WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2022 – 06:21 PM EST

PDB ID	:	1D8W
Title	:	L-RHAMNOSE ISOMERASE
Authors	:	Korndorfer, I.P.; Matthews, B.W.
Deposited on	:	1999-10-26
Resolution	:	1.60 Å(reported)

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 ⓘ

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

The reported resolution of this entry is 1.60 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	Percentile Ranks	Value
Rfree		0.230
Clashscore		18
Ramachandran outliers		0.3%
Sidechain outliers		5.1%
RSRZ outliers		1.3%

Worse — *Better*

▉ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
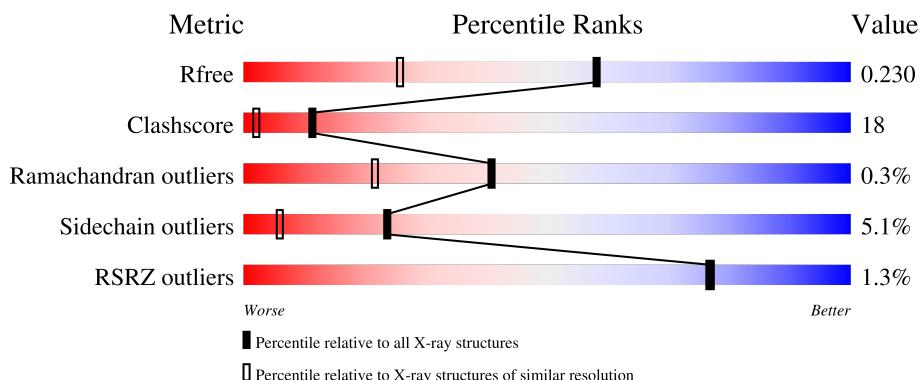
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	426	% 62% 25% 7% · 6%
1	B	426	64% 24% 6% 6%
1	C	426	% 57% 30% 6% · 6%
1	D	426	2% 59% 27% 8% · 5%

W O R L D W I D E
wwPDB
PROTEIN DATA BANK
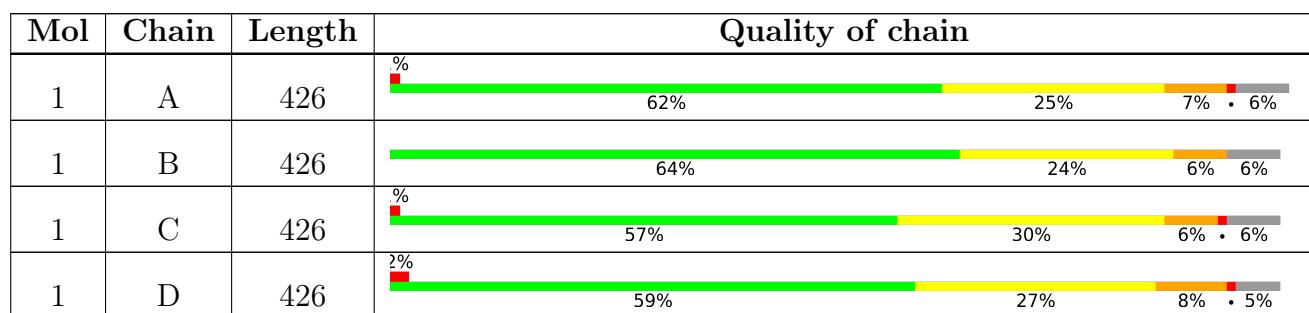
2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 14687 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
1	A	402	Total	C	N	O	S	Se	0	0	0
			3219	2037	571	598	5	8			
1	B	402	Total	C	N	O	S	Se	0	0	0
			3218	2037	570	598	5	8			
1	C	401	Total	C	N	O	S	Se	0	0	0
			3211	2033	569	596	5	8			
1	D	403	Total	C	N	O	S	Se	0	0	0
			3226	2042	571	599	5	9			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MSE	MET	modified residue	UNP P32170
A	45	MSE	MET	modified residue	UNP P32170
A	91	MSE	MET	modified residue	UNP P32170
A	190	MSE	MET	modified residue	UNP P32170
A	198	MSE	MET	modified residue	UNP P32170
A	254	MSE	MET	modified residue	UNP P32170
A	285	MSE	MET	modified residue	UNP P32170
A	353	MSE	MET	modified residue	UNP P32170
A	398	MSE	MET	modified residue	UNP P32170
B	9	MSE	MET	modified residue	UNP P32170
B	45	MSE	MET	modified residue	UNP P32170
B	91	MSE	MET	modified residue	UNP P32170
B	190	MSE	MET	modified residue	UNP P32170
B	198	MSE	MET	modified residue	UNP P32170
B	254	MSE	MET	modified residue	UNP P32170
B	285	MSE	MET	modified residue	UNP P32170
B	353	MSE	MET	modified residue	UNP P32170
B	398	MSE	MET	modified residue	UNP P32170
C	9	MSE	MET	modified residue	UNP P32170
C	45	MSE	MET	modified residue	UNP P32170
C	91	MSE	MET	modified residue	UNP P32170

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Chain	Residue	Modelled	Actual	Comment	Reference
C	190	MSE	MET	modified residue	UNP P32170
C	198	MSE	MET	modified residue	UNP P32170
C	254	MSE	MET	modified residue	UNP P32170
C	285	MSE	MET	modified residue	UNP P32170
C	353	MSE	MET	modified residue	UNP P32170
C	398	MSE	MET	modified residue	UNP P32170
D	9	MSE	MET	modified residue	UNP P32170
D	45	MSE	MET	modified residue	UNP P32170
D	91	MSE	MET	modified residue	UNP P32170
D	190	MSE	MET	modified residue	UNP P32170
D	198	MSE	MET	modified residue	UNP P32170
D	254	MSE	MET	modified residue	UNP P32170
D	285	MSE	MET	modified residue	UNP P32170
D	353	MSE	MET	modified residue	UNP P32170
D	398	MSE	MET	modified residue	UNP P32170
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	8	HIS	-	expression tag	UNP P32170

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	424	Total 424	O 424	0	0
3	B	518	Total 518	O 518	0	0
3	C	475	Total 475	O 475	0	0
3	D	392	Total 392	O 392	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: L-RHAMNOSE ISOMERASE
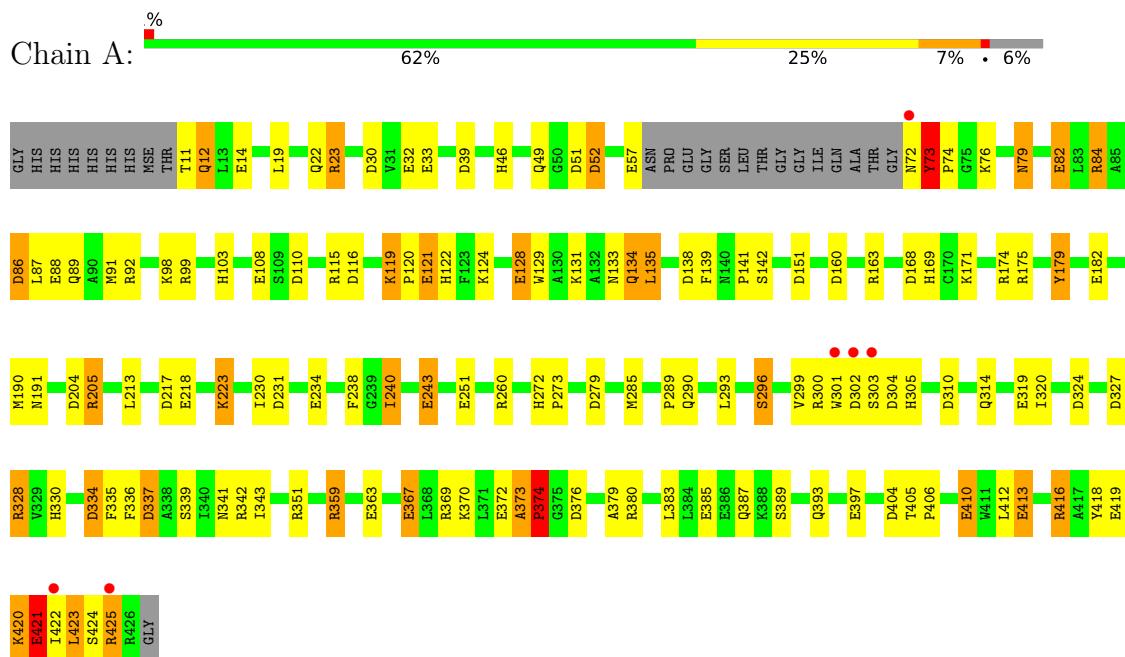
Chain A:

• Molecule 1: L-RHAMNOSE ISOMERASE

Chain B:

• Molecule 1: L-RHAMNOSE ISOMERASE

Chain C:

• Molecule 1: L-RHAMNOSE ISOMERASE

Chain D:
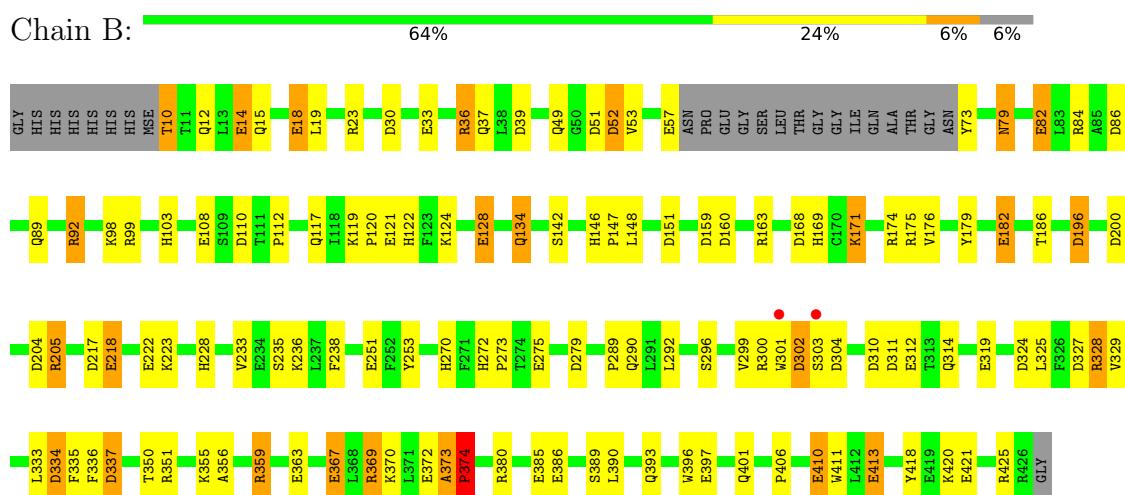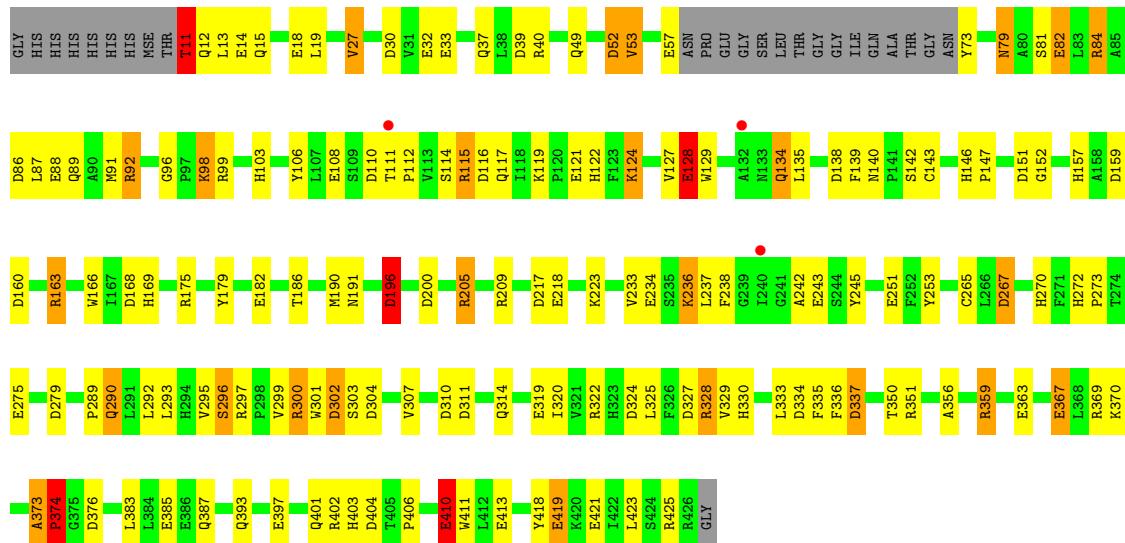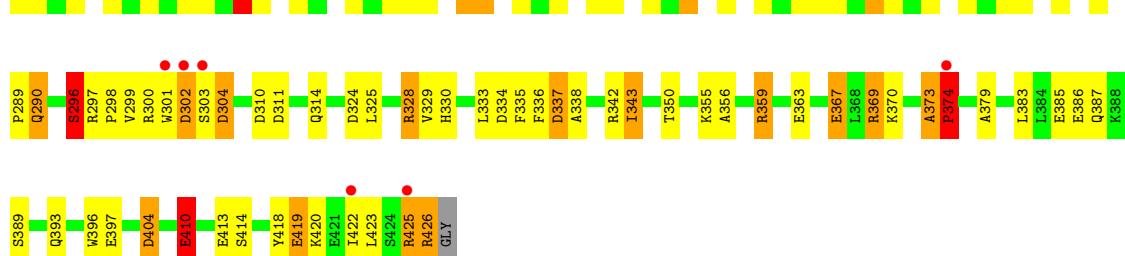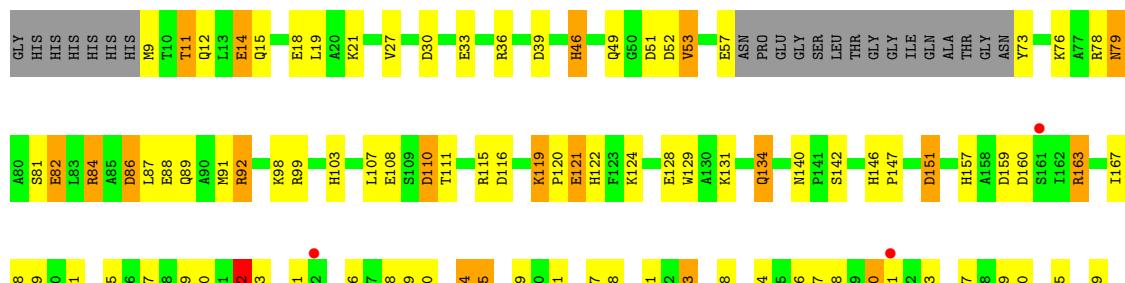
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	169.85Å 163.10Å 78.15Å 90.00° 110.32° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 28.81 – 1.60	Depositor EDS
% Data completeness (in resolution range)	95.7 (30.00-1.60) 96.5 (28.81-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.87 (at 1.60Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.174 , 0.241 0.172 , 0.230	Depositor DCC
R_{free} test set	12796 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	17.2	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 90.5	EDS
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14687	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1   Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	1.12	22/3289 (0.7%)	1.65	67/4451 (1.5%)
1	B	1.16	24/3288 (0.7%)	1.71	62/4450 (1.4%)
1	C	1.15	22/3281 (0.7%)	1.78	64/4440 (1.4%)
1	D	1.09	19/3296 (0.6%)	1.67	72/4460 (1.6%)
All	All	1.13	87/13154 (0.7%)	1.70	265/17801 (1.5%)

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	GLU	CD-OE2	9.35	1.35	1.25
1	C	359	ARG	CZ-NH1	8.74	1.44	1.33
1	B	218	GLU	CD-OE2	7.99	1.34	1.25
1	B	385	GLU	CD-OE2	7.88	1.34	1.25
1	B	413	GLU	CD-OE2	7.84	1.34	1.25
1	C	363	GLU	CD-OE2	7.79	1.34	1.25
1	B	182	GLU	CD-OE2	7.65	1.34	1.25
1	D	14	GLU	CD-OE2	7.62	1.34	1.25
1	C	182	GLU	CD-OE2	7.58	1.33	1.25
1	C	108	GLU	CD-OE2	7.55	1.33	1.25
1	A	57	GLU	CD-OE2	7.52	1.33	1.25
1	B	372	GLU	CD-OE2	7.45	1.33	1.25
1	D	182	GLU	CD-OE2	7.38	1.33	1.25
1	C	128	GLU	CD-OE2	7.33	1.33	1.25
1	A	218	GLU	CD-OE2	7.10	1.33	1.25
1	D	386	GLU	CD-OE2	7.09	1.33	1.25
1	D	108	GLU	CD-OE2	7.05	1.33	1.25
1	B	82	GLU	CD-OE2	7.05	1.33	1.25
1	A	367	GLU	CD-OE2	6.98	1.33	1.25
1	A	363	GLU	CD-OE2	6.91	1.33	1.25
1	A	182	GLU	CD-OE2	6.85	1.33	1.25
1	D	218	GLU	CD-OE2	6.84	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	363	GLU	CD-OE2	6.79	1.33	1.25
1	B	251	GLU	CD-OE2	6.78	1.33	1.25
1	A	410	GLU	CD-OE2	6.76	1.33	1.25
1	B	421	GLU	CD-OE2	6.73	1.33	1.25
1	A	413	GLU	CD-OE2	6.69	1.33	1.25
1	C	14	GLU	CD-OE2	6.68	1.33	1.25
1	C	319	GLU	CD-OE2	6.55	1.32	1.25
1	D	57	GLU	CD-OE2	6.54	1.32	1.25
1	D	275	GLU	CD-OE2	6.53	1.32	1.25
1	C	367	GLU	CD-OE2	6.42	1.32	1.25
1	D	397	GLU	CD-OE2	6.41	1.32	1.25
1	D	128	GLU	CD-OE2	6.38	1.32	1.25
1	B	359	ARG	CZ-NH1	6.38	1.41	1.33
1	A	421	GLU	CD-OE2	6.38	1.32	1.25
1	D	33	GLU	CD-OE2	6.32	1.32	1.25
1	C	421	GLU	CD-OE2	6.31	1.32	1.25
1	D	419	GLU	CD-OE2	6.30	1.32	1.25
1	C	275	GLU	CD-OE2	6.29	1.32	1.25
1	A	128	GLU	CD-OE2	6.29	1.32	1.25
1	A	33	GLU	CD-OE2	6.18	1.32	1.25
1	D	413	GLU	CD-OE2	6.18	1.32	1.25
1	A	385	GLU	CD-OE2	6.18	1.32	1.25
1	B	312	GLU	CD-OE2	6.17	1.32	1.25
1	B	222	GLU	CD-OE2	6.15	1.32	1.25
1	B	18	GLU	CD-OE2	6.13	1.32	1.25
1	D	363	GLU	CD-OE2	6.12	1.32	1.25
1	C	397	GLU	CD-OE2	6.10	1.32	1.25
1	C	18	GLU	CD-OE2	5.98	1.32	1.25
1	C	218	GLU	CD-OE2	5.96	1.32	1.25
1	A	319	GLU	CD-OE2	5.92	1.32	1.25
1	C	33	GLU	CD-OE2	5.87	1.32	1.25
1	D	367	GLU	CD-OE2	5.79	1.32	1.25
1	C	410	GLU	CD-OE2	5.76	1.31	1.25
1	C	251	GLU	CD-OE2	5.76	1.31	1.25
1	A	121	GLU	CD-OE2	5.74	1.31	1.25
1	A	251	GLU	CD-OE2	5.73	1.31	1.25
1	D	18	GLU	CD-OE2	5.69	1.31	1.25
1	B	397	GLU	CD-OE2	5.67	1.31	1.25
1	C	32	GLU	CD-OE2	5.60	1.31	1.25
1	B	57	GLU	CD-OE2	5.57	1.31	1.25
1	C	385	GLU	CD-OE2	5.57	1.31	1.25
1	D	385	GLU	CD-OE1	-5.52	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	GLU	CD-OE2	5.52	1.31	1.25
1	A	397	GLU	CD-OE1	-5.51	1.19	1.25
1	B	319	GLU	CD-OE2	5.51	1.31	1.25
1	D	82	GLU	CD-OE2	5.49	1.31	1.25
1	B	367	GLU	CD-OE2	5.45	1.31	1.25
1	C	82	GLU	CD-OE2	5.45	1.31	1.25
1	A	108	GLU	CD-OE1	-5.45	1.19	1.25
1	D	121	GLU	CD-OE2	5.38	1.31	1.25
1	A	374	PRO	CA-C	-5.38	1.42	1.52
1	B	374	PRO	CA-C	-5.37	1.42	1.52
1	C	57	GLU	CD-OE2	5.33	1.31	1.25
1	D	410	GLU	CD-OE2	5.33	1.31	1.25
1	B	108	GLU	CD-OE2	5.30	1.31	1.25
1	A	32	GLU	CD-OE2	5.29	1.31	1.25
1	A	372	GLU	CD-OE2	5.29	1.31	1.25
1	A	14	GLU	CD-OE2	5.29	1.31	1.25
1	B	386	GLU	CD-OE2	5.27	1.31	1.25
1	C	209	ARG	NE-CZ	5.26	1.39	1.33
1	C	419	GLU	CD-OE1	-5.19	1.20	1.25
1	A	82	GLU	CD-OE2	5.13	1.31	1.25
1	B	14	GLU	CD-OE1	-5.11	1.20	1.25
1	B	410	GLU	CD-OE2	5.10	1.31	1.25
1	A	397	GLU	CD-OE2	5.07	1.31	1.25

