



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:58 PM UTC

PDB ID : 3RHM / pdb_00003rhm
Title : Crystal structure of the E673Q mutant of C-Terminal domain of 10'FORMYLTETRAHYDROFOLATE DEHYDROGENASE
Authors : Tsybovsky, Y.
Deposited on : 2011-04-11
Resolution : 2.38 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

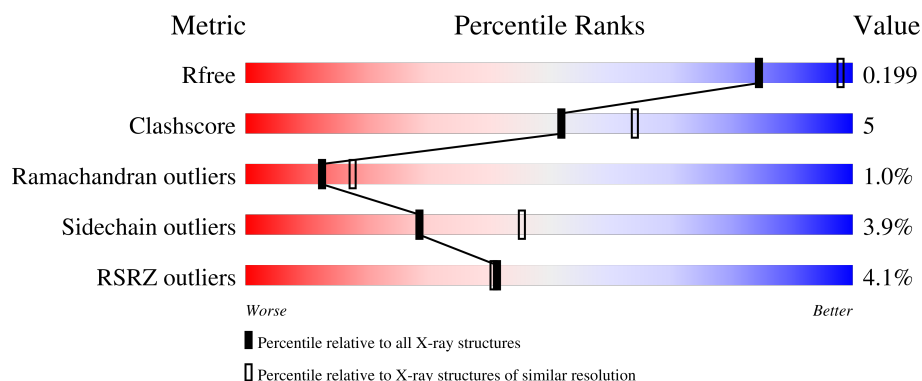
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	4% 78% 15% ...
1	B	517	4% 78% 16% ..
1	C	517	3% 75% 18% ..
1	D	517	4% 76% 18% ...

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16121 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	3	6	0
			3826	2436	657	715	18			
1	B	498	Total	C	N	O	S	3	5	0
			3817	2429	657	713	18			
1	C	498	Total	C	N	O	S	0	3	0
			3806	2424	652	712	18			
1	D	498	Total	C	N	O	S	0	6	0
			3825	2435	656	716	18			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	MET	-	expression tag	UNP Q5HZB2
A	387	ARG	-	expression tag	UNP Q5HZB2
A	388	GLY	-	expression tag	UNP Q5HZB2
A	389	SER	-	expression tag	UNP Q5HZB2
A	390	HIS	-	expression tag	UNP Q5HZB2
A	391	HIS	-	expression tag	UNP Q5HZB2
A	392	HIS	-	expression tag	UNP Q5HZB2
A	393	HIS	-	expression tag	UNP Q5HZB2
A	394	HIS	-	expression tag	UNP Q5HZB2
A	395	THR	-	expression tag	UNP Q5HZB2
A	396	THR	-	expression tag	UNP Q5HZB2
A	673	GLN	GLU	engineered mutation	UNP Q5HZB2
B	386	MET	-	expression tag	UNP Q5HZB2
B	387	ARG	-	expression tag	UNP Q5HZB2
B	388	GLY	-	expression tag	UNP Q5HZB2
B	389	SER	-	expression tag	UNP Q5HZB2
B	390	HIS	-	expression tag	UNP Q5HZB2
B	391	HIS	-	expression tag	UNP Q5HZB2
B	392	HIS	-	expression tag	UNP Q5HZB2
B	393	HIS	-	expression tag	UNP Q5HZB2
B	394	HIS	-	expression tag	UNP Q5HZB2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	395	THR	-	expression tag	UNP Q5HQB2
B	396	THR	-	expression tag	UNP Q5HQB2
B	673	GLN	GLU	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	673	GLN	GLU	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	673	GLN	GLU	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		
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	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	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		
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		

