



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:31 PM UTC

PDB ID : 3LCX / pdb_00003lcx
Title : L-KDO aldolase
Authors : Chou, C.-Y.; Huang, K.-F.; Wang, A.H.-J.; Ko, T.-P.
Deposited on : 2010-01-12
Resolution : 1.98 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

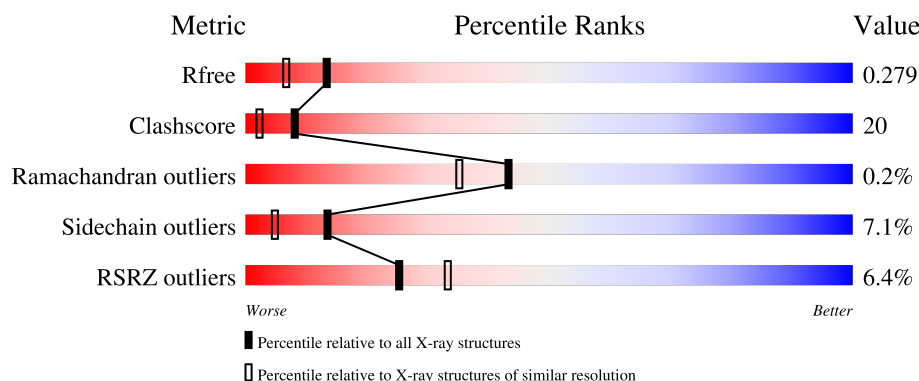
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	A	319	 3% 62% 26% 9%
1	B	319	 7% 56% 31% 9%
1	C	319	 11% 51% 34% 6% 9%
1	D	319	 2% 62% 24% 9%

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
2	SO4	C	1798	-	-	X	-
2	SO4	D	1796	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9754 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 N-acetylneuraminate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	71	0	0
			2234	1425	380	418	11			
1	B	291	Total	C	N	O	S	70	0	0
			2234	1425	380	418	11			
1	C	291	Total	C	N	O	S	68	0	0
			2234	1425	380	418	11			
1	D	291	Total	C	N	O	S	54	0	0
			2234	1425	380	418	11			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP P0A6L4
A	-20	GLY	-	expression tag	UNP P0A6L4
A	-19	HIS	-	expression tag	UNP P0A6L4
A	-18	HIS	-	expression tag	UNP P0A6L4
A	-17	HIS	-	expression tag	UNP P0A6L4
A	-16	HIS	-	expression tag	UNP P0A6L4
A	-15	HIS	-	expression tag	UNP P0A6L4
A	-14	HIS	-	expression tag	UNP P0A6L4
A	-13	HIS	-	expression tag	UNP P0A6L4
A	-12	HIS	-	expression tag	UNP P0A6L4
A	-11	HIS	-	expression tag	UNP P0A6L4
A	-10	HIS	-	expression tag	UNP P0A6L4
A	-9	SER	-	expression tag	UNP P0A6L4
A	-8	SER	-	expression tag	UNP P0A6L4
A	-7	GLY	-	expression tag	UNP P0A6L4
A	-6	HIS	-	expression tag	UNP P0A6L4
A	-5	ILE	-	expression tag	UNP P0A6L4
A	-4	GLU	-	expression tag	UNP P0A6L4
A	-3	GLY	-	expression tag	UNP P0A6L4
A	-2	ARG	-	expression tag	UNP P0A6L4
A	-1	HIS	-	expression tag	UNP P0A6L4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP P0A6L4
A	60	ALA	GLU	engineered mutation	UNP P0A6L4
A	98	HIS	TYR	engineered mutation	UNP P0A6L4
A	115	LEU	PHE	engineered mutation	UNP P0A6L4
A	150	GLY	ASP	engineered mutation	UNP P0A6L4
A	153	TYR	ASN	engineered mutation	UNP P0A6L4
A	251	ILE	VAL	engineered mutation	UNP P0A6L4
A	265	ILE	VAL	engineered mutation	UNP P0A6L4
A	281	CYS	TYR	engineered mutation	UNP P0A6L4
B	-21	MET	-	expression tag	UNP P0A6L4
B	-20	GLY	-	expression tag	UNP P0A6L4
B	-19	HIS	-	expression tag	UNP P0A6L4
B	-18	HIS	-	expression tag	UNP P0A6L4
B	-17	HIS	-	expression tag	UNP P0A6L4
B	-16	HIS	-	expression tag	UNP P0A6L4
B	-15	HIS	-	expression tag	UNP P0A6L4
B	-14	HIS	-	expression tag	UNP P0A6L4
B	-13	HIS	-	expression tag	UNP P0A6L4
B	-12	HIS	-	expression tag	UNP P0A6L4
B	-11	HIS	-	expression tag	UNP P0A6L4
B	-10	HIS	-	expression tag	UNP P0A6L4
B	-9	SER	-	expression tag	UNP P0A6L4
B	-8	SER	-	expression tag	UNP P0A6L4
B	-7	GLY	-	expression tag	UNP P0A6L4
B	-6	HIS	-	expression tag	UNP P0A6L4
B	-5	ILE	-	expression tag	UNP P0A6L4
B	-4	GLU	-	expression tag	UNP P0A6L4
B	-3	GLY	-	expression tag	UNP P0A6L4
B	-2	ARG	-	expression tag	UNP P0A6L4
B	-1	HIS	-	expression tag	UNP P0A6L4
B	0	MET	-	expression tag	UNP P0A6L4
B	60	ALA	GLU	engineered mutation	UNP P0A6L4
B	98	HIS	TYR	engineered mutation	UNP P0A6L4
B	115	LEU	PHE	engineered mutation	UNP P0A6L4
B	150	GLY	ASP	engineered mutation	UNP P0A6L4
B	153	TYR	ASN	engineered mutation	UNP P0A6L4
B	251	ILE	VAL	engineered mutation	UNP P0A6L4
B	265	ILE	VAL	engineered mutation	UNP P0A6L4
B	281	CYS	TYR	engineered mutation	UNP P0A6L4
C	-21	MET	-	expression tag	UNP P0A6L4
C	-20	GLY	-	expression tag	UNP P0A6L4
C	-19	HIS	-	expression tag	UNP P0A6L4

