



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:36 PM UTC

PDB ID : 3RHP / pdb_00003rhp
Title : Crystal structure of the C707A mutant of the C-Terminal domain of 10'FOR MYLTETRAHYDROFOLATE DEHYDROGENASE
Authors : Tsybovsky, Y.
Deposited on : 2011-04-11
Resolution : 2.50 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

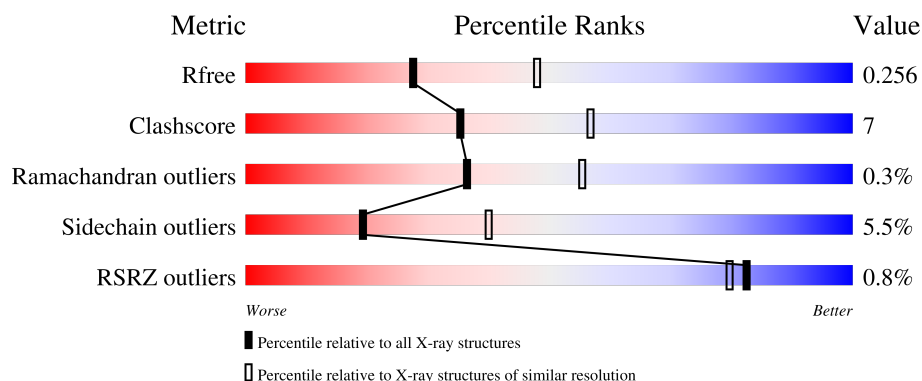
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	517	% 72% 21% • •
1	B	517	% 73% 22% • •
1	C	517	% 72% 23% • •
1	D	517	% 74% 21% • •

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	3	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16351 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 Aldehyde dehydrogenase 1 family, member L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	12	0
			3867	2461	659	727	20			
1	B	498	Total	C	N	O	S	0	11	0
			3871	2461	664	726	20			
1	C	498	Total	C	N	O	S	0	11	0
			3866	2457	669	720	20			
1	D	498	Total	C	N	O	S	0	13	0
			3889	2473	667	729	20			

There are 48 discrepancies between the modelled and reference sequences:

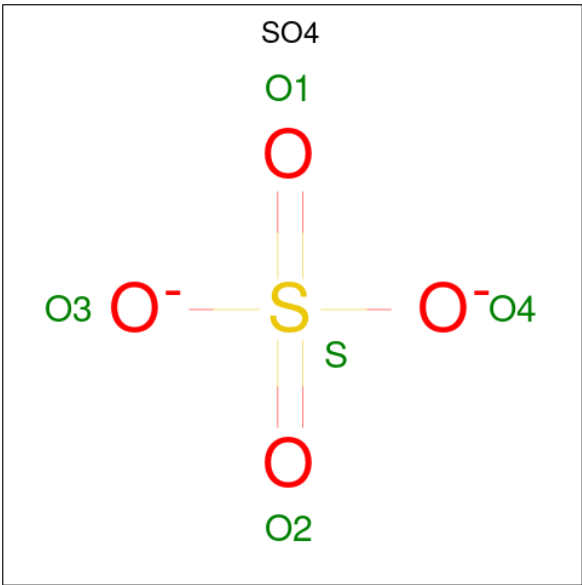
Chain	Residue	Modelled	Actual	Comment	Reference
A	386	MET	-	expression tag	UNP Q5HQB2
A	387	ARG	-	expression tag	UNP Q5HQB2
A	388	GLY	-	expression tag	UNP Q5HQB2
A	389	SER	-	expression tag	UNP Q5HQB2
A	390	HIS	-	expression tag	UNP Q5HQB2
A	391	HIS	-	expression tag	UNP Q5HQB2
A	392	HIS	-	expression tag	UNP Q5HQB2
A	393	HIS	-	expression tag	UNP Q5HQB2
A	394	HIS	-	expression tag	UNP Q5HQB2
A	395	THR	-	expression tag	UNP Q5HQB2
A	396	THR	-	expression tag	UNP Q5HQB2
A	707	ALA	CYS	engineered mutation	UNP Q5HQB2
B	386	MET	-	expression tag	UNP Q5HQB2
B	387	ARG	-	expression tag	UNP Q5HQB2
B	388	GLY	-	expression tag	UNP Q5HQB2
B	389	SER	-	expression tag	UNP Q5HQB2
B	390	HIS	-	expression tag	UNP Q5HQB2
B	391	HIS	-	expression tag	UNP Q5HQB2
B	392	HIS	-	expression tag	UNP Q5HQB2
B	393	HIS	-	expression tag	UNP Q5HQB2
B	394	HIS	-	expression tag	UNP Q5HQB2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	395	THR	-	expression tag	UNP Q5HQB2
B	396	THR	-	expression tag	UNP Q5HQB2
B	707	ALA	CYS	engineered mutation	UNP Q5HQB2
C	386	MET	-	expression tag	UNP Q5HQB2
C	387	ARG	-	expression tag	UNP Q5HQB2
C	388	GLY	-	expression tag	UNP Q5HQB2
C	389	SER	-	expression tag	UNP Q5HQB2
C	390	HIS	-	expression tag	UNP Q5HQB2
C	391	HIS	-	expression tag	UNP Q5HQB2
C	392	HIS	-	expression tag	UNP Q5HQB2
C	393	HIS	-	expression tag	UNP Q5HQB2
C	394	HIS	-	expression tag	UNP Q5HQB2
C	395	THR	-	expression tag	UNP Q5HQB2
C	396	THR	-	expression tag	UNP Q5HQB2
C	707	ALA	CYS	engineered mutation	UNP Q5HQB2
D	386	MET	-	expression tag	UNP Q5HQB2
D	387	ARG	-	expression tag	UNP Q5HQB2
D	388	GLY	-	expression tag	UNP Q5HQB2
D	389	SER	-	expression tag	UNP Q5HQB2
D	390	HIS	-	expression tag	UNP Q5HQB2
D	391	HIS	-	expression tag	UNP Q5HQB2
D	392	HIS	-	expression tag	UNP Q5HQB2
D	393	HIS	-	expression tag	UNP Q5HQB2
D	394	HIS	-	expression tag	UNP Q5HQB2
D	395	THR	-	expression tag	UNP Q5HQB2
D	396	THR	-	expression tag	UNP Q5HQB2
D	707	ALA	CYS	engineered mutation	UNP Q5HQB2

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



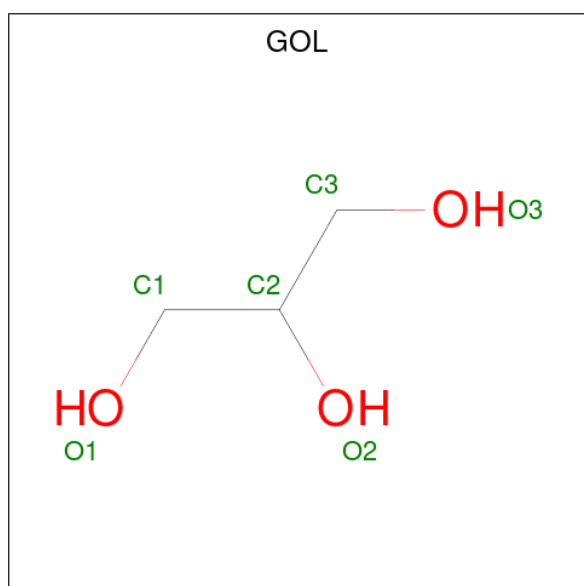
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	B	1	Total	O	S	0	0
			5	4	1		
			Total	O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

