



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:32 AM UTC

PDB ID : 7AC0 / pdb_00007ac0
Title : Epoxide hydrolase CorEH without ligand
Authors : Palm, G.J.; Lammers, M.; Berndt, L.
Deposited on : 2020-09-09
Resolution : 2.18 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

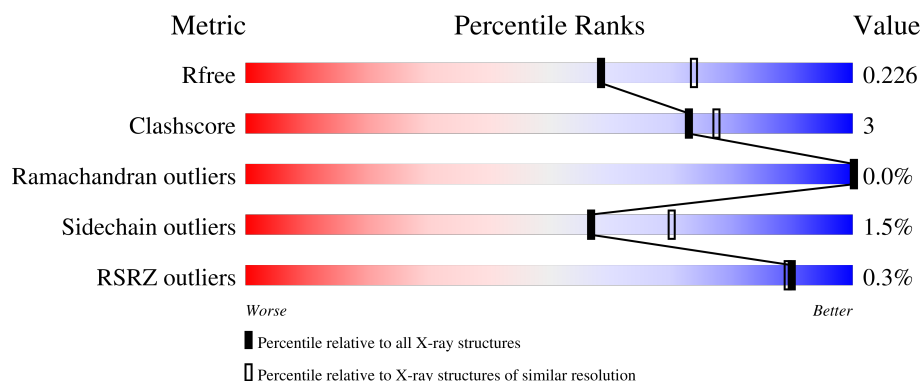
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	304	 83% 11% 7%
1	BBB	304	 81% 12% 7%
1	CCC	304	 78% 15% 7%
1	DDD	304	 79% 14% 7%
1	EEE	304	 83% 10% 7%

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Mol	Chain	Length	Quality of chain
1	FFF	304	 82% 12% 7%
1	GGG	304	 86% 8% 7%
1	HHH	304	 82% 11% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 36845 atoms, of which 17583 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 Soluble epoxide hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	284	Total	C	H	N	O	S	62	2	0
			4467	1465	2198	381	414	9			
1	BBB	283	Total	C	H	N	O	S	61	2	0
			4459	1462	2195	380	413	9			
1	CCC	284	Total	C	H	N	O	S	62	5	0
			4515	1479	2224	384	419	9			
1	DDD	284	Total	C	H	N	O	S	62	0	0
			4443	1457	2185	381	412	8			
1	EEE	283	Total	C	H	N	O	S	61	0	0
			4435	1454	2182	380	411	8			
1	FFF	284	Total	C	H	N	O	S	62	1	0
			4462	1462	2197	381	413	9			
1	GGG	284	Total	C	H	N	O	S	62	2	0
			4473	1466	2202	381	415	9			
1	HHH	283	Total	C	H	N	O	S	61	3	0
			4470	1466	2200	380	415	9			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-17	MET	-	initiating methionine	UNP O52866
AAA	-16	GLY	-	expression tag	UNP O52866
AAA	-15	SER	-	expression tag	UNP O52866
AAA	-14	SER	-	expression tag	UNP O52866
AAA	-13	HIS	-	expression tag	UNP O52866
AAA	-12	HIS	-	expression tag	UNP O52866
AAA	-11	HIS	-	expression tag	UNP O52866
AAA	-10	HIS	-	expression tag	UNP O52866
AAA	-9	HIS	-	expression tag	UNP O52866
AAA	-8	HIS	-	expression tag	UNP O52866
AAA	-7	GLY	-	expression tag	UNP O52866
AAA	-6	LEU	-	expression tag	UNP O52866
AAA	-5	VAL	-	expression tag	UNP O52866

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-4	PRO	-	expression tag	UNP O52866
AAA	-3	ARG	-	expression tag	UNP O52866
AAA	-2	GLY	-	expression tag	UNP O52866
AAA	-1	SER	-	expression tag	UNP O52866
AAA	0	HIS	-	expression tag	UNP O52866
BBB	-17	MET	-	initiating methionine	UNP O52866
BBB	-16	GLY	-	expression tag	UNP O52866
BBB	-15	SER	-	expression tag	UNP O52866
BBB	-14	SER	-	expression tag	UNP O52866
BBB	-13	HIS	-	expression tag	UNP O52866
BBB	-12	HIS	-	expression tag	UNP O52866
BBB	-11	HIS	-	expression tag	UNP O52866
BBB	-10	HIS	-	expression tag	UNP O52866
BBB	-9	HIS	-	expression tag	UNP O52866
BBB	-8	HIS	-	expression tag	UNP O52866
BBB	-7	GLY	-	expression tag	UNP O52866
BBB	-6	LEU	-	expression tag	UNP O52866
BBB	-5	VAL	-	expression tag	UNP O52866
BBB	-4	PRO	-	expression tag	UNP O52866
BBB	-3	ARG	-	expression tag	UNP O52866
BBB	-2	GLY	-	expression tag	UNP O52866
BBB	-1	SER	-	expression tag	UNP O52866
BBB	0	HIS	-	expression tag	UNP O52866
CCC	-17	MET	-	initiating methionine	UNP O52866
CCC	-16	GLY	-	expression tag	UNP O52866
CCC	-15	SER	-	expression tag	UNP O52866
CCC	-14	SER	-	expression tag	UNP O52866
CCC	-13	HIS	-	expression tag	UNP O52866
CCC	-12	HIS	-	expression tag	UNP O52866
CCC	-11	HIS	-	expression tag	UNP O52866
CCC	-10	HIS	-	expression tag	UNP O52866
CCC	-9	HIS	-	expression tag	UNP O52866
CCC	-8	HIS	-	expression tag	UNP O52866
CCC	-7	GLY	-	expression tag	UNP O52866
CCC	-6	LEU	-	expression tag	UNP O52866
CCC	-5	VAL	-	expression tag	UNP O52866
CCC	-4	PRO	-	expression tag	UNP O52866
CCC	-3	ARG	-	expression tag	UNP O52866
CCC	-2	GLY	-	expression tag	UNP O52866
CCC	-1	SER	-	expression tag	UNP O52866
CCC	0	HIS	-	expression tag	UNP O52866
DDD	-17	MET	-	initiating methionine	UNP O52866

