



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:52 PM UTC

PDB ID : 2Q4X / pdb_00002q4x
Title : Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At3g16990
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-31
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 ⓘ 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

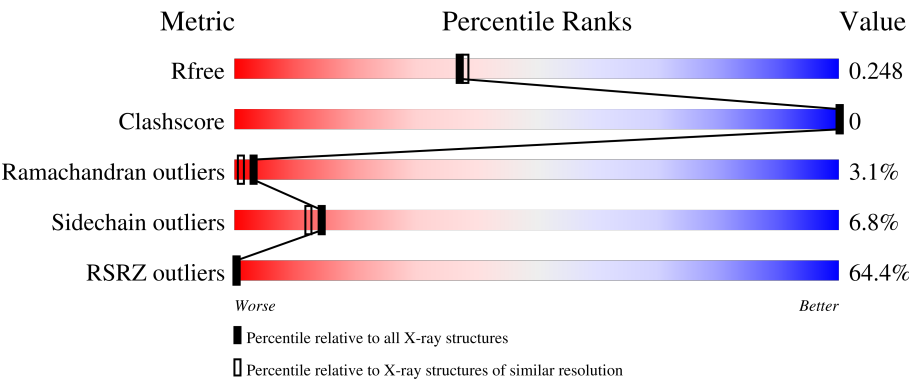
1 Overall quality at a glance i

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	1-A	221	57% 89%8%
1	1-B	221	65% 89%6%5%
1	2-A	221	90%8%
1	2-B	221	87%8%5%
1	3-A	221	88%9%

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Mol	Chain	Length	Quality of chain
1	3-B	221	 86% 9% 5%
1	4-A	221	 88% 9% .
1	4-B	221	 90% 5% 5%
1	5-A	221	 88% 9% .
1	5-B	221	 88% 7% 5%
1	6-A	221	 88% 9% . .
1	6-B	221	 87% 7% . 5%
1	7-A	221	 90% 7% .
1	7-B	221	 85% 10% 5%
1	8-A	221	 88% 9% .
1	8-B	221	 87% 9% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HMH	1-A	1300	-	X	-	-
3	HMH	1-B	1301	-	X	-	-
3	HMH	2-A	1300	-	X	-	-
3	HMH	2-B	1301	-	X	-	-
3	HMH	3-A	1300	-	X	-	-
3	HMH	3-B	1301	-	X	-	-
3	HMH	4-A	1300	-	X	-	-
3	HMH	4-B	1301	-	X	-	-
3	HMH	5-A	1300	-	X	-	-
3	HMH	5-B	1301	-	X	-	-
3	HMH	6-A	1300	-	X	-	-
3	HMH	6-B	1301	-	X	-	-
3	HMH	7-A	1300	-	X	-	-
3	HMH	7-B	1301	-	X	-	-
3	HMH	8-A	1300	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30952 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 Seed maturation protein PM36 homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	215	Total	C	N	O	S	Se	0	0	0
			1714	1087	291	327	5	4			
1	2-A	215	Total	C	N	O	S	Se	0	0	0
			1714	1087	291	327	5	4			
1	3-A	215	Total	C	N	O	S	Se	0	0	0
			1714	1087	291	327	5	4			
1	4-A	215	Total	C	N	O	S	Se	0	0	0
			1714	1087	291	327	5	4			
1	5-A	215	Total	C	N	O	S	Se	0	0	0
			1714	1087	291	327	5	4			
1	6-A	215	Total	C	N	O	S	Se	0	0	0
			1714	1087	291	327	5	4			
1	7-A	215	Total	C	N	O	S	Se	0	0	0
			1714	1087	291	327	5	4			
1	8-A	215	Total	C	N	O	S	Se	0	0	0
			1714	1087	291	327	5	4			
1	1-B	211	Total	C	N	O	S	Se	0	0	0
			1688	1072	289	318	5	4			
1	2-B	211	Total	C	N	O	S	Se	0	0	0
			1688	1072	289	318	5	4			
1	3-B	211	Total	C	N	O	S	Se	0	0	0
			1688	1072	289	318	5	4			
1	4-B	211	Total	C	N	O	S	Se	0	0	0
			1688	1072	289	318	5	4			
1	5-B	211	Total	C	N	O	S	Se	0	0	0
			1688	1072	289	318	5	4			
1	6-B	211	Total	C	N	O	S	Se	0	0	0
			1688	1072	289	318	5	4			
1	7-B	211	Total	C	N	O	S	Se	0	0	0
			1688	1072	289	318	5	4			
1	8-B	211	Total	C	N	O	S	Se	0	0	0
			1688	1072	289	318	5	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9ASY9
A	21	ALA	SER	engineered mutation	UNP Q9ASY9
A	75	MSE	MET	modified residue	UNP Q9ASY9
A	123	MSE	MET	modified residue	UNP Q9ASY9
A	133	MSE	MET	modified residue	UNP Q9ASY9
A	216	MSE	MET	modified residue	UNP Q9ASY9
B	1	MSE	MET	modified residue	UNP Q9ASY9
B	21	ALA	SER	engineered mutation	UNP Q9ASY9
B	75	MSE	MET	modified residue	UNP Q9ASY9
B	123	MSE	MET	modified residue	UNP Q9ASY9
B	133	MSE	MET	modified residue	UNP Q9ASY9
B	216	MSE	MET	modified residue	UNP Q9ASY9

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	1	Total O S 5 4 1	0	0
2	2-A	1	Total O S 5 4 1	0	0
2	3-A	1	Total O S 5 4 1	0	0
2	4-A	1	Total O S 5 4 1	0	0
2	5-A	1	Total O S 5 4 1	0	0

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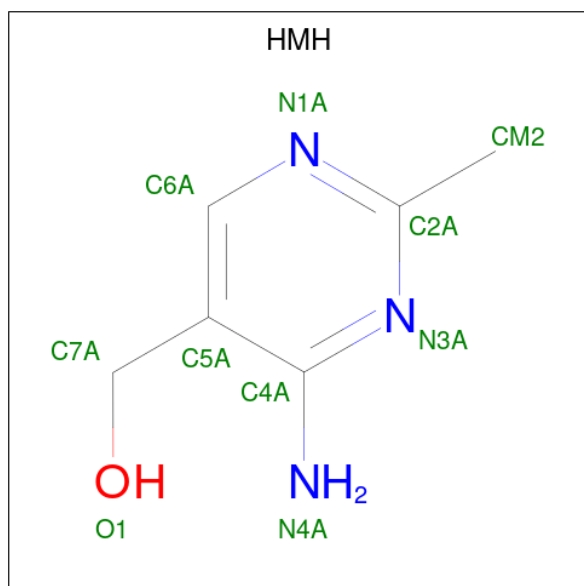
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	6-A	1	Total	O	S	0	0
			5	4	1		
2	7-A	1	Total	O	S	0	0
			5	4	1		
2	8-A	1	Total	O	S	0	0
			5	4	1		
2	1-B	1	Total	O	S	0	0
			5	4	1		
2	2-B	1	Total	O	S	0	0
			5	4	1		
2	3-B	1	Total	O	S	0	0
			5	4	1		
2	4-B	1	Total	O	S	0	0
			5	4	1		
2	5-B	1	Total	O	S	0	0
			5	4	1		
2	6-B	1	Total	O	S	0	0
			5	4	1		
2	7-B	1	Total	O	S	0	0
			5	4	1		
2	8-B	1	Total	O	S	0	0
			5	4	1		
2	1-B	1	Total	O	S	0	0
			5	4	1		
2	2-B	1	Total	O	S	0	0
			5	4	1		
2	3-B	1	Total	O	S	0	0
			5	4	1		
2	4-B	1	Total	O	S	0	0
			5	4	1		
2	5-B	1	Total	O	S	0	0
			5	4	1		
2	6-B	1	Total	O	S	0	0
			5	4	1		
2	7-B	1	Total	O	S	0	0
			5	4	1		
2	8-B	1	Total	O	S	0	0
			5	4	1		
2	1-B	1	Total	O	S	0	0
			5	4	1		
2	2-B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	3-B	1	Total	O	S	0	0
			5	4	1		
2	4-B	1	Total	O	S	0	0
			5	4	1		
2	5-B	1	Total	O	S	0	0
			5	4	1		
2	6-B	1	Total	O	S	0	0
			5	4	1		
2	7-B	1	Total	O	S	0	0
			5	4	1		
2	8-B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 4-AMINO-5-HYDROXYMETHYL-2-METHYLPYRIMIDINE (CCD ID: HMH) (formula: C₆H₉N₃O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	1-A	1	Total	C	N	O	0	0
			10	6	3	1		
3	2-A	1	Total	C	N	O	0	0
			10	6	3	1		
3	3-A	1	Total	C	N	O	0	0
			10	6	3	1		
3	4-A	1	Total	C	N	O	0	0
			10	6	3	1		
3	5-A	1	Total	C	N	O	0	0
			10	6	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	6-A	1	Total	C	N	O	0	0
			10	6	3	1		
3	7-A	1	Total	C	N	O	0	0
			10	6	3	1		
3	8-A	1	Total	C	N	O	0	0
			10	6	3	1		
3	1-B	1	Total	C	N	O	0	0
			10	6	3	1		
3	2-B	1	Total	C	N	O	0	0
			10	6	3	1		
3	3-B	1	Total	C	N	O	0	0
			10	6	3	1		
3	4-B	1	Total	C	N	O	0	0
			10	6	3	1		
3	5-B	1	Total	C	N	O	0	0
			10	6	3	1		
3	6-B	1	Total	C	N	O	0	0
			10	6	3	1		
3	7-B	1	Total	C	N	O	0	0
			10	6	3	1		
3	8-B	1	Total	C	N	O	0	0
			10	6	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	213	Total	O	0	0
			213	213		
4	2-A	214	Total	O	0	0
			214	214		
4	3-A	214	Total	O	0	0
			214	214		
4	4-A	214	Total	O	0	0
			214	214		
4	5-A	213	Total	O	0	0
			213	213		
4	6-A	214	Total	O	0	0
			214	214		
4	7-A	214	Total	O	0	0
			214	214		
4	8-A	214	Total	O	0	0
			214	214		

