D	115	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	D	369	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	C	231	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	C	116	ASP	CB-CG-OD1	8.17	125.65	118.30
1	C	39	ASP	CB-CG-OD2	-8.16	110.95	118.30
1	D	211	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	D	374	PRO	CA-N-CD	-8.14	100.11	111.50
1	C	300	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	D	30	ASP	CB-CG-OD1	8.05	125.54	118.30
1	A	160	ASP	CB-CG-OD2	-8.03	111.07	118.30
1	C	231	ASP	CB-CG-OD1	8.02	125.52	118.30
1	B	374	PRO	CA-N-CD	-8.02	100.27	111.50
1	B	196	ASP	CB-CG-OD2	-7.96	111.14	118.30
1	D	39	ASP	CB-CG-OD2	-7.96	111.14	118.30
1	C	151	ASP	CB-CG-OD2	-7.94	111.16	118.30
1	B	51	ASP	CB-CG-OD1	7.91	125.42	118.30
1	C	160	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	D	260	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	B	40	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	D	200	ASP	CB-CG-OD1	7.80	125.32	118.30
1	A	92	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	B	327	ASP	CB-CG-OD1	7.80	125.32	118.30
1	D	380	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	D	151	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	C	110	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	D	116	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	B	327	ASP	CB-CG-OD2	-7.65	111.42	118.30
1	D	73	TYR	CB-CG-CD1	-7.65	116.41	121.00
1	A	378	THR	CA-CB-CG2	-7.62	101.73	112.40
1	A	297	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	D	376	ASP	CB-CG-OD1	7.59	125.13	118.30
1	B	151	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	C	300	ARG	NE-CZ-NH2	-7.57	116.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	267	ASP	CB-CG-OD2	7.56	125.10	118.30
1	B	39	ASP	CB-CG-OD1	7.55	125.10	118.30
1	D	267	ASP	CB-CG-OD1	-7.55	111.50	118.30
1	A	115	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	324	ASP	CB-CG-OD1	7.49	125.04	118.30
1	D	205	ARG	CD-NE-CZ	7.40	133.95	123.60
1	C	279	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	260	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	A	30	ASP	CB-CG-OD2	-7.26	111.76	118.30
1	C	304	ASP	CB-CG-OD1	7.23	124.81	118.30
1	A	302	ASP	CB-CG-OD1	7.23	124.80	118.30
1	A	73	TYR	CB-CG-CD1	-7.21	116.67	121.00
1	C	204	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	211	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	328	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	327	ASP	CB-CG-OD1	7.10	124.69	118.30
1	C	52	ASP	CB-CG-OD1	7.09	124.68	118.30
1	B	196	ASP	CB-CG-OD1	7.05	124.64	118.30
1	A	92	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	D	217	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	D	310	ASP	CB-CG-OD1	6.96	124.56	118.30
1	C	209	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	425	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	329	VAL	CG1-CB-CG2	-6.90	99.86	110.90
1	A	369	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	B	160	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	A	327	ASP	CB-CG-OD2	-6.88	112.10	118.30
1	A	163	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	D	311	ASP	CB-CG-OD2	-6.86	112.12	118.30
1	C	160	ASP	CB-CG-OD1	6.84	124.46	118.30
1	B	51	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	D	231	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	C	324	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	376	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	175	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	C	92	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	D	51	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	A	359	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	163	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	168	ASP	CB-CG-OD1	6.72	124.34	118.30
1	C	196	ASP	CB-CG-OD1	6.69	124.32	118.30
1	D	84	ARG	NE-CZ-NH2	-6.64	116.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	334	ASP	CB-CG-OD2	-6.62	112.35	118.30
1	C	110	ASP	CB-CG-OD1	6.55	124.19	118.30
1	D	304	ASP	CB-CG-OD1	6.54	124.19	118.30
1	C	327	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	A	416	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	160	ASP	CB-CG-OD1	6.50	124.15	118.30
1	B	205	ARG	CD-NE-CZ	6.48	132.67	123.60
1	A	209	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	D	310	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	A	135	LEU	CB-CA-C	-6.41	98.02	110.20
1	B	138	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	C	159	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	304	ASP	CB-CG-OD1	6.40	124.06	118.30
1	D	160	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	C	327	ASP	CB-CG-OD1	6.36	124.03	118.30
1	C	200	ASP	CB-CG-OD1	6.33	124.00	118.30
1	C	376	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	A	110	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	A	52	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	D	39	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	404	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	C	138	ASP	CB-CG-OD1	6.24	123.91	118.30
1	A	426	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	B	279	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	D	160	ASP	CB-CG-OD1	6.19	123.87	118.30
1	D	297	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	C	73	TYR	CB-CG-CD1	-6.15	117.31	121.00
1	C	168	ASP	CB-CG-OD1	6.11	123.80	118.30
1	C	404	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	295	VAL	CG1-CB-CG2	-6.11	101.13	110.90
1	D	36	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	84	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	369	ARG	CD-NE-CZ	6.04	132.06	123.60
1	B	168	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	A	116	ASP	CB-CG-OD1	6.03	123.72	118.30
1	B	86	ASP	CB-CG-OD1	6.03	123.72	118.30
1	D	334	ASP	N-CA-CB	6.02	121.44	110.60
1	A	217	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	B	204	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	D	228	HIS	CB-CA-C	-5.97	98.46	110.40
1	D	287	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	A	267	ASP	CB-CG-OD1	-5.96	112.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	302	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	187	PRO	N-CA-CB	5.92	110.41	103.30
1	D	300	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	D	52	ASP	CB-CG-OD1	5.91	123.62	118.30
1	C	138	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	C	304	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	D	110	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	A	351	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	C	39	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	151	ASP	CB-CG-OD1	5.80	123.52	118.30
1	D	40	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	D	302	ASP	CB-CG-OD1	5.80	123.52	118.30
1	D	159	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	337	ASP	CB-CG-OD1	5.78	123.51	118.30
1	D	151	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	111	THR	CA-CB-CG2	-5.78	104.31	112.40
1	B	231	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	337	ASP	CB-CG-OD1	5.77	123.50	118.30
1	C	179	TYR	CB-CG-CD2	-5.77	117.54	121.00
1	D	369	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	151	ASP	CB-CG-OD1	5.75	123.48	118.30
1	D	196	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	C	328	ARG	N-CA-CB	-5.74	100.26	110.60
1	B	117	GLN	CB-CA-C	-5.74	98.92	110.40
1	A	52	ASP	CB-CG-OD1	5.72	123.45	118.30
1	D	86	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	B	110	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	C	51	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	D	311	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	267	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	217	ASP	CB-CG-OD1	5.62	123.36	118.30
1	C	36	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	369	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	300	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	200	ASP	CB-CG-OD1	5.54	123.28	118.30
1	C	115	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	342	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	198	MET	CB-CA-C	-5.49	99.43	110.40
1	C	294	HIS	CA-CB-CG	-5.49	104.27	113.60
1	C	154	THR	CA-CB-CG2	-5.47	104.74	112.40
1	B	337	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	C	404	ASP	CB-CG-OD2	-5.45	113.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	159	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	140	ASN	CB-CG-OD1	-5.44	110.71	121.60
1	D	342	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	D	138	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	A	200	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	389	SER	N-CA-CB	5.41	118.62	110.50
1	B	200	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	C	376	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	159	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	B	376	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	D	138	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	328	ARG	CD-NE-CZ	5.36	131.10	123.60
1	D	91	MET	CA-CB-CG	-5.34	104.22	113.30
1	A	300	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	D	340	ILE	CA-CB-CG1	-5.32	100.89	111.00
1	A	117	GLN	CB-CA-C	-5.32	99.77	110.40
1	C	302	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	426	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	52	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	328	ARG	N-CA-CB	-5.30	101.06	110.60
1	C	135	LEU	CB-CA-C	-5.28	100.17	110.20
1	D	11	THR	N-CA-CB	5.26	120.30	110.30
1	A	84	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	231	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	C	387	GLN	CB-CA-C	5.22	120.84	110.40
1	B	116	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	B	86	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	417	ALA	N-CA-CB	-5.20	102.82	110.10
1	B	168	ASP	CB-CG-OD1	5.18	122.96	118.30
1	C	111	THR	CA-CB-CG2	-5.16	105.18	112.40
1	B	267	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	380	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	302	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	C	140	ASN	CB-CA-C	-5.13	100.13	110.40
1	D	16	ALA	CB-CA-C	5.13	117.79	110.10
1	B	406	PRO	N-CA-CB	5.11	109.43	103.30
1	D	173	SER	N-CA-CB	5.11	118.16	110.50
1	A	110	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	231	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	279	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	C	40	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	B	304	ASP	CB-CG-OD1	5.07	122.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	402	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	B	198	MET	CG-SD-CE	-5.05	92.11	100.20
1	B	91	MET	CA-CB-CG	-5.04	104.73	113.30
1	C	209	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	B	23	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	419	GLU	CG-CD-OE2	-5.01	108.28	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3309	0	3231	116	0
1	B	3309	0	3231	137	0
1	C	3309	0	3231	126	0
1	D	3309	0	3231	142	0
2	A	11	0	11	4	0
2	B	11	0	12	0	0
2	C	11	0	12	2	0
2	D	11	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	250	0	0	11	0
5	B	286	0	0	15	0
5	C	263	0	0	9	0
5	D	244	0	0	8	0
All	All	14331	0	12971	499	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 19.