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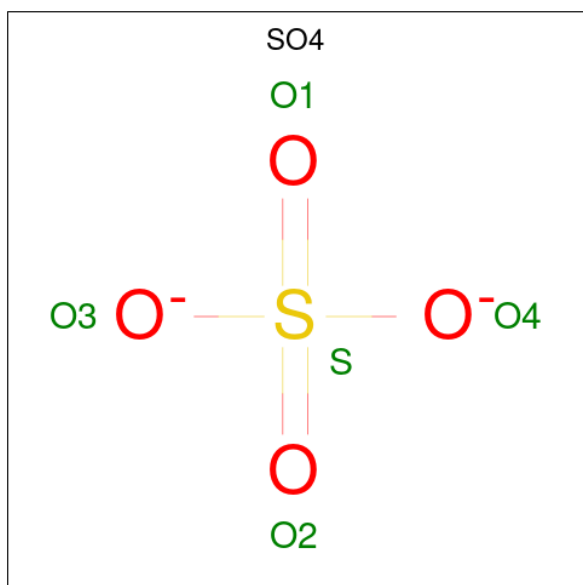
Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	HIS	-	expression tag	UNP P0A6L4
C	-17	HIS	-	expression tag	UNP P0A6L4
C	-16	HIS	-	expression tag	UNP P0A6L4
C	-15	HIS	-	expression tag	UNP P0A6L4
C	-14	HIS	-	expression tag	UNP P0A6L4
C	-13	HIS	-	expression tag	UNP P0A6L4
C	-12	HIS	-	expression tag	UNP P0A6L4
C	-11	HIS	-	expression tag	UNP P0A6L4
C	-10	HIS	-	expression tag	UNP P0A6L4
C	-9	SER	-	expression tag	UNP P0A6L4
C	-8	SER	-	expression tag	UNP P0A6L4
C	-7	GLY	-	expression tag	UNP P0A6L4
C	-6	HIS	-	expression tag	UNP P0A6L4
C	-5	ILE	-	expression tag	UNP P0A6L4
C	-4	GLU	-	expression tag	UNP P0A6L4
C	-3	GLY	-	expression tag	UNP P0A6L4
C	-2	ARG	-	expression tag	UNP P0A6L4
C	-1	HIS	-	expression tag	UNP P0A6L4
C	0	MET	-	expression tag	UNP P0A6L4
C	60	ALA	GLU	engineered mutation	UNP P0A6L4
C	98	HIS	TYR	engineered mutation	UNP P0A6L4
C	115	LEU	PHE	engineered mutation	UNP P0A6L4
C	150	GLY	ASP	engineered mutation	UNP P0A6L4
C	153	TYR	ASN	engineered mutation	UNP P0A6L4
C	251	ILE	VAL	engineered mutation	UNP P0A6L4
C	265	ILE	VAL	engineered mutation	UNP P0A6L4
C	281	CYS	TYR	engineered mutation	UNP P0A6L4
D	-21	MET	-	expression tag	UNP P0A6L4
D	-20	GLY	-	expression tag	UNP P0A6L4
D	-19	HIS	-	expression tag	UNP P0A6L4
D	-18	HIS	-	expression tag	UNP P0A6L4
D	-17	HIS	-	expression tag	UNP P0A6L4
D	-16	HIS	-	expression tag	UNP P0A6L4
D	-15	HIS	-	expression tag	UNP P0A6L4
D	-14	HIS	-	expression tag	UNP P0A6L4
D	-13	HIS	-	expression tag	UNP P0A6L4
D	-12	HIS	-	expression tag	UNP P0A6L4
D	-11	HIS	-	expression tag	UNP P0A6L4
D	-10	HIS	-	expression tag	UNP P0A6L4
D	-9	SER	-	expression tag	UNP P0A6L4
D	-8	SER	-	expression tag	UNP P0A6L4
D	-7	GLY	-	expression tag	UNP P0A6L4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	HIS	-	expression tag	UNP P0A6L4
D	-5	ILE	-	expression tag	UNP P0A6L4
D	-4	GLU	-	expression tag	UNP P0A6L4
D	-3	GLY	-	expression tag	UNP P0A6L4
D	-2	ARG	-	expression tag	UNP P0A6L4
D	-1	HIS	-	expression tag	UNP P0A6L4
D	0	MET	-	expression tag	UNP P0A6L4
D	60	ALA	GLU	engineered mutation	UNP P0A6L4
D	98	HIS	TYR	engineered mutation	UNP P0A6L4
D	115	LEU	PHE	engineered mutation	UNP P0A6L4
D	150	GLY	ASP	engineered mutation	UNP P0A6L4
D	153	TYR	ASN	engineered mutation	UNP P0A6L4
D	251	ILE	VAL	engineered mutation	UNP P0A6L4
D	265	ILE	VAL	engineered mutation	UNP P0A6L4
D	281	CYS	TYR	engineered mutation	UNP P0A6L4

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



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

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

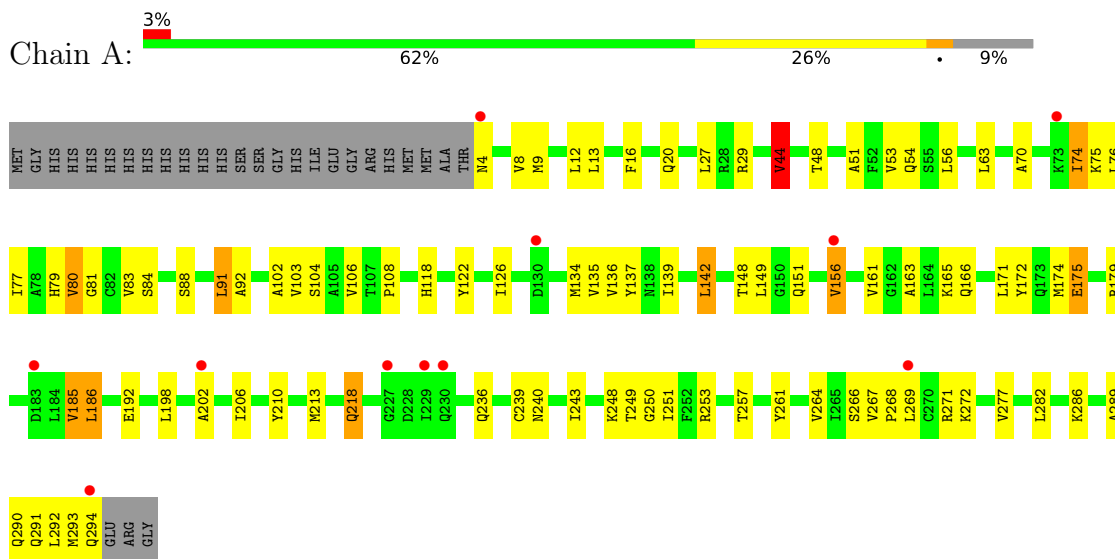
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	226	Total	O	0	0
			226	226		
3	B	174	Total	O	0	0
			174	174		
3	C	173	Total	O	0	0
			173	173		
3	D	205	Total	O	0	0
			205	205		

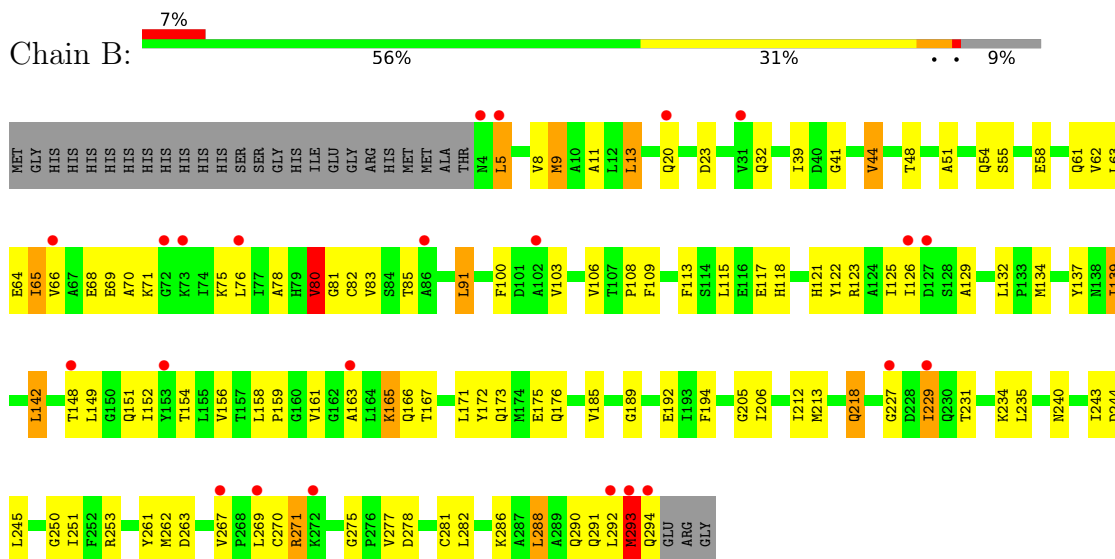
3 Residue-property plots [i](#)

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.