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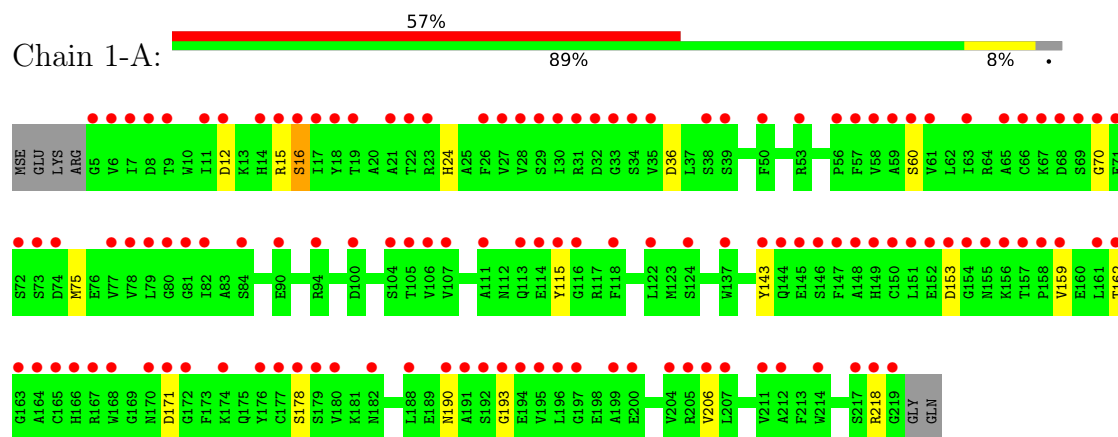
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-B	214	Total 214	O 214	0	0
4	2-B	213	Total 213	O 213	0	0
4	3-B	213	Total 213	O 213	0	0
4	4-B	213	Total 213	O 213	0	0
4	5-B	214	Total 214	O 214	0	0
4	6-B	213	Total 213	O 213	0	0
4	7-B	213	Total 213	O 213	0	0
4	8-B	213	Total 213	O 213	0	0

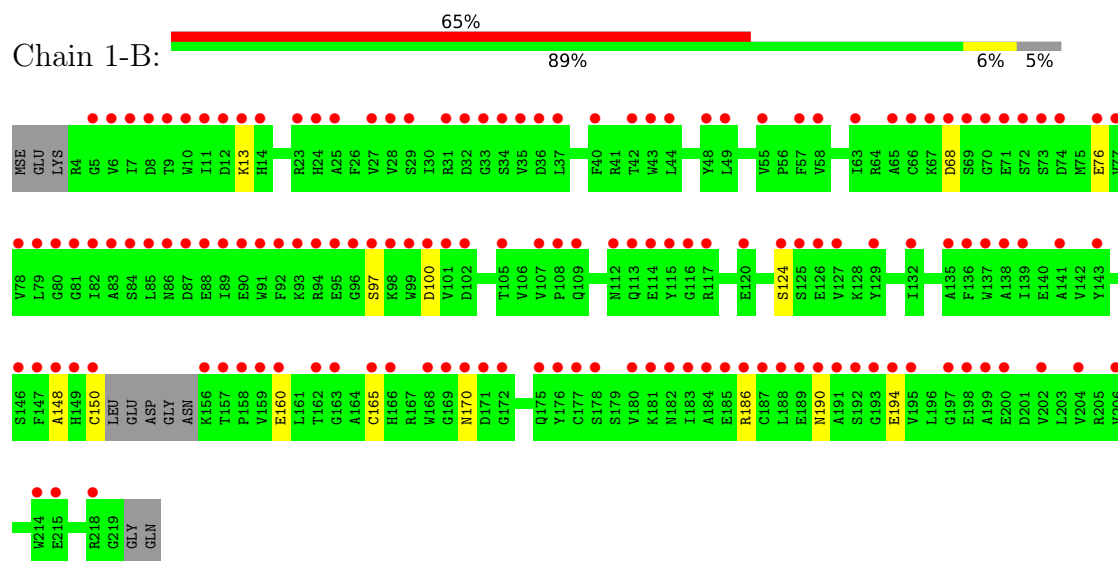
3 Residue-property plots [i](#)

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.

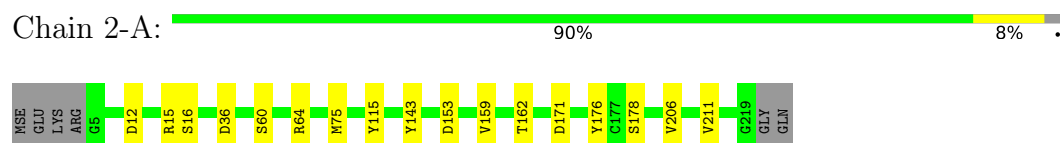
- Molecule 1: Seed maturation protein PM36 homolog



- Molecule 1: Seed maturation protein PM36 homolog

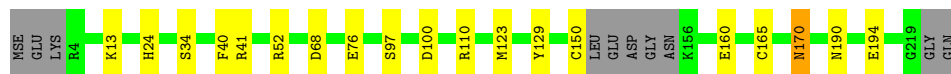


- Molecule 1: Seed maturation protein PM36 homolog



- Molecule 1: Seed maturation protein PM36 homolog

Chain 2-B:  87% 8% 5%



- Molecule 1: Seed maturation protein PM36 homolog

Chain 3-A:  88% 9% .



- Molecule 1: Seed maturation protein PM36 homolog

Chain 3-B:  86% 9% 5%



- Molecule 1: Seed maturation protein PM36 homolog

Chain 4-A:  88% 9% .



- Molecule 1: Seed maturation protein PM36 homolog

Chain 4-B:  90% 5% 5%



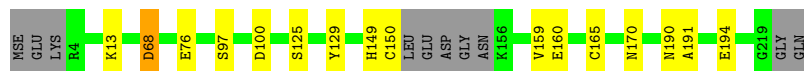
- Molecule 1: Seed maturation protein PM36 homolog

Chain 5-A:  88% 9% .



- Molecule 1: Seed maturation protein PM36 homolog

Chain 5-B:  88% 7% 5%



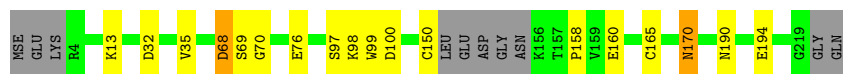
- Molecule 1: Seed maturation protein PM36 homolog

Chain 6-A:  88% 9% . .



- Molecule 1: Seed maturation protein PM36 homolog

Chain 6-B:  87% 7% . 5%



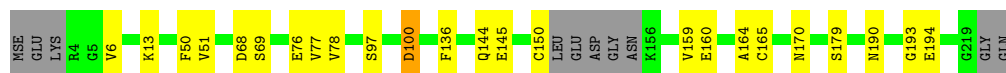
- Molecule 1: Seed maturation protein PM36 homolog

Chain 7-A:  90% 7% .



- Molecule 1: Seed maturation protein PM36 homolog

Chain 7-B:  85% 10% 5%



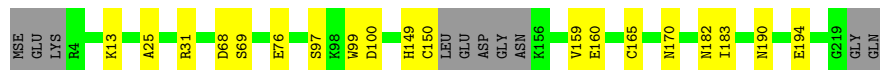
- Molecule 1: Seed maturation protein PM36 homolog

Chain 8-A:  88% 9% .