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	-16	GLY	-	expression tag	UNP O52866
DDD	-15	SER	-	expression tag	UNP O52866
DDD	-14	SER	-	expression tag	UNP O52866
DDD	-13	HIS	-	expression tag	UNP O52866
DDD	-12	HIS	-	expression tag	UNP O52866
DDD	-11	HIS	-	expression tag	UNP O52866
DDD	-10	HIS	-	expression tag	UNP O52866
DDD	-9	HIS	-	expression tag	UNP O52866
DDD	-8	HIS	-	expression tag	UNP O52866
DDD	-7	GLY	-	expression tag	UNP O52866
DDD	-6	LEU	-	expression tag	UNP O52866
DDD	-5	VAL	-	expression tag	UNP O52866
DDD	-4	PRO	-	expression tag	UNP O52866
DDD	-3	ARG	-	expression tag	UNP O52866
DDD	-2	GLY	-	expression tag	UNP O52866
DDD	-1	SER	-	expression tag	UNP O52866
DDD	0	HIS	-	expression tag	UNP O52866
EEE	-17	MET	-	initiating methionine	UNP O52866
EEE	-16	GLY	-	expression tag	UNP O52866
EEE	-15	SER	-	expression tag	UNP O52866
EEE	-14	SER	-	expression tag	UNP O52866
EEE	-13	HIS	-	expression tag	UNP O52866
EEE	-12	HIS	-	expression tag	UNP O52866
EEE	-11	HIS	-	expression tag	UNP O52866
EEE	-10	HIS	-	expression tag	UNP O52866
EEE	-9	HIS	-	expression tag	UNP O52866
EEE	-8	HIS	-	expression tag	UNP O52866
EEE	-7	GLY	-	expression tag	UNP O52866
EEE	-6	LEU	-	expression tag	UNP O52866
EEE	-5	VAL	-	expression tag	UNP O52866
EEE	-4	PRO	-	expression tag	UNP O52866
EEE	-3	ARG	-	expression tag	UNP O52866
EEE	-2	GLY	-	expression tag	UNP O52866
EEE	-1	SER	-	expression tag	UNP O52866
EEE	0	HIS	-	expression tag	UNP O52866
FFF	-17	MET	-	initiating methionine	UNP O52866
FFF	-16	GLY	-	expression tag	UNP O52866
FFF	-15	SER	-	expression tag	UNP O52866
FFF	-14	SER	-	expression tag	UNP O52866
FFF	-13	HIS	-	expression tag	UNP O52866
FFF	-12	HIS	-	expression tag	UNP O52866
FFF	-11	HIS	-	expression tag	UNP O52866

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Chain	Residue	Modelled	Actual	Comment	Reference
FFF	-10	HIS	-	expression tag	UNP O52866
FFF	-9	HIS	-	expression tag	UNP O52866
FFF	-8	HIS	-	expression tag	UNP O52866
FFF	-7	GLY	-	expression tag	UNP O52866
FFF	-6	LEU	-	expression tag	UNP O52866
FFF	-5	VAL	-	expression tag	UNP O52866
FFF	-4	PRO	-	expression tag	UNP O52866
FFF	-3	ARG	-	expression tag	UNP O52866
FFF	-2	GLY	-	expression tag	UNP O52866
FFF	-1	SER	-	expression tag	UNP O52866
FFF	0	HIS	-	expression tag	UNP O52866
GGG	-17	MET	-	initiating methionine	UNP O52866
GGG	-16	GLY	-	expression tag	UNP O52866
GGG	-15	SER	-	expression tag	UNP O52866
GGG	-14	SER	-	expression tag	UNP O52866
GGG	-13	HIS	-	expression tag	UNP O52866
GGG	-12	HIS	-	expression tag	UNP O52866
GGG	-11	HIS	-	expression tag	UNP O52866
GGG	-10	HIS	-	expression tag	UNP O52866
GGG	-9	HIS	-	expression tag	UNP O52866
GGG	-8	HIS	-	expression tag	UNP O52866
GGG	-7	GLY	-	expression tag	UNP O52866
GGG	-6	LEU	-	expression tag	UNP O52866
GGG	-5	VAL	-	expression tag	UNP O52866
GGG	-4	PRO	-	expression tag	UNP O52866
GGG	-3	ARG	-	expression tag	UNP O52866
GGG	-2	GLY	-	expression tag	UNP O52866
GGG	-1	SER	-	expression tag	UNP O52866
GGG	0	HIS	-	expression tag	UNP O52866
HHH	-17	MET	-	initiating methionine	UNP O52866
HHH	-16	GLY	-	expression tag	UNP O52866
HHH	-15	SER	-	expression tag	UNP O52866
HHH	-14	SER	-	expression tag	UNP O52866
HHH	-13	HIS	-	expression tag	UNP O52866
HHH	-12	HIS	-	expression tag	UNP O52866
HHH	-11	HIS	-	expression tag	UNP O52866
HHH	-10	HIS	-	expression tag	UNP O52866
HHH	-9	HIS	-	expression tag	UNP O52866
HHH	-8	HIS	-	expression tag	UNP O52866
HHH	-7	GLY	-	expression tag	UNP O52866
HHH	-6	LEU	-	expression tag	UNP O52866
HHH	-5	VAL	-	expression tag	UNP O52866