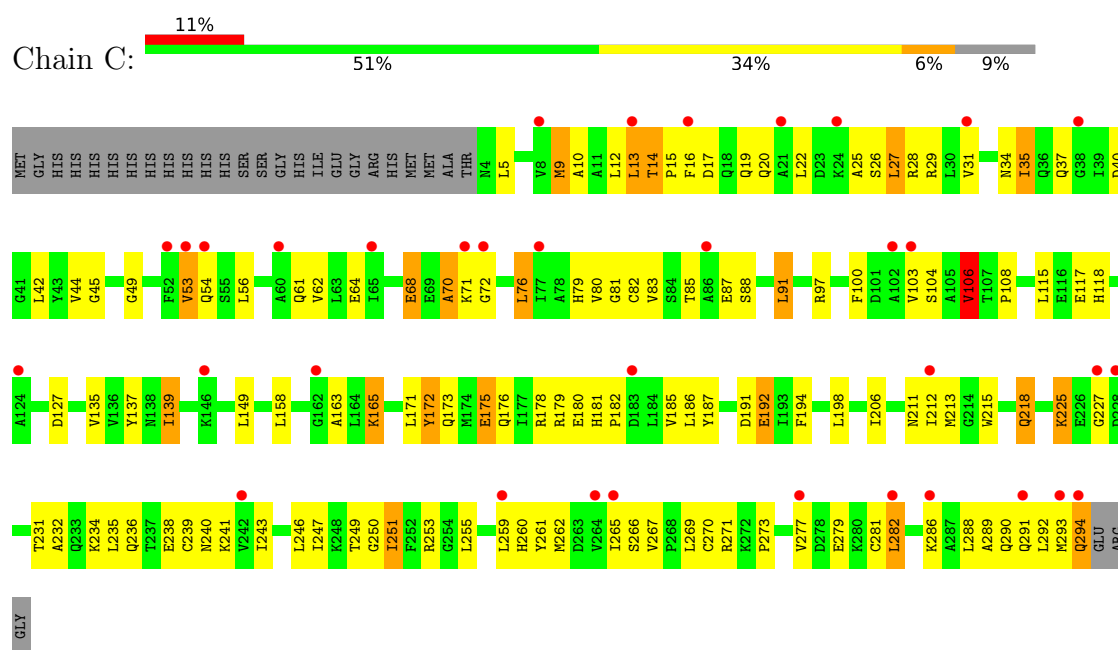
- Molecule 1: N-acetylneuraminate lyase



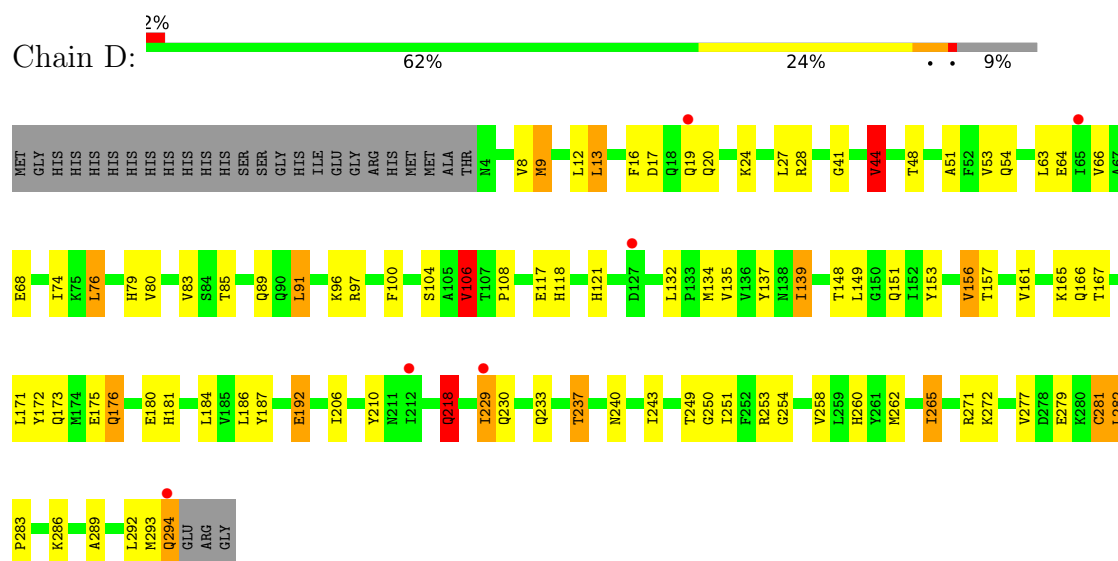
- Molecule 1: N-acetylneuraminate lyase



- Molecule 1: N-acetylneuraminate lyase



- Molecule 1: N-acetylneuraminate lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.81Å 120.81Å 196.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.98 30.00 – 1.98	Depositor EDS
% Data completeness (in resolution range)	88.2 (30.00-1.98) 92.9 (30.00-1.98)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 1.98Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.279 0.234 , 0.279	Depositor DCC
R_{free} test set	5790 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9754	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.78	1/2273 (0.0%)	1.11	11/3076 (0.4%)
1	B	0.72	2/2273 (0.1%)	1.13	21/3076 (0.7%)
1	C	0.67	3/2273 (0.1%)	1.14	19/3076 (0.6%)
1	D	0.76	3/2273 (0.1%)	1.12	13/3076 (0.4%)
All	All	0.73	9/9092 (0.1%)	1.12	64/12304 (0.5%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	LEU	C-N	10.35	1.48	1.33
1	B	281	CYS	C-N	-8.10	1.23	1.33
1	C	281	CYS	C-N	-8.04	1.23	1.33
1	C	282	LEU	C-N	6.60	1.49	1.33
1	D	156	VAL	CA-CB	6.09	1.61	1.54
1	A	53	VAL	CA-CB	6.04	1.60	1.54
1	D	134	MET	SD-CE	5.56	1.93	1.79
1	D	281	CYS	C-N	-5.40	1.26	1.33
1	C	68	GLU	C-N	-5.05	1.25	1.33

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	251	ILE	N-CA-C	10.26	120.25	110.30
1	D	106	VAL	CB-CA-C	-9.24	98.52	111.28
1	B	251	ILE	N-CA-C	8.81	118.85	110.30
1	A	251	ILE	N-CA-C	8.66	118.70	110.30
1	C	83	VAL	N-CA-C	-8.23	102.03	111.00
1	C	267	VAL	CA-C-N	8.08	129.94	119.84
1	C	267	VAL	C-N-CA	8.08	129.94	119.84
1	B	172	TYR	N-CA-C	-8.00	101.64	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	172	TYR	N-CA-C	-7.63	102.30	111.69
1	D	172	TYR	N-CA-C	-7.58	102.36	111.69
1	A	81	GLY	N-CA-C	7.49	121.72	111.54
1	D	251	ILE	N-CA-C	7.24	117.37	110.42
1	A	44	VAL	N-CA-C	7.20	118.96	108.53
1	B	81	GLY	N-CA-C	7.19	120.20	111.93
1	C	139	ILE	CA-C-N	7.11	128.73	119.84
1	C	139	ILE	C-N-CA	7.11	128.73	119.84
1	A	250	GLY	N-CA-C	-6.86	96.92	113.18
1	B	80	VAL	N-CA-CB	-6.86	103.44	112.36
1	A	266	SER	N-CA-C	6.84	118.82	111.36
1	B	11	ALA	N-CA-C	-6.82	98.10	108.67
1	D	44	VAL	N-CA-C	6.72	119.11	108.89
1	D	12	LEU	N-CA-C	6.71	120.09	110.10
1	D	250	GLY	N-CA-C	-6.64	97.44	113.18
1	C	12	LEU	N-CA-C	6.59	119.28	109.59
1	B	126	ILE	N-CA-C	-6.57	104.12	110.42
1	A	12	LEU	N-CA-C	6.56	119.80	109.96
1	D	139	ILE	CA-C-N	6.50	126.00	119.24
1	D	139	ILE	C-N-CA	6.50	126.00	119.24
1	B	282	LEU	O-C-N	-6.41	114.35	120.70
1	C	44	VAL	N-CA-C	6.29	117.53	108.48
1	C	282	LEU	O-C-N	-6.23	114.72	120.51
1	C	81	GLY	N-CA-C	6.11	119.84	111.54
1	B	270	CYS	N-CA-C	-6.10	101.43	110.46
1	B	109	PHE	N-CA-C	5.97	119.39	109.96
1	C	165	LYS	N-CA-C	-5.96	98.02	108.20
1	D	83	VAL	N-CA-C	-5.88	104.78	110.72
1	C	250	GLY	N-CA-C	-5.86	99.29	113.18
1	C	106	VAL	CB-CA-C	-5.81	102.54	111.08
1	A	53	VAL	N-CA-C	-5.79	105.74	111.88
1	C	82	CYS	N-CA-C	-5.74	100.77	108.86
1	A	136	VAL	N-CA-C	-5.72	102.20	109.58
1	A	172	TYR	N-CA-C	-5.72	104.66	111.69
1	D	184	LEU	N-CA-C	5.65	118.44	109.96
1	A	83	VAL	N-CA-C	-5.55	105.31	110.53
1	B	69	GLU	N-CA-C	5.54	118.25	111.82
1	B	139	ILE	CA-C-N	5.54	125.63	119.32
1	B	139	ILE	C-N-CA	5.54	125.63	119.32
1	C	158	LEU	N-CA-C	-5.54	102.80	109.83
1	B	288	LEU	N-CA-C	-5.51	105.19	111.14
1	B	82	CYS	N-CA-C	-5.48	100.73	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	225	LYS	N-CA-C	-5.43	105.28	111.14
1	C	70	ALA	N-CA-C	5.37	122.80	114.64
1	B	151	GLN	N-CA-C	-5.34	105.62	111.82
1	B	250	GLY	N-CA-C	-5.27	100.68	113.18
1	D	218	GLN	N-CA-C	-5.27	105.53	111.28
1	B	275	GLY	CA-C-N	5.24	125.22	120.03
1	B	275	GLY	C-N-CA	5.24	125.22	120.03
1	A	185	VAL	N-CA-C	-5.22	101.95	108.84
1	D	176	GLN	N-CA-C	-5.17	105.72	111.36
1	B	83	VAL	N-CA-C	-5.16	105.36	110.62
1	B	244	ASP	N-CA-C	-5.12	105.59	111.07
1	B	165	LYS	N-CA-C	-5.10	99.48	108.20
1	C	232	ALA	N-CA-C	-5.02	105.72	111.14
1	D	265	ILE	N-CA-C	5.01	115.18	108.17