All (499) 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:398:MET:HE2	1:C:402:ARG:HE	1.02	1.17
1:B:398:MET:HE2	1:B:402:ARG:HE	1.02	1.16
1:A:421:GLU:HG3	1:A:422:ILE:HG12	1.31	1.13
1:A:398:MET:HE2	1:A:402:ARG:HE	1.12	1.06
1:A:393:GLN:NE2	1:D:393:GLN:HE22	1.53	1.05
1:A:393:GLN:HE22	1:D:393:GLN:NE2	1.57	1.02
1:D:142:SER:H	1:D:169:HIS:HE1	1.12	0.98
1:D:398:MET:HE2	1:D:402:ARG:HE	1.27	0.97
1:C:114:SER:HB3	1:C:117:GLN:HG3	1.47	0.96
1:D:421:GLU:HG3	1:D:422:ILE:HG12	1.47	0.95
1:C:398:MET:HE2	1:C:402:ARG:NE	1.81	0.95
1:B:79:ASN:ND2	1:B:82:GLU:H	1.65	0.94
1:B:393:GLN:HE22	1:C:393:GLN:NE2	1.65	0.94
1:A:119:LYS:H	1:A:122:HIS:HD2	1.14	0.94
1:B:398:MET:HE2	1:B:402:ARG:NE	1.83	0.93
1:B:393:GLN:HE22	1:C:393:GLN:HE22	1.08	0.93
1:A:393:GLN:HE22	1:D:393:GLN:HE22	1.00	0.92
1:C:79:ASN:ND2	1:C:82:GLU:H	1.67	0.92
1:B:393:GLN:NE2	1:C:393:GLN:HE22	1.69	0.91
1:D:398:MET:HE2	1:D:402:ARG:NE	1.85	0.91
1:A:369:ARG:HH11	1:A:369:ARG:HG3	1.32	0.91
1:C:119:LYS:H	1:C:122:HIS:CD2	1.89	0.91
1:A:119:LYS:H	1:A:122:HIS:CD2	1.88	0.91
1:A:398:MET:HE2	1:A:402:ARG:NE	1.85	0.90
1:C:119:LYS:H	1:C:122:HIS:HD2	1.08	0.90
1:D:119:LYS:H	1:D:122:HIS:CD2	1.91	0.89
1:B:119:LYS:H	1:B:122:HIS:HD2	1.17	0.89
1:A:55:GLY:HA3	1:A:105:ILE:HD12	1.53	0.89
1:B:421:GLU:HG3	1:B:422:ILE:HG12	1.55	0.89
1:D:369:ARG:HG3	1:D:369:ARG:HH11	1.37	0.89
1:B:63:LEU:HD21	1:B:67:ILE:HD12	1.55	0.87
1:B:114:SER:HB3	1:B:117:GLN:HG3	1.59	0.85
1:B:295:VAL:HG12	1:B:307:VAL:HG21	1.57	0.85
1:B:369:ARG:HG3	1:B:369:ARG:HH11	1.43	0.84
1:A:142:SER:H	1:A:169:HIS:HE1	1.23	0.84
1:B:119:LYS:H	1:B:122:HIS:CD2	1.95	0.84
1:A:79:ASN:ND2	1:A:82:GLU:H	1.74	0.84
1:A:45:MET:CE	1:A:98:LYS:HD2	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:GLN:HE21	1:D:359:ARG:HH11	1.24	0.82
1:D:76:LYS:HE3	5:D:4537:HOH:O	1.81	0.81
1:D:119:LYS:H	1:D:122:HIS:HD2	1.25	0.81
1:B:45:MET:CE	1:B:98:LYS:HD2	2.09	0.81
1:C:76:LYS:HE3	5:C:3486:HOH:O	1.79	0.80
1:C:142:SER:H	1:C:169:HIS:HE1	1.28	0.80
1:A:114:SER:HB3	1:A:117:GLN:HG3	1.62	0.80
1:C:205:ARG:HD2	5:C:3580:HOH:O	1.80	0.80
1:A:124:LYS:O	1:A:128:GLU:HG3	1.81	0.80
1:D:134:GLN:HA	1:D:134:GLN:HE21	1.45	0.80
1:B:205:ARG:HD2	5:B:2606:HOH:O	1.79	0.80
1:B:134:GLN:HA	1:B:134:GLN:HE21	1.47	0.80
1:B:33:GLU:HG2	5:B:2491:HOH:O	1.82	0.79
1:A:314:GLN:HE21	1:A:359:ARG:HH11	1.31	0.79
1:D:142:SER:N	1:D:169:HIS:HE1	1.80	0.79
1:A:367:GLU:HG3	5:A:1491:HOH:O	1.83	0.79
1:A:393:GLN:HB2	5:A:1692:HOH:O	1.82	0.79
1:D:367:GLU:HG3	5:D:4501:HOH:O	1.81	0.79
1:D:398:MET:CE	1:D:402:ARG:HG3	2.13	0.79
1:A:45:MET:HE3	1:A:98:LYS:HD2	1.63	0.78
1:B:295:VAL:HG12	1:B:307:VAL:CG2	2.14	0.78
1:D:18:GLU:O	1:D:22:GLN:HG3	1.83	0.78
1:B:336:PHE:HB2	5:B:2744:HOH:O	1.82	0.78
1:C:134:GLN:HE21	1:C:134:GLN:HA	1.47	0.77
1:D:142:SER:H	1:D:169:HIS:CE1	2.01	0.77
1:A:63:LEU:HD21	1:A:67:ILE:HD12	1.66	0.77
1:D:205:ARG:HD2	5:D:4553:HOH:O	1.84	0.77
1:B:142:SER:H	1:B:169:HIS:HE1	1.30	0.77
1:B:269:GLY:HA2	1:B:298:PRO:HG3	1.66	0.77
1:D:45:MET:CE	1:D:98:LYS:HD2	2.14	0.77
1:D:398:MET:HE2	1:D:402:ARG:HG3	1.64	0.76
1:D:373:ALA:HB3	1:D:374:PRO:HD2	1.69	0.75
1:C:45:MET:CE	1:C:98:LYS:HD2	2.16	0.75
1:D:49:GLN:HE22	1:D:337:ASP:H	1.32	0.74
1:B:45:MET:HE3	1:B:98:LYS:HD2	1.69	0.74
1:C:49:GLN:HE22	1:C:337:ASP:H	1.35	0.73
1:D:79:ASN:ND2	1:D:82:GLU:H	1.86	0.73
1:A:142:SER:N	1:A:169:HIS:HE1	1.87	0.73
1:A:76:LYS:HE3	5:A:1503:HOH:O	1.89	0.72
1:D:295:VAL:HG12	1:D:307:VAL:HG21	1.71	0.72
1:D:63:LEU:HD21	1:D:67:ILE:HD12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:GLN:NE2	5:D:4524:HOH:O	2.23	0.71
1:A:121:GLU:HA	1:A:124:LYS:HE3	1.72	0.71
1:A:63:LEU:HD21	1:A:67:ILE:CD1	2.21	0.70
1:B:142:SER:N	1:B:169:HIS:HE1	1.89	0.70
1:A:205:ARG:HD2	5:A:1537:HOH:O	1.91	0.69