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Chain	Residue	Modelled	Actual	Comment	Reference
HHH	-4	PRO	-	expression tag	UNP O52866
HHH	-3	ARG	-	expression tag	UNP O52866
HHH	-2	GLY	-	expression tag	UNP O52866
HHH	-1	SER	-	expression tag	UNP O52866
HHH	0	HIS	-	expression tag	UNP O52866

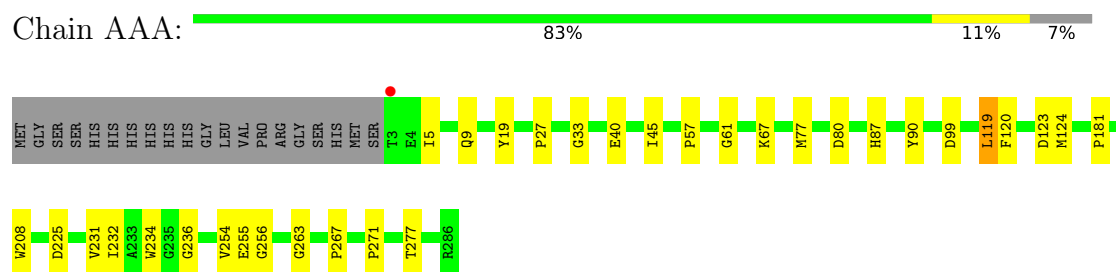
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	175	Total O 179 179	0	4
2	BBB	113	Total O 114 114	0	1
2	CCC	193	Total O 194 194	0	1
2	DDD	100	Total O 101 101	0	1
2	EEE	141	Total O 142 142	0	1
2	FFF	84	Total O 84 84	0	0
2	GGG	182	Total O 183 183	0	1
2	HHH	124	Total O 124 124	0	0

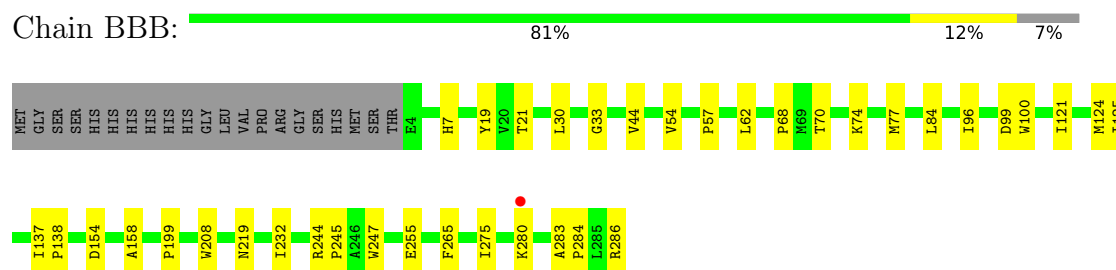
3 Residue-property plots [i](#)

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.