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	A	2234	0	2270	77	0
1	B	2234	0	2270	82	0
1	C	2234	0	2270	120	0
1	D	2234	0	2270	73	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	2	0
2	D	10	0	0	2	0
3	A	226	0	0	3	1
3	B	174	0	0	4	0
3	C	173	0	0	8	0
3	D	205	0	0	5	0
All	All	9754	0	9080	339	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 20.

All (339) 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:A:70:ALA:HB1	1:A:74:ILE:HD11	1.35	1.03
1:A:84:SER:HB2	1:D:53:VAL:HG23	1.45	0.96
1:B:5:LEU:HD23	1:B:5:LEU:H	1.31	0.92
1:C:218:GLN:HE21	1:C:218:GLN:HA	1.34	0.92
1:A:218:GLN:HE21	1:A:218:GLN:HA	1.34	0.91
1:A:267:VAL:HG12	1:A:269:LEU:HD23	1.53	0.90
1:C:286:LYS:O	1:C:290:GLN:HG2	1.72	0.90
1:A:192:GLU:HG3	1:A:243:ILE:HG21	1.55	0.89
1:C:79:HIS:HE1	1:C:106:VAL:H	1.21	0.86
1:D:79:HIS:HE1	1:D:106:VAL:H	1.21	0.86
1:A:139:ILE:HD11	1:A:142:LEU:HD22	1.56	0.85
1:B:20:GLN:NE2	1:B:271:ARG:HA	1.91	0.85
1:A:70:ALA:HB1	1:A:74:ILE:CD1	2.06	0.85
1:B:64:GLU:O	1:B:68:GLU:HG3	1.78	0.82
1:C:282:LEU:O	1:C:286:LYS:HG3	1.80	0.81
1:B:137:TYR:CE1	1:B:165:LYS:HD3	2.15	0.80
1:A:74:ILE:HD13	1:A:74:ILE:H	1.46	0.80
1:C:236:GLN:HE21	1:C:240:ASN:ND2	1.81	0.79
1:C:9:MET:HE2	1:C:40:ASP:HB2	1.65	0.78
1:C:236:GLN:HE21	1:C:240:ASN:HD21	1.30	0.77
1:B:80:VAL:HG22	1:B:91:LEU:HB3	1.66	0.77
1:C:261:TYR:CE2	1:C:286:LYS:HG2	2.18	0.77
1:C:192:GLU:HG3	1:C:243:ILE:HG21	1.67	0.76
1:D:229:ILE:HD13	1:D:229:ILE:H	1.51	0.76
1:B:218:GLN:HE21	1:B:218:GLN:HA	1.51	0.75
1:A:20:GLN:HE22	1:A:272:LYS:H	1.32	0.74
1:C:22:LEU:HD23	1:C:61:GLN:OE1	1.87	0.73
1:A:218:GLN:HA	1:A:218:GLN:NE2	2.04	0.72
1:B:267:VAL:CG1	1:B:269:LEU:HD23	2.20	0.72
1:C:180:GLU:HG3	3:C:1604:HOH:O	1.89	0.72
1:A:51:ALA:HA	1:A:54:GLN:HE21	1.54	0.72
1:B:292:LEU:C	1:B:294:GLN:H	1.96	0.72
1:A:79:HIS:HE1	1:A:106:VAL:H	1.38	0.71
1:D:192:GLU:HG3	1:D:243:ILE:HG21	1.71	0.71
1:B:267:VAL:HG12	1:B:269:LEU:HD23	1.72	0.69
1:A:74:ILE:HD13	1:A:74:ILE:N	2.05	0.69
1:C:291:GLN:O	1:C:294:GLN:HG2	1.91	0.69
1:B:115:LEU:HD12	3:B:1226:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:GLN:HE21	1:C:269:LEU:HD11	1.58	0.69
1:C:218:GLN:HA	1:C:218:GLN:NE2	2.08	0.69
1:D:253:ARG:HD3	1:D:277:VAL:HG22	1.74	0.69
1:D:9:MET:HG3	1:D:41:GLY:C	2.18	0.69
1:D:16:PHE:CE2	1:D:271:ARG:HG3	2.27	0.68
1:A:137:TYR:CE1	1:A:165:LYS:HD3	2.28	0.68
1:A:253:ARG:HD3	1:A:277:VAL:HG22	1.75	0.68
1:B:286:LYS:O	1:B:290:GLN:HG2	1.93	0.68
1:D:108:PRO:HD2	1:D:118:HIS:HD2	1.58	0.68
1:A:236:GLN:HE21	1:A:240:ASN:HD21	1.41	0.68
1:A:70:ALA:CB	1:A:74:ILE:HD11	2.20	0.68
1:D:173:GLN:HA	1:D:176:GLN:HE21	1.57	0.68
1:D:229:ILE:HD13	1:D:229:ILE:N	2.08	0.67
1:C:53:VAL:O	1:C:53:VAL:HG13	1.94	0.67
1:C:282:LEU:HD12	1:C:282:LEU:N	2.09	0.67
1:D:249:THR:O	1:D:253:ARG:HD2	1.96	0.66
1:C:15:PRO:HB3	1:C:265:ILE:HG23	1.77	0.65
1:B:212:ILE:HD12	1:B:292:LEU:HD11	1.78	0.65
1:C:213:MET:HE1	1:C:239:CYS:HA	1.79	0.65
1:A:108:PRO:HD2	1:A:118:HIS:HD2	1.61	0.65
1:C:137:TYR:CE1	1:C:165:LYS:HD3	2.32	0.64
1:C:80:VAL:HG13	1:C:91:LEU:HB3	1.80	0.64
1:D:13:LEU:HD13	1:D:48:THR:CG2	2.28	0.64
1:A:9:MET:HE1	1:A:75:LYS:HB2	1.80	0.64
1:D:279:GLU:HA	1:D:282:LEU:HD22	1.80	0.64
1:C:15:PRO:HG3	1:C:265:ILE:CD1	2.28	0.63
1:A:13:LEU:HD13	1:A:48:THR:HG22	1.79	0.63
1:B:5:LEU:HD23	1:B:5:LEU:N	2.09	0.63
1:D:13:LEU:HD13	1:D:48:THR:HG22	1.80	0.63
1:D:96:LYS:HD3	1:D:132:LEU:HD13	1.80	0.63
1:D:289:ALA:O	1:D:293:MET:HG3	1.99	0.63
1:C:236:GLN:NE2	1:C:240:ASN:HD21	1.96	0.63
1:A:192:GLU:CG	1:A:243:ILE:HG21	2.28	0.63
1:C:218:GLN:HE21	1:C:218:GLN:CA	2.09	0.63
1:B:20:GLN:HE22	1:B:271:ARG:HA	1.62	0.63
1:A:267:VAL:CG1	1:A:269:LEU:HD23	2.27	0.62
1:C:25:ALA:C	1:C:29:ARG:HH21	2.07	0.62
1:C:31:VAL:O	1:C:35:ILE:HD13	1.99	0.62
1:B:5:LEU:H	1:B:5:LEU:CD2	2.11	0.61
1:C:289:ALA:O	1:C:293:MET:HG3	2.00	0.61