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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	C	1	Total	O	S	0	0
			5	4	1		
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		
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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

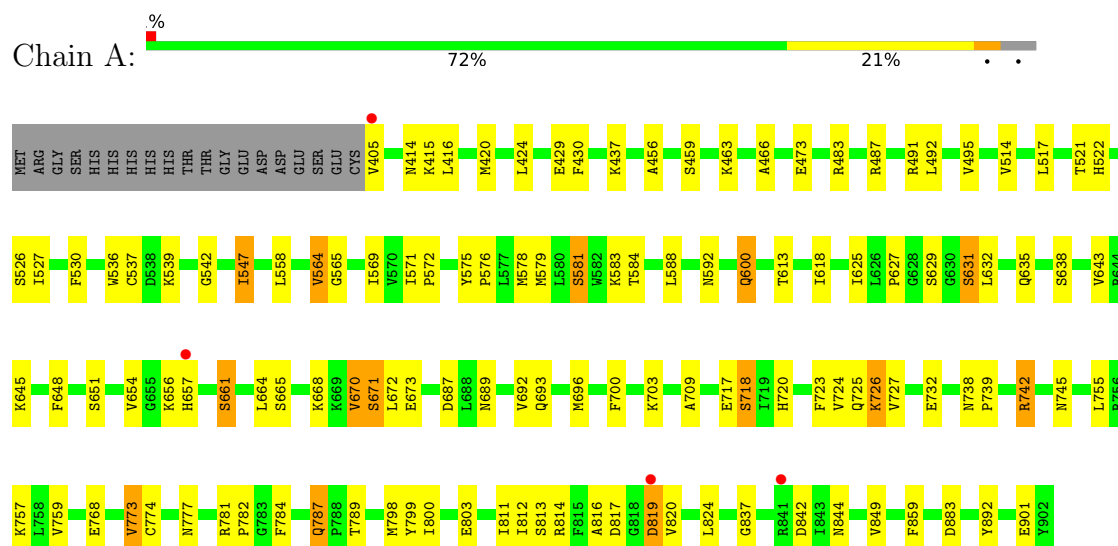
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	176	Total	O	0	0
			176	176		
4	B	170	Total	O	0	0
			170	170		
4	C	185	Total	O	0	0
			185	185		
4	D	183	Total	O	0	0
			183	183		

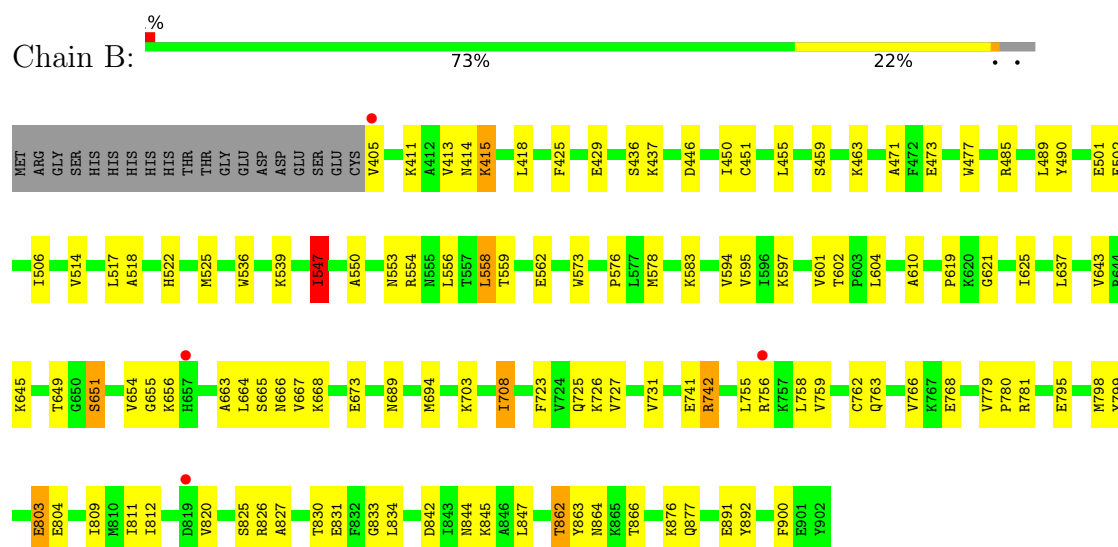
3 Residue-property plots

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: Aldehyde dehydrogenase 1 family, member L1