All (265) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	359	ARG	NE-CZ-NH2	-33.88	103.36	120.30
1	B	328	ARG	NE-CZ-NH1	27.62	134.11	120.30
1	C	359	ARG	NE-CZ-NH1	26.19	133.40	120.30
1	D	205	ARG	NE-CZ-NH1	26.08	133.34	120.30
1	C	328	ARG	NE-CZ-NH1	24.38	132.49	120.30
1	C	328	ARG	NE-CZ-NH2	-23.67	108.47	120.30
1	D	205	ARG	NE-CZ-NH2	-23.21	108.69	120.30
1	A	205	ARG	NE-CZ-NH1	21.82	131.21	120.30
1	B	205	ARG	NE-CZ-NH1	21.57	131.09	120.30
1	B	359	ARG	NE-CZ-NH2	-21.53	109.53	120.30
1	B	328	ARG	NE-CZ-NH2	-21.16	109.72	120.30
1	A	328	ARG	NE-CZ-NH2	-19.55	110.52	120.30
1	A	205	ARG	NE-CZ-NH2	-19.54	110.53	120.30
1	B	205	ARG	NE-CZ-NH2	-18.66	110.97	120.30
1	D	328	ARG	NE-CZ-NH1	17.49	129.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	359	ARG	NE-CZ-NH1	17.14	128.87	120.30
1	C	205	ARG	NE-CZ-NH1	17.13	128.87	120.30
1	C	205	ARG	NE-CZ-NH2	-16.93	111.83	120.30
1	A	373	ALA	C-N-CD	-15.95	85.52	120.60
1	A	328	ARG	NE-CZ-NH1	15.83	128.22	120.30
1	D	373	ALA	C-N-CD	-15.54	86.42	120.60
1	C	373	ALA	C-N-CD	-14.77	88.10	120.60
1	B	373	ALA	C-N-CD	-14.66	88.34	120.60
1	C	425	ARG	NE-CZ-NH2	-14.33	113.14	120.30
1	D	359	ARG	NE-CZ-NH1	13.55	127.08	120.30
1	B	328	ARG	CD-NE-CZ	13.19	142.07	123.60
1	A	23	ARG	NE-CZ-NH1	12.89	126.75	120.30
1	D	328	ARG	NE-CZ-NH2	-12.76	113.92	120.30
1	B	374	PRO	CA-N-CD	-12.64	93.80	111.50
1	D	359	ARG	NE-CZ-NH2	-12.63	113.98	120.30
1	A	205	ARG	CD-NE-CZ	12.39	140.94	123.60
1	A	23	ARG	NE-CZ-NH2	-12.11	114.25	120.30
1	B	163	ARG	NE-CZ-NH1	11.61	126.10	120.30
1	A	359	ARG	NE-CZ-NH2	-11.45	114.57	120.30
1	C	328	ARG	CD-NE-CZ	11.21	139.30	123.60
1	D	217	ASP	CB-CG-OD2	-11.20	108.22	118.30
1	A	376	ASP	CB-CG-OD2	-10.82	108.56	118.30
1	D	175	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	A	337	ASP	CB-CG-OD2	-10.77	108.61	118.30
1	C	92	ARG	NE-CZ-NH1	10.67	125.63	120.30
1	A	374	PRO	CA-N-CD	-10.51	96.79	111.50
1	D	163	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	D	374	PRO	CA-N-CD	-10.04	97.45	111.50
1	A	351	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	D	116	ASP	CB-CG-OD1	9.84	127.15	118.30
1	C	159	ASP	CB-CG-OD2	-9.67	109.59	118.30
1	C	374	PRO	CA-N-CD	-9.57	98.10	111.50
1	B	168	ASP	CB-CG-OD1	9.48	126.84	118.30
1	A	175	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	A	351	ARG	NE-CZ-NH1	9.05	124.82	120.30
1	B	163	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	B	304	ASP	CB-CG-OD2	-9.00	110.20	118.30
1	D	426	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	B	337	ASP	CB-CG-OD1	8.85	126.27	118.30
1	C	310	ASP	CB-CG-OD1	8.77	126.19	118.30
1	D	30	ASP	CB-CG-OD1	8.77	126.19	118.30
1	C	196	ASP	CB-CG-OD2	-8.75	110.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	168	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	C	337	ASP	CB-CG-OD2	-8.71	110.46	118.30
1	D	204	ASP	CB-CG-OD2	-8.68	110.49	118.30
1	A	52	ASP	CB-CG-OD1	8.57	126.02	118.30
1	B	110	ASP	CB-CG-OD2	-8.50	110.65	118.30
1	B	175	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	B	51	ASP	CB-CG-OD1	8.46	125.91	118.30
1	B	39	ASP	CB-CG-OD1	8.42	125.88	118.30
1	C	337	ASP	CB-CG-OD1	8.39	125.85	118.30
1	D	328	ARG	CD-NE-CZ	8.37	135.31	123.60
1	A	359	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	C	175	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	C	311	ASP	CB-CG-OD2	-8.25	110.87	118.30
1	A	337	ASP	CB-CG-OD1	8.20	125.68	118.30
1	B	52	ASP	CB-CG-OD1	8.19	125.67	118.30
1	D	92	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	D	337	ASP	CB-CG-OD2	-7.97	111.13	118.30
1	B	304	ASP	CB-CG-OD1	7.96	125.47	118.30
1	A	376	ASP	CB-CG-OD1	7.96	125.47	118.30
1	D	36	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	A	30	ASP	CB-CG-OD1	7.91	125.42	118.30
1	A	39	ASP	CB-CG-OD2	-7.87	111.22	118.30
1	D	36	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	D	404	ASP	CB-CG-OD1	7.83	125.35	118.30
1	A	328	ARG	CD-NE-CZ	7.81	134.53	123.60
1	B	205	ARG	CD-NE-CZ	7.79	134.50	123.60
1	C	310	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	D	205	ARG	CD-NE-CZ	7.74	134.44	123.60
1	A	39	ASP	CB-CG-OD1	7.68	125.22	118.30
1	A	138	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	D	311	ASP	CB-CG-OD1	7.56	125.11	118.30
1	B	30	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	B	39	ASP	CB-CG-OD2	-7.55	111.51	118.30
1	D	30	ASP	CB-CG-OD2	-7.53	111.53	118.30
1	B	302	ASP	CB-CG-OD1	7.52	125.07	118.30
1	A	163	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	D	311	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	D	302	ASP	CB-CG-OD1	7.49	125.04	118.30
1	D	310	ASP	CB-CG-OD1	7.48	125.03	118.30
1	C	425	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	B	99	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	C	404	ASP	CB-CG-OD2	-7.46	111.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	159	ASP	CB-CG-OD1	7.43	124.99	118.30
1	C	39	ASP	CB-CG-OD1	7.41	124.97	118.30
1	D	51	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	116	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	342	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	B	159	ASP	CB-CG-OD1	7.37	124.93	118.30
1	C	217	ASP	CB-CG-OD2	-7.35	111.69	118.30
1	B	159	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	C	138	ASP	CB-CG-OD1	7.25	124.83	118.30
1	A	302	ASP	CB-CG-OD1	7.25	124.82	118.30
1	A	327	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	B	160	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	C	30	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	D	204	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	175	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	D	209	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	D	159	ASP	CB-CG-OD2	-7.11	111.91	118.30
1	C	302	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	116	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	D	116	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	D	39	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	B	23	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	B	351	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	C	86	ASP	CB-CG-OD2	-6.94	112.06	118.30
1	A	334	ASP	CB-CG-OD1	6.93	124.54	118.30
1	C	160	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	B	30	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	151	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	C	30	ASP	CB-CG-OD1	6.86	124.47	118.30
1	B	311	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	C	52	ASP	CB-CG-OD1	6.79	124.41	118.30
1	D	337	ASP	CB-CG-OD1	6.78	124.40	118.30
1	D	198	MSE	CG-SE-CE	-6.77	84.01	98.90
1	D	159	ASP	CB-CG-OD1	6.76	124.39	118.30
1	D	168	ASP	CB-CG-OD1	6.76	124.39	118.30
1	A	30	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	C	138	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	A	52	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	C	110	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	A	168	ASP	CB-CG-OD1	6.64	124.28	118.30
1	D	51	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	324	ASP	CB-CG-OD2	-6.57	112.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	217	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	380	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	A	51	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	D	217	ASP	CB-CG-OD1	6.53	124.18	118.30
1	D	200	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	404	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	C	151	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	D	168	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	C	279	ASP	CB-CG-OD1	6.48	124.13	118.30
1	D	279	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	B	52	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	C	205	ARG	CD-NE-CZ	6.46	132.64	123.60
1	A	310	ASP	CB-CG-OD1	6.45	124.10	118.30
1	C	84	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	404	ASP	CB-CG-OD1	6.43	124.08	118.30
1	B	324	ASP	CB-CG-OD1	6.43	124.08	118.30
1	A	310	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	B	112	PRO	N-CA-CB	6.37	110.94	103.30
1	C	39	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	B	51	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	A	179	TYR	CB-CG-CD2	-6.31	117.22	121.00
1	B	200	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	C	163	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	C	322	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	D	110	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	D	342	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	334	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	51	ASP	CB-CG-OD1	6.13	123.81	118.30
1	B	196	ASP	CB-CG-OD1	6.13	123.81	118.30
1	B	23	ARG	CG-CD-NE	-6.12	98.94	111.80
1	D	211	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	163	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	B	369	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	D	160	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	C	217	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	110	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	B	175	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	C	92	ARG	CB-CA-C	-6.01	98.37	110.40
1	D	304	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	B	302	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	C	334	ASP	CB-CG-OD1	5.98	123.68	118.30
1	B	279	ASP	CB-CG-OD1	5.98	123.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	204	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	D	175	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	B	86	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	C	311	ASP	CB-CG-OD1	5.95	123.65	118.30
1	C	168	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	D	310	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	D	404	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	A	204	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	B	337	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	C	135	LEU	CB-CA-C	-5.90	99.00	110.20
1	A	327	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	416	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	C	52	ASP	CB-CG-OD2	-5.87	113.01	118.30
1	D	369	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	B	151	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	73	TYR	N-CA-C	5.80	126.66	111.00
1	C	402	ARG	CD-NE-CZ	-5.79	115.49	123.60
1	A	84	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	217	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	86	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	D	163	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	99	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	B	160	ASP	CB-CG-OD1	5.74	123.46	118.30
1	C	200	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	84	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	D	296	SER	N-CA-CB	5.68	119.03	110.50
1	D	304	ASP	CB-CG-OD1	5.67	123.41	118.30
1	D	342	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	D	111	THR	CA-CB-CG2	-5.66	104.48	112.40
1	C	324	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	C	351	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	174	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	D	334	ASP	CB-CG-OD1	5.63	123.36	118.30