1:D:218:GLN:HE21	1:D:218:GLN:HA	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HD13	1:B:115:LEU:C	2.25	0.61
1:C:192:GLU:HG3	1:C:243:ILE:HD13	1.82	0.61
1:B:113:PHE:CZ	1:C:273:PRO:HG2	2.35	0.61
1:D:79:HIS:HE1	1:D:106:VAL:N	1.96	0.61
1:A:236:GLN:HE21	1:A:240:ASN:ND2	1.99	0.60
1:C:28:ARG:HD2	3:C:1669:HOH:O	2.01	0.60
1:C:80:VAL:HG13	1:C:91:LEU:CB	2.32	0.60
1:B:115:LEU:HD11	1:B:154:THR:HG21	1.84	0.60
1:C:53:VAL:O	1:C:53:VAL:CG1	2.49	0.60
1:C:70:ALA:O	1:C:72:GLY:N	2.35	0.60
1:A:149:LEU:HD23	1:A:149:LEU:O	2.01	0.60
1:D:272:LYS:HE3	3:D:1697:HOH:O	2.02	0.60
1:B:9:MET:HG3	1:B:41:GLY:C	2.28	0.59
1:B:229:ILE:C	1:B:229:ILE:HD13	2.28	0.59
1:B:262:MET:O	1:B:263:ASP:HB2	2.02	0.59
1:C:192:GLU:CG	1:C:243:ILE:HG21	2.30	0.59
1:A:171:LEU:HD12	1:C:171:LEU:HD12	1.84	0.59
1:C:282:LEU:H	1:C:282:LEU:CD1	2.15	0.59
1:A:240:ASN:OD1	1:C:175:GLU:HG2	2.02	0.59
1:C:261:TYR:CD2	1:C:286:LYS:HA	2.38	0.59
1:C:282:LEU:HD12	1:C:282:LEU:H	1.66	0.59
1:D:80:VAL:HB	1:D:91:LEU:HB3	1.85	0.59
1:C:243:ILE:O	1:C:247:ILE:HG12	2.02	0.59
1:A:108:PRO:HD2	1:A:118:HIS:CD2	2.37	0.58
1:A:13:LEU:HD13	1:A:48:THR:CG2	2.33	0.58
1:C:9:MET:CE	1:C:40:ASP:HB2	2.32	0.58
1:A:20:GLN:HB3	1:A:271:ARG:HD2	1.85	0.58
1:B:171:LEU:HD12	1:D:171:LEU:HD12	1.84	0.58
1:D:229:ILE:H	1:D:229:ILE:CD1	2.16	0.58
1:A:79:HIS:HE1	1:A:106:VAL:N	2.01	0.57
1:B:192:GLU:HG3	1:B:243:ILE:HG21	1.86	0.57
1:B:262:MET:HA	1:B:293:MET:HE1	1.85	0.57
1:C:97:ARG:NH1	2:C:1798:SO4:S	2.77	0.57
1:C:165:LYS:HE2	1:C:206:ILE:HG21	1.85	0.57
1:D:51:ALA:HA	1:D:54:GLN:HE21	1.69	0.57
1:C:20:GLN:HG2	1:C:269:LEU:HD21	1.87	0.57
1:A:291:GLN:HG3	1:A:292:LEU:N	2.18	0.57
1:A:8:VAL:HG13	1:A:210:TYR:CE2	2.39	0.57
1:C:97:ARG:NH2	3:C:1590:HOH:O	2.38	0.57
1:C:108:PRO:HD2	1:C:118:HIS:HD2	1.70	0.56
1:D:108:PRO:HD2	1:D:118:HIS:CD2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:PRO:HB3	3:C:1720:HOH:O	2.05	0.56
1:C:173:GLN:HA	1:C:176:GLN:HE21	1.71	0.56
1:D:258:VAL:O	1:D:262:MET:HG3	2.06	0.56
1:B:23:ASP:OD1	1:B:23:ASP:C	2.49	0.56
1:B:137:TYR:CD1	1:B:165:LYS:HD3	2.40	0.56
1:C:26:SER:N	1:C:29:ARG:HH21	2.03	0.56
1:D:192:GLU:HA	1:D:240:ASN:HD21	1.71	0.55
1:C:294:GLN:HG3	1:C:294:GLN:O	2.05	0.55
1:D:281:CYS:SG	3:D:1546:HOH:O	2.58	0.55
1:A:139:ILE:CD1	1:A:142:LEU:HD22	2.31	0.55
1:B:108:PRO:HD2	1:B:118:HIS:HD2	1.71	0.55
1:B:156:VAL:HA	1:B:161:VAL:HG11	1.87	0.55
1:A:106:VAL:HA	1:A:137:TYR:HB3	1.88	0.55
1:A:122:TYR:O	1:A:126:ILE:HG13	2.07	0.55
1:B:9:MET:O	1:B:206:ILE:HA	2.07	0.55
1:A:84:SER:CB	1:D:53:VAL:HG23	2.27	0.55
1:C:56:LEU:HD11	1:C:87:GLU:HG2	1.89	0.55
1:A:148:THR:OG1	1:A:151:GLN:HG3	2.06	0.54
1:C:165:LYS:HE2	1:C:206:ILE:CG2	2.36	0.54
1:C:163:ALA:HB2	1:C:185:VAL:HB	1.88	0.54
1:D:85:THR:OG1	1:D:121:HIS:HD2	1.91	0.54
1:D:96:LYS:HD3	1:D:132:LEU:CD1	2.37	0.54
1:B:175:GLU:HG2	1:D:240:ASN:OD1	2.08	0.54
1:C:80:VAL:CG1	1:C:88:SER:O	2.55	0.54
1:C:19:GLN:CD	1:C:19:GLN:N	2.66	0.54
1:B:227:GLY:HA2	1:D:229:ILE:HD12	1.89	0.54
1:C:192:GLU:CD	1:C:192:GLU:H	2.16	0.54
1:D:253:ARG:HG3	1:D:254:GLY:N	2.23	0.54
1:A:20:GLN:HE22	1:A:272:LYS:N	2.03	0.53
1:B:8:VAL:HG12	1:B:39:ILE:HD11	1.89	0.53
1:D:180:GLU:HG3	3:D:1175:HOH:O	2.09	0.53
1:D:181:HIS:HE1	3:D:1046:HOH:O	1.91	0.53
1:B:13:LEU:HD13	1:B:48:THR:HG22	1.90	0.53
1:D:121:HIS:HE1	3:D:1396:HOH:O	1.91	0.53
1:C:288:LEU:HA	1:C:291:GLN:HG2	1.90	0.53
1:A:149:LEU:HD21	3:A:1302:HOH:O	2.08	0.53
1:B:261:TYR:CD2	1:B:286:LYS:HA	2.44	0.53
1:C:282:LEU:N	1:C:282:LEU:CD1	2.72	0.53
1:D:97:ARG:NH1	2:D:1796:SO4:S	2.81	0.53
1:D:79:HIS:CE1	1:D:106:VAL:H	2.12	0.53
1:C:175:GLU:OE2	1:C:179:ARG:NH2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:ARG:NH1	2:D:1796:SO4:O1	2.42	0.52
1:A:249:THR:O	1:A:253:ARG:HD2	2.10	0.52
1:A:289:ALA:O	1:A:293:MET:HG3	2.09	0.52
1:C:14:THR:CG2	1:C:49:GLY:O	2.57	0.52