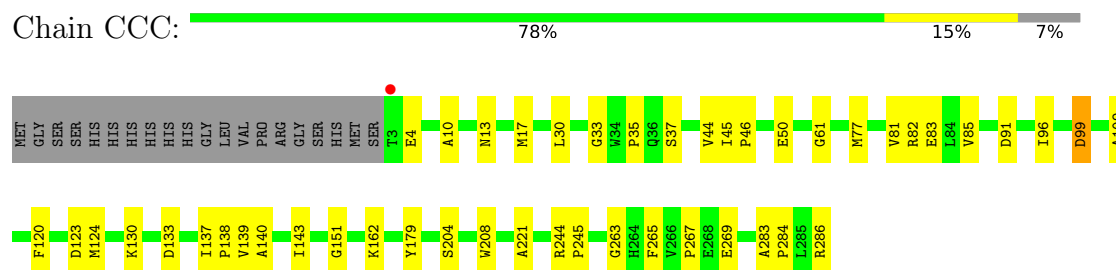
- Molecule 1: Soluble epoxide hydrolase



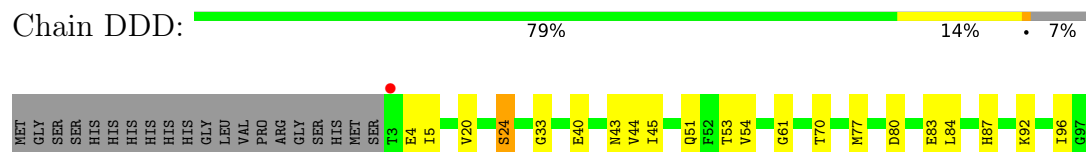
- Molecule 1: Soluble epoxide hydrolase



- Molecule 1: Soluble epoxide hydrolase



- Molecule 1: Soluble epoxide hydrolase





- Molecule 1: Soluble epoxide hydrolase

Chain EEE: 83% 10% 7%



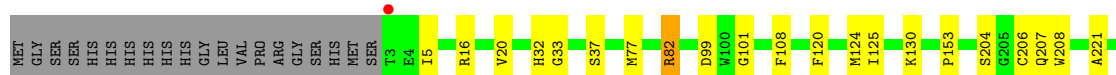
- Molecule 1: Soluble epoxide hydrolase

Chain FFF: 82% 12% 7%



- Molecule 1: Soluble epoxide hydrolase

Chain GGG: 86% 8% 7%



- Molecule 1: Soluble epoxide hydrolase

Chain HHH: 82% 11% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.02Å 156.57Å 112.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.39 – 2.18 47.39 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.39-2.18) 99.7 (47.39-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.173 , 0.226 0.173 , 0.226	Depositor DCC
R_{free} test set	6415 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36845	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	AAA	1.21	8/2343 (0.3%)	1.45	7/3191 (0.2%)
1	BBB	1.19	6/2338 (0.3%)	1.41	7/3184 (0.2%)
1	CCC	1.21	9/2374 (0.4%)	1.45	12/3232 (0.4%)
1	DDD	1.18	3/2326 (0.1%)	1.47	10/3169 (0.3%)
1	EEE	1.16	2/2321 (0.1%)	1.45	9/3162 (0.3%)
1	FFF	1.19	2/2336 (0.1%)	1.49	9/3182 (0.3%)
1	GGG	1.17	3/2345 (0.1%)	1.41	4/3194 (0.1%)
1	HHH	1.14	2/2347 (0.1%)	1.43	5/3196 (0.2%)
All	All	1.18	35/18730 (0.2%)	1.44	63/25510 (0.2%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	7	HIS	CE1-NE2	8.97	1.41	1.32
1	CCC	99	ASP	C-O	7.63	1.32	1.24
1	AAA	271	PRO	C-O	-7.23	1.14	1.24
1	BBB	68	PRO	C-O	-6.38	1.15	1.23
1	AAA	181	PRO	C-O	-6.32	1.17	1.23
1	FFF	174	THR	C-O	6.26	1.31	1.23
1	AAA	254	VAL	C-O	-6.14	1.17	1.24
1	AAA	263	GLY	C-O	5.99	1.29	1.23
1	CCC	17	MET	C-O	5.96	1.31	1.24
1	CCC	83[A]	GLU	C-O	5.89	1.31	1.24
1	CCC	83[B]	GLU	C-O	5.89	1.31	1.24
1	AAA	9	GLN	C-O	5.78	1.30	1.23
1	FFF	165	ASN	C-O	5.68	1.30	1.24
1	CCC	267	PRO	C-O	-5.53	1.17	1.24
1	DDD	24	SER	C-O	5.51	1.29	1.23
1	HHH	98	HIS	CE1-NE2	5.51	1.38	1.32
1	BBB	199	PRO	C-O	-5.50	1.16	1.24
1	GGG	204	SER	C-O	5.48	1.30	1.24
1	DDD	213	LEU	C-O	5.47	1.31	1.24
1	CCC	50	GLU	C-O	-5.43	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	87	HIS	C-O	-5.42	1.17	1.24
1	DDD	154	ASP	C-O	5.33	1.30	1.24
1	CCC	10	ALA	C-O	5.31	1.30	1.23
1	GGG	37	SER	C-O	5.23	1.30	1.24
1	BBB	154	ASP	C-O	5.22	1.30	1.24
1	AAA	124	MET	C-O	5.20	1.30	1.23
1	BBB	158	ALA	C-O	5.18	1.30	1.24
1	HHH	80	ASP	C-O	5.15	1.30	1.24
1	GGG	32	HIS	CE1-NE2	5.14	1.37	1.32
1	EEE	234	TRP	C-O	5.11	1.29	1.24
1	BBB	219	ASN	C-O	5.07	1.30	1.24
1	CCC	37	SER	C-O	-5.05	1.18	1.24
1	EEE	120	PHE	C-O	5.03	1.30	1.24
1	CCC	109	ALA	C-O	5.01	1.30	1.24
1	AAA	277	THR	C-O	5.01	1.29	1.24