1	D	300	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	C	302	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	D	426	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	267	ASP	CB-CG-OD1	5.56	123.30	118.30
1	C	106	TYR	CB-CG-CD2	5.54	124.33	121.00
1	C	115	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	C	11	THR	CA-CB-OG1	5.48	120.52	109.00
1	A	160	ASP	CB-CG-OD1	5.46	123.22	118.30
1	D	84	ARG	NE-CZ-NH1	5.46	123.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	151	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	C	86	ASP	CB-CG-OD1	5.44	123.19	118.30
1	D	297	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	279	ASP	CB-CG-OD1	5.40	123.16	118.30
1	D	86	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	C	168	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	302	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	B	128	GLU	N-CA-CB	5.37	120.27	110.60
1	D	39	ASP	CB-CG-OD1	5.36	123.12	118.30
1	C	297	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	C	296	SER	N-CA-CB	5.34	118.52	110.50
1	B	327	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	D	302	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	174	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	D	110	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	135	LEU	CB-CG-CD2	-5.27	102.04	111.00
1	A	168	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	C	334	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	B	200	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	324	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	A	279	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	174	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	300	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	217	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	D	425	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	D	99	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	B	310	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	A	296	SER	N-CA-CB	5.14	118.21	110.50
1	C	110	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	140	ASN	CB-CA-C	-5.10	100.20	110.40
1	A	141	PRO	N-CA-CB	5.10	109.42	103.30
1	D	160	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	231	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	C	376	ASP	CB-CG-OD1	5.07	122.86	118.30
1	C	300	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	196	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	B	374	PRO	CA-CB-CG	-5.03	94.45	104.00
1	B	380	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	D	57	GLU	N-CA-CB	5.02	119.64	110.60
1	A	243	GLU	CG-CD-OE1	5.02	128.34	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	3219	0	3145	135	0
1	B	3218	0	3146	102	0
1	C	3211	0	3139	129	0
1	D	3226	0	3155	120	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	424	0	0	16	0
3	B	518	0	0	24	0
3	C	475	0	0	26	2
3	D	392	0	0	20	0
All	All	14687	0	12585	452	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (452) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:THR:HG22	1:B:15:GLN:HG3	1.23	1.19
1:B:10:THR:HG23	1:B:14:GLU:HB3	1.35	1.08
1:A:22:GLN:NE2	1:D:12:GLN:HE22	1.50	1.08
1:C:11:THR:HG23	1:C:15:GLN:HE21	1.21	1.04
1:A:142:SER:H	1:A:169:HIS:HE1	1.02	1.00
1:D:142:SER:H	1:D:169:HIS:HE1	1.06	0.99
1:A:22:GLN:HE22	1:D:12:GLN:NE2	1.63	0.97
1:D:182:GLU:HG3	1:D:228:HIS:CE1	2.05	0.92
1:A:22:GLN:HE22	1:D:12:GLN:HE22	1.04	0.92
1:A:119:LYS:H	1:A:122:HIS:HD2	1.16	0.91
1:C:142:SER:H	1:C:169:HIS:HE1	1.08	0.91
1:D:236:LYS:HG3	1:D:270:HIS:CE1	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:LYS:H	1:D:122:HIS:HD2	1.13	0.90
1:D:49:GLN:HE22	1:D:337:ASP:H	1.19	0.89
1:C:11:THR:HG23	1:C:15:GLN:NE2	1.88	0.88
1:A:49:GLN:HE22	1:A:337:ASP:H	1.17	0.87
1:D:88:GLU:HA	1:D:91:MSE:HE3	1.52	0.87
1:D:296:SER:HB2	1:D:335:PHE:HB3	1.55	0.86
1:B:49:GLN:HE22	1:B:337:ASP:H	1.21	0.86
1:A:314:GLN:HE21	1:A:359:ARG:HH11	1.23	0.86
1:B:119:LYS:H	1:B:122:HIS:HD2	1.23	0.85
1:D:269:GLY:HA2	1:D:298:PRO:HG3	1.58	0.85
1:B:142:SER:H	1:B:169:HIS:HE1	1.22	0.85
1:A:171:LYS:HE3	3:A:593:HOH:O	1.79	0.82
1:A:205:ARG:HD2	3:A:573:HOH:O	1.80	0.81
1:B:289:PRO:O	1:B:328:ARG:HD2	1.80	0.81
1:C:119:LYS:H	1:C:122:HIS:HD2	1.22	0.81
1:A:290:GLN:NE2	1:A:330:HIS:NE2	2.29	0.81
1:A:119:LYS:H	1:A:122:HIS:CD2	1.99	0.80
1:D:119:LYS:H	1:D:122:HIS:CD2	1.99	0.80
1:C:119:LYS:H	1:C:122:HIS:CD2	2.00	0.80
1:A:418:TYR:CE1	1:A:422:ILE:HD12	2.17	0.79
1:B:10:THR:CG2	1:B:15:GLN:HG3	2.08	0.79
1:A:142:SER:H	1:A:169:HIS:CE1	1.95	0.79
1:B:236:LYS:HE3	1:B:302:ASP:OD2	1.84	0.78
1:B:393:GLN:HB2	3:B:753:HOH:O	1.82	0.78
1:D:76:LYS:HE3	3:D:499:HOH:O	1.83	0.77
1:B:290:GLN:HG3	3:B:844:HOH:O	1.85	0.77
1:C:304:ASP:HB3	1:C:336:PHE:H	1.50	0.77
1:B:119:LYS:H	1:B:122:HIS:CD2	2.03	0.76
1:B:205:ARG:HD2	3:B:592:HOH:O	1.83	0.76
1:B:389:SER:HA	1:C:393:GLN:HG2	1.67	0.76
1:B:73:TYR:N	3:B:502:HOH:O	2.18	0.76
1:C:325:LEU:HB3	1:C:329:VAL:HG23	1.67	0.76
1:C:289:PRO:O	1:C:328:ARG:HD2	1.86	0.76
1:D:221:SER:O	1:D:223:LYS:HE2	1.87	0.75
1:A:92:ARG:HD3	3:A:832:HOH:O	1.86	0.75
1:B:314:GLN:HE21	1:B:359:ARG:HH11	1.31	0.75
1:C:73:TYR:N	3:C:672:HOH:O	2.20	0.75
1:D:404:ASP:HB2	3:D:824:HOH:O	1.85	0.75
1:D:205:ARG:HD2	3:D:452:HOH:O	1.87	0.75
1:B:325:LEU:HB3	1:B:329:VAL:HG23	1.68	0.74
1:B:373:ALA:HB3	1:B:374:PRO:HD2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:GLU:HA	1:A:124:LYS:HG3	1.68	0.74
1:D:367:GLU:HG3	3:D:694:HOH:O	1.86	0.74
1:D:373:ALA:HB3	1:D:374:PRO:HD2	1.70	0.73
1:B:36:ARG:HD2	3:B:483:HOH:O	1.88	0.73
1:D:314:GLN:HE21	1:D:359:ARG:HH11	1.35	0.73
1:A:373:ALA:HB3	1:A:374:PRO:HD2	1.71	0.73
1:A:425:ARG:HG3	1:A:425:ARG:HH11	1.53	0.72
1:A:293:LEU:HD12	1:A:320:ILE:HD11	1.71	0.72
1:C:242:ALA:HB2	3:C:797:HOH:O	1.88	0.72
1:C:393:GLN:HB2	3:C:926:HOH:O	1.89	0.72
1:D:73:TYR:N	3:D:494:HOH:O	2.22	0.72
1:A:11:THR:N	3:A:451:HOH:O	2.23	0.71
1:D:87:LEU:C	1:D:91:MSE:HE2	2.11	0.71
1:C:49:GLN:HE22	1:C:337:ASP:H	1.35	0.71
1:B:33:GLU:HG2	3:B:798:HOH:O	1.91	0.71
1:B:92:ARG:HD3	3:B:888:HOH:O	1.89	0.71
1:D:134:GLN:HA	1:D:134:GLN:HE21	1.55	0.71
1:C:236:LYS:HE3	1:C:302:ASP:OD2	1.90	0.70
1:C:290:GLN:HB2	3:C:829:HOH:O	1.90	0.70
1:D:142:SER:H	1:D:169:HIS:CE1	1.99	0.70
1:C:142:SER:H	1:C:169:HIS:CE1	2.01	0.70
1:C:205:ARG:HD2	3:C:756:HOH:O	1.91	0.70
1:C:314:GLN:HE21	1:C:359:ARG:HH11	1.37	0.69
1:C:142:SER:N	1:C:169:HIS:HE1	1.87	0.69
1:B:10:THR:CG2	1:B:14:GLU:HB3	2.19	0.69
1:B:182:GLU:HG3	1:B:228:HIS:CE1	2.28	0.69
1:D:79:ASN:ND2	1:D:82:GLU:H	1.92	0.68
1:C:79:ASN:ND2	1:C:82:GLU:H	1.92	0.68
1:D:134:GLN:HE21	1:D:134:GLN:CA	2.07	0.68
1:A:303:SER:HB2	1:A:305:HIS:CE1	2.27	0.68
1:B:329:VAL:HB	3:B:702:HOH:O	1.93	0.68
1:C:367:GLU:HG3	3:C:895:HOH:O	1.94	0.68
1:D:9:MSE:N	3:D:840:HOH:O	2.27	0.67
1:C:11:THR:N	3:C:633:HOH:O	2.26	0.67
1:A:88:GLU:O	1:A:92:ARG:HG2	1.95	0.67
1:A:289:PRO:O	1:A:328:ARG:HD2	1.95	0.67
1:D:199:LYS:HB2	1:D:241:GLY:O	1.95	0.67
1:D:142:SER:N	1:D:169:HIS:HE1	1.88	0.67
1:D:289:PRO:O	1:D:328:ARG:HD2	1.94	0.67
1:B:218:GLU:HG3	3:B:908:HOH:O	1.93	0.67
1:A:425:ARG:HD3	1:A:425:ARG:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:LYS:HE3	1:D:302:ASP:OD2	1.95	0.67
1:A:300:ARG:HD2	1:C:238:PHE:CD1	2.31	0.66
1:D:12:GLN:HG3	3:D:454:HOH:O	1.96	0.66
1:D:88:GLU:HA	1:D:91:MSE:CE	2.23	0.66
1:C:359:ARG:NH2	3:C:886:HOH:O	2.28	0.66
1:D:89:GLN:NE2	3:D:510:HOH:O	2.29	0.66
1:A:142:SER:N	1:A:169:HIS:HE1	1.84	0.66
1:C:410:GLU:HG3	3:C:946:HOH:O	1.96	0.66
1:A:121:GLU:HA	1:A:124:LYS:CG	2.26	0.66
1:B:236:LYS:HA	1:B:270:HIS:HD1	1.60	0.66
1:C:290:GLN:HG3	1:C:328:ARG:O	1.96	0.65
1:A:290:GLN:HG3	3:A:795:HOH:O	1.96	0.65
1:D:420:LYS:HG3	3:D:736:HOH:O	1.96	0.65
1:C:327:ASP:HB2	3:C:1483:HOH:O	1.95	0.65
1:D:92:ARG:NH2	3:D:513:HOH:O	2.29	0.65
1:D:325:LEU:O	1:D:329:VAL:HG12	1.97	0.65
1:B:413:GLU:HG3	3:B:929:HOH:O	1.96	0.64
1:A:19:LEU:HD23	1:D:12:GLN:NE2	2.12	0.64
1:B:325:LEU:HB3	1:B:329:VAL:CG2	2.27	0.64
1:C:134:GLN:HE21	1:C:134:GLN:HA	1.63	0.64
1:D:89:GLN:HG3	1:D:418:TYR:CE1	2.33	0.64
1:B:389:SER:CA	1:C:393:GLN:HG2	2.28	0.64
1:A:22:GLN:CD	1:D:12:GLN:HE22	1.99	0.64
1:A:73:TYR:CG	1:A:74:PRO:HD2	2.33	0.64
1:D:419:GLU:HG3	1:D:423:LEU:HD12	1.78	0.64
1:A:79:ASN:ND2	1:A:82:GLU:H	1.96	0.63
1:A:314:GLN:NE2	1:A:359:ARG:HD3	2.13	0.63
1:D:223:LYS:HE3	3:D:597:HOH:O	1.97	0.63
1:B:142:SER:N	1:B:169:HIS:HE1	1.95	0.63
1:A:424:SER:OG	1:A:425:ARG:NE	2.32	0.63
1:A:290:GLN:OE1	1:A:328:ARG:HA	1.98	0.63
1:B:292:LEU:HD21	3:B:668:HOH:O	1.98	0.63
1:C:52:ASP:HA	1:C:336:PHE:CZ	2.33	0.63
1:B:236:LYS:HA	1:B:270:HIS:ND1	2.14	0.62
1:B:410:GLU:H	1:B:410:GLU:CD	2.02	0.62
1:C:373:ALA:HB3	1:C:374:PRO:HD2	1.81	0.62
1:B:235:SER:O	1:B:270:HIS:ND1	2.33	0.62
1:A:420:LYS:HB3	1:A:421:GLU:OE1	2.00	0.62
1:A:11:THR:HB	3:A:452:HOH:O	1.98	0.62
1:C:296:SER:HB2	1:C:335:PHE:HB3	1.80	0.62
1:D:89:GLN:HG3	1:D:418:TYR:CD1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:GLN:HA	1:A:134:GLN:HE21	1.64	0.61
1:D:374:PRO:HD3	3:D:787:HOH:O	1.98	0.61
1:D:324:ASP:HB2	3:D:663:HOH:O	2.00	0.61
1:D:304:ASP:HB3	1:D:336:PHE:H	1.65	0.61
1:B:19:LEU:HD23	1:C:12:GLN:HE21	1.65	0.61
1:B:393:GLN:NE2	1:C:393:GLN:OE1	2.33	0.61
1:C:27:VAL:HG21	3:C:922:HOH:O	2.00	0.60
1:D:89:GLN:OE1	1:D:92:ARG:NH1	2.34	0.60
1:B:236:LYS:CA	1:B:270:HIS:HD1	2.15	0.60
1:A:304:ASP:HB3	1:A:336:PHE:H	1.66	0.60
1:C:292:LEU:HD21	3:C:831:HOH:O	2.00	0.60
1:C:410:GLU:CD	1:C:410:GLU:H	2.04	0.59
1:D:387:GLN:HG2	3:D:714:HOH:O	2.03	0.59
1:A:134:GLN:HA	1:A:134:GLN:NE2	2.16	0.59
1:A:300:ARG:HD3	3:A:658:HOH:O	2.01	0.59
1:C:238:PHE:HB2	1:C:243:GLU:HA	1.84	0.59
1:D:86:ASP:HB3	1:D:343:ILE:HD11	1.83	0.59
1:A:72:ASN:OD1	1:A:339:SER:HA	2.02	0.59
1:A:230:ILE:HD13	1:A:290:GLN:NE2	2.17	0.59
1:A:52:ASP:HA	1:A:336:PHE:CZ	2.37	0.58
1:C:37:GLN:OE1	1:C:40:ARG:HD3	2.02	0.58
1:A:230:ILE:HD13	1:A:290:GLN:HE21	1.69	0.58
1:D:419:GLU:HA	1:D:423:LEU:HB2	1.86	0.58
1:A:128:GLU:HG3	3:A:530:HOH:O	2.03	0.58
1:C:304:ASP:HB3	1:C:336:PHE:N	2.18	0.58
1:B:142:SER:H	1:B:169:HIS:CE1	2.12	0.57
1:A:393:GLN:HG2	1:D:389:SER:HA	1.85	0.57
1:C:325:LEU:HB3	1:C:329:VAL:CG2	2.32	0.57
1:D:237:LEU:HB2	3:D:775:HOH:O	2.04	0.57
1:A:134:GLN:HE21	1:A:134:GLN:CA	2.18	0.57
1:A:373:ALA:CB	1:A:374:PRO:HD2	2.32	0.57
1:C:99:ARG:HH12	1:C:186:THR:CG2	2.16	0.57
1:C:336:PHE:HB2	3:C:662:HOH:O	2.05	0.57
1:D:373:ALA:CB	1:D:374:PRO:HD2	2.31	0.57
1:A:92:ARG:NH1	3:A:503:HOH:O	2.38	0.56
1:C:89:GLN:NE2	3:C:696:HOH:O	2.38	0.56
1:B:124:LYS:HD3	1:B:179:TYR:OH	2.04	0.56
1:B:272:HIS:HB3	1:B:273:PRO:HD2	1.88	0.56
1:A:410:GLU:CD	1:A:410:GLU:H	2.07	0.56
1:C:88:GLU:HA	1:C:91:MSE:CE	2.36	0.56
1:C:290:GLN:HG2	1:C:330:HIS:NE2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:GLU:HA	1:A:413:GLU:OE1	2.06	0.55
1:B:19:LEU:HD23	1:C:12:GLN:NE2	2.21	0.55
1:C:413:GLU:HG3	3:C:1725:HOH:O	2.07	0.55
1:A:89:GLN:O	1:A:92:ARG:HG3	2.05	0.55
1:A:343:ILE:HD12	1:A:343:ILE:N	2.22	0.55
1:B:121:GLU:HB3	3:B:545:HOH:O	2.07	0.55
1:C:369:ARG:NH1	1:D:204:ASP:OD2	2.40	0.55
1:C:92:ARG:NH2	3:C:699:HOH:O	2.40	0.55
1:D:290:GLN:NE2	3:D:642:HOH:O	2.40	0.54
1:A:52:ASP:HA	1:A:336:PHE:CE1	2.43	0.54
1:A:412:LEU:HG	1:A:416:ARG:HD2	1.89	0.54
1:B:182:GLU:HG3	1:B:228:HIS:ND1	2.22	0.54
1:C:383:LEU:O	1:C:387:GLN:HG2	2.08	0.54
1:A:296:SER:HB2	1:A:335:PHE:HB3	1.89	0.54
1:D:314:GLN:HE21	1:D:359:ARG:NH1	2.03	0.54
1:A:379:ALA:O	1:A:383:LEU:HG	2.08	0.54