1:C:247:ILE:HD13	1:C:251:ILE:HD11	1.92	0.52
1:C:20:GLN:NE2	1:C:269:LEU:HD11	2.25	0.52
1:C:137:TYR:CD1	1:C:165:LYS:HD3	2.44	0.52
1:A:137:TYR:CD1	1:A:165:LYS:HD3	2.45	0.52
1:B:117:GLU:OE2	1:C:253:ARG:NH2	2.42	0.52
1:B:231:THR:O	1:B:235:LEU:HG	2.10	0.52
1:A:56:LEU:HD22	1:A:91:LEU:HD22	1.91	0.52
1:A:149:LEU:HD23	1:A:149:LEU:C	2.35	0.52
1:A:4:ASN:HB2	3:A:1249:HOH:O	2.09	0.52
1:B:122:TYR:HD1	1:B:134:MET:HE3	1.75	0.52
1:A:74:ILE:CD1	1:A:74:ILE:N	2.73	0.51
1:D:53:VAL:O	1:D:53:VAL:HG22	2.09	0.51
1:B:253:ARG:NH2	1:C:117:GLU:OE2	2.43	0.51
1:C:14:THR:HG21	1:C:54:GLN:HE22	1.76	0.51
1:B:173:GLN:HA	1:B:176:GLN:HE21	1.76	0.51
1:D:139:ILE:O	1:D:139:ILE:HG23	2.11	0.51
1:B:294:GLN:O	1:B:294:GLN:HG3	2.10	0.51
1:B:13:LEU:HD13	1:B:48:THR:CG2	2.41	0.50
1:C:25:ALA:HA	3:C:1669:HOH:O	2.11	0.50
1:B:61:GLN:O	1:B:65:ILE:HD12	2.12	0.50
1:B:106:VAL:HA	1:B:137:TYR:HB3	1.94	0.50
1:A:253:ARG:NH2	1:D:117:GLU:OE2	2.45	0.50
1:B:108:PRO:HD2	1:B:118:HIS:CD2	2.47	0.50
1:A:257:THR:HG22	1:A:261:TYR:CE2	2.47	0.50
1:C:212:ILE:HG13	1:C:213:MET:HG2	1.93	0.49
1:C:246:LEU:HD13	1:C:255:LEU:HD21	1.94	0.49
1:B:5:LEU:N	1:B:5:LEU:CD2	2.73	0.49
1:B:148:THR:O	1:B:152:ILE:HG13	2.11	0.49
1:D:44:VAL:HG22	1:D:63:LEU:HD23	1.94	0.49
1:C:15:PRO:HG3	1:C:265:ILE:HD13	1.94	0.49
1:A:84:SER:HB2	1:D:53:VAL:CG2	2.31	0.49
1:D:104:SER:HB2	1:D:135:VAL:HB	1.93	0.49
1:D:137:TYR:CE1	1:D:165:LYS:HD3	2.47	0.49
1:B:212:ILE:HG13	1:B:213:MET:HG2	1.94	0.49
1:C:247:ILE:CD1	1:C:251:ILE:HD11	2.42	0.49
1:B:5:LEU:O	1:B:9:MET:HE1	2.13	0.49
1:B:277:VAL:HG12	1:B:278:ASP:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ALA:CB	1:C:29:ARG:HH21	2.26	0.49
1:B:159:PRO:HG2	3:B:1533:HOH:O	2.13	0.49
1:B:55:SER:OG	1:B:58:GLU:HG3	2.13	0.49
1:B:292:LEU:O	1:B:294:GLN:N	2.43	0.49
1:B:129:ALA:O	1:B:132:LEU:HD13	2.13	0.48
1:C:106:VAL:HG13	1:C:137:TYR:CD2	2.48	0.48
1:B:85:THR:OG1	1:B:121:HIS:HD2	1.96	0.48
1:B:152:ILE:O	1:B:156:VAL:HG22	2.13	0.48
1:C:64:GLU:O	1:C:68:GLU:HG3	2.12	0.48
1:C:49:GLY:O	1:C:54:GLN:NE2	2.47	0.48
1:D:282:LEU:N	1:D:283:PRO:HD2	2.28	0.48
1:A:80:VAL:HG21	1:A:92:ALA:HA	1.96	0.48
1:A:293:MET:O	1:A:294:GLN:HB2	2.12	0.48
1:B:291:GLN:O	1:B:294:GLN:HB3	2.14	0.47
1:D:260:HIS:HD2	1:D:265:ILE:O	1.97	0.47
1:A:103:VAL:CG1	1:A:104:SER:N	2.78	0.47
1:A:218:GLN:HE21	1:A:218:GLN:CA	2.09	0.47
1:A:261:TYR:CE2	1:A:286:LYS:HG2	2.50	0.47
1:B:245:LEU:HD23	1:B:288:LEU:HD22	1.97	0.47
1:A:44:VAL:HG22	1:A:63:LEU:HD23	1.96	0.47
1:A:80:VAL:HG22	1:A:91:LEU:HB3	1.97	0.47
1:B:167:THR:HA	1:B:189:GLY:HA3	1.97	0.47
1:C:45:GLY:O	1:C:79:HIS:HD2	1.97	0.47
1:C:103:VAL:CG1	1:C:104:SER:N	2.77	0.47
1:A:248:LYS:NZ	3:A:1459:HOH:O	2.41	0.47
1:B:78:ALA:HB2	1:B:100:PHE:CD2	2.50	0.46
1:B:121:HIS:HE1	3:B:1416:HOH:O	1.97	0.46
1:C:261:TYR:CZ	1:C:286:LYS:HG2	2.50	0.46
1:D:156:VAL:HA	1:D:161:VAL:HG11	1.96	0.46
1:D:9:MET:O	1:D:206:ILE:HA	2.16	0.46
1:D:229:ILE:N	1:D:229:ILE:CD1	2.77	0.46
1:D:262:MET:HE3	1:D:292:LEU:HB2	1.97	0.46
1:B:212:ILE:HD12	1:B:292:LEU:CD1	2.45	0.46
1:C:9:MET:O	1:C:206:ILE:HA	2.14	0.46
1:C:27:LEU:HD11	1:C:62:VAL:HG13	1.97	0.46
1:A:9:MET:O	1:A:206:ILE:HA	2.16	0.46
1:B:51:ALA:HA	1:B:54:GLN:HE21	1.80	0.46
1:B:192:GLU:HA	1:B:240:ASN:HD21	1.81	0.46
1:C:194:PHE:CE2	1:C:198:LEU:HD11	2.51	0.46
1:D:148:THR:OG1	1:D:151:GLN:HG3	2.15	0.46
1:C:135:VAL:HG22	1:C:163:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:GLU:O	1:C:282:LEU:HD13	2.14	0.46
1:B:121:HIS:CE1	1:B:125:ILE:HD11	2.51	0.46
1:C:240:ASN:N	1:C:240:ASN:HD22	2.14	0.46
1:D:20:GLN:HB3	1:D:271:ARG:HD2	1.98	0.46
1:B:163:ALA:HB2	1:B:185:VAL:HB	1.98	0.45
1:C:249:THR:O	1:C:253:ARG:HD2	2.15	0.45
1:C:238:GLU:OE2	1:C:241:LYS:NZ	2.49	0.45
1:A:253:ARG:HD3	1:A:277:VAL:CG2	2.46	0.45
1:B:139:ILE:HD11	1:B:142:LEU:HD22	1.97	0.45
1:D:17:ASP:OD1	1:D:19:GLN:N	2.48	0.45