- Molecule 1: Seed maturation protein PM36 homolog

Chain 8-B:  87% 9% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	62.70Å 62.70Å 287.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.04 – 2.10 28.04 – 2.10	Depositor EDS
% Data completeness (in resolution range)	86.4 (28.04-2.10) 86.4 (28.04-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.46 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.136 , 0.231 0.154 , 0.248	Depositor DCC
R_{free} test set	1519 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.05 , 72.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	30952	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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

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

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	1-A	0.39	0/1749	0.33	0/2362
1	1-B	0.39	0/1722	0.34	0/2323
1	2-A	0.39	0/1749	0.33	0/2362
1	2-B	0.39	0/1722	0.34	0/2323
1	3-A	0.39	0/1749	0.33	0/2362
1	3-B	0.39	0/1722	0.34	0/2323
1	4-A	0.39	0/1749	0.33	0/2362
1	4-B	0.39	0/1722	0.34	0/2323
1	5-A	0.39	0/1749	0.33	0/2362
1	5-B	0.39	0/1722	0.34	0/2323
1	6-A	0.39	0/1749	0.33	0/2362
1	6-B	0.39	0/1722	0.34	0/2323
1	7-A	0.39	0/1749	0.33	0/2362
1	7-B	0.39	0/1722	0.34	0/2323
1	8-A	0.39	0/1749	0.33	0/2362
1	8-B	0.39	0/1722	0.34	0/2323
All	All	0.39	0/27768	0.33	0/37480

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2-A	0	1
1	2-B	0	1
1	3-B	0	1
1	4-B	0	1
1	5-B	0	1
1	6-A	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2-A	176	TYR	Sidechain
1	2-B	129	TYR	Sidechain
1	3-B	129	TYR	Sidechain
1	4-B	129	TYR	Sidechain
1	5-B	129	TYR	Sidechain
1	6-A	143	TYR	Sidechain

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	1-A	1714	0	1642	0	0
1	1-B	1688	0	1624	0	0
1	2-A	1714	0	1642	0	0
1	2-B	1688	0	1624	0	0
1	3-A	1714	0	1642	0	0
1	3-B	1688	0	1624	0	0
1	4-A	1714	0	1642	0	0
1	4-B	1688	0	1624	0	0
1	5-A	1714	0	1642	0	0
1	5-B	1688	0	1624	0	0
1	6-A	1714	0	1642	0	0
1	6-B	1688	0	1624	0	0
1	7-A	1714	0	1642	0	0
1	7-B	1688	0	1624	0	0
1	8-A	1714	0	1642	0	0
1	8-B	1688	0	1624	0	0
2	1-A	5	0	0	0	0
2	1-B	15	0	0	0	0
2	2-A	5	0	0	0	0
2	2-B	15	0	0	0	0
2	3-A	5	0	0	0	0
2	3-B	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	4-A	5	0	0	0	0
2	4-B	15	0	0	0	0
2	5-A	5	0	0	0	0
2	5-B	15	0	0	0	0
2	6-A	5	0	0	0	0
2	6-B	15	0	0	0	0
2	7-A	5	0	0	0	0
2	7-B	15	0	0	0	0
2	8-A	5	0	0	0	0
2	8-B	15	0	0	0	0
3	1-A	10	0	8	0	0
3	1-B	10	0	9	0	0
3	2-A	10	0	8	0	0
3	2-B	10	0	9	0	0
3	3-A	10	0	8	0	0
3	3-B	10	0	9	0	0
3	4-A	10	0	8	0	0
3	4-B	10	0	8	0	0
3	5-A	10	0	9	0	0
3	5-B	10	0	9	0	0
3	6-A	10	0	9	0	0
3	6-B	10	0	8	0	0
3	7-A	10	0	8	0	0
3	7-B	10	0	9	0	0
3	8-A	10	0	8	0	0
3	8-B	10	0	9	0	0
4	1-A	213	0	0	0	0
4	1-B	214	0	0	0	0
4	2-A	214	0	0	0	0
4	2-B	213	0	0	0	0
4	3-A	214	0	0	0	0
4	3-B	213	0	0	0	0
4	4-A	214	0	0	0	0
4	4-B	213	0	0	0	0
4	5-A	213	0	0	0	0
4	5-B	214	0	0	0	0
4	6-A	214	0	0	0	0
4	6-B	213	0	0	0	0
4	7-A	214	0	0	0	0
4	7-B	213	0	0	0	0
4	8-A	214	0	0	0	0
4	8-B	213	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	30952	0	26264	0	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 0.

There are no clashes within the asymmetric unit.

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	1-A	213/221 (96%)	192 (90%)	15 (7%)	6 (3%)	4	1
1	1-B	207/221 (94%)	190 (92%)	14 (7%)	3 (1%)	9	5
1	2-A	213/221 (96%)	203 (95%)	8 (4%)	2 (1%)	14	10
1	2-B	207/221 (94%)	179 (86%)	20 (10%)	8 (4%)	2	0
1	3-A	213/221 (96%)	181 (85%)	26 (12%)	6 (3%)	4	1
1	3-B	207/221 (94%)	175 (84%)	23 (11%)	9 (4%)	2	0
1	4-A	213/221 (96%)	186 (87%)	19 (9%)	8 (4%)	2	1
1	4-B	207/221 (94%)	184 (89%)	21 (10%)	2 (1%)	12	9
1	5-A	213/221 (96%)	191 (90%)	16 (8%)	6 (3%)	4	1
1	5-B	207/221 (94%)	184 (89%)	18 (9%)	5 (2%)	4	2
1	6-A	213/221 (96%)	190 (89%)	15 (7%)	8 (4%)	2	1
1	6-B	207/221 (94%)	181 (87%)	17 (8%)	9 (4%)	2	0
1	7-A	213/221 (96%)	188 (88%)	21 (10%)	4 (2%)	6	3
1	7-B	207/221 (94%)	165 (80%)	28 (14%)	14 (7%)	1	0
1	8-A	213/221 (96%)	188 (88%)	19 (9%)	6 (3%)	4	1
1	8-B	207/221 (94%)	179 (86%)	20 (10%)	8 (4%)	2	0
All	All	3360/3536 (95%)	2956 (88%)	300 (9%)	104 (3%)	3	1

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	190	ASN
1	1-A	193	GLY
1	2-B	170	ASN
1	3-B	124	SER
1	4-A	73	SER
1	4-A	122	LEU
1	5-A	184	ALA
1	5-B	159	VAL
1	6-B	98	LYS
1	7-B	50	PHE
1	7-B	51	VAL
1	7-B	69	SER
1	7-B	136	PHE
1	7-B	145	GLU
1	7-B	179	SER
1	8-A	6	VAL
1	8-B	159	VAL
1	8-B	182	ASN
1	1-A	218	ARG
1	1-B	148	ALA
1	1-B	186	ARG
1	3-A	73	SER
1	3-A	158	PRO
1	3-A	218	ARG
1	3-B	104	SER
1	3-B	187	CYS
1	4-A	6	VAL
1	4-A	75	MSE
1	4-A	218	ARG
1	4-B	13	LYS
1	5-B	191	ALA
1	6-A	6	VAL
1	6-A	8	ASP
1	6-A	64	ARG
1	6-A	206	VAL
1	6-B	35	VAL
1	6-B	69	SER
1	6-B	158	PRO
1	7-A	65	ALA
1	7-A	69	SER
1	7-B	77	VAL
1	7-B	78	VAL

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Mol	Chain	Res	Type
1	7-B	144	GLN
1	7-B	164	ALA
1	8-A	120	GLU
1	8-B	31	ARG
1	8-B	69	SER
1	1-A	16	SER
1	2-B	41	ARG
1	2-B	123	MSE
1	3-B	25	ALA
1	3-B	68	ASP
1	4-B	14	HIS
1	5-A	13	LYS
1	5-A	14	HIS
1	5-A	185	GLU
1	5-B	149	HIS
1	6-A	9	THR
1	6-B	99	TRP
1	7-A	206	VAL
1	8-A	119	LEU
1	8-B	25	ALA
1	8-B	149	HIS
1	8-B	183	ILE
1	1-B	124	SER
1	2-A	64	ARG
1	2-B	24	HIS
1	2-B	34	SER
1	3-A	100	ASP
1	3-A	187	CYS
1	3-B	23	ARG
1	3-B	167	ARG
1	4-A	64	ARG
1	5-A	181	LYS
1	5-B	125	SER
1	6-A	7	ILE
1	6-B	32	ASP
1	6-B	170	ASN
1	7-A	146	SER
1	7-B	100	ASP
1	8-A	7	ILE
1	8-B	99	TRP
1	1-A	24	HIS
1	1-A	70	GLY

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Mol	Chain	Res	Type
1	2-B	40	PHE
1	2-B	110	ARG
1	4-A	121	ASP
1	5-B	68	ASP
1	6-A	38	SER
1	6-B	68	ASP
1	7-B	193	GLY
1	8-A	184	ALA
1	2-B	52	ARG
1	3-A	102	ASP
1	3-B	99	TRP
1	5-A	81	GLY
1	3-B	6	VAL
1	6-A	63	ILE
1	6-B	70	GLY
1	7-B	6	VAL
1	7-B	159	VAL
1	8-A	183	ILE
1	4-A	183	ILE
1	2-A	211	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	1-A	184/184 (100%)	170 (92%)	14 (8%)	12	9
1	1-B	181/184 (98%)	170 (94%)	11 (6%)	17	15
1	2-A	184/184 (100%)	170 (92%)	14 (8%)	12	9
1	2-B	181/184 (98%)	170 (94%)	11 (6%)	17	15
1	3-A	184/184 (100%)	170 (92%)	14 (8%)	12	9
1	3-B	181/184 (98%)	170 (94%)	11 (6%)	17	15
1	4-A	184/184 (100%)	170 (92%)	14 (8%)	12	9
1	4-B	181/184 (98%)	170 (94%)	11 (6%)	17	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5-A	184/184 (100%)	170 (92%)	14 (8%)	12	9
1	5-B	181/184 (98%)	170 (94%)	11 (6%)	17	15
1	6-A	184/184 (100%)	170 (92%)	14 (8%)	12	9
1	6-B	181/184 (98%)	170 (94%)	11 (6%)	17	15
1	7-A	184/184 (100%)	170 (92%)	14 (8%)	12	9
1	7-B	181/184 (98%)	170 (94%)	11 (6%)	17	15
1	8-A	184/184 (100%)	170 (92%)	14 (8%)	12	9
1	8-B	181/184 (98%)	170 (94%)	11 (6%)	17	15
All	All	2920/2944 (99%)	2720 (93%)	200 (7%)	14	12