1:B:121:GLU:HA	1:B:124:LYS:HE3	1.74	0.69
1:C:114:SER:HB3	1:C:117:GLN:CG	2.20	0.69
1:C:295:VAL:HG12	1:C:307:VAL:HG21	1.73	0.69
1:A:369:ARG:HG3	1:A:369:ARG:NH1	2.04	0.69
1:B:289:PRO:O	1:B:328:ARG:HD2	1.92	0.69
1:D:11:THR:N	5:D:4498:HOH:O	2.26	0.69
1:D:63:LEU:HD21	1:D:67:ILE:CD1	2.23	0.69
1:D:365:THR:O	1:D:369:ARG:HB2	1.92	0.68
1:B:63:LEU:HD21	1:B:67:ILE:CD1	2.23	0.68
1:D:314:GLN:NE2	1:D:359:ARG:HD3	2.09	0.67
1:C:295:VAL:HG12	1:C:307:VAL:CG2	2.24	0.67
1:A:373:ALA:HB3	1:A:374:PRO:HD2	1.75	0.67
1:B:139:PHE:HE2	1:B:173:SER:HB3	1.59	0.67
1:C:314:GLN:HE21	1:C:359:ARG:HH11	1.43	0.67
1:C:421:GLU:HG3	1:C:422:ILE:HG12	1.75	0.67
1:D:369:ARG:HG3	1:D:369:ARG:NH1	2.05	0.67
1:C:45:MET:HE2	1:C:98:LYS:HB3	1.77	0.66
1:C:121:GLU:HA	1:C:124:LYS:CE	2.25	0.66
1:B:139:PHE:CE2	1:B:173:SER:HB3	2.31	0.66
1:D:134:GLN:HE21	1:D:134:GLN:CA	2.08	0.66
1:D:289:PRO:O	1:D:328:ARG:HD2	1.96	0.66
1:A:89:GLN:NE2	5:A:1481:HOH:O	2.29	0.66
1:C:63:LEU:HD21	1:C:67:ILE:HD12	1.78	0.66
1:B:121:GLU:HA	1:B:124:LYS:CE	2.25	0.65
1:A:79:ASN:HD21	1:A:82:GLU:H	1.43	0.65
1:D:121:GLU:HA	1:D:124:LYS:HE3	1.78	0.65
1:B:373:ALA:HB3	1:B:374:PRO:HD2	1.77	0.65
1:C:373:ALA:HB3	1:C:374:PRO:HD2	1.79	0.65
1:D:314:GLN:HE22	1:D:359:ARG:HD3	1.60	0.65
1:B:49:GLN:HE22	1:B:337:ASP:H	1.44	0.65
1:C:369:ARG:HH11	1:D:204:ASP:HB2	1.62	0.65
1:A:142:SER:H	1:A:169:HIS:CE1	2.10	0.64
1:A:365:THR:O	1:A:369:ARG:HB2	1.96	0.64
1:A:314:GLN:NE2	1:A:359:ARG:HH11	1.95	0.64
1:B:18:GLU:O	1:B:22:GLN:HG3	1.98	0.64
1:C:55:GLY:HA3	1:C:105:ILE:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:HIS:CG	1:C:147:PRO:HD2	2.33	0.64
1:C:421:GLU:HB2	5:C:3721:HOH:O	1.96	0.64
1:B:45:MET:HE2	1:B:98:LYS:HB3	1.79	0.64
1:C:18:GLU:O	1:C:22:GLN:HG3	1.97	0.64
1:D:119:LYS:HB3	1:D:120:PRO:HD2	1.80	0.63
1:A:124:LYS:HD3	1:A:179:TYR:OH	1.98	0.63
1:B:124:LYS:O	1:B:128:GLU:HG3	1.97	0.63
1:C:142:SER:N	1:C:169:HIS:HE1	1.97	0.63
1:C:119:LYS:N	1:C:122:HIS:HD2	1.90	0.62
1:D:295:VAL:HG12	1:D:307:VAL:CG2	2.29	0.62
1:C:387:GLN:OE1	5:C:3593:HOH:O	2.16	0.62
1:C:406:PRO:HG2	1:C:411:TRP:HB3	1.82	0.62
1:D:398:MET:HE2	1:D:402:ARG:CG	2.28	0.62
1:C:387:GLN:HG2	5:C:3570:HOH:O	1.99	0.62
1:A:289:PRO:O	1:A:328:ARG:HD2	2.00	0.62
1:C:170:CYS:O	1:C:174:ARG:HG3	2.00	0.61
1:B:370:LYS:O	1:B:374:PRO:HD2	2.00	0.61
1:D:124:LYS:O	1:D:128:GLU:HG3	2.01	0.61
1:A:121:GLU:HA	1:A:124:LYS:CE	2.29	0.61
1:A:134:GLN:HA	1:A:134:GLN:HE21	1.65	0.61
1:B:421:GLU:HB2	5:B:2722:HOH:O	1.99	0.61
1:D:55:GLY:HA3	1:D:105:ILE:HD12	1.82	0.61
1:D:79:ASN:HD22	1:D:81:SER:N	1.98	0.61
1:B:45:MET:CE	1:B:98:LYS:HB3	2.31	0.61
1:B:79:ASN:HD21	1:B:82:GLU:H	1.47	0.61
1:A:295:VAL:HG12	1:A:307:VAL:HG21	1.83	0.60
1:D:398:MET:CE	1:D:402:ARG:HE	2.08	0.60
1:B:369:ARG:HG3	1:B:369:ARG:NH1	2.11	0.60
1:C:314:GLN:HE22	1:C:359:ARG:HD3	1.66	0.60
1:A:71:GLY:HA3	1:A:339:SER:HA	1.83	0.60
1:B:367:GLU:HG3	5:B:2509:HOH:O	2.02	0.60
1:B:369:ARG:NE	5:B:2500:HOH:O	2.34	0.60
1:C:370:LYS:O	1:C:374:PRO:HD2	2.02	0.60
1:A:207:ALA:HB3	1:A:208:PRO:HD3	1.83	0.60
1:C:314:GLN:NE2	1:C:359:ARG:HD3	2.17	0.60
1:D:79:ASN:HD21	1:D:82:GLU:H	1.49	0.60
1:D:314:GLN:HE21	1:D:359:ARG:NH1	1.99	0.60
1:C:120:PRO:HB3	1:C:179:TYR:CD2	2.37	0.60
1:A:314:GLN:HE21	1:A:359:ARG:NH1	1.98	0.60
1:A:406:PRO:HG2	1:A:411:TRP:HB3	1.85	0.59
1:C:119:LYS:N	1:C:122:HIS:CD2	2.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:LYS:O	1:C:128:GLU:HG3	2.01	0.59
1:A:314:GLN:HE22	1:A:359:ARG:HD3	1.66	0.59
1:C:45:MET:CE	1:C:98:LYS:HB3	2.32	0.59
1:C:79:ASN:HD21	1:C:82:GLU:H	1.46	0.59
1:C:121:GLU:HA	1:C:124:LYS:HE3	1.83	0.59
1:A:393:GLN:HE22	1:D:393:GLN:CD	2.06	0.59
1:A:55:GLY:CA	1:A:105:ILE:HD12	2.31	0.59
1:B:393:GLN:HG2	1:C:389:SER:C	2.23	0.59
1:D:416:ARG:O	1:D:419:GLU:HB3	2.03	0.59