1:D:165:LYS:HA	1:D:187:TYR:HB2	1.99	0.45
1:B:20:GLN:HB3	1:B:271:ARG:HD2	1.99	0.45
1:C:253:ARG:HD3	1:C:277:VAL:HG22	1.98	0.45
1:D:41:GLY:HA2	1:D:74:ILE:HB	1.98	0.45
1:C:139:ILE:HG23	1:C:139:ILE:O	2.16	0.45
1:C:269:LEU:HD12	1:C:270:CYS:O	2.17	0.45
1:C:231:THR:O	1:C:235:LEU:HG	2.17	0.45
1:D:85:THR:O	1:D:89:GLN:HG3	2.17	0.45
1:D:139:ILE:HD12	1:D:167:THR:HG21	1.99	0.45
1:A:156:VAL:HA	1:A:161:VAL:HG11	1.98	0.44
1:D:230:GLN:HA	1:D:230:GLN:HE21	1.82	0.44
1:D:76:LEU:HB3	1:D:100:PHE:CD2	2.52	0.44
1:D:233:GLN:O	1:D:237:THR:HG23	2.18	0.44
1:A:91:LEU:HD12	1:A:91:LEU:HA	1.92	0.44
1:B:139:ILE:HG23	1:B:139:ILE:O	2.17	0.44
1:D:153:TYR:O	1:D:157:THR:HG23	2.18	0.44
1:C:13:LEU:CD2	1:C:211:ASN:ND2	2.81	0.44
1:C:106:VAL:HA	1:C:137:TYR:HB3	1.99	0.44
1:C:215:TRP:CZ2	1:C:292:LEU:HD12	2.52	0.44
1:B:123:ARG:NH2	3:B:1218:HOH:O	2.51	0.44
1:D:64:GLU:O	1:D:68:GLU:HG3	2.18	0.43
1:C:16:PHE:CE1	1:C:271:ARG:HD3	2.54	0.43
1:D:24:LYS:O	1:D:28:ARG:HG3	2.18	0.43
1:D:230:GLN:HA	1:D:230:GLN:NE2	2.34	0.43
1:A:80:VAL:CG1	1:A:88:SER:O	2.66	0.43
1:C:212:ILE:HG22	1:C:259:LEU:CD2	2.49	0.43
1:A:198:LEU:HA	1:A:202:ALA:HB3	2.01	0.43
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.80	0.43
1:B:32:GLN:HA	1:B:32:GLN:NE2	2.33	0.43
1:B:218:GLN:HA	1:B:218:GLN:NE2	2.28	0.43
1:D:8:VAL:HG13	1:D:210:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ALA:HB3	1:C:29:ARG:NH2	2.34	0.43
1:C:79:HIS:CE1	1:C:106:VAL:H	2.14	0.43
1:B:192:GLU:HG3	1:B:243:ILE:HD13	2.00	0.43
1:C:127:ASP:OD1	1:C:127:ASP:C	2.61	0.43
1:A:135:VAL:HG22	1:A:163:ALA:HB3	2.00	0.43
1:B:75:LYS:C	1:B:76:LEU:HD22	2.44	0.43
1:C:10:ALA:HB3	1:C:42:LEU:CD2	2.49	0.43
1:C:97:ARG:NH1	2:C:1798:SO4:O3	2.52	0.43
1:B:165:LYS:HE2	1:B:206:ILE:HB	2.00	0.42
1:C:181:HIS:HE1	3:C:1336:HOH:O	2.01	0.42
1:C:191:ASP:OD1	1:C:191:ASP:N	2.52	0.42
1:B:194:PHE:HE1	1:B:205:GLY:HA3	1.84	0.42
1:C:13:LEU:HD23	1:C:211:ASN:ND2	2.34	0.42
1:C:14:THR:HG23	1:C:49:GLY:O	2.19	0.42
1:A:163:ALA:HB2	1:A:185:VAL:HB	2.00	0.42
1:C:10:ALA:HB3	1:C:42:LEU:HD23	2.00	0.42
1:C:85:THR:O	1:C:88:SER:HB2	2.18	0.42
1:C:260:HIS:HD2	1:C:266:SER:O	2.02	0.42
1:D:167:THR:O	1:D:167:THR:HG22	2.19	0.42
1:A:213:MET:HE1	1:A:239:CYS:HA	2.01	0.42
1:C:163:ALA:CB	1:C:185:VAL:HB	2.49	0.42
1:C:259:LEU:HD23	1:C:259:LEU:HA	1.83	0.42
1:D:192:GLU:H	1:D:192:GLU:CD	2.26	0.42
1:D:17:ASP:OD1	1:D:17:ASP:C	2.63	0.42
1:A:16:PHE:CE2	1:A:271:ARG:HG3	2.54	0.42
1:A:20:GLN:NE2	1:A:271:ARG:HA	2.35	0.42
1:B:70:ALA:O	1:B:71:LYS:C	2.63	0.42
1:D:230:GLN:HE21	1:D:230:GLN:CA	2.33	0.42
1:B:44:VAL:CG2	1:B:63:LEU:HD23	2.49	0.42
1:B:132:LEU:HD12	1:B:132:LEU:N	2.35	0.41
1:C:212:ILE:HG22	1:C:259:LEU:HD21	2.02	0.41
1:A:77:ILE:HG12	1:A:102:ALA:HB3	2.01	0.41
1:C:28:ARG:NH2	3:C:1670:HOH:O	2.44	0.41
1:C:262:MET:HE2	1:C:292:LEU:HB2	2.02	0.41
1:B:8:VAL:HG12	1:B:39:ILE:CD1	2.50	0.41
1:B:62:VAL:O	1:B:66:VAL:HG12	2.20	0.41
1:D:294:GLN:CG	1:D:294:GLN:O	2.68	0.41
1:A:122:TYR:HD1	1:A:134:MET:HE3	1.86	0.41
1:C:15:PRO:HB3	1:C:265:ILE:CG2	2.46	0.41
1:B:121:HIS:O	1:B:125:ILE:HG13	2.21	0.41
1:C:28:ARG:NE	3:C:1670:HOH:O	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:VAL:HG12	1:A:104:SER:N	2.35	0.41
1:C:17:ASP:O	1:C:269:LEU:HD23	2.20	0.41
1:C:225:LYS:C	1:C:227:GLY:H	2.29	0.41
1:C:76:LEU:HB3	1:C:100:PHE:CD2	2.56	0.41
1:D:104:SER:CB	1:D:135:VAL:HB	2.51	0.41
1:A:174:MET:SD	1:A:186:LEU:HD13	2.61	0.40
1:A:29:ARG:HD2	1:A:264:VAL:O	2.21	0.40
1:A:192:GLU:HB3	1:C:172:TYR:CD1	2.56	0.40
1:C:165:LYS:HA	1:C:187:TYR:HB2	2.02	0.40
1:C:178:ARG:HA	1:C:178:ARG:HD3	1.94	0.40
1:B:292:LEU:C	1:B:294:GLN:N	2.63	0.40
1:A:175:GLU:OE2	1:A:179:ARG:NH2	2.46	0.40
1:A:192:GLU:H	1:A:192:GLU:CD	2.27	0.40
1:C:34:ASN:HA	1:C:37:GLN:HE21	1.85	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)
3:A:1786:HOH:O	3:A:1786:HOH:O[4_555]	1.66	0.54