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	12	ASP
1	1-A	15	ARG
1	1-A	16	SER
1	1-A	36	ASP
1	1-A	60	SER
1	1-A	75	MSE
1	1-A	115	TYR
1	1-A	143	TYR
1	1-A	153	ASP
1	1-A	159	VAL
1	1-A	162	THR
1	1-A	171	ASP
1	1-A	178	SER
1	1-A	206	VAL
1	1-B	13	LYS
1	1-B	68	ASP
1	1-B	76	GLU
1	1-B	97	SER
1	1-B	100	ASP
1	1-B	150	CYS
1	1-B	160	GLU
1	1-B	165	CYS
1	1-B	170	ASN
1	1-B	190	ASN
1	1-B	194	GLU
1	2-A	12	ASP

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Mol	Chain	Res	Type
1	2-A	15	ARG
1	2-A	16	SER
1	2-A	36	ASP
1	2-A	60	SER
1	2-A	75	MSE
1	2-A	115	TYR
1	2-A	143	TYR
1	2-A	153	ASP
1	2-A	159	VAL
1	2-A	162	THR
1	2-A	171	ASP
1	2-A	178	SER
1	2-A	206	VAL
1	2-B	13	LYS
1	2-B	68	ASP
1	2-B	76	GLU
1	2-B	97	SER
1	2-B	100	ASP
1	2-B	150	CYS
1	2-B	160	GLU
1	2-B	165	CYS
1	2-B	170	ASN
1	2-B	190	ASN
1	2-B	194	GLU
1	3-A	12	ASP
1	3-A	15	ARG
1	3-A	16	SER
1	3-A	36	ASP
1	3-A	60	SER
1	3-A	75	MSE
1	3-A	115	TYR
1	3-A	143	TYR
1	3-A	153	ASP
1	3-A	159	VAL
1	3-A	162	THR
1	3-A	171	ASP
1	3-A	178	SER
1	3-A	206	VAL
1	3-B	13	LYS
1	3-B	68	ASP
1	3-B	76	GLU
1	3-B	97	SER

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Mol	Chain	Res	Type
1	3-B	100	ASP
1	3-B	150	CYS
1	3-B	160	GLU
1	3-B	165	CYS
1	3-B	170	ASN
1	3-B	190	ASN
1	3-B	194	GLU
1	4-A	12	ASP
1	4-A	15	ARG
1	4-A	16	SER
1	4-A	36	ASP
1	4-A	60	SER
1	4-A	75	MSE
1	4-A	115	TYR
1	4-A	143	TYR
1	4-A	153	ASP
1	4-A	159	VAL
1	4-A	162	THR
1	4-A	171	ASP
1	4-A	178	SER
1	4-A	206	VAL
1	4-B	13	LYS
1	4-B	68	ASP
1	4-B	76	GLU
1	4-B	97	SER
1	4-B	100	ASP
1	4-B	150	CYS
1	4-B	160	GLU
1	4-B	165	CYS
1	4-B	170	ASN
1	4-B	190	ASN
1	4-B	194	GLU
1	5-A	12	ASP
1	5-A	15	ARG
1	5-A	16	SER
1	5-A	36	ASP
1	5-A	60	SER
1	5-A	75	MSE
1	5-A	115	TYR
1	5-A	143	TYR
1	5-A	153	ASP
1	5-A	159	VAL

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Mol	Chain	Res	Type
1	5-A	162	THR
1	5-A	171	ASP
1	5-A	178	SER
1	5-A	206	VAL
1	5-B	13	LYS
1	5-B	68	ASP
1	5-B	76	GLU
1	5-B	97	SER
1	5-B	100	ASP
1	5-B	150	CYS
1	5-B	160	GLU
1	5-B	165	CYS
1	5-B	170	ASN
1	5-B	190	ASN
1	5-B	194	GLU
1	6-A	12	ASP
1	6-A	15	ARG
1	6-A	16	SER
1	6-A	36	ASP
1	6-A	60	SER
1	6-A	75	MSE
1	6-A	115	TYR
1	6-A	143	TYR
1	6-A	153	ASP
1	6-A	159	VAL
1	6-A	162	THR
1	6-A	171	ASP
1	6-A	178	SER
1	6-A	206	VAL
1	6-B	13	LYS
1	6-B	68	ASP
1	6-B	76	GLU
1	6-B	97	SER
1	6-B	100	ASP
1	6-B	150	CYS
1	6-B	160	GLU
1	6-B	165	CYS
1	6-B	170	ASN
1	6-B	190	ASN
1	6-B	194	GLU
1	7-A	12	ASP
1	7-A	15	ARG

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Mol	Chain	Res	Type
1	7-A	16	SER
1	7-A	36	ASP
1	7-A	60	SER
1	7-A	75	MSE
1	7-A	115	TYR
1	7-A	143	TYR
1	7-A	153	ASP
1	7-A	159	VAL
1	7-A	162	THR
1	7-A	171	ASP
1	7-A	178	SER
1	7-A	206	VAL
1	7-B	13	LYS
1	7-B	68	ASP
1	7-B	76	GLU
1	7-B	97	SER
1	7-B	100	ASP
1	7-B	150	CYS
1	7-B	160	GLU
1	7-B	165	CYS
1	7-B	170	ASN
1	7-B	190	ASN
1	7-B	194	GLU
1	8-A	12	ASP
1	8-A	15	ARG
1	8-A	16	SER
1	8-A	36	ASP
1	8-A	60	SER
1	8-A	75	MSE
1	8-A	115	TYR
1	8-A	143	TYR
1	8-A	153	ASP
1	8-A	159	VAL
1	8-A	162	THR
1	8-A	171	ASP
1	8-A	178	SER
1	8-A	206	VAL
1	8-B	13	LYS
1	8-B	68	ASP
1	8-B	76	GLU
1	8-B	97	SER
1	8-B	100	ASP

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Mol	Chain	Res	Type
1	8-B	150	CYS
1	8-B	160	GLU
1	8-B	165	CYS
1	8-B	170	ASN
1	8-B	190	ASN
1	8-B	194	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	155	ASN
1	1-A	166	HIS
1	1-A	175	GLN
1	1-B	86	ASN
1	1-B	112	ASN
1	1-B	170	ASN
1	1-B	182	ASN
1	1-B	190	ASN
1	2-A	112	ASN
1	2-A	155	ASN
1	2-B	112	ASN
1	2-B	113	GLN
1	3-A	113	GLN
1	3-A	166	HIS
1	3-B	24	HIS
1	3-B	166	HIS
1	4-A	24	HIS
1	4-A	112	ASN
1	4-A	155	ASN
1	4-A	182	ASN
1	4-B	86	ASN
1	4-B	144	GLN
1	4-B	182	ASN
1	5-A	113	GLN
1	5-A	155	ASN
1	5-B	182	ASN
1	6-A	166	HIS
1	6-B	113	GLN
1	6-B	144	GLN
1	6-B	175	GLN
1	6-B	182	ASN
1	7-A	109	GLN

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Mol	Chain	Res	Type
1	7-A	155	ASN
1	7-B	14	HIS
1	7-B	144	GLN
1	8-A	113	GLN
1	8-A	144	GLN
1	8-A	155	ASN
1	8-A	166	HIS
1	8-B	24	HIS
1	8-B	112	ASN
1	8-B	175	GLN
1	8-B	190	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