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	44	VAL	CA-C-N	7.42	126.27	120.33
1	CCC	44	VAL	C-N-CA	7.42	126.27	120.33
1	DDD	265	PHE	CA-C-N	6.60	124.40	120.24
1	DDD	265	PHE	C-N-CA	6.60	124.40	120.24
1	BBB	265	PHE	CA-C-N	6.57	125.58	120.33
1	BBB	265	PHE	C-N-CA	6.57	125.58	120.33
1	DDD	44	VAL	N-CA-C	-6.22	106.70	111.62
1	EEE	136	PRO	CA-C-N	6.14	125.24	120.33
1	EEE	136	PRO	C-N-CA	6.14	125.24	120.33
1	DDD	44	VAL	CA-C-N	5.92	126.11	120.43
1	DDD	44	VAL	C-N-CA	5.92	126.11	120.43
1	DDD	101	GLY	CA-C-N	5.82	126.41	119.94
1	DDD	101	GLY	C-N-CA	5.82	126.41	119.94
1	CCC	4	GLU	CA-C-N	5.78	128.84	120.98
1	CCC	4	GLU	C-N-CA	5.78	128.84	120.98
1	CCC	263	GLY	CA-C-N	5.70	128.39	120.29
1	CCC	263	GLY	C-N-CA	5.70	128.39	120.29
1	CCC	13	ASN	CA-C-O	-5.63	115.31	121.84
1	CCC	140	ALA	CA-C-N	5.60	128.05	120.44
1	CCC	140	ALA	C-N-CA	5.60	128.05	120.44
1	AAA	236	GLY	CA-C-N	5.59	128.04	120.38
1	AAA	236	GLY	C-N-CA	5.59	128.04	120.38
1	BBB	275	ILE	CA-C-N	5.59	128.08	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	275	ILE	C-N-CA	5.59	128.08	120.54
1	CCC	133	ASP	CA-CB-CG	5.49	118.09	112.60
1	FFF	44	VAL	N-CA-C	-5.44	107.49	111.90
1	HHH	211	THR	CA-C-N	5.43	126.93	120.14
1	HHH	211	THR	C-N-CA	5.43	126.93	120.14
1	AAA	45	ILE	O-C-N	-5.43	116.94	120.42
1	FFF	211	THR	CA-C-N	5.38	126.92	120.13
1	FFF	211	THR	C-N-CA	5.38	126.92	120.13
1	AAA	225	ASP	CA-CB-CG	5.33	117.93	112.60
1	AAA	5	ILE	CA-C-O	-5.30	114.98	121.13
1	EEE	265	PHE	CA-C-N	5.28	124.56	120.33
1	EEE	265	PHE	C-N-CA	5.28	124.56	120.33
1	HHH	99	ASP	CA-CB-CG	5.26	117.86	112.60
1	GGG	239	PHE	CB-CA-C	5.22	120.82	110.42
1	GGG	101	GLY	CA-C-N	5.22	125.74	120.00
1	GGG	101	GLY	C-N-CA	5.22	125.74	120.00
1	FFF	223	ALA	CA-C-O	-5.16	115.97	122.63
1	FFF	78	ALA	CA-C-O	-5.15	115.09	120.55
1	HHH	38	TRP	CA-C-N	5.14	127.69	120.28
1	HHH	38	TRP	C-N-CA	5.14	127.69	120.28
1	CCC	265	PHE	CA-C-N	5.13	123.47	120.24
1	CCC	265	PHE	C-N-CA	5.13	123.47	120.24
1	FFF	277	THR	CA-C-N	5.11	127.39	120.65
1	FFF	277	THR	C-N-CA	5.11	127.39	120.65
1	AAA	119	LEU	CA-C-N	5.11	130.37	123.11
1	AAA	119	LEU	C-N-CA	5.11	130.37	123.11
1	EEE	123	ASP	CB-CA-C	5.11	120.08	112.06
1	GGG	108	PHE	N-CA-C	-5.09	105.64	111.14
1	EEE	67	LYS	CB-CA-C	5.08	119.53	111.15
1	EEE	263	GLY	CA-C-N	5.07	127.08	120.28
1	EEE	263	GLY	C-N-CA	5.07	127.08	120.28
1	FFF	86	SER	CA-C-N	5.07	127.33	120.38
1	FFF	86	SER	C-N-CA	5.07	127.33	120.38
1	DDD	43	ASN	CA-C-N	5.06	128.52	123.16
1	DDD	43	ASN	C-N-CA	5.06	128.52	123.16
1	EEE	215	GLU	CA-C-O	-5.05	115.49	120.90
1	BBB	44	VAL	N-CA-C	-5.04	107.81	111.90
1	DDD	129	ILE	CA-C-O	-5.01	117.30	120.66
1	BBB	84	LEU	CA-C-N	5.01	126.88	120.56
1	BBB	84	LEU	C-N-CA	5.01	126.88	120.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2269	2198	2188	10	0
1	BBB	2264	2195	2186	15	0
1	CCC	2291	2224	2218	17	0
1	DDD	2258	2185	2173	19	1
1	EEE	2253	2182	2171	18	0
1	FFF	2265	2197	2187	18	0
1	GGG	2271	2202	2193	9	1
1	HHH	2270	2200	2192	14	0
2	AAA	179	0	0	0	0
2	BBB	114	0	0	1	0
2	CCC	194	0	0	3	0
2	DDD	101	0	0	1	0
2	EEE	142	0	0	2	0
2	FFF	84	0	0	0	0
2	GGG	183	0	0	2	0
2	HHH	124	0	0	0	0
All	All	19262	17583	17508	114	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (114) 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:BBB:30:LEU:HD22	1:BBB:96:ILE:HD12	1.66	0.76
1:HHH:77[A]:MET:HE1	1:HHH:208:TRP:CZ2	2.25	0.71
1:EEE:77:MET:HE1	1:EEE:208:TRP:CZ2	2.27	0.70
1:GGG:16:ARG:HD3	2:GGG:367:HOH:O	1.91	0.69
1:DDD:83:GLU:OE1	2:DDD:301:HOH:O	2.09	0.68
2:EEE:348:HOH:O	1:FFF:137:ILE:HD12	1.94	0.67
1:DDD:130:LYS:HG2	1:DDD:220:LEU:HD23	1.77	0.67
1:CCC:82[B]:ARG:HD2	2:CCC:343:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:99:ASP:O	1:EEE:124:MET:HG2	1.97	0.65
1:BBB:77[A]:MET:HE1	1:BBB:208:TRP:CZ2	2.32	0.64
1:DDD:24:SER:HA	1:DDD:53:THR:OG1	1.98	0.64
1:FFF:214:ARG:O	1:FFF:217:THR:OG1	2.19	0.61
1:EEE:144:ASN:HD21	1:FFF:152:ASN:ND2	1.99	0.61
1:CCC:286:ARG:NH1	2:CCC:303:HOH:O	2.33	0.60
1:EEE:30:LEU:HD22	1:EEE:96:ILE:HD12	1.85	0.58
1:BBB:286:ARG:NE	2:BBB:301:HOH:O	1.96	0.58
1:FFF:77[A]:MET:HE1	1:FFF:208:TRP:CE2	2.39	0.57
1:FFF:77[A]:MET:HE1	1:FFF:208:TRP:CZ2	2.40	0.56
1:GGG:33:GLY:HA3	1:GGG:99:ASP:HB3	1.88	0.56
1:BBB:244:ARG:HB2	1:BBB:245:PRO:HD3	1.87	0.55
1:HHH:74:LYS:HE2	1:HHH:100:TRP:CE3	2.43	0.54
1:EEE:170:ARG:HH21	1:FFF:152:ASN:HD21	1.55	0.54