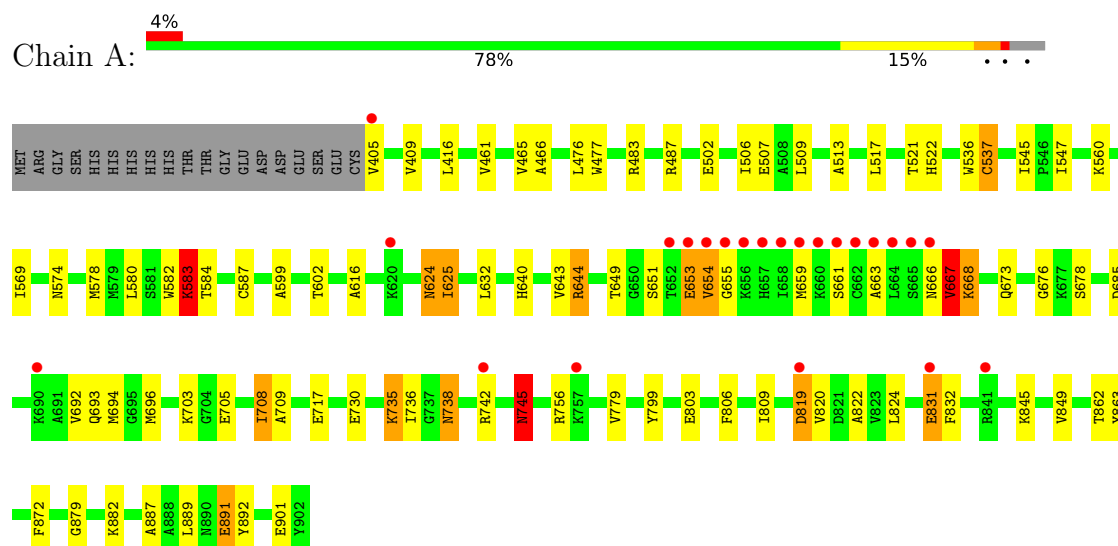
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	179	Total	O	0	0
			179	179		
4	B	156	Total	O	0	0
			156	156		
4	C	179	Total	O	0	0
			179	179		
4	D	169	Total	O	0	0
			169	169		

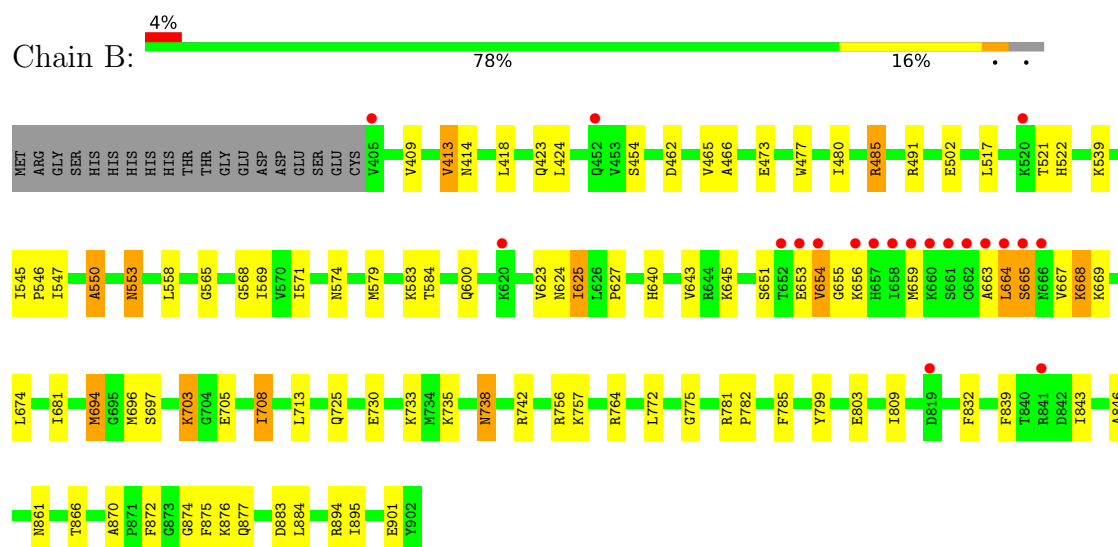
3 Residue-property plots

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.