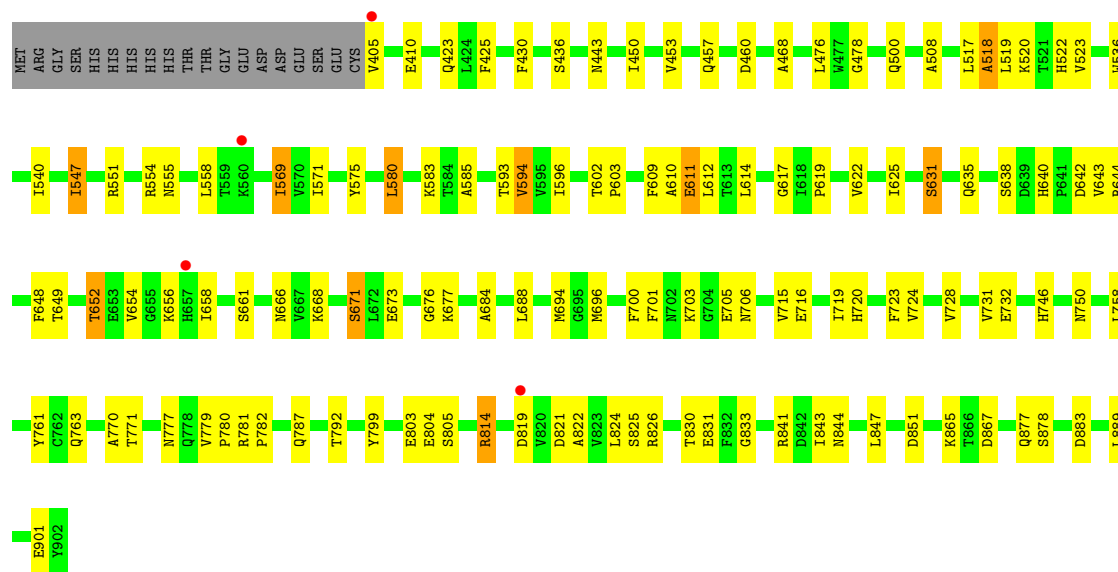


- Molecule 1: Aldehyde dehydrogenase 1 family, member L1

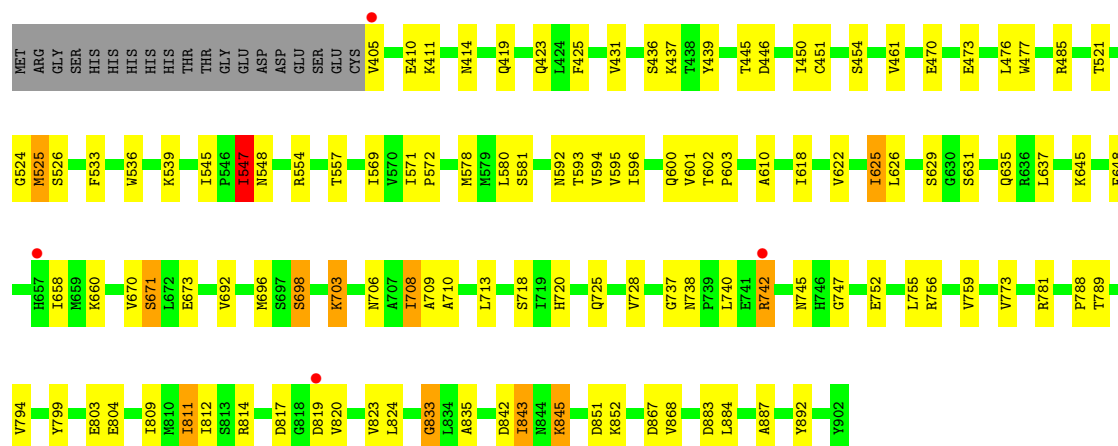
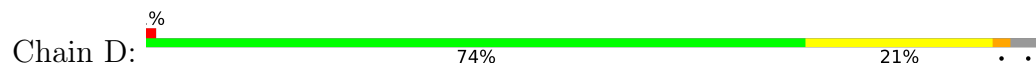


- Molecule 1: Aldehyde dehydrogenase 1 family, member L1





- Molecule 1: Aldehyde dehydrogenase 1 family, member L1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	261.40Å 194.90Å 97.11Å 90.00° 108.70° 90.00°	Depositor
Resolution (Å)	48.97 – 2.50 48.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.97-2.50) 98.1 (48.97-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.213 , 0.257 0.214 , 0.256	Depositor DCC
R_{free} test set	7861 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16351	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	1.29	10/3985 (0.3%)	1.33	15/5394 (0.3%)
1	B	1.27	9/3993 (0.2%)	1.33	21/5403 (0.4%)
1	C	1.39	10/3991 (0.3%)	1.40	24/5400 (0.4%)
1	D	1.34	13/4015 (0.3%)	1.34	26/5430 (0.5%)
All	All	1.32	42/15984 (0.3%)	1.35	86/21627 (0.4%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	547	ILE	CA-CB	9.99	1.65	1.54
1	B	827	ALA	CA-CB	-8.19	1.39	1.53
1	D	596	ILE	CA-CB	-7.61	1.45	1.54
1	A	709	ALA	CA-CB	-7.36	1.41	1.53
1	B	811	ILE	CA-C	7.25	1.59	1.53
1	D	521	THR	CA-C	7.23	1.57	1.52
1	C	468	ALA	C-O	-6.83	1.16	1.24
1	C	715	VAL	C-O	-6.77	1.16	1.24
1	D	545	ILE	CA-CB	6.60	1.62	1.54
1	D	725	GLN	CA-CB	6.54	1.63	1.53
1	B	725	GLN	CA-CB	6.52	1.63	1.53
1	B	547	ILE	CA-CB	6.44	1.61	1.54
1	A	495	VAL	CA-CB	6.42	1.61	1.54
1	C	585	ALA	C-O	-6.38	1.16	1.24
1	C	780	PRO	CA-C	6.32	1.58	1.52
1	D	602	THR	CA-CB	6.20	1.63	1.53
1	D	709	ALA	CA-CB	-6.14	1.43	1.53
1	D	625	ILE	CA-CB	-5.91	1.47	1.54
1	A	759	VAL	CA-CB	5.90	1.61	1.54
1	D	759	VAL	CA-CB	5.89	1.60	1.54
1	C	770	ALA	CA-CB	-5.80	1.43	1.53
1	A	725	GLN	CA-CB	5.72	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	819	ASP	N-CA	5.70	1.52	1.45
1	B	602	THR	CA-CB	5.69	1.60	1.53
1	C	518	ALA	CA-CB	-5.67	1.44	1.53
1	D	658	ILE	CA-CB	5.61	1.60	1.54
1	A	514	VAL	CA-CB	-5.44	1.47	1.54
1	A	670	VAL	CA-C	5.42	1.59	1.52
1	D	738	ASN	CB-CG	5.40	1.65	1.52
1	B	708	ILE	CA-CB	5.33	1.61	1.54
1	D	742	ARG	CG-CD	5.30	1.68	1.52
1	C	508	ALA	CA-CB	-5.29	1.45	1.53
1	C	520	LYS	C-O	-5.26	1.17	1.24
1	A	466	ALA	N-CA	5.26	1.53	1.46
1	C	746	HIS	C-O	5.23	1.29	1.23
1	A	527	ILE	CA-CB	5.21	1.60	1.54
1	A	491	ARG	CB-CG	5.17	1.68	1.52
1	B	514	VAL	CA-CB	-5.16	1.48	1.54
1	A	456	ALA	CA-CB	-5.13	1.45	1.53
1	B	562	GLU	CA-C	5.08	1.59	1.52
1	B	559	THR	N-CA	5.04	1.52	1.46
1	D	809	ILE	C-O	5.01	1.30	1.24