1:DDD:143:ILE:HD12	1:DDD:146:ILE:HD13	1.88	0.54
1:CCC:77[A]:MET:HE1	1:CCC:208:TRP:CZ2	2.43	0.53
1:EEE:232:ILE:HA	1:EEE:255:GLU:O	2.08	0.53
1:BBB:137:ILE:HB	1:BBB:138:PRO:HD3	1.91	0.52
1:AAA:234:TRP:CE2	1:AAA:256:GLY:HA2	2.45	0.51
1:CCC:77[A]:MET:HE1	1:CCC:208:TRP:CE2	2.45	0.51
1:CCC:244:ARG:HB3	1:CCC:245:PRO:HD3	1.92	0.50
1:DDD:45:ILE:HG12	1:DDD:54:VAL:HG11	1.92	0.50
1:HHH:266:VAL:N	1:HHH:267:PRO:CD	2.74	0.50
1:FFF:232:ILE:HA	1:FFF:255:GLU:O	2.12	0.50
1:BBB:33:GLY:HA3	1:BBB:99:ASP:HB3	1.94	0.49
1:FFF:19:TYR:HA	1:FFF:57:PRO:HA	1.94	0.49
1:CCC:91:ASP:OD1	2:CCC:301:HOH:O	2.19	0.49
1:FFF:231:VAL:O	1:FFF:254:VAL:HA	2.12	0.48
1:CCC:33:GLY:HA3	1:CCC:99:ASP:HB3	1.94	0.48
1:BBB:74:LYS:HE2	1:BBB:100:TRP:CE3	2.49	0.47
1:AAA:27:PRO:HG3	1:AAA:90:TYR:CD1	2.49	0.47
1:CCC:81:VAL:O	1:CCC:85:VAL:HG23	2.14	0.47
1:DDD:33:GLY:HA3	1:DDD:99:ASP:HB3	1.97	0.47
1:DDD:96:ILE:HA	1:DDD:120:PHE:O	2.14	0.47
1:BBB:62:LEU:HD22	1:BBB:208:TRP:CH2	2.49	0.47
1:CCC:179:TYR:HB3	1:CCC:269:GLU:OE2	2.14	0.47
1:CCC:30:LEU:HD22	1:CCC:96:ILE:HD12	1.95	0.47
1:EEE:170:ARG:HH21	1:FFF:152:ASN:ND2	2.12	0.47
1:HHH:232:ILE:HA	1:HHH:255:GLU:O	2.14	0.46
1:EEE:30:LEU:CD2	1:EEE:96:ILE:HD12	2.46	0.46
1:AAA:33:GLY:HA3	1:AAA:99:ASP:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:61:GLY:HA3	1:CCC:204:SER:HB3	1.97	0.46
1:HHH:124:MET:HG3	1:HHH:125:ILE:O	2.16	0.46
1:AAA:61:GLY:HA2	1:AAA:67:LYS:HG2	1.98	0.46
1:GGG:5:ILE:HG23	1:GGG:20:VAL:HB	1.97	0.46
1:HHH:96:ILE:HA	1:HHH:120:PHE:O	2.16	0.46
1:AAA:119:LEU:O	1:AAA:231:VAL:HA	2.17	0.45
1:CCC:139:VAL:O	1:CCC:143:ILE:HG12	2.16	0.45
1:EEE:59:LEU:O	1:EEE:60:ARG:C	2.58	0.45
1:HHH:143:ILE:O	1:HHH:146:ILE:HG12	2.15	0.45
1:GGG:207:GLN:NE2	2:GGG:309:HOH:O	2.50	0.45
1:DDD:266:VAL:N	1:DDD:267:PRO:CD	2.80	0.45
1:EEE:77:MET:HE1	1:EEE:208:TRP:CE2	2.51	0.45
1:CCC:283:ALA:N	1:CCC:284:PRO:CD	2.80	0.45
1:DDD:77:MET:HE1	1:DDD:208:TRP:CE2	2.51	0.45
1:CCC:45:ILE:N	1:CCC:46:PRO:CD	2.80	0.45
1:GGG:153:PRO:HB3	1:GGG:206:CYS:HB3	1.99	0.44
1:HHH:189:ILE:O	1:HHH:193:VAL:HG23	2.18	0.44
1:EEE:152:ASN:ND2	1:FFF:144:ASN:HD21	2.16	0.44
1:DDD:40:GLU:OE1	1:DDD:98:HIS:ND1	2.50	0.44
1:EEE:75:ARG:NH1	2:EEE:302:HOH:O	2.31	0.44
1:EEE:273:PHE:CD1	1:EEE:273:PHE:C	2.95	0.44
1:BBB:77[A]:MET:HE1	1:BBB:208:TRP:CE2	2.53	0.44
1:HHH:61:GLY:HA2	1:HHH:67:LYS:HG2	1.98	0.44
1:BBB:232:ILE:HA	1:BBB:255:GLU:O	2.17	0.44
1:EEE:74:LYS:HE2	1:EEE:100:TRP:CE3	2.52	0.44
1:BBB:283:ALA:N	1:BBB:284:PRO:CD	2.81	0.44
1:EEE:21:THR:HA	1:EEE:54:VAL:O	2.18	0.44
1:EEE:34:TRP:CE2	1:EEE:35:PRO:HB3	2.53	0.44
1:HHH:185:SER:O	1:HHH:189:ILE:HG13	2.18	0.44
1:GGG:130:LYS:HD2	1:GGG:221:ALA:HA	1.99	0.43
1:DDD:61:GLY:HA3	1:DDD:204:SER:HB3	2.01	0.43
1:FFF:74:LYS:HE2	1:FFF:100:TRP:CE3	2.53	0.43
1:GGG:244:ARG:HB2	1:GGG:245:PRO:HD3	2.01	0.43
1:CCC:137:ILE:N	1:CCC:138:PRO:HD2	2.34	0.43
1:DDD:283:ALA:HB3	1:DDD:284:PRO:HD3	2.00	0.43
1:GGG:77[A]:MET:HE1	1:GGG:208:TRP:CZ2	2.54	0.43
1:BBB:124:MET:HG3	1:BBB:125:ILE:O	2.18	0.42
1:DDD:5:ILE:HD12	1:DDD:5:ILE:H	1.84	0.42
1:DDD:5:ILE:CG2	1:DDD:20:VAL:HB	2.49	0.42
1:CCC:130:LYS:HD2	1:CCC:221:ALA:HA	2.00	0.42
1:BBB:21:THR:HA	1:BBB:54:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:142:MET:HE1	1:DDD:240:LEU:HD23	2.02	0.42
1:FFF:29:VAL:C	1:FFF:30:LEU:HD23	2.45	0.42
1:CCC:99:ASP:O	1:CCC:124:MET:HG2	2.19	0.42
1:HHH:77[A]:MET:HE1	1:HHH:208:TRP:CE2	2.54	0.41
1:HHH:29:VAL:C	1:HHH:30:LEU:HD23	2.44	0.41
1:AAA:19:TYR:HA	1:AAA:57:PRO:HA	2.01	0.41
1:AAA:40:GLU:OE1	1:AAA:267:PRO:HG2	2.20	0.41
1:AAA:77[A]:MET:HE1	1:AAA:208:TRP:CZ2	2.56	0.41
1:HHH:37:SER:C	1:HHH:39:TYR:N	2.78	0.41
1:DDD:84:LEU:O	1:DDD:87:HIS:HB3	2.21	0.41
1:DDD:155:TRP:CE3	1:EEE:199:PRO:HG2	2.54	0.41
1:HHH:244:ARG:CB	1:HHH:245:PRO:HD3	2.50	0.41
1:DDD:92:LYS:HD2	1:DDD:117:GLU:CD	2.46	0.41
1:FFF:33:GLY:HA3	1:FFF:99:ASP:HB3	2.03	0.41
1:BBB:121:ILE:HG21	1:BBB:247:TRP:CZ2	2.55	0.41
1:EEE:144:ASN:HD21	1:FFF:152:ASN:HD22	1.69	0.41
1:GGG:124:MET:HG3	1:GGG:125:ILE:O	2.21	0.41
1:FFF:137:ILE:HB	1:FFF:138:PRO:HD3	2.03	0.41
1:BBB:19:TYR:HA	1:BBB:57:PRO:HA	2.03	0.40
1:DDD:77:MET:O	1:DDD:80:ASP:HB2	2.21	0.40
1:FFF:283:ALA:N	1:FFF:284:PRO:CD	2.84	0.40
1:FFF:26:TYR:CE2	1:FFF:285:LEU:HD13	2.56	0.40
1:AAA:232:ILE:HG22	1:AAA:255:GLU:HB2	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:24:SER:HG	1:GGG:82:ARG:HH12[4_557]	1.27	0.33