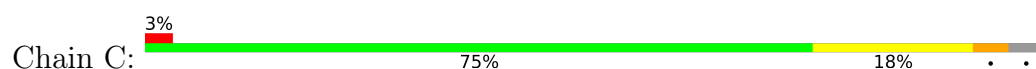
- Molecule 1: Aldehyde dehydrogenase 1 family, member L1

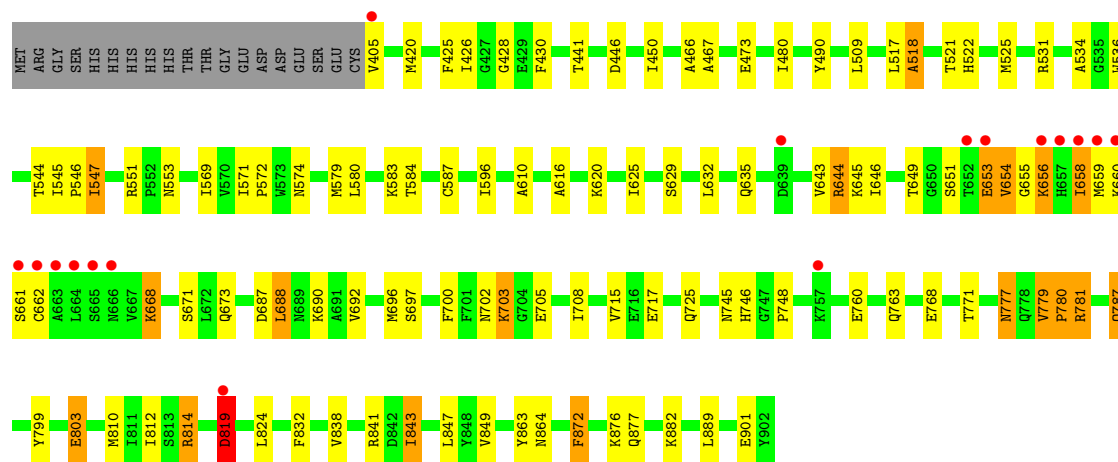


- Molecule 1: Aldehyde dehydrogenase 1 family, member L1

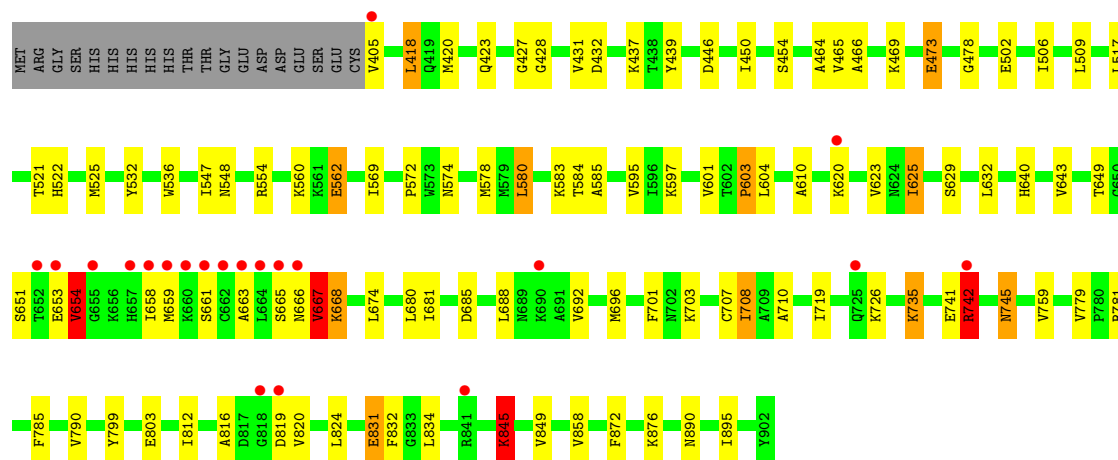
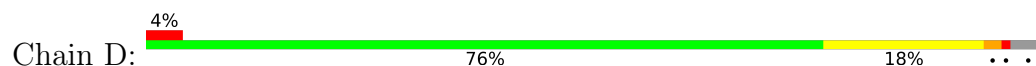


- Molecule 1: Aldehyde dehydrogenase 1 family, member L1





- 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	261.61Å 193.72Å 97.31Å 90.00° 109.05° 90.00°	Depositor
Resolution (Å)	49.81 – 2.38 49.81 – 2.38	Depositor EDS
% Data completeness (in resolution range)	96.7 (49.81-2.38) 96.7 (49.81-2.38)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.171 , 0.202 0.169 , 0.199	Depositor DCC
R_{free} test set	8869 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16121	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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, GOL