1:C:292:LEU:HD11	3:C:831:HOH:O	2.06	0.53
1:B:79:ASN:ND2	1:B:82:GLU:H	2.06	0.53
1:B:314:GLN:NE2	1:B:359:ARG:HD3	2.23	0.53
1:C:273:PRO:HD3	3:C:818:HOH:O	2.07	0.53
1:D:236:LYS:HG3	1:D:270:HIS:ND1	2.23	0.53
1:A:213:LEU:HD11	1:A:260:ARG:NH2	2.24	0.53
1:D:21:LYS:HE2	3:D:471:HOH:O	2.07	0.53
1:B:186:THR:HG22	3:B:579:HOH:O	2.08	0.53
1:C:401:GLN:NE2	3:C:932:HOH:O	2.40	0.53
1:B:49:GLN:HE22	1:B:337:ASP:N	2.00	0.53
1:B:367:GLU:HG3	3:B:865:HOH:O	2.07	0.53
1:C:99:ARG:HH12	1:C:186:THR:HG21	1.74	0.53
1:D:146:HIS:CG	1:D:147:PRO:HD2	2.43	0.53
1:B:296:SER:HB2	1:B:335:PHE:HB3	1.90	0.53
1:C:234:GLU:HB2	1:C:265:CYS:HB3	1.89	0.53
1:B:134:GLN:HA	1:B:134:GLN:HE21	1.74	0.53
1:D:52:ASP:HA	1:D:336:PHE:CE1	2.44	0.53
1:A:367:GLU:HG3	3:A:709:HOH:O	2.08	0.53
1:C:121:GLU:HA	1:C:124:LYS:CG	2.40	0.53
1:D:52:ASP:HA	1:D:336:PHE:CZ	2.44	0.52
1:B:171:LYS:NZ	3:B:572:HOH:O	2.41	0.52
1:C:114:SER:OG	1:C:116:ASP:OD1	2.26	0.52
1:A:285:MSE:HB2	3:A:853:HOH:O	2.09	0.52
1:B:79:ASN:C	1:B:79:ASN:HD22	2.13	0.52
1:B:359:ARG:NH2	3:B:720:HOH:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:LYS:NZ	1:D:183:GLN:OE1	2.43	0.52
1:A:393:GLN:HG2	1:D:389:SER:C	2.29	0.52
1:A:405:THR:HG23	1:A:406:PRO:HD2	1.90	0.52
1:B:373:ALA:CB	1:B:374:PRO:HD2	2.32	0.52
1:C:272:HIS:HB3	1:C:273:PRO:HD2	1.91	0.52
1:A:121:GLU:O	1:A:124:LYS:HG3	2.10	0.52
1:C:383:LEU:HD13	3:C:921:HOH:O	2.09	0.52
1:D:121:GLU:HA	1:D:124:LYS:CG	2.40	0.52
1:C:27:VAL:HG23	1:C:27:VAL:O	2.10	0.52
1:C:406:PRO:HG2	1:C:411:TRP:HB3	1.92	0.52
1:B:89:GLN:HG3	1:B:418:TYR:CE1	2.45	0.52
1:C:267:ASP:HB3	1:C:270:HIS:CG	2.45	0.51
1:D:304:ASP:O	1:D:335:PHE:HB2	2.10	0.51
1:C:121:GLU:O	1:C:124:LYS:HG3	2.11	0.51
1:B:121:GLU:HA	1:B:124:LYS:HE3	1.92	0.51
1:C:333:LEU:HD11	1:C:350:THR:OG1	2.10	0.51
1:A:22:GLN:NE2	1:D:12:GLN:NE2	2.30	0.51
1:C:114:SER:HB3	1:C:117:GLN:HG3	1.91	0.51
1:C:11:THR:CG2	1:C:15:GLN:HE21	2.09	0.51
1:D:27:VAL:HG22	1:D:27:VAL:O	2.11	0.51
1:B:296:SER:HB3	1:B:334:ASP:O	2.11	0.51
1:D:290:GLN:HG3	1:D:328:ARG:O	2.11	0.51
1:D:304:ASP:HB3	1:D:336:PHE:N	2.26	0.51
1:C:146:HIS:CG	1:C:147:PRO:HD2	2.46	0.50
1:D:121:GLU:HA	1:D:124:LYS:HG3	1.92	0.50
1:D:115:ARG:O	1:D:169:HIS:HD2	1.94	0.50
1:D:336:PHE:CZ	1:D:338:ALA:HB2	2.46	0.50
1:D:177:SER:O	1:D:180:PHE:HB2	2.12	0.50
1:A:296:SER:HB3	1:A:334:ASP:O	2.12	0.50
1:A:300:ARG:CZ	1:C:237:LEU:HD21	2.42	0.49
1:A:84:ARG:HD2	1:A:129:TRP:CD1	2.48	0.49
1:A:425:ARG:HH11	1:A:425:ARG:CG	2.23	0.49
1:D:355:LYS:HE3	1:D:396:TRP:NE1	2.27	0.49
1:B:18:GLU:HG3	3:B:935:HOH:O	2.12	0.49
1:C:236:LYS:HE2	1:C:238:PHE:O	2.13	0.49
1:B:367:GLU:HG3	3:B:729:HOH:O	2.12	0.49
1:C:111:THR:HB	1:C:112:PRO:HD2	1.94	0.49
1:A:314:GLN:HE22	1:A:359:ARG:HD3	1.78	0.49
1:C:295:VAL:HG23	1:C:307:VAL:HG21	1.94	0.49
1:A:405:THR:CG2	1:A:406:PRO:HD2	2.43	0.48
1:C:134:GLN:HE21	1:C:134:GLN:CA	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:LEU:HD22	1:C:401:GLN:NE2	2.28	0.48
1:C:89:GLN:HG3	1:C:418:TYR:CE1	2.48	0.48
1:C:115:ARG:O	1:C:169:HIS:HD2	1.97	0.48
1:C:124:LYS:O	1:C:128:GLU:HG3	2.13	0.48
1:A:370:LYS:O	1:A:374:PRO:HG2	2.14	0.48
1:B:89:GLN:NE2	3:B:519:HOH:O	2.46	0.48
1:D:53:VAL:HG12	1:D:53:VAL:O	2.13	0.48
1:A:121:GLU:CA	1:A:124:LYS:HG3	2.40	0.48
1:C:139:PHE:O	1:C:190:MSE:HA	2.13	0.48
1:A:131:LYS:NZ	3:A:531:HOH:O	2.47	0.48
1:C:233:VAL:HB	1:C:253:TYR:CD1	2.49	0.48
1:A:370:LYS:O	1:A:374:PRO:HD2	2.14	0.48
1:B:389:SER:C	1:C:393:GLN:HG2	2.33	0.48
1:A:49:GLN:HE22	1:A:337:ASP:N	1.98	0.47
1:B:33:GLU:OE1	1:B:36:ARG:NE	2.46	0.47
1:B:236:LYS:HB2	1:B:270:HIS:CE1	2.49	0.47
1:C:87:LEU:C	1:C:91:MSE:HE2	2.35	0.47
1:A:12:GLN:HB3	1:D:19:LEU:HD22	1.96	0.47
1:A:134:GLN:NE2	1:A:134:GLN:CA	2.77	0.47
1:A:304:ASP:HB3	1:A:336:PHE:N	2.29	0.47
1:A:213:LEU:HD11	1:A:260:ARG:CZ	2.44	0.47
1:C:157:HIS:O	1:C:163:ARG:HD3	2.14	0.47
1:D:379:ALA:O	1:D:383:LEU:HG	2.15	0.47
1:C:370:LYS:O	1:C:374:PRO:HD2	2.14	0.47
1:B:233:VAL:HB	1:B:253:TYR:CD1	2.50	0.47
1:A:115:ARG:O	1:A:169:HIS:HD2	1.98	0.46
1:B:301:TRP:NE1	1:D:240:ILE:HD12	2.30	0.46
1:D:370:LYS:O	1:D:374:PRO:HG2	2.15	0.46
1:A:89:GLN:NE2	1:A:92:ARG:HD2	2.30	0.46
1:C:127:VAL:HG21	1:C:179:TYR:CE2	2.50	0.46
1:A:223:LYS:HE2	3:A:599:HOH:O	2.15	0.46
1:D:11:THR:HG23	1:D:15:GLN:NE2	2.29	0.46
1:D:119:LYS:N	1:D:122:HIS:CD2	2.78	0.46
1:A:213:LEU:HD12	1:A:213:LEU:O	2.15	0.46
1:A:303:SER:HB2	1:A:305:HIS:HE1	1.76	0.46
1:A:46:HIS:NE2	1:A:335:PHE:O	2.48	0.46
1:A:272:HIS:HB3	1:A:273:PRO:HD2	1.97	0.46
1:C:290:GLN:HG2	1:C:330:HIS:CD2	2.50	0.46
1:C:370:LYS:O	1:C:374:PRO:HG2	2.16	0.46
1:C:373:ALA:CB	1:C:374:PRO:HD2	2.40	0.46
1:C:152:GLY:O	1:C:196:ASP:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LYS:NZ	3:A:528:HOH:O	2.45	0.46
1:A:406:PRO:HD3	3:A:871:HOH:O	2.15	0.46
1:A:425:ARG:CG	1:A:425:ARG:NH1	2.79	0.46
1:C:119:LYS:N	1:C:122:HIS:CD2	2.78	0.45
1:D:84:ARG:HD2	1:D:129:TRP:CD1	2.51	0.45
1:D:301:TRP:O	1:D:303:SER:N	2.47	0.45
1:A:87:LEU:C	1:A:91:MSE:HE2	2.36	0.45
1:A:139:PHE:O	1:A:190:MSE:HA	2.16	0.45
1:B:12:GLN:HE21	1:C:19:LEU:CD2	2.29	0.45
1:A:238:PHE:HB3	1:C:300:ARG:HD2	1.98	0.45
1:A:393:GLN:HG2	1:D:389:SER:CA	2.45	0.45
1:A:119:LYS:N	1:A:122:HIS:CD2	2.76	0.45
1:D:89:GLN:CG	1:D:418:TYR:CE1	2.99	0.45
1:D:410:GLU:H	1:D:410:GLU:CD	2.19	0.45
1:A:22:GLN:OE1	1:D:12:GLN:OE1	2.34	0.45
1:A:73:TYR:CD2	1:A:74:PRO:HD2	2.52	0.45
1:B:374:PRO:HD2	3:B:733:HOH:O	2.17	0.45
1:C:223:LYS:HD3	1:C:223:LYS:HA	1.80	0.45
1:B:52:ASP:HA	1:B:336:PHE:CZ	2.52	0.45
1:C:84:ARG:HD2	1:C:129:TRP:CD1	2.51	0.45
1:B:120:PRO:HB3	1:B:179:TYR:CD2	2.51	0.45
1:C:27:VAL:HB	3:C:897:HOH:O	2.17	0.45
1:D:267:ASP:HB3	1:D:270:HIS:CG	2.52	0.45
1:B:10:THR:HG22	1:B:15:GLN:CG	2.17	0.44
1:D:9:MSE:HA	3:D:818:HOH:O	2.17	0.44
1:A:121:GLU:HA	1:A:124:LYS:CD	2.48	0.44
1:A:133:ASN:O	1:A:134:GLN:HB2	2.18	0.44
1:A:314:GLN:HE21	1:A:359:ARG:NH1	2.04	0.44
1:B:120:PRO:HB3	1:B:179:TYR:CG	2.52	0.44
1:B:374:PRO:CD	3:B:733:HOH:O	2.65	0.44
1:D:299:VAL:C	1:D:301:TRP:H	2.21	0.44
1:B:119:LYS:N	1:B:122:HIS:HD2	2.04	0.44
1:B:121:GLU:HA	1:B:124:LYS:HG2	1.98	0.44
1:B:301:TRP:CE2	1:D:240:ILE:HD12	2.53	0.44
1:A:419:GLU:HA	1:A:423:LEU:HB2	1.99	0.44
1:A:425:ARG:HG3	1:A:425:ARG:NH1	2.26	0.44
1:D:191:ASN:HD21	1:D:234:GLU:HB2	1.83	0.44
1:D:370:LYS:O	1:D:374:PRO:HD2	2.17	0.44
1:C:236:LYS:HA	1:C:270:HIS:HB3	2.00	0.44
1:D:373:ALA:CB	1:D:374:PRO:CD	2.95	0.44
1:A:19:LEU:CD2	1:D:12:GLN:NE2	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLN:NE2	1:A:336:PHE:HA	2.33	0.44
1:B:389:SER:HA	1:C:393:GLN:CG	2.44	0.44
1:C:314:GLN:HE22	1:C:356:ALA:HA	1.83	0.44
1:B:301:TRP:NE1	1:B:303:SER:HB3	2.33	0.44
1:C:143:CYS:HA	1:C:166:TRP:CZ3	2.52	0.44
1:C:393:GLN:OE1	3:C:926:HOH:O	2.21	0.44
1:D:78:ARG:NH2	1:D:426:ARG:HG2	2.33	0.44
1:A:76:LYS:HE3	3:A:490:HOH:O	2.18	0.43
1:A:119:LYS:N	1:A:122:HIS:HD2	1.98	0.43
1:A:135:LEU:HD23	1:A:135:LEU:HA	1.67	0.43
1:A:389:SER:C	1:D:393:GLN:HG2	2.38	0.43
1:B:236:LYS:CA	1:B:270:HIS:ND1	2.78	0.43
1:B:370:LYS:O	1:B:374:PRO:HG2	2.18	0.43
1:C:52:ASP:HA	1:C:336:PHE:CE1	2.53	0.43
1:A:343:ILE:N	1:A:343:ILE:CD1	2.81	0.43
1:A:393:GLN:HE22	1:D:393:GLN:HE22	1.67	0.43
1:B:301:TRP:O	1:B:303:SER:N	2.45	0.43
1:B:314:GLN:HE22	1:B:359:ARG:HD3	1.83	0.43
1:D:299:VAL:N	1:D:303:SER:OG	2.46	0.43
1:D:134:GLN:CA	1:D:134:GLN:NE2	2.78	0.43
1:A:92:ARG:HD2	1:A:92:ARG:HH11	1.62	0.43
1:A:373:ALA:CB	1:A:374:PRO:CD	2.96	0.43
1:B:236:LYS:CB	1:B:270:HIS:ND1	2.80	0.43
1:A:240:ILE:HD12	1:A:240:ILE:HA	1.69	0.43
1:C:84:ARG:O	1:C:88:GLU:HG3	2.18	0.43
1:C:191:ASN:HD21	1:C:234:GLU:HB2	1.84	0.43
1:D:120:PRO:HB3	1:D:179:TYR:CD2	2.54	0.43
1:C:96:GLY:HA2	1:C:403:HIS:CE1	2.54	0.43
1:A:418:TYR:O	1:A:422:ILE:HB	2.19	0.43
1:B:355:LYS:HE3	1:B:396:TRP:NE1	2.34	0.43
1:D:301:TRP:NE1	1:D:303:SER:HB3	2.34	0.43
1:C:314:GLN:HE21	1:C:359:ARG:NH1	2.13	0.43
1:A:299:VAL:N	1:A:303:SER:OG	2.49	0.43
1:C:11:THR:O	1:C:15:GLN:HG3	2.19	0.43
1:C:88:GLU:HA	1:C:91:MSE:HE3	2.01	0.43
1:A:300:ARG:HB3	1:C:238:PHE:CE1	2.53	0.42
1:A:341:ASN:HD21	1:A:423:LEU:HD12	1.84	0.42
1:B:12:GLN:NE2	1:C:19:LEU:HD23	2.34	0.42
1:B:299:VAL:N	1:B:303:SER:OG	2.46	0.42
1:D:240:ILE:HD12	1:D:240:ILE:HA	1.83	0.42
1:C:299:VAL:C	1:C:301:TRP:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:TRP:NE1	1:A:303:SER:HB3	2.34	0.42
1:B:176:VAL:O	1:B:179:TYR:HB3	2.19	0.42
1:C:96:GLY:O	1:C:98:LYS:HD3	2.19	0.42
1:A:343:ILE:HD13	1:A:423:LEU:HD11	2.01	0.42
1:C:370:LYS:HG3	3:C:902:HOH:O	2.19	0.42
1:C:419:GLU:HA	1:C:423:LEU:HB2	2.01	0.42
1:B:37:GLN:HG2	3:B:487:HOH:O	2.19	0.42
1:C:140:ASN:ND2	1:C:191:ASN:HB3	2.34	0.42
1:D:91:MSE:HE1	1:D:129:TRP:CZ2	2.55	0.42
1:D:234:GLU:OE2	1:D:267:ASP:HB2	2.20	0.42
1:D:329:VAL:O	1:D:329:VAL:HG13	2.19	0.42
1:A:12:GLN:H	1:A:12:GLN:HG2	1.50	0.42
1:D:46:HIS:NE2	1:D:335:PHE:O	2.51	0.42
1:D:314:GLN:NE2	1:D:359:ARG:HH11	2.09	0.42
1:A:86:ASP:OD1	1:A:418:TYR:OH	2.30	0.42
1:A:120:PRO:HB3	1:A:179:TYR:CG	2.55	0.42
1:D:269:GLY:HA2	1:D:298:PRO:CG	2.40	0.42
1:B:119:LYS:N	1:B:122:HIS:CD2	2.82	0.42
1:D:151:ASP:HB2	3:D:548:HOH:O	2.18	0.42
1:D:157:HIS:O	1:D:163:ARG:HD3	2.19	0.42
1:B:236:LYS:HG3	1:B:270:HIS:ND1	2.35	0.42
1:D:167:ILE:HG22	1:D:171:LYS:HD2	2.02	0.42
1:A:79:ASN:C	1:A:79:ASN:HD22	2.24	0.41
1:A:314:GLN:NE2	1:A:359:ARG:HH11	2.02	0.41
1:C:383:LEU:HB3	3:C:921:HOH:O	2.20	0.41
1:A:393:GLN:NE2	1:D:393:GLN:HE22	2.17	0.41
1:A:422:ILE:C	1:A:424:SER:H	2.23	0.41
1:B:333:LEU:HD11	1:B:350:THR:OG1	2.20	0.41
1:A:383:LEU:O	1:A:387:GLN:HG2	2.19	0.41
1:C:88:GLU:HA	1:C:91:MSE:HE2	2.02	0.41
1:D:374:PRO:CD	3:D:698:HOH:O	2.67	0.41
1:A:300:ARG:CD	1:C:238:PHE:CD1	3.02	0.41
1:B:49:GLN:NE2	1:B:336:PHE:HA	2.35	0.41
1:D:314:GLN:HE22	1:D:356:ALA:HA	1.86	0.41
1:B:406:PRO:HG2	1:B:411:TRP:HB3	2.02	0.41
1:A:121:GLU:C	1:A:124:LYS:HG3	2.41	0.41
1:A:393:GLN:HG2	1:D:389:SER:O	2.20	0.41
1:C:314:GLN:HG2	3:C:1801:HOH:O	2.20	0.41
1:D:91:MSE:HE1	1:D:129:TRP:HZ2	1.84	0.41
1:B:19:LEU:CD2	1:C:12:GLN:HE21	2.33	0.41
1:B:299:VAL:C	1:B:301:TRP:H	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:GLN:HE22	1:B:356:ALA:HA	1.85	0.41
1:C:299:VAL:N	1:C:303:SER:OG	2.47	0.41
1:A:23:ARG:HA	1:A:23:ARG:HD2	1.74	0.41
1:C:293:LEU:HD12	1:C:320:ILE:HD11	2.02	0.41
1:D:333:LEU:HD11	1:D:350:THR:OG1	2.20	0.41
1:A:301:TRP:O	1:A:303:SER:N	2.48	0.41
1:C:89:GLN:HG3	1:C:418:TYR:CD1	2.56	0.41
1:C:236:LYS:HG3	1:C:270:HIS:CE1	2.56	0.41
1:A:88:GLU:HA	1:A:91:MSE:HE3	2.02	0.41
1:C:243:GLU:CD	1:C:243:GLU:H	2.24	0.41
1:C:301:TRP:NE1	1:C:303:SER:HB3	2.34	0.41
1:B:146:HIS:CG	1:B:147:PRO:HD2	2.56	0.40
1:B:425:ARG:NH2	3:B:783:HOH:O	2.24	0.40
1:D:236:LYS:HE2	1:D:238:PHE:O	2.20	0.40
1:C:205:ARG:HG2	1:C:245:TYR:CD1	2.56	0.40
1:C:374:PRO:CD	3:C:902:HOH:O	2.70	0.40
1:A:299:VAL:C	1:A:301:TRP:H	2.23	0.40
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.90	0.40
1:C:301:TRP:O	1:C:303:SER:N	2.48	0.40
1:B:236:LYS:HE2	1:B:238:PHE:O	2.21	0.40
1:B:390:LEU:HD23	1:B:390:LEU:HA	1.88	0.40
1:C:134:GLN:CA	1:C:134:GLN:NE2	2.84	0.40
1:C:373:ALA:CB	1:C:374:PRO:CD	2.98	0.40
1:D:267:ASP:HB3	1:D:270:HIS:HB2	2.02	0.40
1:A:84:ARG:HD2	1:A:129:TRP:CG	2.56	0.40
1:A:191:ASN:HD21	1:A:234:GLU:HB2	1.87	0.40
1:B:89:GLN:HG3	1:B:418:TYR:CD1	2.57	0.40
1:B:370:LYS:O	1:B:374:PRO:HD2	2.22	0.40
1:B:420:LYS:HD2	3:B:777:HOH:O	2.21	0.40
1:D:290:GLN:HG2	1:D:330:HIS:NE2	2.37	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:660:HOH:O	3:C:660:HOH:O[2_556]	0.96	1.24
3:C:934:HOH:O	3:C:934:HOH:O[2_556]	2.06	0.14