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	781[A]	ARG	CA-C-N	-10.15	110.47	120.52
1	C	781[A]	ARG	C-N-CA	-10.15	110.47	120.52
1	C	781[B]	ARG	CA-C-N	-10.15	110.47	120.52
1	C	781[B]	ARG	C-N-CA	-10.15	110.47	120.52
1	D	781[A]	ARG	CA-C-N	-9.31	108.20	119.84
1	D	781[A]	ARG	C-N-CA	-9.31	108.20	119.84
1	D	781[B]	ARG	CA-C-N	-9.31	108.20	119.84
1	D	781[B]	ARG	C-N-CA	-9.31	108.20	119.84
1	B	811	ILE	N-CA-C	9.17	119.85	106.55
1	C	777	ASN	N-CA-C	8.77	122.83	109.23
1	B	820	VAL	N-CA-C	8.65	119.23	110.23
1	C	443	ASN	CA-C-N	-8.61	110.47	120.89
1	C	443	ASN	C-N-CA	-8.61	110.47	120.89
1	C	779	VAL	CA-C-N	-8.48	109.79	120.23
1	C	779	VAL	C-N-CA	-8.48	109.79	120.23
1	D	618	ILE	N-CA-C	-8.45	101.37	108.63
1	B	811	ILE	N-CA-CB	-8.08	104.22	112.06
1	D	812	ILE	N-CA-C	7.99	120.08	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	811	ILE	N-CA-C	7.96	118.15	106.85
1	B	763	GLN	N-CA-C	-7.95	102.20	111.03
1	D	473	GLU	N-CA-C	7.90	119.89	111.28
1	B	812	ILE	N-CA-C	7.76	119.76	108.58
1	C	596	ILE	N-CA-C	-7.28	97.92	108.11
1	B	826	ARG	N-CA-C	-7.21	103.35	111.07
1	A	820	VAL	N-CA-C	7.08	117.60	110.23
1	C	594	VAL	N-CA-C	6.76	118.08	108.42
1	D	747	GLY	CA-C-N	6.75	126.71	120.03
1	D	747	GLY	C-N-CA	6.75	126.71	120.03
1	B	578	MET	N-CA-C	-6.72	103.88	111.14
1	A	420	MET	CA-C-N	-6.71	113.39	120.03
1	A	420	MET	C-N-CA	-6.71	113.39	120.03
1	D	708	ILE	N-CA-C	6.62	118.51	112.29
1	D	594	VAL	N-CA-C	6.59	117.05	108.35
1	A	812	ILE	N-CA-C	6.57	117.58	107.99
1	C	723	PHE	N-CA-C	6.44	117.96	111.07
1	D	887	ALA	N-CA-C	6.44	119.12	111.33
1	B	795[A]	GLU	N-CA-C	-6.38	99.76	109.85
1	B	795[B]	GLU	N-CA-C	-6.38	99.76	109.85
1	D	820	VAL	N-CA-C	6.29	116.92	110.82
1	A	842	ASP	N-CA-C	6.08	117.90	109.15
1	D	737	GLY	N-CA-C	6.07	119.61	110.75
1	C	878	SER	N-CA-C	-5.88	106.10	113.28
1	A	811	ILE	N-CA-C	5.83	115.13	106.85
1	A	564	VAL	CB-CA-C	-5.81	102.85	112.26
1	B	601	VAL	N-CA-C	5.80	120.55	113.00
1	B	604	LEU	N-CA-C	5.79	117.39	111.14
1	B	781[A]	ARG	CA-C-N	-5.75	112.66	119.84
1	B	781[A]	ARG	C-N-CA	-5.75	112.66	119.84
1	B	781[B]	ARG	CA-C-N	-5.75	112.66	119.84
1	B	781[B]	ARG	C-N-CA	-5.75	112.66	119.84
1	D	533	PHE	N-CA-C	5.69	118.25	111.71
1	C	523	VAL	N-CA-C	-5.64	106.31	111.67
1	D	789	THR	N-CA-C	5.58	118.57	109.59
1	D	773	VAL	N-CA-C	5.58	118.06	111.09
1	C	625	ILE	N-CA-C	5.53	116.08	108.12
1	B	594	VAL	N-CA-C	5.43	115.52	108.35
1	D	835	ALA	N-CA-C	5.42	116.50	108.86
1	C	851	ASP	CB-CA-C	-5.38	101.86	110.79
1	A	844	ASN	N-CA-C	5.37	116.94	111.14
1	C	883	ASP	N-CA-C	-5.37	101.13	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	542	GLY	N-CA-C	-5.28	104.95	112.55
1	C	575	TYR	CA-CB-CG	5.26	123.38	113.90
1	C	611	GLU	N-CA-C	-5.24	105.47	111.07
1	A	787	GLN	N-CA-C	5.24	117.02	109.48
1	B	803[A]	GLU	N-CA-C	5.23	118.75	109.96
1	B	803[B]	GLU	N-CA-C	5.23	118.75	109.96
1	B	812	ILE	CB-CA-C	-5.23	104.43	110.91
1	D	436	SER	N-CA-C	5.21	119.21	112.86
1	D	670	VAL	N-CA-C	5.17	116.17	108.46
1	A	742	ARG	CA-C-N	5.17	128.17	120.31
1	A	742	ARG	C-N-CA	5.17	128.17	120.31
1	D	625	ILE	N-CA-C	5.17	115.34	108.11
1	A	787	GLN	CA-C-N	-5.16	114.00	119.98
1	A	787	GLN	C-N-CA	-5.16	114.00	119.98
1	D	618	ILE	CA-C-N	-5.11	114.67	119.89
1	D	618	ILE	C-N-CA	-5.11	114.67	119.89
1	C	450	ILE	N-CA-C	-5.10	105.88	110.82
1	B	862	THR	N-CA-C	-5.09	101.71	108.74
1	C	825	SER	CB-CA-C	-5.09	102.89	110.88
1	B	473	GLU	N-CA-C	5.07	116.89	111.36
1	C	780	PRO	CB-CA-C	5.05	117.07	111.56
1	D	851	ASP	CB-CA-C	-5.05	102.92	110.90
1	A	618	ILE	CB-CA-C	-5.05	102.17	111.36
1	D	601	VAL	N-CA-C	5.04	119.28	112.98
1	C	602	THR	N-CA-C	5.02	115.99	108.76
1	C	666	ASN	N-CA-C	5.01	118.47	111.56

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	A	3867	0	3861	61	0
1	B	3871	0	3869	55	0
1	C	3866	0	3867	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3889	0	3898	60	0
2	A	30	0	0	0	0
2	B	35	0	0	0	0
2	C	35	0	0	2	0
2	D	20	0	0	1	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0
3	C	6	0	8	1	0
3	D	6	0	8	0	0
4	A	176	0	0	2	0
4	B	170	0	0	6	0
4	C	185	0	0	7	0
4	D	183	0	0	7	0
All	All	16351	0	15527	230	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 7.