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	AAA	284/304 (93%)	270 (95%)	14 (5%)	0	100	100
1	BBB	283/304 (93%)	268 (95%)	15 (5%)	0	100	100
1	CCC	287/304 (94%)	274 (96%)	12 (4%)	1 (0%)	36	39
1	DDD	282/304 (93%)	267 (95%)	15 (5%)	0	100	100
1	EEE	281/304 (92%)	264 (94%)	17 (6%)	0	100	100
1	FFF	283/304 (93%)	270 (95%)	13 (5%)	0	100	100
1	GGG	284/304 (93%)	270 (95%)	14 (5%)	0	100	100
1	HHH	284/304 (93%)	269 (95%)	15 (5%)	0	100	100
All	All	2268/2432 (93%)	2152 (95%)	115 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CCC	151	GLY

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	AAA	238/254 (94%)	236 (99%)	2 (1%)	73	83
1	BBB	238/254 (94%)	236 (99%)	2 (1%)	73	83
1	CCC	242/254 (95%)	238 (98%)	4 (2%)	53	66
1	DDD	236/254 (93%)	230 (98%)	6 (2%)	42	53
1	EEE	236/254 (93%)	233 (99%)	3 (1%)	61	74
1	FFF	238/254 (94%)	233 (98%)	5 (2%)	47	59
1	GGG	239/254 (94%)	237 (99%)	2 (1%)	73	83
1	HHH	239/254 (94%)	235 (98%)	4 (2%)	53	66
All	All	1906/2032 (94%)	1878 (98%)	28 (2%)	57	70