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/426 (93%)	379 (95%)	17 (4%)	2 (0%)	29	11
1	B	398/426 (93%)	385 (97%)	13 (3%)	0	100	100
1	C	397/426 (93%)	382 (96%)	14 (4%)	1 (0%)	41	21
1	D	399/426 (94%)	388 (97%)	10 (2%)	1 (0%)	41	21
All	All	1592/1704 (93%)	1534 (96%)	54 (3%)	4 (0%)	41	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	LEU
1	A	73	TYR
1	C	53	VAL
1	D	53	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/350 (98%)	327 (96%)	15 (4%)	28	8
1	B	342/350 (98%)	326 (95%)	16 (5%)	26	7
1	C	341/350 (97%)	326 (96%)	15 (4%)	28	8
1	D	343/350 (98%)	319 (93%)	24 (7%)	15	3
All	All	1368/1400 (98%)	1298 (95%)	70 (5%)	24	6

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	73	TYR
1	A	79	ASN
1	A	98	LYS
1	A	103	HIS
1	A	119	LYS
1	A	134	GLN
1	A	223	LYS
1	A	240	ILE
1	A	243	GLU
1	A	369	ARG
1	A	374	PRO
1	A	420	LYS
1	A	421	GLU
1	A	425	ARG
1	B	10	THR
1	B	36	ARG
1	B	53	VAL
1	B	79	ASN
1	B	92	ARG
1	B	98	LYS
1	B	103	HIS
1	B	117	GLN
1	B	128	GLU
1	B	134	GLN
1	B	171	LYS
1	B	196	ASP
1	B	223	LYS
1	B	369	ARG
1	B	374	PRO
1	B	401	GLN
1	C	11	THR
1	C	27	VAL
1	C	53	VAL
1	C	79	ASN
1	C	81	SER
1	C	98	LYS
1	C	103	HIS
1	C	124	LYS
1	C	128	GLU
1	C	134	GLN
1	C	196	ASP