All (230) 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:D:756:ARG:NH2	4:D:1159:HOH:O	1.88	1.04
1:C:841[B]:ARG:HG2	1:C:841[B]:ARG:HH11	1.42	0.82
1:A:773:VAL:O	1:A:774:CYS:HB3	1.81	0.78
1:B:799:TYR:CE2	1:B:803[B]:GLU:HG3	2.18	0.78
1:B:414:ASN:O	1:B:415:LYS:HB2	1.84	0.76
1:B:727:VAL:O	1:B:731:VAL:HG23	1.87	0.75
1:C:684:ALA:HA	1:C:719:ILE:HD13	1.69	0.75
1:D:756:ARG:NE	4:D:1161:HOH:O	2.23	0.70
1:C:500:GLN:OE1	4:C:1093:HOH:O	2.08	0.70
1:C:457:GLN:O	1:C:460:ASP:HB2	1.92	0.69
1:A:547:ILE:HD13	1:A:547:ILE:H	1.57	0.69
1:A:720:HIS:CD2	1:A:814:ARG:HG3	2.27	0.69
1:C:593:THR:HG22	1:C:622:VAL:HG13	1.75	0.68
1:A:459:SER:O	1:A:463:LYS:HG3	1.94	0.68
1:B:414:ASN:OD1	1:B:742:ARG:NH2	2.28	0.67
1:B:780:PRO:O	4:B:1071:HOH:O	2.12	0.67
1:D:423:GLN:HA	1:D:454:SER:OG	1.95	0.66
1:D:794:VAL:HG21	1:D:811:ILE:HG23	1.77	0.66
1:D:718:SER:HB3	1:D:817:ASP:OD1	1.97	0.65
1:B:844:ASN:ND2	1:C:841[B]:ARG:HH12	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:631:SER:O	1:D:635:GLN:HB2	1.98	0.64
1:B:689:ASN:OD1	1:B:726:LYS:NZ	2.29	0.64
1:D:842:ASP:HB3	1:D:845:LYS:HB2	1.79	0.64
1:C:841[B]:ARG:HG2	1:C:841[B]:ARG:NH1	2.09	0.64
1:B:558:LEU:HD12	1:B:558:LEU:C	2.23	0.63
1:C:551:ARG:NH2	2:C:3:SO4:O4	2.31	0.63
1:A:558:LEU:C	1:A:558:LEU:HD12	2.23	0.63
1:C:518:ALA:HA	1:C:522:HIS:HB2	1.83	0.61
1:B:539:LYS:HD3	1:D:536:TRP:CE2	2.37	0.59
1:D:868:VAL:HG13	4:D:1017:HOH:O	2.03	0.58
1:D:600:GLN:NE2	1:D:629:SER:HA	2.18	0.58
1:A:569:ILE:HD12	1:A:571:ILE:HD11	1.86	0.58
1:D:526:SER:OG	1:D:578:MET:HA	2.03	0.58
1:A:777:ASN:O	1:A:787:GLN:HG3	2.04	0.58
1:A:824:LEU:HD21	1:A:849:VAL:HG13	1.85	0.58
1:C:831:GLU:HB2	4:C:1119:HOH:O	2.03	0.57
1:A:564:VAL:HG23	1:A:565:GLY:N	2.19	0.57
1:A:692:VAL:HG21	1:A:726:LYS:HB3	1.87	0.57
1:A:799:TYR:CE2	1:A:803[A]:GLU:HG3	2.40	0.57
1:D:804:GLU:HA	4:D:1046:HOH:O	2.03	0.57
1:C:540:ILE:HD11	1:C:889:LEU:HD22	1.87	0.56
1:A:651:SER:OG	1:A:654:VAL:HG23	2.06	0.56
1:B:762:CYS:O	1:B:766:VAL:HG23	2.05	0.56
1:D:470:GLU:HG3	4:D:1032:HOH:O	2.06	0.56
1:B:536:TRP:CE2	1:D:539:LYS:HD3	2.41	0.56
1:C:547:ILE:HB	1:D:867:ASP:CG	2.30	0.56
1:C:643:VAL:O	1:C:668:LYS:HE3	2.06	0.56
1:D:580:LEU:C	1:D:580:LEU:HD23	2.31	0.56
1:C:671:SER:HB2	4:C:1098:HOH:O	2.05	0.55
1:A:720:HIS:O	1:A:724:VAL:HG23	2.07	0.55
1:A:781[B]:ARG:HB2	1:A:782:PRO:HD2	1.88	0.55
1:C:640:HIS:CE1	1:C:642:ASP:HB2	2.42	0.55
1:A:671:SER:O	1:A:672:LEU:HD23	2.06	0.55
1:A:517:LEU:HD23	1:A:521:THR:HB	1.89	0.55
1:D:445:THR:O	1:D:445:THR:HG22	2.06	0.55
1:C:684:ALA:N	1:C:716:GLU:OE2	2.32	0.55
1:A:539:LYS:HD3	1:C:536:TRP:CE2	2.41	0.54
1:C:558:LEU:C	1:C:558:LEU:HD12	2.32	0.54
1:A:837:GLY:HA2	1:A:859:PHE:O	2.08	0.54
1:A:414:ASN:O	1:A:415:LYS:HB2	2.06	0.54
1:A:781[B]:ARG:HB2	1:A:782:PRO:CD	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:VAL:O	1:B:668:LYS:HE3	2.07	0.54
1:D:883:ASP:O	1:D:884:LEU:HB2	2.08	0.54
1:C:569:ILE:HG13	1:C:571:ILE:HD11	1.91	0.53
1:A:521:THR:O	1:A:522:HIS:C	2.52	0.53
1:A:718:SER:HB3	1:A:817:ASP:OD1	2.09	0.53
1:D:799:TYR:CE2	1:D:803[A]:GLU:HG3	2.44	0.53
1:C:799:TYR:CE2	1:C:803[A]:GLU:HG3	2.44	0.52
1:D:592:ASN:ND2	1:D:892:TYR:HB3	2.24	0.52
1:D:692:VAL:O	1:D:696:MET:HG2	2.09	0.52
1:B:842:ASP:C	1:B:842:ASP:OD2	2.53	0.52
1:D:450:ILE:O	1:D:451:CYS:HB3	2.10	0.51
1:A:638:SER:HB3	1:A:661:SER:HB2	1.92	0.51
1:C:901:GLU:HG3	4:C:1040:HOH:O	2.11	0.51
1:D:811:ILE:O	1:D:811:ILE:HG22	2.09	0.51
1:C:867:ASP:CG	1:D:547:ILE:HB	2.35	0.51
1:C:676:GLY:O	1:C:804:GLU:HG3	2.11	0.51
1:C:554:ARG:NE	2:C:3:SO4:O1	2.35	0.51
1:A:424:LEU:O	1:A:430:PHE:HA	2.12	0.50
1:C:453:VAL:HG21	1:C:603:PRO:HG2	1.94	0.50
1:B:651:SER:OG	1:B:654:VAL:HG23	2.12	0.50
1:B:863:TYR:CD2	1:B:864:ASN:N	2.79	0.50
1:D:477:TRP:CH2	1:D:485:ARG:HG3	2.46	0.50
1:B:891:GLU:HB3	4:B:1056:HOH:O	2.10	0.50
1:D:698:SER:OG	1:D:710:ALA:HB3	2.12	0.50
1:C:654:VAL:O	1:C:658:ILE:HG12	2.12	0.50
1:B:758:LEU:HD22	1:B:809:ILE:HD11	1.94	0.49
1:A:631:SER:O	1:A:632:LEU:C	2.51	0.49
1:B:708:ILE:HG22	1:B:834:LEU:HG	1.95	0.49
1:C:571:ILE:HD12	1:C:580:LEU:HA	1.94	0.49
1:D:425:PHE:CD2	1:D:610:ALA:HB1	2.47	0.49
1:D:706:ASN:C	1:D:706:ASN:HD22	2.20	0.49
1:D:554:ARG:NE	2:D:2:SO4:O4	2.37	0.48
1:B:550:ALA:O	1:B:553:ASN:HB2	2.12	0.48
1:C:833:GLY:HA2	4:C:1013:HOH:O	2.14	0.48
1:C:644:ARG:HB3	4:C:1044:HOH:O	2.13	0.48
1:C:724:VAL:O	1:C:728:VAL:HG23	2.13	0.47
1:D:580:LEU:HD23	1:D:581:SER:N	2.30	0.47
1:A:656:LYS:HG2	1:B:663:ALA:O	2.14	0.47
1:D:720:HIS:CD2	1:D:814:ARG:HG3	2.49	0.47
1:A:547:ILE:H	1:A:547:ILE:CD1	2.27	0.47
1:A:632:LEU:C	1:A:632:LEU:HD23	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:758:LEU:HD23	1:C:758:LEU:HA	1.51	0.47
1:C:425:PHE:CD2	1:C:610:ALA:HB1	2.50	0.46
1:A:583:LYS:HE2	1:A:883:ASP:OD2	2.15	0.46
1:A:687:ASP:OD2	4:A:1162:HOH:O	2.20	0.46
1:A:696:MET:HE3	1:A:700:PHE:HE2	1.80	0.46
1:B:595:VAL:HG11	1:B:637:LEU:HD21	1.98	0.46
1:B:831:GLU:O	1:B:877:GLN:HB2	2.16	0.46
1:D:571:ILE:CG2	1:D:572:PRO:HD2	2.46	0.46
1:D:595:VAL:HG11	1:D:637:LEU:HD21	1.97	0.46
1:B:525:MET:HE1	1:B:866:THR:OG1	2.16	0.46
1:B:554:ARG:HH22	1:D:852:LYS:HE2	1.80	0.46
1:A:816:ALA:HB3	1:A:819:ASP:HB2	1.98	0.46
1:B:554:ARG:NH2	1:D:852:LYS:HE2	2.30	0.46
1:C:617:GLY:O	1:C:619:PRO:HD3	2.16	0.46