1:A:128:GLU:HG2	5:A:1473:HOH:O	2.04	0.58
1:B:55:GLY:HA3	1:B:105:ILE:HD12	1.84	0.58
1:D:139:PHE:CE2	1:D:173:SER:HB3	2.39	0.58
1:D:387:GLN:HG2	5:D:4582:HOH:O	2.04	0.58
1:A:123:PHE:HA	5:A:1622:HOH:O	2.04	0.58
1:C:120:PRO:HB3	1:C:179:TYR:CG	2.38	0.58
1:B:142:SER:H	1:B:169:HIS:CE1	2.17	0.58
1:B:114:SER:HB3	1:B:117:GLN:CG	2.34	0.58
1:D:37:GLN:OE1	1:D:40:ARG:HD3	2.03	0.58
1:A:295:VAL:HG12	1:A:307:VAL:CG2	2.33	0.58
1:C:63:LEU:HD21	1:C:67:ILE:CD1	2.34	0.57
1:C:368:LEU:HD21	1:C:383:LEU:HB3	1.85	0.57
1:D:45:MET:HE2	1:D:98:LYS:HB3	1.86	0.57
1:B:389:SER:C	1:C:393:GLN:HG2	2.25	0.57
1:B:167:ILE:HG22	1:B:171:LYS:HD2	1.87	0.57
1:D:285:MET:CE	1:D:325:LEU:HD21	2.34	0.57
1:D:121:GLU:HA	1:D:124:LYS:CE	2.34	0.57
1:D:406:PRO:HG2	1:D:411:TRP:HB3	1.86	0.57
1:D:225:ASN:HB3	1:D:228:HIS:ND1	2.20	0.57
1:D:45:MET:CE	1:D:98:LYS:HB3	2.35	0.56
1:B:146:HIS:CG	1:B:147:PRO:HD2	2.40	0.56
1:D:114:SER:HB3	1:D:117:GLN:HG3	1.88	0.56
1:A:314:GLN:NE2	1:A:359:ARG:HD3	2.21	0.56
1:B:151:ASP:HB2	5:B:2652:HOH:O	2.05	0.56
1:D:139:PHE:HE2	1:D:173:SER:HB3	1.70	0.55
1:C:116:ASP:OD1	1:C:117:GLN:HG2	2.07	0.55
1:D:79:ASN:ND2	1:D:81:SER:HB2	2.22	0.55
1:D:119:LYS:O	1:D:122:HIS:N	2.36	0.55
1:D:314:GLN:NE2	1:D:359:ARG:HH11	1.99	0.55
1:B:225:ASN:HB3	1:B:228:HIS:ND1	2.22	0.55
1:A:24:PHE:O	1:A:27:VAL:HG22	2.07	0.54
1:A:71:GLY:HA3	1:A:339:SER:CA	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASN:HD22	1:B:81:SER:N	2.05	0.54
1:C:152:GLY:O	1:C:196:ASP:HA	2.06	0.54
1:D:285:MET:HE3	1:D:325:LEU:HD21	1.89	0.54
1:D:157:HIS:O	1:D:163:ARG:HD3	2.07	0.54
1:A:49:GLN:HE22	1:A:337:ASP:H	1.55	0.54
1:A:393:GLN:CD	1:D:393:GLN:HE22	2.08	0.54
1:B:79:ASN:HD22	1:B:82:GLU:H	1.50	0.54
1:B:406:PRO:HG2	1:B:411:TRP:HB3	1.89	0.54
1:A:299:VAL:HG12	1:C:243:GLU:HB3	1.89	0.54
1:C:290:GLN:HG2	1:C:330:HIS:NE2	2.22	0.54
1:B:207:ALA:HB3	1:B:208:PRO:HD3	1.90	0.54
1:A:45:MET:HE3	1:A:98:LYS:CB	2.38	0.54
1:C:289:PRO:O	1:C:328:ARG:HD2	2.08	0.54
1:D:146:HIS:CG	1:D:147:PRO:HD2	2.43	0.54
1:A:114:SER:HB3	1:A:117:GLN:CG	2.35	0.53
1:C:181:GLY:HA2	1:C:186:THR:O	2.08	0.53
1:A:79:ASN:ND2	1:A:82:GLU:HG3	2.23	0.53
1:A:141:PRO:HD2	1:A:191:ASN:O	2.07	0.53
1:B:314:GLN:HE21	1:B:359:ARG:HH11	1.56	0.53
1:D:45:MET:HE1	1:D:98:LYS:HD2	1.87	0.53
1:A:121:GLU:CA	1:A:124:LYS:HE3	2.38	0.53
1:A:370:LYS:O	1:A:374:PRO:HD2	2.09	0.53
1:C:383:LEU:HD23	1:C:383:LEU:N	2.23	0.53
1:A:120:PRO:HB3	1:A:179:TYR:CG	2.43	0.53
1:D:181:GLY:HA2	1:D:186:THR:O	2.08	0.53
1:A:119:LYS:N	1:A:122:HIS:CD2	2.69	0.53
1:B:79:ASN:ND2	1:B:82:GLU:N	2.47	0.53
1:B:398:MET:HE3	1:B:402:ARG:HG3	1.90	0.53
1:C:369:ARG:NH1	1:D:204:ASP:HB2	2.23	0.53
1:C:45:MET:HE1	1:C:98:LYS:HD2	1.91	0.52
1:B:120:PRO:HB3	1:B:179:TYR:CD2	2.44	0.52
1:C:37:GLN:OE1	1:C:40:ARG:HD3	2.10	0.52
1:A:79:ASN:C	1:A:79:ASN:HD22	2.13	0.52
1:A:270:HIS:NE2	2:A:1462:RNS:O2	2.41	0.52
1:B:57:GLU:HB2	5:B:2633:HOH:O	2.08	0.52
1:C:398:MET:HE3	1:C:402:ARG:HG3	1.92	0.52
1:C:225:ASN:OD1	1:C:226:PRO:HD2	2.10	0.52
1:D:45:MET:HE3	1:D:98:LYS:CB	2.40	0.52
1:A:18:GLU:O	1:A:22:GLN:HG3	2.10	0.52
1:D:37:GLN:O	1:D:40:ARG:HB2	2.10	0.51
1:D:373:ALA:CB	1:D:374:PRO:HD2	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:MET:CE	1:A:98:LYS:HB3	2.40	0.51
1:B:120:PRO:HB3	1:B:179:TYR:CG	2.45	0.51
1:C:45:MET:HE3	1:C:98:LYS:CB	2.40	0.51
1:B:89:GLN:NE2	5:B:2507:HOH:O	2.43	0.51
1:D:370:LYS:O	1:D:374:PRO:HD2	2.10	0.51
1:A:45:MET:HE3	1:A:98:LYS:CD	2.38	0.51
1:C:267:ASP:HA	1:C:294:HIS:HB2	1.92	0.51
1:C:390:LEU:HB3	1:C:391:PRO:HD2	1.92	0.51
1:A:121:GLU:HA	1:A:124:LYS:CG	2.41	0.51
1:B:152:GLY:O	1:B:196:ASP:HA	2.10	0.51
1:C:79:ASN:HD22	1:C:81:SER:N	2.09	0.51
1:D:89:GLN:HG2	1:D:418:TYR:CE1	2.46	0.51
1:A:84:ARG:HD2	1:A:129:TRP:CD1	2.46	0.51