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Mol	Chain	Res	Type
1	C	236	LYS
1	C	290	GLN
1	C	374	PRO
1	C	410	GLU
1	D	11	THR
1	D	14	GLU
1	D	46	HIS
1	D	79	ASN
1	D	81	SER
1	D	98	LYS
1	D	103	HIS
1	D	107	LEU
1	D	110	ASP
1	D	119	LYS
1	D	134	GLN
1	D	182	GLU
1	D	223	LYS
1	D	240	ILE
1	D	243	GLU
1	D	290	GLN
1	D	296	SER
1	D	343	ILE
1	D	369	ARG
1	D	374	PRO
1	D	410	GLU
1	D	414	SER
1	D	422	ILE
1	D	425	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	79	ASN
1	A	89	GLN
1	A	122	HIS
1	A	125	ASN
1	A	134	GLN
1	A	140	ASN
1	A	169	HIS
1	A	191	ASN
1	A	290	GLN

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Mol	Chain	Res	Type
1	A	314	GLN
1	A	387	GLN
1	A	401	GLN
1	B	12	GLN
1	B	22	GLN
1	B	49	GLN
1	B	79	ASN
1	B	89	GLN
1	B	122	HIS
1	B	125	ASN
1	B	134	GLN
1	B	140	ASN
1	B	169	HIS
1	B	191	ASN
1	B	314	GLN
1	C	12	GLN
1	C	15	GLN
1	C	49	GLN
1	C	79	ASN
1	C	89	GLN
1	C	122	HIS
1	C	125	ASN
1	C	134	GLN
1	C	140	ASN
1	C	169	HIS
1	C	191	ASN
1	C	314	GLN
1	C	401	GLN
1	D	12	GLN
1	D	49	GLN
1	D	79	ASN
1	D	122	HIS
1	D	125	ASN
1	D	134	GLN
1	D	140	ASN
1	D	169	HIS
1	D	191	ASN
1	D	314	GLN