1:A:781[A]:ARG:HB2	1:A:782:PRO:CD	2.45	0.46
1:B:583:LYS:HE3	1:B:649:THR:OG1	2.16	0.46
1:C:547:ILE:HD11	1:C:555:ASN:HB3	1.98	0.46
1:D:706:ASN:C	1:D:706:ASN:ND2	2.74	0.46
1:A:693:GLN:HA	1:A:693:GLN:OE1	2.16	0.45
1:A:781[A]:ARG:HB2	1:A:782:PRO:HD2	1.98	0.45
1:D:706:ASN:ND2	1:D:708:ILE:H	2.13	0.45
1:A:592:ASN:HD21	1:A:892:TYR:HB3	1.81	0.45
1:D:593:THR:HG22	1:D:622:VAL:HA	1.99	0.45
1:B:450:ILE:O	1:B:451:CYS:HB3	2.16	0.45
1:A:600:GLN:NE2	1:A:629:SER:HA	2.31	0.44
1:A:768[B]:GLU:CD	1:A:798:MET:HG2	2.42	0.44
1:B:411:LYS:HD3	4:B:1154:HOH:O	2.17	0.44
1:B:833:GLY:HA2	4:B:1027:HOH:O	2.18	0.44
1:C:700:PHE:O	1:C:701:PHE:C	2.59	0.44
1:C:720:HIS:O	1:C:724:VAL:HG23	2.16	0.44
1:D:439:TYR:OH	1:D:603:PRO:HG3	2.18	0.44
1:A:575:TYR:O	1:A:576:PRO:C	2.58	0.44
1:A:901:GLU:HB3	1:B:862:THR:HB	1.98	0.44
1:B:866:THR:OG1	3:B:10:GOL:H11	2.17	0.44
1:A:530:PHE:CE1	1:A:581:SER:HB3	2.52	0.44
1:D:547:ILE:HD12	1:D:557:THR:OG1	2.18	0.44
1:B:755:LEU:O	1:B:759:VAL:HG23	2.18	0.44
1:B:803[A]:GLU:HG3	1:B:804:GLU:N	2.32	0.44
1:C:688:LEU:HD12	1:C:688:LEU:HA	1.75	0.44
1:D:425:PHE:CG	1:D:610:ALA:HB1	2.53	0.44
1:A:774:CYS:O	1:A:789:THR:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:631:SER:O	1:C:635:GLN:HB3	2.18	0.44
1:B:501:GLU:HB2	4:B:1017:HOH:O	2.18	0.43
1:D:648:PHE:CD2	1:D:648:PHE:C	2.96	0.43
1:A:643:VAL:O	1:A:668:LYS:HE3	2.18	0.43
1:D:571:ILE:HG23	1:D:572:PRO:HD2	2.00	0.43
1:D:755:LEU:C	1:D:755:LEU:HD13	2.43	0.43
1:C:476:LEU:C	1:C:478:GLY:H	2.25	0.43
1:D:713:LEU:HD12	1:D:713:LEU:N	2.33	0.43
1:A:689:ASN:OD1	1:A:726:LYS:NZ	2.51	0.43
1:C:705:GLU:OE1	1:C:750:ASN:HB2	2.18	0.43
1:C:831:GLU:HB3	1:C:877:GLN:HG3	2.01	0.43
1:A:483:ARG:HB3	1:D:548:ASN:HD21	1.84	0.43
1:C:638:SER:HB3	1:C:661:SER:HB2	2.00	0.43
1:B:446:ASP:OD2	1:B:446:ASP:C	2.60	0.43
1:D:410:GLU:HG3	1:D:419[B]:GLN:NE2	2.34	0.43
1:D:446:ASP:OD2	1:D:446:ASP:C	2.62	0.43
1:A:648:PHE:C	1:A:648:PHE:CD2	2.96	0.43
1:C:583:LYS:HE2	1:C:649:THR:OG1	2.19	0.43
1:C:865:LYS:O	1:C:865:LYS:HG3	2.18	0.43
1:D:414:ASN:HB2	1:D:740:LEU:HD22	2.00	0.43
1:A:592:ASN:ND2	1:A:892:TYR:HB3	2.34	0.43
1:C:843:ILE:HG23	1:C:844:ASN:N	2.33	0.43
1:C:847:LEU:HD23	1:C:847:LEU:HA	1.76	0.43
1:A:536:TRP:O	1:A:537:CYS:C	2.61	0.42
1:A:635:GLN:OE1	1:A:657[A]:HIS:NE2	2.50	0.42
1:A:768[B]:GLU:OE2	1:A:800:ILE:HG12	2.19	0.42
1:D:671:SER:HB2	4:D:1092:HOH:O	2.18	0.42
1:B:547:ILE:HD13	1:B:547:ILE:H	1.84	0.42
1:B:876:LYS:HE2	4:B:1008:HOH:O	2.20	0.42
1:D:423:GLN:HB3	1:D:431:VAL:O	2.19	0.42
1:B:471:ALA:HB2	1:B:621:GLY:HA3	2.00	0.42
1:B:573:TRP:O	1:B:576:PRO:HD3	2.18	0.42
1:B:655:GLY:O	1:B:656:LYS:C	2.61	0.42
1:B:666:ASN:O	1:B:667:VAL:CG2	2.67	0.42
1:C:423:GLN:HB2	1:C:430:PHE:HB3	2.00	0.42
1:B:645:LYS:HE3	1:B:892:TYR:CE1	2.54	0.42
1:C:609:PHE:O	1:C:612:LEU:HB2	2.19	0.42
1:C:706:ASN:HD21	3:C:8:GOL:H31	1.84	0.42
1:D:571:ILE:HD12	1:D:580:LEU:HA	2.02	0.42
1:A:572:PRO:HG2	1:A:579:MET:HG3	2.02	0.42
1:C:569:ILE:HD13	1:C:594:VAL:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:833:GLY:HA2	4:D:1022:HOH:O	2.20	0.42
1:B:723:PHE:O	1:B:727:VAL:HG23	2.20	0.42
1:C:720:HIS:CD2	1:C:814:ARG:HG3	2.54	0.42
1:B:847:LEU:HD23	1:B:847:LEU:HA	1.75	0.42
1:C:821:ASP:HA	1:C:824:LEU:HD12	2.02	0.41
1:A:738:ASN:OD1	1:A:739:PRO:HD2	2.19	0.41
1:B:459:SER:O	1:B:463:LYS:HG3	2.20	0.41
1:B:477:TRP:CH2	1:B:485:ARG:HG3	2.55	0.41
1:B:768[B]:GLU:HG3	1:B:798:MET:HG2	2.02	0.41
1:C:536:TRP:CG	1:C:889:LEU:HD11	2.55	0.41
1:C:648:PHE:CD2	1:C:648:PHE:C	2.98	0.41
1:D:823:VAL:HG13	1:D:824:LEU:N	2.35	0.41
1:A:424:LEU:CD2	1:A:627:PRO:HD2	2.51	0.41
1:A:782:PRO:HG2	4:A:1109:HOH:O	2.20	0.41
1:B:489:LEU:HD23	1:B:489:LEU:HA	1.83	0.41
1:B:425:PHE:CD2	1:B:610:ALA:HB1	2.55	0.41
1:C:831:GLU:OE1	1:C:877:GLN:HG3	2.20	0.41
1:D:752:GLU:HG2	1:D:756:ARG:HH21	1.84	0.41
1:A:664:LEU:HD23	1:A:664:LEU:HA	1.86	0.41
1:B:518:ALA:HA	1:B:522:HIS:HB2	2.01	0.41
1:C:677:LYS:HA	4:C:1097:HOH:O	2.20	0.41
1:A:755:LEU:HD22	1:A:784:PHE:HB3	2.02	0.41
1:B:799:TYR:CD2	1:B:803[B]:GLU:HG3	2.55	0.41
1:C:611:GLU:O	1:C:614:LEU:HB2	2.20	0.41
1:C:822:ALA:O	1:C:826:ARG:HG3	2.21	0.41
1:D:571:ILE:CD1	1:D:580:LEU:HA	2.51	0.41
1:A:492:LEU:HD13	1:A:613:THR:HA	2.03	0.41
1:C:696:MET:HE3	1:C:731:VAL:HG22	2.01	0.41
1:B:547:ILE:HD13	1:B:547:ILE:N	2.36	0.40
1:D:525:MET:O	1:D:526:SER:C	2.61	0.40
1:B:490[A]:TYR:O	1:B:490[A]:TYR:CD2	2.73	0.40
1:C:652:THR:HG22	1:C:656:LYS:HE3	2.04	0.40
1:A:526:SER:OG	1:A:578:MET:HA	2.21	0.40
1:A:584:THR:HG22	1:A:588:LEU:HG	2.03	0.40
1:B:502:GLU:O	1:B:506:ILE:HG13	2.21	0.40
1:B:900:PHE:HD2	1:D:843:ILE:HD11	1.86	0.40
1:D:461:VAL:HA	1:D:626:LEU:HD11	2.03	0.40
1:A:723:PHE:O	1:A:727:VAL:HG23	2.22	0.40
1:C:761:TYR:CZ	1:C:805:SER:HB3	2.56	0.40
1:D:569:ILE:HD13	1:D:569:ILE:HG21	1.88	0.40
1:A:670:VAL:HG22	1:A:671:SER:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:771:THR:HB	1:C:792:THR:OG1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	507/517 (98%)	484 (96%)	23 (4%)	0	100	100
1	B	507/517 (98%)	477 (94%)	29 (6%)	1 (0%)	43	63
1	C	507/517 (98%)	479 (94%)	27 (5%)	1 (0%)	43	63
1	D	509/517 (98%)	470 (92%)	36 (7%)	3 (1%)	21	38
All	All	2030/2068 (98%)	1910 (94%)	115 (6%)	5 (0%)	36	63