48 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	5-B	1402	-	4,4,4	0.47	0	6,6,6	0.17	0
2	SO4	3-A	1401	-	4,4,4	0.35	0	6,6,6	0.46	0
2	SO4	4-A	1401	-	4,4,4	0.64	0	6,6,6	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	2-B	1404	-	4,4,4	0.46	0	6,6,6	0.22	0
2	SO4	1-B	1402	-	4,4,4	0.43	0	6,6,6	0.22	0
2	SO4	2-B	1403	-	4,4,4	0.52	0	6,6,6	0.11	0
2	SO4	1-A	1403	-	4,4,4	0.41	0	6,6,6	0.19	0
3	HMH	7-A	1300	-	10,10,10	2.50	4 (40%)	12,13,13	3.13	9 (75%)
3	HMH	6-A	1300	-	10,10,10	2.71	3 (30%)	12,13,13	2.77	8 (66%)
2	SO4	4-B	1403	-	4,4,4	0.39	0	6,6,6	0.17	0
2	SO4	6-B	1404	-	4,4,4	0.52	0	6,6,6	0.20	0
3	HMH	3-A	1300	-	10,10,10	2.57	5 (50%)	12,13,13	3.30	8 (66%)
2	SO4	4-B	1402	-	4,4,4	0.39	0	6,6,6	0.27	0
2	SO4	5-B	1403	-	4,4,4	0.40	0	6,6,6	0.21	0
2	SO4	7-B	1404	-	4,4,4	0.34	0	6,6,6	0.38	0
2	SO4	7-B	1403	-	4,4,4	0.52	0	6,6,6	0.24	0
2	SO4	5-B	1404	-	4,4,4	0.50	0	6,6,6	0.20	0
2	SO4	2-B	1402	-	4,4,4	0.52	0	6,6,6	0.23	0
2	SO4	1-B	1404	-	4,4,4	0.48	0	6,6,6	0.26	0
3	HMH	5-B	1301	-	10,10,10	2.32	4 (40%)	12,13,13	2.79	7 (58%)
2	SO4	6-B	1402	-	4,4,4	0.45	0	6,6,6	0.20	0
2	SO4	6-A	1401	-	4,4,4	0.36	0	6,6,6	0.54	0
3	HMH	2-A	1300	-	10,10,10	2.40	5 (50%)	12,13,13	3.23	9 (75%)
2	SO4	6-B	1403	-	4,4,4	0.39	0	6,6,6	0.14	0
2	SO4	2-A	1401	-	4,4,4	0.48	0	6,6,6	0.42	0
2	SO4	7-B	1402	-	4,4,4	0.43	0	6,6,6	0.19	0
2	SO4	3-B	1403	-	4,4,4	0.52	0	6,6,6	0.20	0
2	SO4	4-B	1404	-	4,4,4	0.48	0	6,6,6	0.24	0
3	HMH	4-B	1301	-	10,10,10	1.50	3 (30%)	12,13,13	2.64	8 (66%)
2	SO4	3-B	1404	-	4,4,4	0.48	0	6,6,6	0.28	0
2	SO4	8-B	1402	-	4,4,4	0.48	0	6,6,6	0.21	0
3	HMH	2-B	1301	-	10,10,10	1.97	3 (30%)	12,13,13	2.44	9 (75%)
3	HMH	5-A	1300	-	10,10,10	2.78	4 (40%)	12,13,13	3.15	7 (58%)
3	HMH	8-A	1300	-	10,10,10	2.58	6 (60%)	12,13,13	3.19	8 (66%)
3	HMH	6-B	1301	-	10,10,10	2.00	4 (40%)	12,13,13	2.82	8 (66%)
2	SO4	5-A	1401	-	4,4,4	0.52	0	6,6,6	0.38	0
2	SO4	7-A	1401	-	4,4,4	0.59	0	6,6,6	0.53	0
2	SO4	8-B	1404	-	4,4,4	0.50	0	6,6,6	0.19	0
3	HMH	3-B	1301	-	10,10,10	1.72	3 (30%)	12,13,13	2.74	8 (66%)
3	HMH	8-B	1301	-	10,10,10	1.84	3 (30%)	12,13,13	2.39	7 (58%)
2	SO4	8-A	1401	-	4,4,4	0.46	0	6,6,6	0.35	0
3	HMH	4-A	1300	-	10,10,10	2.44	7 (70%)	12,13,13	3.24	9 (75%)
3	HMH	1-B	1301	-	10,10,10	1.80	3 (30%)	12,13,13	2.66	9 (75%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	8-B	1403	-	4,4,4	0.42	0	6,6,6	0.17	0
3	HMH	7-B	1301	-	10,10,10	2.02	4 (40%)	12,13,13	2.75	8 (66%)
3	HMH	1-A	1300	-	10,10,10	2.47	5 (50%)	12,13,13	3.31	8 (66%)
2	SO4	1-B	1401	-	4,4,4	0.42	0	6,6,6	0.29	0
2	SO4	3-B	1402	-	4,4,4	0.41	0	6,6,6	0.17	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HMH	5-A	1300	-	-	0/2/2/2	0/1/1/1
3	HMH	8-A	1300	-	-	0/2/2/2	0/1/1/1
3	HMH	6-B	1301	-	-	0/2/2/2	0/1/1/1
3	HMH	2-B	1301	-	-	0/2/2/2	0/1/1/1
3	HMH	3-B	1301	-	-	0/2/2/2	0/1/1/1
3	HMH	4-B	1301	-	-	0/2/2/2	0/1/1/1
3	HMH	4-A	1300	-	-	0/2/2/2	0/1/1/1
3	HMH	1-B	1301	-	-	0/2/2/2	0/1/1/1
3	HMH	7-A	1300	-	-	0/2/2/2	0/1/1/1
3	HMH	5-B	1301	-	-	0/2/2/2	0/1/1/1
3	HMH	8-B	1301	-	-	0/2/2/2	0/1/1/1
3	HMH	6-A	1300	-	-	0/2/2/2	0/1/1/1
3	HMH	7-B	1301	-	-	0/2/2/2	0/1/1/1
3	HMH	1-A	1300	-	-	0/2/2/2	0/1/1/1
3	HMH	3-A	1300	-	-	0/2/2/2	0/1/1/1
3	HMH	2-A	1300	-	-	0/2/2/2	0/1/1/1

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	6-A	1300	HMH	C4A-N3A	5.53	1.42	1.35
3	3-A	1300	HMH	C4A-N3A	4.53	1.41	1.35
3	7-A	1300	HMH	C4A-N3A	4.53	1.41	1.35
3	5-A	1300	HMH	C6A-N1A	4.51	1.43	1.34
3	8-A	1300	HMH	C4A-N3A	4.50	1.41	1.35
3	5-A	1300	HMH	C6A-C5A	4.45	1.46	1.37
3	6-A	1300	HMH	C6A-C5A	4.44	1.46	1.37
3	4-A	1300	HMH	C6A-C5A	4.39	1.46	1.37
3	2-A	1300	HMH	C6A-C5A	4.13	1.45	1.37
3	5-A	1300	HMH	C4A-N3A	4.12	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-A	1300	HMH	C6A-C5A	4.11	1.45	1.37
3	5-B	1301	HMH	C4A-N3A	3.94	1.40	1.35
3	7-A	1300	HMH	C6A-C5A	3.93	1.45	1.37
3	2-A	1300	HMH	C4A-N3A	3.73	1.40	1.35
3	8-A	1300	HMH	C6A-N1A	3.62	1.41	1.34
3	2-B	1301	HMH	C4A-N4A	3.60	1.43	1.34
3	3-A	1300	HMH	C6A-N1A	3.58	1.41	1.34
3	8-B	1301	HMH	C6A-C5A	3.51	1.44	1.37
3	6-B	1301	HMH	C5A-C4A	-3.44	1.37	1.42
3	1-A	1300	HMH	C5A-C4A	-3.38	1.37	1.42
3	5-B	1301	HMH	C6A-N1A	3.37	1.41	1.34
3	6-A	1300	HMH	C2A-N3A	3.33	1.39	1.34
3	3-A	1300	HMH	C2A-N1A	3.33	1.39	1.34
3	7-B	1301	HMH	C6A-C5A	3.30	1.44	1.37
3	7-B	1301	HMH	C6A-N1A	3.29	1.41	1.34
3	4-A	1300	HMH	C5A-C4A	-3.27	1.37	1.42
3	5-B	1301	HMH	C4A-N4A	3.25	1.42	1.34
3	7-A	1300	HMH	C4A-N4A	3.24	1.42	1.34
3	3-A	1300	HMH	C6A-C5A	3.21	1.44	1.37
3	8-A	1300	HMH	C6A-C5A	3.20	1.44	1.37
3	1-B	1301	HMH	C4A-N4A	3.16	1.42	1.34
3	8-A	1300	HMH	C2A-N1A	3.15	1.39	1.34
3	3-B	1301	HMH	C6A-N1A	3.05	1.40	1.34
3	7-B	1301	HMH	C5A-C4A	-3.03	1.37	1.42
3	1-A	1300	HMH	C6A-N1A	3.01	1.40	1.34
3	2-B	1301	HMH	C6A-C5A	2.97	1.43	1.37
3	2-B	1301	HMH	C4A-N3A	2.96	1.39	1.35
3	6-B	1301	HMH	C6A-C5A	2.91	1.43	1.37
3	1-A	1300	HMH	C2A-N1A	2.85	1.38	1.34
3	3-B	1301	HMH	C6A-C5A	2.84	1.43	1.37
3	4-B	1301	HMH	C6A-C5A	2.78	1.43	1.37
3	5-A	1300	HMH	C2A-N1A	2.74	1.38	1.34
3	6-B	1301	HMH	C6A-N1A	2.71	1.39	1.34
3	3-B	1301	HMH	C5A-C4A	-2.70	1.38	1.42
3	4-A	1300	HMH	C2A-N1A	2.68	1.38	1.34
3	1-B	1301	HMH	C4A-N3A	2.67	1.38	1.35
3	4-A	1300	HMH	C4A-N3A	2.64	1.38	1.35
3	1-B	1301	HMH	C6A-C5A	2.64	1.43	1.37
3	2-A	1300	HMH	C4A-N4A	2.64	1.41	1.34
3	7-A	1300	HMH	C2A-N1A	2.64	1.38	1.34
3	8-B	1301	HMH	C7A-C5A	2.64	1.57	1.51
3	5-B	1301	HMH	C6A-C5A	2.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-A	1300	HMH	C5A-C4A	-2.57	1.38	1.42
3	1-A	1300	HMH	C4A-N3A	2.54	1.38	1.35
3	2-A	1300	HMH	C2A-N1A	2.53	1.38	1.34
3	8-B	1301	HMH	C6A-N1A	2.39	1.39	1.34
3	4-A	1300	HMH	C6A-N1A	2.26	1.39	1.34
3	4-A	1300	HMH	C4A-N4A	2.23	1.39	1.34
3	7-B	1301	HMH	C4A-N3A	2.22	1.38	1.35
3	4-B	1301	HMH	C6A-N1A	2.16	1.38	1.34
3	4-B	1301	HMH	C4A-N4A	2.12	1.39	1.34
3	8-A	1300	HMH	C5A-C4A	-2.11	1.39	1.42
3	4-A	1300	HMH	O1-C7A	-2.09	1.32	1.41
3	6-B	1301	HMH	C4A-N4A	2.04	1.39	1.34
3	3-A	1300	HMH	C5A-C4A	-2.02	1.39	1.42
3	8-A	1300	HMH	C4A-N4A	2.01	1.39	1.34