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7   Other polymers ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9
1	A	394/426 (92%)	-0.26	6 (1%) 73	73	12, 21, 48, 96	0
1	B	394/426 (92%)	-0.38	2 (0%) 91	90	12, 19, 42, 62	0
1	C	393/426 (92%)	-0.34	3 (0%) 86	86	11, 20, 45, 69	0
1	D	394/426 (92%)	-0.20	9 (2%) 60	59	14, 22, 49, 87	0
All	All	1575/1704 (92%)	-0.29	20 (1%) 77	77	11, 21, 48, 96	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	301	TRP	3.8
1	A	425	ARG	3.6
1	D	425	ARG	3.2
1	B	301	TRP	3.2
1	D	241	GLY	3.0
1	A	422	ILE	3.0
1	A	302	ASP	2.8
1	A	72	ASN	2.8
1	A	301	TRP	2.6
1	D	303	SER	2.5
1	B	303	SER	2.4
1	C	111	THR	2.3
1	D	192	ILE	2.2
1	D	302	ASP	2.2
1	D	161	SER	2.2
1	D	374	PRO	2.1
1	A	303	SER	2.1
1	C	240	ILE	2.1
1	D	422	ILE	2.1
1	C	132	ALA	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	C	450	1/1	0.96	0.06	40,40,40,40	1
2	ZN	D	450	1/1	0.97	0.05	39,39,39,39	1
2	ZN	A	450	1/1	0.98	0.06	31,31,31,31	1
2	ZN	B	450	1/1	0.99	0.04	26,26,26,26	1

6.5 Other polymers ⓘ

There are no such residues in this entry.