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	1.63	26/3921 (0.7%)	1.31	13/5309 (0.2%)
1	B	1.60	26/3914 (0.7%)	1.33	23/5300 (0.4%)
1	C	1.73	40/3892 (1.0%)	1.38	16/5271 (0.3%)
1	D	1.65	34/3921 (0.9%)	1.33	23/5309 (0.4%)
All	All	1.66	126/15648 (0.8%)	1.34	75/21189 (0.4%)

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	A	0	1
1	D	0	1
All	All	0	2

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	565	GLY	C-O	9.96	1.29	1.24
1	D	759	VAL	CA-CB	9.63	1.66	1.54
1	D	667	VAL	CA-CB	9.50	1.67	1.54
1	A	560	LYS	CG-CD	-9.49	1.24	1.52
1	C	466	ALA	CA-CB	8.92	1.67	1.53
1	D	562	GLU	CA-C	7.99	1.60	1.52
1	D	834	LEU	N-CA	-7.73	1.36	1.46
1	C	780	PRO	CA-C	7.71	1.60	1.52
1	B	665	SER	N-CA	7.67	1.56	1.46
1	A	667	VAL	CA-CB	7.62	1.64	1.54
1	D	665	SER	CA-C	7.56	1.62	1.52
1	A	879	GLY	C-O	7.42	1.27	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	779	VAL	CA-C	7.22	1.59	1.52
1	C	746	HIS	N-CA	-7.20	1.37	1.46
1	B	667	VAL	CA-CB	6.87	1.62	1.54
1	C	518	ALA	CA-CB	-6.80	1.42	1.53
1	C	426	ILE	CA-CB	-6.78	1.45	1.54
1	C	546	PRO	CA-C	6.73	1.59	1.53
1	D	585	ALA	CA-CB	-6.72	1.42	1.53
1	C	446	ASP	CA-C	-6.70	1.45	1.52
1	D	623	VAL	C-O	-6.67	1.17	1.24
1	C	653	GLU	CA-C	6.62	1.61	1.52
1	D	583	LYS	CA-C	-6.56	1.41	1.52
1	C	760	GLU	CG-CD	6.52	1.68	1.52
1	C	779	VAL	CA-CB	-6.49	1.45	1.54
1	B	713	LEU	N-CA	-6.39	1.38	1.46
1	B	782	PRO	CA-C	6.37	1.60	1.52
1	A	599	ALA	CA-CB	6.35	1.63	1.53
1	B	875	PHE	CA-C	6.32	1.61	1.53
1	C	534	ALA	CA-CB	-6.29	1.43	1.53
1	B	735	LYS	N-CA	-6.25	1.38	1.46
1	D	473	GLU	C-O	-6.22	1.16	1.24
1	C	787	GLN	CA-C	-6.22	1.46	1.53
1	D	710	ALA	N-CA	-6.20	1.38	1.46
1	B	681	ILE	C-O	6.19	1.30	1.24
1	B	466	ALA	CA-CB	6.19	1.62	1.53
1	D	597	LYS	N-CA	-6.18	1.39	1.46
1	A	831	GLU	CG-CD	6.13	1.67	1.52
1	D	432	ASP	CA-C	-6.11	1.44	1.53
1	A	584	THR	C-O	6.11	1.31	1.24
1	B	664	LEU	CA-C	6.08	1.60	1.52
1	B	874	GLY	N-CA	6.06	1.50	1.44
1	B	665	SER	CA-C	6.04	1.60	1.52
1	C	571	ILE	CA-CB	6.04	1.61	1.54
1	D	466	ALA	CA-CB	6.03	1.62	1.53
1	C	547	ILE	CA-CB	5.99	1.60	1.54
1	B	846	ALA	CA-CB	-5.98	1.44	1.53
1	C	646	ILE	C-N	-5.97	1.30	1.33
1	B	550	ALA	CA-CB	5.97	1.59	1.52
1	C	745	ASN	C-O	-5.95	1.16	1.24
1	B	870	ALA	CA-CB	-5.91	1.43	1.52
1	D	595	VAL	C-O	-5.89	1.17	1.24
1	A	602	THR	CA-CB	5.88	1.60	1.53
1	B	546	PRO	CA-C	5.85	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	545	ILE	CA-CB	-5.84	1.50	1.54
1	C	587	CYS	N-CA	-5.82	1.39	1.46