1:B:45:MET:HE3	1:B:98:LYS:CD	2.40	0.51
1:C:369:ARG:HH11	1:C:369:ARG:HG3	1.75	0.51
1:B:267:ASP:HA	1:B:294:HIS:HB2	1.94	0.50
1:A:236:LYS:NZ	2:A:1462:RNS:O1	2.28	0.50
1:B:119:LYS:N	1:B:122:HIS:CD2	2.75	0.50
1:C:236:LYS:HE2	1:C:238:PHE:O	2.12	0.50
1:A:57:GLU:HB2	5:A:1623:HOH:O	2.11	0.50
1:C:142:SER:H	1:C:169:HIS:CE1	2.18	0.50
1:D:84:ARG:HD2	1:D:129:TRP:CD1	2.47	0.50
1:D:234:GLU:OE2	1:D:267:ASP:HB2	2.12	0.50
1:D:398:MET:HE2	1:D:402:ARG:CD	2.41	0.50
1:B:45:MET:HE3	1:B:98:LYS:CB	2.42	0.49
1:B:213:LEU:HD11	1:B:260:ARG:NH2	2.27	0.49
1:B:301:TRP:O	1:B:303:SER:N	2.37	0.49
1:C:121:GLU:HA	1:C:124:LYS:CG	2.42	0.49
1:A:299:VAL:CG1	1:C:243:GLU:HB3	2.43	0.49
1:C:234:GLU:OE2	1:C:267:ASP:HB2	2.12	0.49
1:A:233:VAL:HB	1:A:253:TYR:CD1	2.47	0.49
1:C:370:LYS:O	1:C:374:PRO:HG2	2.12	0.49
1:C:134:GLN:HE21	1:C:134:GLN:CA	2.18	0.49
1:D:115:ARG:O	1:D:169:HIS:HD2	1.95	0.49
1:D:141:PRO:HD2	1:D:191:ASN:O	2.12	0.49
1:D:387:GLN:OE1	5:D:4638:HOH:O	2.19	0.49
1:A:270:HIS:HE1	2:A:1462:RNS:H2	1.77	0.49
1:A:387:GLN:HG2	5:A:1587:HOH:O	2.13	0.49
1:D:151:ASP:HB2	5:D:4606:HOH:O	2.12	0.49
1:A:410:GLU:CD	1:A:410:GLU:H	2.15	0.49
5:A:1650:HOH:O	1:D:377:TYR:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:MET:HE3	1:D:98:LYS:HD2	1.95	0.49
1:D:207:ALA:HB3	1:D:208:PRO:HD3	1.94	0.49
1:A:115:ARG:O	1:A:169:HIS:HD2	1.95	0.48
1:A:419:GLU:O	1:A:424:SER:HB3	2.13	0.48
1:C:119:LYS:O	1:C:122:HIS:N	2.27	0.48
1:D:373:ALA:CB	1:D:374:PRO:CD	2.91	0.48
1:B:370:LYS:O	1:B:374:PRO:HG2	2.13	0.48
1:C:204:ASP:HB2	1:D:369:ARG:NH1	2.29	0.48
1:D:84:ARG:O	1:D:88:GLU:HG3	2.14	0.48
1:B:318:SER:O	1:B:322:ARG:HG3	2.14	0.48
1:C:124:LYS:HD3	1:C:179:TYR:OH	2.14	0.48
1:A:393:GLN:HG2	1:D:389:SER:C	2.34	0.48
1:C:213:LEU:HD11	1:C:260:ARG:NH2	2.29	0.48
1:B:243:GLU:HB3	1:D:299:VAL:HG12	1.94	0.48
1:A:393:GLN:NE2	1:D:393:GLN:NE2	2.29	0.47
1:B:57:GLU:HG2	5:B:2668:HOH:O	2.14	0.47
1:C:96:GLY:HA2	1:C:403:HIS:CE1	2.48	0.47
1:B:96:GLY:HA2	1:B:403:HIS:CE1	2.49	0.47
1:B:79:ASN:ND2	1:B:81:SER:HB2	2.29	0.47
1:A:17:TRP:CH2	1:A:31:VAL:HG23	2.49	0.47
1:B:121:GLU:HA	1:B:124:LYS:CG	2.45	0.47
1:B:121:GLU:HB3	5:B:2645:HOH:O	2.13	0.47
1:B:234:GLU:OE2	1:B:267:ASP:HB2	2.14	0.47
1:B:368:LEU:HD21	1:B:383:LEU:HB3	1.95	0.47
1:D:46:HIS:ND1	1:D:333:LEU:HB2	2.29	0.47
1:D:370:LYS:O	1:D:374:PRO:HG2	2.14	0.47
1:A:213:LEU:HD11	1:A:260:ARG:NH2	2.30	0.47
1:B:384:LEU:O	1:B:387:GLN:HB3	2.15	0.47
1:C:46:HIS:NE2	1:C:49:GLN:HB2	2.29	0.47
1:C:115:ARG:O	1:C:169:HIS:HD2	1.98	0.47
1:A:45:MET:HE2	1:A:98:LYS:HB3	1.96	0.47
1:A:304:ASP:HB3	1:A:336:PHE:H	1.79	0.47
1:C:79:ASN:HD22	1:C:82:GLU:H	1.54	0.47
1:C:383:LEU:HA	1:C:383:LEU:HD22	1.17	0.47
1:D:383:LEU:N	1:D:383:LEU:HD23	2.29	0.47
1:D:108:GLU:OE2	1:D:125:ASN:HB2	2.15	0.47
1:D:152:GLY:O	1:D:196:ASP:HA	2.15	0.47
1:A:134:GLN:HE21	1:A:134:GLN:CA	2.28	0.46
1:A:89:GLN:HG3	1:A:418:TYR:CG	2.50	0.46
1:A:146:HIS:CG	1:A:147:PRO:HD2	2.49	0.46
1:D:17:TRP:CH2	1:D:31:VAL:HG23	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ASN:ND2	1:D:82:GLU:HG3	2.30	0.46
1:D:265:CYS:HA	1:D:292:LEU:O	2.15	0.46
1:A:373:ALA:CB	1:A:374:PRO:HD2	2.39	0.46
1:A:418:TYR:O	1:A:422:ILE:HB	2.15	0.46
1:B:157:HIS:O	1:B:163:ARG:HD3	2.16	0.46
1:D:84:ARG:HD2	1:D:129:TRP:CG	2.50	0.46
1:D:176:VAL:O	1:D:179:TYR:HB3	2.16	0.46
1:A:119:LYS:N	1:A:122:HIS:HD2	1.97	0.46
1:A:351:ARG:O	1:A:355:LYS:HG3	2.16	0.46
1:D:290:GLN:HG2	1:D:330:HIS:NE2	2.30	0.46
1:A:89:GLN:HG3	1:A:418:TYR:CD1	2.50	0.46
1:D:45:MET:HE3	1:D:98:LYS:CG	2.46	0.46
1:C:70:THR:N	5:C:3529:HOH:O	2.28	0.46
1:C:46:HIS:ND1	1:C:333:LEU:HB2	2.31	0.45
1:B:365:THR:O	1:B:369:ARG:HB2	2.16	0.45
1:D:383:LEU:HD22	1:D:383:LEU:HA	1.51	0.45
1:B:398:MET:HE3	1:B:402:ARG:CG	2.46	0.45