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	289/319 (91%)	285 (99%)	4 (1%)	0	100	100
1	B	289/319 (91%)	281 (97%)	7 (2%)	1 (0%)	36	27
1	C	289/319 (91%)	275 (95%)	13 (4%)	1 (0%)	36	27
1	D	289/319 (91%)	283 (98%)	6 (2%)	0	100	100
All	All	1156/1276 (91%)	1124 (97%)	30 (3%)	2 (0%)	43	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	71	LYS
1	B	293	MET

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/261 (91%)	224 (94%)	14 (6%)	18	8
1	B	238/261 (91%)	221 (93%)	17 (7%)	13	5
1	C	238/261 (91%)	220 (92%)	18 (8%)	12	4
1	D	238/261 (91%)	219 (92%)	19 (8%)	11	3
All	All	952/1044 (91%)	884 (93%)	68 (7%)	13	5

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	44	VAL
1	A	74	ILE
1	A	76	LEU
1	A	80	VAL
1	A	91	LEU
1	A	142	LEU
1	A	156	VAL
1	A	166	GLN
1	A	175	GLU
1	A	186	LEU
1	A	218	GLN
1	A	268	PRO
1	A	290	GLN
1	B	5	LEU
1	B	9	MET
1	B	13	LEU
1	B	44	VAL

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Mol	Chain	Res	Type
1	B	65	ILE
1	B	80	VAL
1	B	91	LEU
1	B	103	VAL
1	B	142	LEU
1	B	149	LEU
1	B	158	LEU
1	B	166	GLN
1	B	218	GLN
1	B	229	ILE
1	B	234	LYS
1	B	271	ARG
1	B	293	MET
1	C	5	LEU
1	C	9	MET
1	C	13	LEU
1	C	14	THR
1	C	27	LEU
1	C	35	ILE
1	C	53	VAL
1	C	76	LEU
1	C	91	LEU
1	C	106	VAL
1	C	115	LEU
1	C	149	LEU
1	C	175	GLU
1	C	186	LEU
1	C	192	GLU
1	C	218	GLN
1	C	234	LYS
1	C	294	GLN
1	D	9	MET
1	D	13	LEU
1	D	27	LEU
1	D	44	VAL
1	D	66	VAL
1	D	76	LEU
1	D	91	LEU
1	D	106	VAL
1	D	149	LEU
1	D	166	GLN
1	D	175	GLU

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Mol	Chain	Res	Type
1	D	186	LEU
1	D	192	GLU
1	D	218	GLN
1	D	229	ILE
1	D	237	THR
1	D	282	LEU
1	D	286	LYS
1	D	294	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	20	GLN
1	A	34	ASN
1	A	37	GLN
1	A	54	GLN
1	A	61	GLN
1	A	79	HIS
1	A	90	GLN
1	A	118	HIS
1	A	173	GLN
1	A	211	ASN
1	A	218	GLN
1	A	240	ASN
1	B	18	GLN
1	B	20	GLN
1	B	32	GLN
1	B	34	ASN
1	B	37	GLN
1	B	54	GLN
1	B	61	GLN
1	B	89	GLN
1	B	90	GLN
1	B	98	HIS
1	B	118	HIS
1	B	121	HIS
1	B	173	GLN
1	B	176	GLN
1	B	211	ASN
1	B	218	GLN
1	B	230	GLN

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Mol	Chain	Res	Type
1	B	240	ASN
1	B	260	HIS
1	B	294	GLN
1	C	4	ASN
1	C	18	GLN
1	C	34	ASN
1	C	37	GLN
1	C	54	GLN
1	C	79	HIS
1	C	118	HIS
1	C	173	GLN
1	C	176	GLN
1	C	211	ASN
1	C	218	GLN
1	C	240	ASN
1	C	260	HIS
1	C	291	GLN
1	C	294	GLN
1	D	18	GLN
1	D	34	ASN
1	D	54	GLN
1	D	79	HIS
1	D	90	GLN
1	D	118	HIS
1	D	121	HIS
1	D	173	GLN
1	D	176	GLN
1	D	211	ASN
1	D	218	GLN
1	D	230	GLN
1	D	240	ASN
1	D	260	HIS
1	D	290	GLN
1	D	294	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	C	1798	-	4,4,4	0.37	0	6,6,6	0.13	0
2	SO4	C	1794	-	4,4,4	0.39	0	6,6,6	0.30	0
2	SO4	A	1791	-	4,4,4	0.34	0	6,6,6	0.15	0
2	SO4	D	1792	-	4,4,4	0.50	0	6,6,6	0.24	0
2	SO4	B	1793	-	4,4,4	0.38	0	6,6,6	0.24	0
2	SO4	D	1796	-	4,4,4	0.46	0	6,6,6	0.18	0
2	SO4	B	1797	-	4,4,4	0.31	0	6,6,6	0.23	0
2	SO4	A	1795	-	4,4,4	0.32	0	6,6,6	0.10	0

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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1798	SO4	2	0
2	D	1796	SO4	2	0

5.7 Other polymers [i](#)

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	A	291/319 (91%)	0.42	11 (3%) 44 54	17, 40, 56, 72	16 (5%)
1	B	291/319 (91%)	0.88	23 (7%) 18 25	20, 45, 66, 83	16 (5%)
1	C	291/319 (91%)	1.10	35 (12%) 9 12	21, 50, 70, 94	16 (5%)
1	D	291/319 (91%)	0.39	6 (2%) 63 72	20, 39, 55, 68	13 (4%)
All	All	1164/1276 (91%)	0.70	75 (6%) 25 33	17, 44, 65, 94	61 (5%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	ASN	3.9
1	B	153	TYR	3.8
1	B	227	GLY	3.7
1	B	72	GLY	3.6
1	D	229	ILE	3.6
1	B	229	ILE	3.5
1	B	73	LYS	3.5
1	C	16	PHE	3.4
1	C	21	ALA	3.3
1	D	294	GLN	3.3
1	C	13	LEU	3.3
1	C	65	ILE	3.2
1	C	227	GLY	3.1
1	B	267	VAL	3.1
1	C	53	VAL	3.1
1	C	31	VAL	3.1
1	C	293	MET	3.0
1	C	265	ILE	3.0
1	C	294	GLN	2.9
1	C	102	ALA	2.9
1	C	146	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	227	GLY	2.8
1	C	52	PHE	2.7
1	B	66	VAL	2.7
1	C	24	LYS	2.7
1	C	8	VAL	2.7
1	A	4	ASN	2.7
1	C	282	LEU	2.6
1	A	294	GLN	2.6
1	C	72	GLY	2.6
1	C	242	VAL	2.6
1	B	148	THR	2.6
1	B	294	GLN	2.6
1	B	5	LEU	2.5
1	B	127	ASP	2.5
1	C	77	ILE	2.5
1	B	76	LEU	2.5
1	C	38	GLY	2.4
1	A	229	ILE	2.4
1	C	291	GLN	2.4
1	B	293	MET	2.4
1	C	259	LEU	2.4
1	C	183	ASP	2.4
1	D	212	ILE	2.4
1	B	272	LYS	2.4
1	B	20	GLN	2.3
1	C	286	LYS	2.3
1	C	86	ALA	2.3
1	C	54	GLN	2.3
1	D	65	ILE	2.3
1	B	31	VAL	2.3
1	B	163	ALA	2.2
1	C	71	LYS	2.2
1	A	130	ASP	2.2
1	C	124	ALA	2.2
1	A	183	ASP	2.2
1	A	202	ALA	2.2
1	C	277	VAL	2.1
1	A	269	LEU	2.1
1	A	156	VAL	2.1
1	C	162	GLY	2.1
1	C	264	VAL	2.1
1	A	230	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	60	ALA	2.1
1	C	228	ASP	2.1
1	C	103	VAL	2.1
1	B	292	LEU	2.1
1	B	86	ALA	2.1
1	B	102	ALA	2.1
1	A	73	LYS	2.0
1	B	269	LEU	2.0
1	D	127	ASP	2.0
1	B	126	ILE	2.0
1	C	212	ILE	2.0
1	D	19	GLN	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($\text{\AA}^2$)	Q<0.9
2	SO4	B	1797	5/5	0.90	0.15	58,58,59,59	5
2	SO4	C	1798	5/5	0.90	0.14	55,55,57,58	5
2	SO4	A	1795	5/5	0.94	0.11	49,50,51,51	5
2	SO4	C	1794	5/5	0.95	0.08	49,50,52,54	0
2	SO4	D	1796	5/5	0.95	0.08	46,47,49,51	0
2	SO4	B	1793	5/5	0.97	0.06	46,46,49,50	0
2	SO4	D	1792	5/5	0.98	0.06	36,39,40,42	0
2	SO4	A	1791	5/5	0.98	0.08	35,35,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.