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-A	1300	HMH	CM2-C2A-N1A	5.83	123.41	117.20
3	7-A	1300	HMH	N4A-C4A-N3A	5.68	124.68	117.03
3	3-A	1300	HMH	C7A-C5A-C6A	5.64	128.49	119.36
3	2-A	1300	HMH	N4A-C4A-N3A	5.61	124.59	117.03
3	1-A	1300	HMH	CM2-C2A-N1A	5.34	122.88	117.20
3	6-A	1300	HMH	N4A-C4A-N3A	5.31	124.20	117.03
3	1-A	1300	HMH	C7A-C5A-C6A	5.30	127.94	119.36
3	8-A	1300	HMH	C7A-C5A-C6A	5.26	127.88	119.36
3	3-A	1300	HMH	CM2-C2A-N1A	5.07	122.60	117.20
3	5-B	1301	HMH	C7A-C5A-C6A	4.93	127.34	119.36
3	4-A	1300	HMH	C7A-C5A-C6A	4.91	127.30	119.36
3	4-A	1300	HMH	CM2-C2A-N1A	4.90	122.42	117.20
3	1-B	1301	HMH	N4A-C4A-N3A	4.87	123.59	117.03
3	4-A	1300	HMH	N4A-C4A-N3A	4.86	123.58	117.03
3	8-A	1300	HMH	CM2-C2A-N1A	4.77	122.28	117.20
3	5-A	1300	HMH	C7A-C5A-C6A	4.68	126.94	119.36
3	8-A	1300	HMH	N4A-C4A-N3A	4.64	123.29	117.03
3	8-A	1300	HMH	C5A-C4A-N4A	-4.58	115.98	122.14
3	3-A	1300	HMH	N4A-C4A-N3A	4.54	123.15	117.03
3	3-A	1300	HMH	C5A-C4A-N4A	-4.54	116.03	122.14
3	1-A	1300	HMH	N4A-C4A-N3A	4.48	123.07	117.03
3	1-A	1300	HMH	C5A-C4A-N4A	-4.44	116.17	122.14
3	5-B	1301	HMH	N4A-C4A-N3A	4.37	122.93	117.03
3	6-B	1301	HMH	N4A-C4A-N3A	4.36	122.92	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2-A	1300	HMH	C7A-C5A-C6A	4.28	126.28	119.36
3	2-A	1300	HMH	C5A-C4A-N4A	-4.24	116.43	122.14
3	4-A	1300	HMH	C5A-C4A-N4A	-4.14	116.56	122.14
3	6-B	1301	HMH	C7A-C5A-C6A	4.12	126.03	119.36
3	4-B	1301	HMH	C7A-C5A-C6A	4.03	125.89	119.36
3	2-B	1301	HMH	N4A-C4A-N3A	4.03	122.46	117.03
3	2-A	1300	HMH	CM2-C2A-N1A	4.02	121.48	117.20
3	3-B	1301	HMH	CM2-C2A-N1A	3.96	121.42	117.20
3	7-A	1300	HMH	C5A-C4A-N4A	-3.90	116.89	122.14
3	7-B	1301	HMH	CM2-C2A-N1A	3.88	121.34	117.20
3	5-A	1300	HMH	N1A-C2A-N3A	-3.88	119.07	125.53
3	7-B	1301	HMH	C7A-C5A-C6A	3.84	125.57	119.36
3	8-B	1301	HMH	CM2-C2A-N1A	3.79	121.24	117.20
3	5-A	1300	HMH	C6A-N1A-C2A	3.78	122.28	116.07
3	3-B	1301	HMH	C7A-C5A-C6A	3.77	125.46	119.36
3	7-A	1300	HMH	C7A-C5A-C6A	3.77	125.46	119.36
3	5-A	1300	HMH	C5A-C6A-N1A	-3.71	117.80	123.83
3	4-B	1301	HMH	CM2-C2A-N1A	3.69	121.13	117.20
3	7-A	1300	HMH	CM2-C2A-N1A	3.67	121.11	117.20
3	6-B	1301	HMH	C5A-C4A-N4A	-3.61	117.28	122.14
3	6-B	1301	HMH	CM2-C2A-N1A	3.52	120.95	117.20
3	7-B	1301	HMH	N4A-C4A-N3A	3.49	121.73	117.03
3	6-A	1300	HMH	N1A-C2A-N3A	-3.39	119.89	125.53
3	8-B	1301	HMH	C7A-C5A-C6A	3.35	124.79	119.36
3	3-B	1301	HMH	N4A-C4A-N3A	3.32	121.51	117.03
3	5-B	1301	HMH	C5A-C4A-N4A	-3.30	117.70	122.14
3	7-B	1301	HMH	C5A-C4A-N4A	-3.27	117.74	122.14
3	4-B	1301	HMH	N4A-C4A-N3A	3.25	121.41	117.03
3	8-B	1301	HMH	C6A-N1A-C2A	3.24	121.39	116.07
3	1-B	1301	HMH	C7A-C5A-C6A	3.24	124.60	119.36
3	4-B	1301	HMH	C5A-C6A-N1A	-3.24	118.57	123.83
3	7-B	1301	HMH	N1A-C2A-N3A	-3.19	120.22	125.53
3	3-B	1301	HMH	N1A-C2A-N3A	-3.19	120.22	125.53
3	8-B	1301	HMH	C2A-N3A-C4A	3.18	122.99	118.10
3	3-A	1300	HMH	N1A-C2A-N3A	-3.17	120.25	125.53
3	1-B	1301	HMH	C5A-C4A-N4A	-3.15	117.90	122.14
3	6-A	1300	HMH	CM2-C2A-N3A	3.13	121.81	117.13
3	3-B	1301	HMH	C5A-C4A-N4A	-3.12	117.94	122.14
3	3-B	1301	HMH	C5A-C6A-N1A	-3.08	118.82	123.83
3	8-A	1300	HMH	N1A-C2A-N3A	-3.08	120.41	125.53
3	1-A	1300	HMH	C5A-C6A-N1A	-3.07	118.83	123.83
3	5-A	1300	HMH	C2A-N3A-C4A	3.01	122.73	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-A	1300	HMH	N1A-C2A-N3A	-2.99	120.55	125.53
3	6-A	1300	HMH	C2A-N3A-C4A	2.99	122.69	118.10
3	2-B	1301	HMH	C6A-N1A-C2A	2.99	120.97	116.07
3	3-B	1301	HMH	C6A-N1A-C2A	2.96	120.93	116.07
3	2-A	1300	HMH	N1A-C2A-N3A	-2.94	120.64	125.53
3	4-A	1300	HMH	N1A-C2A-N3A	-2.93	120.65	125.53
3	7-A	1300	HMH	N1A-C2A-N3A	-2.91	120.69	125.53
3	5-B	1301	HMH	C2A-N3A-C4A	2.91	122.57	118.10
3	4-A	1300	HMH	C2A-N3A-C4A	2.89	122.55	118.10
3	4-A	1300	HMH	C5A-C6A-N1A	-2.89	119.14	123.83
3	7-A	1300	HMH	C6A-N1A-C2A	2.88	120.80	116.07
3	7-B	1301	HMH	C5A-C6A-N1A	-2.87	119.16	123.83
3	4-B	1301	HMH	C6A-N1A-C2A	2.86	120.78	116.07
3	5-B	1301	HMH	N1A-C2A-N3A	-2.83	120.81	125.53
3	6-A	1300	HMH	C5A-C4A-N4A	-2.82	118.34	122.14
3	7-B	1301	HMH	C2A-N3A-C4A	2.82	122.44	118.10
3	6-B	1301	HMH	N1A-C2A-N3A	-2.82	120.84	125.53
3	7-B	1301	HMH	C6A-N1A-C2A	2.80	120.67	116.07
3	5-B	1301	HMH	CM2-C2A-N1A	2.79	120.17	117.20
3	8-B	1301	HMH	N1A-C2A-N3A	-2.77	120.93	125.53
3	2-A	1300	HMH	C5A-C6A-N1A	-2.77	119.33	123.83
3	6-B	1301	HMH	C5A-C6A-N1A	-2.76	119.34	123.83
3	1-A	1300	HMH	C2A-N3A-C4A	2.74	122.32	118.10
3	1-B	1301	HMH	CM2-C2A-N1A	2.73	120.11	117.20
3	6-A	1300	HMH	C6A-N1A-C2A	2.71	120.53	116.07
3	2-A	1300	HMH	C6A-N1A-C2A	2.68	120.48	116.07
3	3-B	1301	HMH	C2A-N3A-C4A	2.68	122.22	118.10
3	4-B	1301	HMH	C5A-C4A-N4A	-2.66	118.55	122.14
3	2-B	1301	HMH	C5A-C6A-N1A	-2.66	119.50	123.83
3	2-B	1301	HMH	CM2-C2A-N1A	2.66	120.03	117.20
3	4-B	1301	HMH	N1A-C2A-N3A	-2.65	121.12	125.53
3	6-A	1300	HMH	C5A-C4A-N3A	-2.63	117.46	121.31
3	7-A	1300	HMH	C5A-C6A-N1A	-2.62	119.56	123.83
3	5-A	1300	HMH	C5A-C4A-N4A	-2.62	118.62	122.14
3	8-B	1301	HMH	O1-C7A-C5A	2.61	119.22	111.94
3	6-B	1301	HMH	C2A-N3A-C4A	2.61	122.11	118.10
3	1-B	1301	HMH	N1A-C2A-N3A	-2.59	121.23	125.53
3	3-A	1300	HMH	C5A-C6A-N1A	-2.59	119.63	123.83
3	4-B	1301	HMH	C2A-N3A-C4A	2.59	122.07	118.10
3	2-B	1301	HMH	C2A-N3A-C4A	2.56	122.04	118.10
3	8-B	1301	HMH	C5A-C6A-N1A	-2.56	119.66	123.83
3	2-A	1300	HMH	C2A-N3A-C4A	2.56	122.03	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-B	1301	HMH	C6A-N1A-C2A	2.54	120.25	116.07
3	3-A	1300	HMH	C6A-N1A-C2A	2.50	120.18	116.07
3	2-B	1301	HMH	N1A-C2A-N3A	-2.49	121.38	125.53
3	8-A	1300	HMH	C5A-C6A-N1A	-2.48	119.79	123.83
3	7-A	1300	HMH	C6A-C5A-C4A	2.48	118.60	115.55
3	7-A	1300	HMH	C2A-N3A-C4A	2.48	121.91	118.10
3	1-B	1301	HMH	C2A-N3A-C4A	2.46	121.89	118.10
3	2-A	1300	HMH	C6A-C5A-C4A	2.43	118.53	115.55
3	6-B	1301	HMH	C6A-N1A-C2A	2.42	120.04	116.07
3	3-A	1300	HMH	C2A-N3A-C4A	2.39	121.77	118.10
3	8-A	1300	HMH	C6A-N1A-C2A	2.36	119.94	116.07
3	2-B	1301	HMH	C7A-C5A-C6A	2.34	123.15	119.36
3	5-B	1301	HMH	C6A-N1A-C2A	2.33	119.90	116.07
3	8-A	1300	HMH	C2A-N3A-C4A	2.29	121.62	118.10
3	1-B	1301	HMH	C5A-C6A-N1A	-2.28	120.12	123.83
3	1-A	1300	HMH	C6A-N1A-C2A	2.26	119.78	116.07
3	4-A	1300	HMH	C6A-N1A-C2A	2.22	119.72	116.07
3	2-B	1301	HMH	C5A-C4A-N4A	-2.16	119.23	122.14
3	6-A	1300	HMH	C7A-C5A-C6A	2.09	122.74	119.36
3	4-A	1300	HMH	C6A-C5A-C4A	2.07	118.09	115.55
3	2-B	1301	HMH	C5A-C4A-N3A	-2.05	118.31	121.31
3	1-B	1301	HMH	C6A-C5A-C4A	2.00	118.01	115.55