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	436	SER
1	D	524	GLY
1	B	436	SER
1	D	703	LYS
1	D	833	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	415/425 (98%)	388 (94%)	27 (6%)	15	32
1	B	416/425 (98%)	387 (93%)	29 (7%)	14	29
1	C	415/425 (98%)	399 (96%)	16 (4%)	28	55
1	D	419/425 (99%)	399 (95%)	20 (5%)	23	46
All	All	1665/1700 (98%)	1573 (94%)	92 (6%)	19	40

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405	VAL
1	A	416	LEU
1	A	429	GLU
1	A	437	LYS
1	A	473	GLU
1	A	487	ARG
1	A	547	ILE
1	A	581	SER
1	A	600	GLN
1	A	625	ILE
1	A	631	SER
1	A	645	LYS
1	A	661	SER
1	A	665	SER
1	A	671	SER
1	A	673	GLU
1	A	703	LYS
1	A	717	GLU
1	A	718	SER
1	A	726	LYS
1	A	732	GLU
1	A	742	ARG
1	A	745	ASN
1	A	757	LYS
1	A	773	VAL
1	A	813	SER
1	A	819	ASP
1	B	405	VAL
1	B	413	VAL
1	B	415	LYS
1	B	418	LEU
1	B	429	GLU
1	B	437	LYS

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Mol	Chain	Res	Type
1	B	455	LEU
1	B	517	LEU
1	B	547	ILE
1	B	556	LEU
1	B	558	LEU
1	B	597	LYS
1	B	619	PRO
1	B	625	ILE
1	B	651	SER
1	B	664	LEU
1	B	665	SER
1	B	673	GLU
1	B	694[A]	MET
1	B	694[B]	MET
1	B	703	LYS
1	B	741[A]	GLU
1	B	741[B]	GLU
1	B	742	ARG
1	B	756	ARG
1	B	779	VAL
1	B	825	SER
1	B	830	THR
1	B	845	LYS
1	C	405	VAL
1	C	410	GLU
1	C	517	LEU
1	C	519	LEU
1	C	547	ILE
1	C	569	ILE
1	C	580	LEU
1	C	631	SER
1	C	652	THR
1	C	671	SER
1	C	673	GLU
1	C	703	LYS
1	C	732	GLU
1	C	787	GLN
1	C	814	ARG
1	C	830	THR
1	D	405	VAL
1	D	411	LYS
1	D	437	LYS

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Mol	Chain	Res	Type
1	D	476	LEU
1	D	525	MET
1	D	547	ILE
1	D	625	ILE
1	D	645	LYS
1	D	660	LYS
1	D	671	SER
1	D	673	GLU
1	D	698	SER
1	D	703	LYS
1	D	728	VAL
1	D	742	ARG
1	D	745	ASN
1	D	788	PRO
1	D	819	ASP
1	D	843	ILE
1	D	845	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	541	GLN
1	A	555	ASN
1	A	600	GLN
1	A	745	ASN
1	A	750	ASN
1	A	890	ASN
1	B	440	ASN
1	B	457	GLN
1	B	541	GLN
1	B	555	ASN
1	B	600	GLN
1	B	745	ASN
1	B	749	GLN
1	B	844	ASN
1	C	457	GLN
1	C	498	GLN
1	C	541	GLN
1	C	600	GLN
1	C	706	ASN
1	C	749	GLN
1	C	797	HIS

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Mol	Chain	Res	Type
1	C	844	ASN
1	D	474	ASN
1	D	548	ASN
1	D	600	GLN
1	D	706	ASN
1	D	745	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