1:A:51:ASP:OD2	1:A:55:GLY:N	2.44	0.45
1:A:213:LEU:CD1	1:A:256:TYR:HE1	2.30	0.45
1:B:134:GLN:HE21	1:B:134:GLN:CA	2.20	0.45
1:B:389:SER:O	1:C:393:GLN:HG2	2.16	0.45
1:C:13:LEU:HD21	1:C:398:MET:HA	1.99	0.45
1:A:398:MET:O	1:A:402:ARG:HG3	2.16	0.45
1:B:49:GLN:NE2	1:B:336:PHE:HA	2.31	0.45
1:B:213:LEU:HD12	1:B:213:LEU:O	2.16	0.45
1:A:46:HIS:ND1	1:A:46:HIS:N	2.58	0.45
1:B:116:ASP:OD1	1:B:117:GLN:HG2	2.17	0.45
1:C:45:MET:CE	1:C:98:LYS:CB	2.94	0.45
1:C:207:ALA:HB3	1:C:208:PRO:HD3	1.98	0.45
1:D:79:ASN:HD22	1:D:81:SER:H	1.65	0.45
1:D:11:THR:HG23	1:D:12:GLN:N	2.31	0.45
1:A:373:ALA:CB	1:A:374:PRO:CD	2.96	0.45
1:B:78:ARG:N	1:B:82:GLU:OE1	2.46	0.45
1:B:115:ARG:HB3	1:B:169:HIS:CD2	2.52	0.45
1:A:181:GLY:HA2	1:A:186:THR:O	2.17	0.44
1:B:37:GLN:OE1	1:B:40:ARG:HD3	2.18	0.44
1:C:27:VAL:O	1:C:27:VAL:HG23	2.17	0.44
1:B:64:THR:O	1:B:67:ILE:HD11	2.16	0.44
1:B:45:MET:CE	1:B:98:LYS:CB	2.96	0.44
1:B:181:GLY:HA3	1:B:228:HIS:O	2.17	0.44
1:B:335:PHE:C	1:B:336:PHE:CD2	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LYS:HB3	1:C:120:PRO:HD2	1.99	0.44
1:B:181:GLY:HA2	1:B:186:THR:O	2.18	0.44
1:C:216:LEU:O	1:C:220:ILE:HG12	2.18	0.44
1:D:120:PRO:HB3	1:D:179:TYR:CG	2.53	0.44
1:B:211:ARG:NH1	5:B:2642:HOH:O	2.48	0.44
1:C:78:ARG:HB2	1:C:82:GLU:OE1	2.18	0.44
1:C:204:ASP:HB2	1:D:369:ARG:HH11	1.83	0.44
1:B:79:ASN:HD22	1:B:79:ASN:C	2.20	0.44
1:D:27:VAL:O	1:D:27:VAL:HG23	2.16	0.44
1:D:37:GLN:OE1	1:D:37:GLN:HA	2.18	0.44
1:D:119:LYS:CB	1:D:120:PRO:HD2	2.44	0.44
1:D:225:ASN:OD1	1:D:226:PRO:HD2	2.17	0.44
1:B:373:ALA:CB	1:B:374:PRO:CD	2.95	0.43
1:C:295:VAL:HG21	1:C:353:MET:SD	2.58	0.43
1:C:335:PHE:C	1:C:336:PHE:CD2	2.91	0.43
1:D:24:PHE:O	1:D:27:VAL:HG22	2.18	0.43
1:D:63:LEU:HD22	1:D:64:THR:N	2.33	0.43
1:D:86:ASP:HB3	1:D:343:ILE:HD11	1.99	0.43
1:D:269:GLY:HA2	1:D:298:PRO:HG3	1.99	0.43
1:A:213:LEU:CD1	1:A:256:TYR:CE1	3.01	0.43
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.84	0.43
1:D:71:GLY:HA3	1:D:339:SER:CA	2.48	0.43
1:D:390:LEU:HB3	1:D:391:PRO:HD2	2.00	0.43
1:D:408:GLY:O	1:D:411:TRP:HD1	2.01	0.43
1:A:120:PRO:HB3	1:A:179:TYR:CD2	2.53	0.43
1:C:79:ASN:ND2	1:C:82:GLU:N	2.50	0.43
1:C:269:GLY:HA2	1:C:298:PRO:HG3	1.99	0.43
1:B:205:ARG:HG2	1:B:245:TYR:CD1	2.53	0.43
1:C:297:ARG:O	1:C:305:HIS:HB2	2.18	0.43
1:D:405:THR:HG23	1:D:406:PRO:HD2	2.00	0.43
1:C:387:GLN:HB2	5:C:3593:HOH:O	2.18	0.43
1:B:79:ASN:HD21	1:B:82:GLU:N	2.13	0.43
1:B:236:LYS:HE2	1:B:238:PHE:O	2.19	0.43
1:C:139:PHE:HE2	1:C:173:SER:HB3	1.84	0.43
1:B:115:ARG:O	1:B:169:HIS:HD2	2.02	0.43
1:C:71:GLY:HA3	1:C:339:SER:CA	2.48	0.43
1:D:11:THR:CG2	1:D:12:GLN:N	2.81	0.43
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.84	0.43
1:C:373:ALA:CB	1:C:374:PRO:HD2	2.44	0.43
1:D:79:ASN:HD21	1:D:81:SER:HB2	1.84	0.42
1:D:134:GLN:CA	1:D:134:GLN:NE2	2.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:HD12	1:A:213:LEU:O	2.19	0.42
1:A:225:ASN:HB3	1:A:228:HIS:ND1	2.33	0.42
1:C:71:GLY:HA3	1:C:339:SER:HA	2.00	0.42
1:A:76:LYS:HG3	1:A:77:ALA:O	2.18	0.42
1:B:77:ALA:HB2	1:B:86:ASP:OD2	2.18	0.42
1:B:213:LEU:HD12	1:B:213:LEU:C	2.40	0.42
1:B:290:GLN:HG2	1:B:330:HIS:NE2	2.35	0.42
1:C:213:LEU:C	1:C:213:LEU:HD12	2.39	0.42
1:D:355:LYS:HE3	1:D:396:TRP:NE1	2.34	0.42
1:A:79:ASN:HD21	1:A:82:GLU:HG3	1.84	0.42
1:C:398:MET:CE	1:C:402:ARG:CG	2.98	0.42
1:A:116:ASP:HA	1:A:169:HIS:HA	2.00	0.42
1:B:36:ARG:NH2	5:B:2603:HOH:O	2.27	0.42
1:C:84:ARG:HD2	1:C:129:TRP:CD1	2.54	0.42
1:C:373:ALA:HB3	1:C:374:PRO:CD	2.49	0.42
1:D:71:GLY:HA3	1:D:339:SER:HA	2.00	0.42
1:D:119:LYS:N	1:D:122:HIS:CD2	2.73	0.42
1:A:270:HIS:CE1	2:A:1462:RNS:H2	2.55	0.42
1:B:290:GLN:HG3	1:B:328:ARG:HA	2.02	0.42
1:A:45:MET:HE1	1:A:98:LYS:HD2	1.95	0.42
1:B:325:LEU:HA	1:B:325:LEU:HD23	1.62	0.42