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(Å ²)	Q<0.9
1	1-A	211/221 (95%)	2.76	126 (59%) 0 0	2, 3, 4, 7	211 (100%)
1	1-B	207/221 (93%)	2.95	143 (69%) 0 0	1, 3, 5, 7	207 (100%)
1	2-A	0/221	-	-	-	-
1	2-B	0/221	-	-	-	-
1	3-A	0/221	-	-	-	-
1	3-B	0/221	-	-	-	-
1	4-A	0/221	-	-	-	-
1	4-B	0/221	-	-	-	-
1	5-A	0/221	-	-	-	-
1	5-B	0/221	-	-	-	-
1	6-A	0/221	-	-	-	-
1	6-B	0/221	-	-	-	-
1	7-A	0/221	-	-	-	-
1	7-B	0/221	-	-	-	-
1	8-A	0/221	-	-	-	-
1	8-B	0/221	-	-	-	-
All	All	418/3536 (11%)	2.85	269 (64%) 0 0	1, 3, 5, 7	418 (100%)

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	83	ALA	11.2
1	1-A	32	ASP	9.3
1	1-B	84	SER	9.0
1	1-B	87	ASP	9.0
1	1-A	182	ASN	7.7
1	1-A	73	SER	7.3
1	1-A	68	ASP	7.0
1	1-B	86	ASN	6.9
1	1-A	146	SER	6.9
1	1-B	158	PRO	6.8