28 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	A	5	-	4,4,4	0.51	0	6,6,6	1.40	1 (16%)
2	SO4	C	1	-	4,4,4	0.34	0	6,6,6	0.60	0
2	SO4	D	2	-	4,4,4	0.50	0	6,6,6	0.52	0
3	GOL	A	7	-	5,5,5	0.35	0	5,5,5	1.55	1 (20%)
3	GOL	B	10	-	5,5,5	0.38	0	5,5,5	1.99	1 (20%)
2	SO4	C	6	-	4,4,4	0.29	0	6,6,6	0.98	0
2	SO4	C	3	-	4,4,4	0.23	0	6,6,6	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	5	-	4,4,4	0.21	0	6,6,6	0.63	0
2	SO4	B	5	-	4,4,4	0.43	0	6,6,6	0.66	0
2	SO4	D	1	-	4,4,4	0.43	0	6,6,6	0.61	0
3	GOL	D	5	-	5,5,5	0.68	0	5,5,5	1.21	1 (20%)
2	SO4	A	1	-	4,4,4	0.19	0	6,6,6	0.70	0
2	SO4	B	3	-	4,4,4	0.28	0	6,6,6	0.48	0
2	SO4	C	4	-	4,4,4	0.37	0	6,6,6	0.58	0
2	SO4	A	4	-	4,4,4	0.31	0	6,6,6	0.84	0
2	SO4	C	7	-	4,4,4	0.50	0	6,6,6	0.77	0
3	GOL	C	8	-	5,5,5	0.65	0	5,5,5	2.21	2 (40%)
2	SO4	D	3	-	4,4,4	0.28	0	6,6,6	0.77	0
2	SO4	B	6	-	4,4,4	0.32	0	6,6,6	0.48	0
2	SO4	C	2	-	4,4,4	0.30	0	6,6,6	0.62	0
2	SO4	B	9	-	4,4,4	0.38	0	6,6,6	0.54	0
2	SO4	A	3	-	4,4,4	0.50	0	6,6,6	0.71	0
2	SO4	B	8	-	4,4,4	0.32	0	6,6,6	0.53	0
2	SO4	B	4	-	4,4,4	0.24	0	6,6,6	0.50	0
2	SO4	B	7	-	4,4,4	0.18	0	6,6,6	0.85	0
2	SO4	D	4	-	4,4,4	0.24	0	6,6,6	0.55	0
2	SO4	A	6	-	4,4,4	0.32	0	6,6,6	1.38	1 (16%)
2	SO4	A	2	-	4,4,4	0.43	0	6,6,6	0.78	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	GOL	C	8	-	-	3/4/4/4	-
3	GOL	A	7	-	-	2/4/4/4	-
3	GOL	D	5	-	-	2/4/4/4	-
3	GOL	B	10	-	-	2/4/4/4	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	10	GOL	C3-C2-C1	-4.05	96.95	111.80
3	C	8	GOL	C3-C2-C1	-3.62	98.51	111.80
3	A	7	GOL	C3-C2-C1	-3.15	100.25	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6	SO4	O4-S-O3	2.26	121.02	108.54
3	C	8	GOL	O2-C2-C3	2.13	118.00	109.18
3	D	5	GOL	O2-C2-C1	2.08	117.79	109.18
2	A	5	SO4	O2-S-O1	2.06	123.60	109.06

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	7	GOL	C1-C2-C3-O3
3	B	10	GOL	C1-C2-C3-O3
3	C	8	GOL	C1-C2-C3-O3
3	D	5	GOL	O1-C1-C2-C3
3	D	5	GOL	O1-C1-C2-O2
3	A	7	GOL	O2-C2-C3-O3
3	B	10	GOL	O2-C2-C3-O3
3	C	8	GOL	O2-C2-C3-O3
3	C	8	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	SO4	1	0
3	B	10	GOL	1	0
2	C	3	SO4	2	0
3	C	8	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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	498/517 (96%)	-0.42	4 (0%) 82 80	10, 30, 46, 57	30 (6%)
1	B	498/517 (96%)	-0.34	4 (0%) 82 80	12, 32, 45, 62	31 (6%)
1	C	498/517 (96%)	-0.51	4 (0%) 82 80	9, 27, 38, 53	27 (5%)
1	D	498/517 (96%)	-0.41	4 (0%) 82 80	12, 30, 43, 62	32 (6%)
All	All	1992/2068 (96%)	-0.42	16 (0%) 82 80	9, 30, 44, 62	120 (6%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	657[A]	HIS	3.5
1	C	819	ASP	3.2
1	B	405	VAL	3.1
1	D	742	ARG	2.9
1	A	657[A]	HIS	2.9
1	C	657[A]	HIS	2.8
1	C	405	VAL	2.8
1	A	405	VAL	2.7
1	D	405	VAL	2.6
1	A	819	ASP	2.4
1	D	657[A]	HIS	2.3
1	C	560	LYS	2.3
1	B	819	ASP	2.2
1	D	819	ASP	2.2
1	A	841[A]	ARG	2.2
1	B	756	ARG	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	A	4	5/5	0.84	0.20	33,35,36,39	5
2	SO4	A	5	5/5	0.87	0.16	55,56,60,60	5
2	SO4	D	3	5/5	0.88	0.14	34,35,36,37	5
2	SO4	B	7	5/5	0.89	0.16	35,36,39,39	5
2	SO4	D	2	5/5	0.89	0.11	40,40,41,42	5
2	SO4	A	3	5/5	0.89	0.14	41,41,42,44	5
3	GOL	D	5	6/6	0.89	0.12	29,34,43,49	0
2	SO4	A	6	5/5	0.90	0.17	59,59,62,63	5
2	SO4	C	4	5/5	0.90	0.12	33,33,35,35	5
2	SO4	C	6	5/5	0.90	0.15	51,54,56,57	5
2	SO4	B	9	5/5	0.91	0.14	33,33,36,36	5
3	GOL	C	8	6/6	0.92	0.12	34,34,36,39	0
2	SO4	B	8	5/5	0.92	0.14	30,32,35,36	5
2	SO4	C	5	5/5	0.93	0.13	37,38,40,41	5
3	GOL	A	7	6/6	0.93	0.11	39,40,43,49	0
3	GOL	B	10	6/6	0.93	0.14	36,39,43,50	0
2	SO4	C	3	5/5	0.93	0.09	47,49,50,50	5
2	SO4	B	6	5/5	0.93	0.10	42,42,43,44	5
2	SO4	B	5	5/5	0.94	0.08	46,48,49,51	5
2	SO4	C	2	5/5	0.94	0.12	30,31,35,36	5
2	SO4	C	1	5/5	0.95	0.08	42,42,43,46	5
2	SO4	D	1	5/5	0.95	0.08	34,38,39,42	5
2	SO4	A	2	5/5	0.96	0.09	36,36,38,38	5
2	SO4	B	4	5/5	0.96	0.08	25,26,29,31	5
2	SO4	B	3	5/5	0.97	0.07	18,18,21,21	5
2	SO4	C	7	5/5	0.97	0.06	32,34,37,37	5
2	SO4	A	1	5/5	0.97	0.07	25,28,29,30	5
2	SO4	D	4	5/5	0.97	0.10	49,54,54,54	5

6.5 Other polymers [i](#)

There are no such residues in this entry.