1:C:213:LEU:HD12	1:C:213:LEU:O	2.20	0.42
1:C:373:ALA:CB	1:C:374:PRO:CD	2.97	0.42
1:A:89:GLN:CG	1:A:418:TYR:CD1	3.03	0.42
1:C:193:TRP:CD2	2:C:3462:RNS:H3	2.55	0.42
1:D:78:ARG:N	1:D:82:GLU:OE1	2.52	0.42
1:B:374:PRO:CD	5:B:2631:HOH:O	2.67	0.42
1:C:365:THR:O	1:C:369:ARG:HB2	2.20	0.42
1:C:398:MET:HE3	1:C:402:ARG:CG	2.50	0.42
1:D:120:PRO:HB3	1:D:179:TYR:CD2	2.54	0.42
1:D:167:ILE:HG22	1:D:171:LYS:HD2	2.02	0.42
1:D:194:ILE:HD12	1:D:196:ASP:CG	2.39	0.42
1:A:405:THR:HG23	1:A:406:PRO:HD2	2.01	0.42
1:C:13:LEU:HD22	1:C:401:GLN:HE21	1.85	0.42
1:D:368:LEU:HD21	1:D:383:LEU:HB3	2.01	0.42
1:B:45:MET:HE1	1:B:98:LYS:HD2	1.94	0.41
1:B:225:ASN:OD1	1:B:226:PRO:HD2	2.19	0.41
1:B:225:ASN:ND2	1:B:228:HIS:CE1	2.88	0.41
1:B:297:ARG:O	1:B:305:HIS:HB2	2.20	0.41
1:D:106:TYR:CD1	1:D:106:TYR:N	2.88	0.41
1:D:139:PHE:O	1:D:190:MET:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:TRP:CH2	1:B:31:VAL:HG23	2.55	0.41
1:B:398:MET:CE	1:B:402:ARG:HG3	2.50	0.41
1:C:46:HIS:NE2	1:C:335:PHE:O	2.53	0.41
1:C:193:TRP:CZ2	2:C:3462:RNS:H11	2.55	0.41
1:B:393:GLN:HG2	1:C:389:SER:O	2.20	0.41
1:C:277:ILE:HG12	5:C:3544:HOH:O	2.21	0.41
1:D:225:ASN:O	1:D:228:HIS:N	2.38	0.41
1:B:33:GLU:OE1	1:B:36:ARG:NE	2.52	0.41
1:B:216:LEU:O	1:B:220:ILE:HG12	2.19	0.41
1:C:405:THR:HG23	1:C:406:PRO:HD2	2.02	0.41
1:D:79:ASN:HD22	1:D:79:ASN:C	2.24	0.41
1:B:71:GLY:HA3	1:B:339:SER:CA	2.51	0.41
1:B:71:GLY:HA3	1:B:339:SER:HA	2.03	0.41
1:C:121:GLU:HB3	5:C:3672:HOH:O	2.19	0.41
1:C:125:ASN:HA	1:C:128:GLU:HG3	2.02	0.41
1:C:271:PHE:HB3	1:C:275:GLU:OE1	2.20	0.41
1:D:95:PRO:HD3	1:D:405:THR:HG21	2.02	0.41
1:A:293:LEU:HD12	1:A:329:VAL:CG1	2.50	0.41
1:B:37:GLN:OE1	1:B:37:GLN:HA	2.21	0.41
1:B:95:PRO:HD3	1:B:405:THR:HG21	2.02	0.41
1:C:13:LEU:HD22	1:C:401:GLN:NE2	2.36	0.41
1:D:398:MET:HE3	1:D:402:ARG:HG3	1.96	0.41
1:A:384:LEU:HD23	1:A:384:LEU:HA	1.90	0.41
1:B:124:LYS:HD3	1:B:179:TYR:OH	2.21	0.41
1:B:369:ARG:HD2	5:B:2714:HOH:O	2.20	0.41
1:B:398:MET:CE	1:B:402:ARG:CG	2.99	0.41
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.95	0.41
1:C:314:GLN:HE22	1:C:356:ALA:HA	1.86	0.41
1:D:179:TYR:CE1	1:D:183:GLN:HG3	2.56	0.41
1:C:119:LYS:O	1:C:120:PRO:C	2.59	0.41
1:B:11:THR:O	1:B:15:GLN:HG3	2.21	0.40
1:B:83:LEU:HA	1:B:83:LEU:HD12	1.81	0.40
1:B:295:VAL:HG12	1:B:307:VAL:HG22	1.98	0.40
1:C:314:GLN:NE2	1:C:356:ALA:HA	2.36	0.40
1:D:267:ASP:HA	1:D:294:HIS:HB2	2.03	0.40
1:A:393:GLN:HG2	1:D:389:SER:O	2.21	0.40
1:A:424:SER:OG	1:A:425:ARG:HG2	2.21	0.40
1:B:384:LEU:HD23	1:B:384:LEU:HA	1.88	0.40
1:A:46:HIS:NE2	1:A:335:PHE:O	2.54	0.40
1:A:390:LEU:HD23	1:A:390:LEU:HA	1.76	0.40
1:B:19:LEU:HD23	1:B:19:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:TRP:C	1:B:303:SER:N	2.75	0.40
1:B:390:LEU:HD23	1:B:390:LEU:HA	1.96	0.40
1:D:314:GLN:NE2	1:D:356:ALA:HA	2.37	0.40
1:D:418:TYR:HA	1:D:421:GLU:HG2	2.02	0.40
1:A:151:ASP:HB2	5:A:1598:HOH:O	2.20	0.40
1:B:13:LEU:HD21	1:B:398:MET:HA	2.04	0.40
1:B:111:THR:HA	1:B:112:PRO:HD3	1.88	0.40
1:B:178:ALA:HA	1:B:229:HIS:HB2	2.03	0.40
1:D:335:PHE:C	1:D:336:PHE:CD2	2.94	0.40
1:B:314:GLN:NE2	1:B:359:ARG:HD3	2.36	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	414/426 (97%)	397 (96%)	15 (4%)	2 (0%)	29	26
1	B	414/426 (97%)	397 (96%)	14 (3%)	3 (1%)	22	18
1	C	414/426 (97%)	394 (95%)	17 (4%)	3 (1%)	22	18
1	D	414/426 (97%)	395 (95%)	17 (4%)	2 (0%)	29	26
All	All	1656/1704 (97%)	1583 (96%)	63 (4%)	10 (1%)	25	21

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	B	62	SER
1	C	62	SER
1	D	62	SER
1	C	59	PRO

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Mol	Chain	Res	Type
1	D	59	PRO
1	B	53	VAL
1	C	61	GLY
1	A	61	GLY
1	B	61	GLY

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	351/359 (98%)	334 (95%)	17 (5%)	25	24