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Mol	Chain	Res	Type	RSRZ
1	1-A	33	GLY	6.8
1	1-A	116	GLY	6.7
1	1-B	100	ASP	6.7
1	1-B	72	SER	6.6
1	1-A	72	SER	6.6
1	1-A	193	GLY	6.6
1	1-B	150	CYS	6.6
1	1-A	34	SER	6.5
1	1-A	69	SER	6.4
1	1-B	28	VAL	6.4
1	1-B	68	ASP	6.4
1	1-A	29	SER	6.3
1	1-A	70	GLY	6.0
1	1-B	97	SER	5.9
1	1-A	149	HIS	5.9
1	1-A	18	TYR	5.8
1	1-B	159	VAL	5.8
1	1-A	191	ALA	5.8
1	1-A	28	VAL	5.7
1	1-A	5	GLY	5.6
1	1-A	204	VAL	5.6
1	1-A	192	SER	5.5
1	1-B	74	ASP	5.5
1	1-A	219	GLY	5.4
1	1-B	91	TRP	5.3
1	1-A	196	LEU	5.3
1	1-B	157	THR	5.3
1	1-B	182	ASN	5.2
1	1-A	190	ASN	5.2
1	1-B	9	THR	5.2
1	1-B	73	SER	5.2
1	1-B	92	PHE	5.1
1	1-A	154	GLY	5.0
1	1-A	199	ALA	5.0
1	1-B	69	SER	4.9
1	1-B	11	ILE	4.9
1	1-B	80	GLY	4.9
1	1-A	6	VAL	4.9
1	1-B	149	HIS	4.9
1	1-A	12	ASP	4.8
1	1-A	165	CYS	4.8
1	1-B	85	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	1-B	132	ILE	4.8
1	1-B	34	SER	4.8
1	1-A	161	LEU	4.7
1	1-B	194	GLU	4.7
1	1-A	194	GLU	4.7
1	1-B	8	ASP	4.7
1	1-B	190	ASN	4.7
1	1-A	71	GLU	4.6
1	1-A	16	SER	4.6
1	1-B	195	VAL	4.6
1	1-B	165	CYS	4.6
1	1-B	70	GLY	4.5
1	1-A	67	LYS	4.5
1	1-B	117	ARG	4.5
1	1-A	197	GLY	4.5
1	1-A	113	GLN	4.5
1	1-B	5	GLY	4.4
1	1-B	193	GLY	4.3
1	1-B	66	CYS	4.3
1	1-A	218	ARG	4.3
1	1-A	158	PRO	4.3
1	1-B	31	ARG	4.3
1	1-A	30	ILE	4.3
1	1-A	174	LYS	4.2
1	1-A	22	THR	4.2
1	1-A	195	VAL	4.2
1	1-B	166	HIS	4.2
1	1-B	185	GLU	4.1
1	1-A	61	VAL	4.1
1	1-B	175	GLN	4.1
1	1-A	39	SER	4.1
1	1-A	114	GLU	4.1
1	1-B	160	GLU	4.1
1	1-B	95	GLU	4.0
1	1-A	8	ASP	4.0
1	1-B	148	ALA	4.0
1	1-B	184	ALA	4.0
1	1-A	217	SER	4.0
1	1-B	81	GLY	3.9
1	1-B	162	THR	3.9
1	1-B	71	GLU	3.9
1	1-B	76	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	1-A	56	PRO	3.9
1	1-B	48	TYR	3.9
1	1-B	218	ARG	3.9
1	1-B	90	GLU	3.8
1	1-B	156	LYS	3.8
1	1-B	171	ASP	3.8
1	1-B	126	GLU	3.8
1	1-A	179	SER	3.7
1	1-A	31	ARG	3.7
1	1-B	14	HIS	3.7
1	1-B	114	GLU	3.7
1	1-A	150	CYS	3.7
1	1-B	187	CYS	3.7
1	1-A	153	ASP	3.7
1	1-A	162	THR	3.6
1	1-B	109	GLN	3.6
1	1-A	105	THR	3.6
1	1-B	129	TYR	3.6
1	1-B	137	TRP	3.5
1	1-A	122	LEU	3.5
1	1-A	143	TYR	3.5
1	1-B	55	VAL	3.5
1	1-B	105	THR	3.5
1	1-B	176	TYR	3.4
1	1-B	107	VAL	3.4
1	1-B	78	VAL	3.4
1	1-B	191	ALA	3.4
1	1-A	176	TYR	3.3
1	1-B	113	GLN	3.3
1	1-B	98	LYS	3.3
1	1-A	7	ILE	3.3
1	1-A	50	PHE	3.3
1	1-B	147	PHE	3.3
1	1-A	77	VAL	3.2
1	1-A	207	LEU	3.2
1	1-A	81	GLY	3.2
1	1-A	155	ASN	3.2
1	1-B	170	ASN	3.2
1	1-A	27	VAL	3.2
1	1-A	63	ILE	3.2
1	1-A	100	ASP	3.2
1	1-A	124	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	1-B	65	ALA	3.1
1	1-B	146	SER	3.1
1	1-B	67	LYS	3.1
1	1-B	93	LYS	3.1
1	1-A	9	THR	3.1
1	1-A	21	ALA	3.1
1	1-B	124	SER	3.1
1	1-A	211	VAL	3.1
1	1-B	178	SER	3.1
1	1-A	115	TYR	3.0
1	1-A	147	PHE	3.0
1	1-A	58	VAL	3.0
1	1-B	101	VAL	3.0
1	1-A	170	ASN	3.0
1	1-A	145	GLU	3.0
1	1-B	102	ASP	3.0
1	1-A	164	ALA	3.0
1	1-B	29	SER	3.0
1	1-A	163	GLY	2.9
1	1-B	115	TYR	2.9
1	1-B	37	LEU	2.9
1	1-B	169	GLY	2.9
1	1-A	159	VAL	2.9
1	1-B	136	PHE	2.9
1	1-A	78	VAL	2.9
1	1-B	94	ARG	2.9
1	1-B	181	LYS	2.9
1	1-B	127	VAL	2.8
1	1-A	178	SER	2.8
1	1-A	59	ALA	2.8
1	1-B	135	ALA	2.8
1	1-A	106	VAL	2.8
1	1-B	63	ILE	2.8
1	1-B	89	ILE	2.8
1	1-B	125	SER	2.8
1	1-A	166	HIS	2.8
1	1-B	36	ASP	2.8
1	1-B	99	TRP	2.8
1	1-B	96	GLY	2.8
1	1-A	151	LEU	2.8
1	1-A	206	VAL	2.7
1	1-B	27	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	1-A	11	ILE	2.7
1	1-B	198	GLU	2.7
1	1-B	172	GLY	2.7
1	1-B	82	ILE	2.7
1	1-B	177	CYS	2.7
1	1-B	186	ARG	2.7
1	1-B	35	VAL	2.7
1	1-B	202	VAL	2.7
1	1-A	66	CYS	2.7
1	1-B	44	LEU	2.6
1	1-A	168	TRP	2.6
1	1-A	19	THR	2.6
1	1-A	104	SER	2.6
1	1-B	77	VAL	2.6
1	1-A	14	HIS	2.6
1	1-A	148	ALA	2.6
1	1-A	60	SER	2.6
1	1-A	118	PHE	2.6
1	1-A	17	ILE	2.6
1	1-B	204	VAL	2.6
1	1-B	88	GLU	2.6
1	1-B	189	GLU	2.6
1	1-A	177	CYS	2.6
1	1-A	65	ALA	2.6
1	1-B	12	ASP	2.6
1	1-B	49	LEU	2.6
1	1-B	168	TRP	2.6
1	1-B	214	TRP	2.6
1	1-B	57	PHE	2.5
1	1-A	90	GLU	2.5
1	1-B	24	HIS	2.5
1	1-B	13	LYS	2.5
1	1-A	53	ARG	2.5
1	1-A	167	ARG	2.5
1	1-B	32	ASP	2.5
1	1-A	144	GLN	2.5
1	1-A	152	GLU	2.5
1	1-B	200	GLU	2.5
1	1-A	82	ILE	2.5
1	1-A	94	ARG	2.5
1	1-B	23	ARG	2.5
1	1-A	171	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	1-B	79	LEU	2.5
1	1-A	107	VAL	2.4
1	1-B	141	ALA	2.4
1	1-B	6	VAL	2.4
1	1-A	212	ALA	2.4
1	1-A	188	LEU	2.4
1	1-B	188	LEU	2.4
1	1-B	116	GLY	2.4
1	1-A	84	SER	2.4
1	1-B	25	ALA	2.4
1	1-B	197	GLY	2.4
1	1-A	74	ASP	2.4
1	1-A	57	PHE	2.4
1	1-B	40	PHE	2.4
1	1-B	108	PRO	2.4
1	1-B	206	VAL	2.3
1	1-A	157	THR	2.3
1	1-B	163	GLY	2.3
1	1-A	15	ARG	2.3
1	1-B	192	SER	2.3
1	1-B	143	TYR	2.3
1	1-B	7	ILE	2.2
1	1-B	120	GLU	2.2
1	1-A	111	ALA	2.2
1	1-A	38	SER	2.2
1	1-A	137	TRP	2.2
1	1-A	214	TRP	2.2
1	1-B	139	ILE	2.2
1	1-B	58	VAL	2.2
1	1-B	138	ALA	2.2
1	1-B	199	ALA	2.2
1	1-B	10	TRP	2.2
1	1-B	112	ASN	2.1
1	1-B	43	TRP	2.1
1	1-A	26	PHE	2.1
1	1-B	183	ILE	2.1
1	1-A	172	GLY	2.1
1	1-B	33	GLY	2.1
1	1-B	180	VAL	2.1
1	1-A	23	ARG	2.1
1	1-A	79	LEU	2.1
1	1-A	200	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-B	42	THR	2.1
1	1-A	156	LYS	2.1
1	1-A	80	GLY	2.1
1	1-B	215	GLU	2.0
1	1-A	205	ARG	2.0
1	1-A	35	VAL	2.0
1	1-A	180	VAL	2.0

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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HMH	1-A	1300	10/10	0.69	0.16	19,24,25,26	10
2	SO4	2-A	1401	5/5	-	-	27,30,30,31	5
2	SO4	3-A	1401	5/5	-	-	28,30,31,32	5
2	SO4	4-A	1401	5/5	-	-	29,35,36,36	5
2	SO4	5-A	1401	5/5	-	-	24,25,27,27	5
2	SO4	6-A	1401	5/5	-	-	26,28,30,31	5
2	SO4	7-A	1401	5/5	-	-	26,28,29,29	5
2	SO4	8-A	1401	5/5	-	-	25,25,26,28	5
3	HMH	1-B	1301	10/10	0.80	0.15	15,19,23,33	10
2	SO4	1-B	1404	5/5	0.81	0.21	66,67,68,69	5
2	SO4	2-B	1402	5/5	-	-	23,24,26,26	5
2	SO4	3-B	1402	5/5	-	-	22,22,23,24	5
2	SO4	4-B	1402	5/5	-	-	24,24,26,26	5
2	SO4	5-B	1402	5/5	-	-	21,25,26,27	5
2	SO4	6-B	1402	5/5	-	-	22,22,25,25	5
2	SO4	7-B	1402	5/5	-	-	22,23,25,25	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	8-B	1402	5/5	-	-	21,22,23,25	5
2	SO4	2-B	1403	5/5	-	-	58,58,59,59	5
2	SO4	3-B	1403	5/5	-	-	60,60,61,61	5
2	SO4	4-B	1403	5/5	-	-	61,62,62,63	5
2	SO4	5-B	1403	5/5	-	-	58,61,61,61	5
2	SO4	6-B	1403	5/5	-	-	57,57,58,58	5
2	SO4	7-B	1403	5/5	-	-	61,62,63,63	5
2	SO4	8-B	1403	5/5	-	-	61,61,62,63	5
2	SO4	1-B	1401	5/5	0.83	0.19	29,29,30,31	5
2	SO4	2-B	1404	5/5	-	-	65,67,68,68	5
2	SO4	3-B	1404	5/5	-	-	68,68,68,69	5
2	SO4	4-B	1404	5/5	-	-	66,67,68,69	5
2	SO4	5-B	1404	5/5	-	-	66,67,68,68	5
2	SO4	6-B	1404	5/5	-	-	67,67,68,69	5
2	SO4	7-B	1404	5/5	-	-	63,64,67,67	5
2	SO4	8-B	1404	5/5	-	-	64,66,67,68	5
2	SO4	1-A	1403	5/5	0.83	0.17	62,62,62,63	5
3	HMH	2-A	1300	10/10	-	-	17,23,25,26	10
3	HMH	3-A	1300	10/10	-	-	21,24,26,28	10
3	HMH	4-A	1300	10/10	-	-	17,23,25,25	10
3	HMH	5-A	1300	10/10	-	-	21,25,27,29	10
3	HMH	6-A	1300	10/10	-	-	14,23,26,27	10
3	HMH	7-A	1300	10/10	-	-	16,21,23,31	10
3	HMH	8-A	1300	10/10	-	-	21,24,26,26	10
2	SO4	1-B	1402	5/5	0.93	0.10	21,21,22,23	5
3	HMH	2-B	1301	10/10	-	-	15,17,21,34	10
3	HMH	3-B	1301	10/10	-	-	23,25,29,32	10
3	HMH	4-B	1301	10/10	-	-	19,21,25,26	10
3	HMH	5-B	1301	10/10	-	-	17,19,21,24	10
3	HMH	6-B	1301	10/10	-	-	19,24,26,26	10
3	HMH	7-B	1301	10/10	-	-	21,25,28,31	10
3	HMH	8-B	1301	10/10	-	-	3,20,23,24	10

6.5 Other polymers [i](#)

There are no such residues in this entry.