1	C	551	ARG	CA-C	5.81	1.60	1.52
1	A	513	ALA	CA-CB	5.79	1.62	1.53
1	A	653	GLU	CA-C	5.78	1.60	1.52
1	D	816	ALA	N-CA	5.75	1.53	1.46
1	B	663	ALA	CA-CB	5.74	1.62	1.53
1	C	545	ILE	C-O	5.74	1.28	1.23
1	B	895	ILE	CA-CB	-5.71	1.47	1.54
1	D	632	LEU	CA-C	5.70	1.59	1.52
1	A	545	ILE	CA-CB	-5.68	1.50	1.54
1	C	810	MET	CA-C	5.68	1.59	1.52
1	A	616	ALA	CA-CB	5.67	1.62	1.53
1	C	467	ALA	CA-CB	-5.66	1.44	1.53
1	D	665	SER	N-CA	5.63	1.53	1.46
1	B	491	ARG	CA-C	5.63	1.60	1.52
1	B	653	GLU	CA-C	5.61	1.60	1.52
1	A	409	VAL	N-CA	-5.61	1.39	1.46
1	D	625	ILE	CA-CB	-5.58	1.47	1.54
1	D	858	VAL	N-CA	-5.57	1.39	1.46
1	C	819	ASP	N-CA	5.56	1.52	1.45
1	B	623	VAL	CA-CB	-5.56	1.47	1.54
1	D	790	VAL	CA-CB	-5.56	1.47	1.54
1	C	430	PHE	N-CA	-5.55	1.39	1.46
1	B	756[A]	ARG	C-O	5.55	1.30	1.24
1	B	756[B]	ARG	C-O	5.55	1.30	1.24
1	A	578	MET	N-CA	-5.55	1.39	1.46
1	D	629	SER	C-O	5.54	1.30	1.24
1	D	742	ARG	CG-CD	5.53	1.69	1.52
1	D	420	MET	C-O	-5.53	1.20	1.25
1	A	779	VAL	N-CA	-5.53	1.40	1.47
1	A	537	CYS	N-CA	5.52	1.52	1.46
1	A	466	ALA	CA-CB	5.51	1.61	1.53
1	C	596	ILE	CA-CB	5.51	1.60	1.54
1	A	809	ILE	C-O	-5.50	1.18	1.24
1	B	708	ILE	C-O	5.50	1.32	1.23
1	A	736	ILE	C-O	-5.49	1.17	1.24
1	A	819	ASP	N-CA	5.46	1.52	1.46
1	A	692	VAL	CA-C	5.45	1.59	1.52
1	D	427	GLY	N-CA	5.45	1.53	1.45
1	D	680	LEU	CA-C	5.42	1.58	1.52
1	C	544	THR	C-O	5.41	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	502	GLU	CD-OE2	5.40	1.35	1.25
1	A	461	VAL	N-CA	-5.37	1.40	1.46
1	C	480	ILE	C-O	-5.36	1.16	1.24
1	D	845	LYS	N-CA	-5.36	1.39	1.46
1	C	661	SER	CA-C	5.35	1.59	1.52
1	C	700	PHE	CA-C	5.33	1.59	1.52
1	C	748	PRO	N-CA	-5.33	1.41	1.46
1	A	831	GLU	CB-CG	5.31	1.68	1.52
1	A	745	ASN	N-CA	-5.29	1.39	1.46
1	D	663	ALA	CA-C	5.29	1.59	1.52
1	C	715	VAL	N-CA	5.26	1.52	1.46
1	D	580	LEU	CA-C	5.23	1.59	1.52
1	C	838	VAL	CA-C	5.22	1.59	1.52
1	A	709	ALA	CA-CB	-5.20	1.45	1.53
1	A	624	ASN	N-CA	-5.19	1.39	1.46
1	C	872	PHE	CA-C	5.18	1.58	1.52
1	C	441	THR	CA-CB	5.17	1.61	1.53
1	D	446	ASP	CA-C	-5.17	1.46	1.52
1	D	681	ILE	CA-CB	-5.11	1.48	1.54
1	C	803[A]	GLU	CA-CB	5.10	1.60	1.53
1	C	803[B]	GLU	CA-CB	5.10	1.60	1.53
1	D	469	LYS	C-O	-5.08	1.18	1.24
1	C	771	THR	CA-C	5.08	1.59	1.52
1	D	418	LEU	CA-C	-5.07	1.46	1.52
1	C	420	MET	C-O	-5.07	1.20	1.25
1	D	707	CYS	CB-SG	5.05	1.98	1.81
1	C	525	MET	C-O	5.05	1.30	1.24
1	C	467	ALA	CA-C	5.02	1.59	1.52
1	C	787	GLN	C-O	-5.02	1.17	1.23
1	A	887	ALA	C-O	-5.00	1.17	1.24