1	B	351/359 (98%)	331 (94%)	20 (6%)	20	18
1	C	351/359 (98%)	332 (95%)	19 (5%)	22	20
1	D	351/359 (98%)	332 (95%)	19 (5%)	22	20
All	All	1404/1436 (98%)	1329 (95%)	75 (5%)	22	20

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	53	VAL
1	A	63	LEU
1	A	79	ASN
1	A	98	LYS
1	A	103	HIS
1	A	134	GLN
1	A	140	ASN
1	A	188	SER
1	A	196	ASP
1	A	223	LYS
1	A	290	GLN
1	A	324	ASP
1	A	336	PHE
1	A	369	ARG
1	A	374	PRO

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Mol	Chain	Res	Type
1	A	383	LEU
1	B	27	VAL
1	B	53	VAL
1	B	63	LEU
1	B	79	ASN
1	B	92	ARG
1	B	98	LYS
1	B	103	HIS
1	B	128	GLU
1	B	134	GLN
1	B	140	ASN
1	B	188	SER
1	B	223	LYS
1	B	290	GLN
1	B	324	ASP
1	B	336	PHE
1	B	346	TRP
1	B	369	ARG
1	B	374	PRO
1	B	383	LEU
1	B	401	GLN
1	C	53	VAL
1	C	63	LEU
1	C	79	ASN
1	C	98	LYS
1	C	103	HIS
1	C	119	LYS
1	C	128	GLU
1	C	134	GLN
1	C	140	ASN
1	C	188	SER
1	C	196	ASP
1	C	223	LYS
1	C	290	GLN
1	C	324	ASP
1	C	336	PHE
1	C	374	PRO
1	C	383	LEU
1	C	401	GLN
1	C	410	GLU
1	D	11	THR
1	D	53	VAL

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Mol	Chain	Res	Type
1	D	63	LEU
1	D	79	ASN
1	D	98	LYS
1	D	103	HIS
1	D	128	GLU
1	D	134	GLN
1	D	173	SER
1	D	196	ASP
1	D	223	LYS
1	D	290	GLN
1	D	324	ASP
1	D	336	PHE
1	D	369	ARG
1	D	374	PRO
1	D	383	LEU
1	D	401	GLN
1	D	425	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	49	GLN
1	A	79	ASN
1	A	122	HIS
1	A	125	ASN
1	A	134	GLN
1	A	169	HIS
1	A	191	ASN
1	A	314	GLN
1	A	393	GLN
1	B	49	GLN
1	B	72	ASN
1	B	79	ASN
1	B	122	HIS
1	B	125	ASN
1	B	134	GLN
1	B	169	HIS
1	B	228	HIS
1	B	314	GLN
1	C	49	GLN
1	C	79	ASN

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Mol	Chain	Res	Type
1	C	122	HIS
1	C	125	ASN
1	C	134	GLN
1	C	169	HIS
1	C	191	ASN
1	C	314	GLN
1	C	387	GLN
1	C	393	GLN
1	D	49	GLN
1	D	79	ASN
1	D	122	HIS
1	D	125	ASN
1	D	134	GLN
1	D	169	HIS
1	D	314	GLN
1	D	387	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	RNS	C	3462	-	8,10,10	1.14	1 (12%)	9,13,13	1.15	1 (11%)
2	RNS	A	1462	4	8,10,10	1.00	1 (12%)	9,13,13	1.84	3 (33%)
2	RNS	D	4462	-	8,10,10	0.87	0	9,13,13	1.00	0
2	RNS	B	2462	-	8,10,10	1.31	2 (25%)	9,13,13	1.27	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RNS	C	3462	-	-	7/12/14/14	-
2	RNS	A	1462	4	-	5/12/14/14	-
2	RNS	D	4462	-	-	8/12/14/14	-
2	RNS	B	2462	-	-	5/12/14/14	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3462	RNS	O5-C5	2.55	1.50	1.43
2	B	2462	RNS	O3-C3	2.14	1.48	1.43
2	B	2462	RNS	O5-C5	2.11	1.48	1.43
2	A	1462	RNS	O5-C5	2.00	1.48	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1462	RNS	O3-C3-C2	3.39	115.38	109.17
2	A	1462	RNS	O3-C3-C4	2.73	115.83	109.47
2	B	2462	RNS	C4-C3-C2	-2.72	108.79	113.54
2	C	3462	RNS	C4-C3-C2	-2.47	109.23	113.54
2	A	1462	RNS	C3-C2-C1	-2.11	104.45	111.10

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1462	RNS	C3-C4-C5-O5
2	B	2462	RNS	C3-C4-C5-C6
2	B	2462	RNS	C3-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
2	B	2462	RNS	O4-C4-C5-O5
2	C	3462	RNS	C3-C4-C5-C6
2	C	3462	RNS	C3-C4-C5-O5
2	C	3462	RNS	O4-C4-C5-O5
2	D	4462	RNS	C3-C4-C5-O5
2	D	4462	RNS	O4-C4-C5-O5
2	A	1462	RNS	O3-C3-C4-O4
2	C	3462	RNS	O3-C3-C4-O4
2	B	2462	RNS	O4-C4-C5-C6
2	C	3462	RNS	C2-C3-C4-O4
2	C	3462	RNS	O4-C4-C5-C6
2	C	3462	RNS	O3-C3-C4-C5
2	A	1462	RNS	O4-C4-C5-O5
2	D	4462	RNS	O2-C2-C3-O3
2	D	4462	RNS	O2-C2-C3-C4
2	D	4462	RNS	C3-C4-C5-C6
2	D	4462	RNS	O4-C4-C5-C6
2	D	4462	RNS	C2-C3-C4-O4
2	A	1462	RNS	O3-C3-C4-C5
2	B	2462	RNS	O3-C3-C4-O4
2	D	4462	RNS	O3-C3-C4-O4
2	A	1462	RNS	C3-C4-C5-C6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3462	RNS	2	0
2	A	1462	RNS	4	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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.