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	120	PHE
1	AAA	123	ASP
1	BBB	70	THR
1	BBB	280	LYS
1	CCC	35	PRO
1	CCC	120	PHE
1	CCC	123	ASP
1	CCC	162	LYS
1	DDD	4	GLU
1	DDD	51	GLN
1	DDD	70	THR
1	DDD	103	SER
1	DDD	120	PHE
1	DDD	182	ASN
1	EEE	120	PHE
1	EEE	162	LYS
1	EEE	249	GLU
1	FFF	3	THR
1	FFF	6	THR
1	FFF	70	THR
1	FFF	86	SER
1	FFF	286	ARG
1	GGG	82	ARG
1	GGG	120	PHE
1	HHH	86	SER
1	HHH	120	PHE
1	HHH	123	ASP
1	HHH	162	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	284/304 (93%)	-0.83	1 (0%) 88 88	15, 28, 43, 59	2 (0%)
1	BBB	283/304 (93%)	-0.46	1 (0%) 88 88	20, 41, 58, 80	2 (0%)
1	CCC	284/304 (93%)	-0.82	1 (0%) 88 88	14, 27, 40, 70	5 (1%)
1	DDD	284/304 (93%)	-0.43	1 (0%) 88 88	27, 42, 61, 88	0
1	EEE	283/304 (93%)	-0.64	0 100 100	24, 35, 51, 65	0
1	FFF	284/304 (93%)	-0.34	1 (0%) 88 88	23, 44, 63, 79	1 (0%)
1	GGG	284/304 (93%)	-0.84	1 (0%) 88 88	15, 28, 40, 63	2 (0%)
1	HHH	283/304 (93%)	-0.66	0 100 100	19, 36, 50, 67	3 (1%)
All	All	2269/2432 (93%)	-0.63	6 (0%) 90 89	14, 35, 55, 88	15 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	3	THR	4.9
1	AAA	3	THR	4.3
1	FFF	3	THR	3.8
1	CCC	3	THR	2.7
1	BBB	280	LYS	2.6
1	GGG	3	THR	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.