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	450	ILE	N-CA-C	-8.93	102.16	110.82
1	B	708	ILE	N-CA-C	8.61	119.58	111.91
1	D	708	ILE	N-CA-C	8.60	120.38	112.29
1	B	473	GLU	N-CA-C	7.81	119.87	111.36
1	A	708	ILE	N-CA-C	7.71	119.53	112.29
1	D	667	VAL	N-CA-CB	7.53	123.65	111.23
1	D	473	GLU	N-CA-C	7.50	119.54	111.36
1	B	480	ILE	N-CA-C	7.23	118.38	110.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	688	LEU	N-CA-C	6.83	118.42	110.97
1	B	725	GLN	N-CA-C	-6.56	104.05	111.07
1	D	473	GLU	CA-CB-CG	-6.53	101.03	114.10
1	D	890	ASN	N-CA-C	6.49	119.17	111.71
1	A	820	VAL	N-CA-CB	6.49	116.96	111.64
1	B	553	ASN	N-CA-C	6.45	118.35	110.41
1	C	696	MET	N-CA-C	6.44	118.30	111.28
1	C	653	GLU	N-CA-C	6.41	118.83	111.02
1	C	531	ARG	NE-CZ-NH2	6.26	124.83	119.20
1	B	653	GLU	CA-C-N	6.25	132.96	121.70
1	B	653	GLU	C-N-CA	6.25	132.96	121.70
1	D	674	LEU	CA-C-N	-6.25	114.25	122.63
1	D	674	LEU	C-N-CA	-6.25	114.25	122.63
1	D	532	TYR	N-CA-C	-6.22	104.42	111.07
1	D	708	ILE	CB-CA-C	-6.19	103.41	111.88
1	C	763	GLN	N-CA-C	-6.10	104.72	111.36
1	B	574	ASN	N-CA-C	6.05	117.87	111.28
1	C	814	ARG	NE-CZ-NH2	-6.01	113.79	119.20
1	B	413	VAL	CB-CA-C	-6.00	102.94	111.40
1	D	831	GLU	N-CA-C	-5.99	105.94	113.18
1	D	574	ASN	N-CA-C	5.91	117.80	111.36
1	C	812	ILE	N-CA-C	5.88	116.40	108.17
1	A	583	LYS	CB-CG-CD	-5.76	98.06	111.30
1	B	733	LYS	CA-C-N	-5.73	113.23	121.42
1	B	733	LYS	C-N-CA	-5.73	113.23	121.42
1	B	409	VAL	N-CA-C	-5.67	99.58	107.80
1	C	644	ARG	NE-CZ-NH2	-5.66	114.11	119.20
1	D	653	GLU	CA-C-N	5.65	131.87	121.70
1	D	653	GLU	C-N-CA	5.65	131.87	121.70
1	B	894	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	A	678	SER	CA-C-N	-5.58	113.48	120.51
1	A	678	SER	C-N-CA	-5.58	113.48	120.51
1	B	708	ILE	CB-CA-C	-5.56	105.79	112.19
1	D	603	PRO	CA-C-N	-5.55	112.89	120.44
1	D	603	PRO	C-N-CA	-5.55	112.89	120.44
1	A	509	LEU	CB-CA-C	-5.53	102.20	110.88
1	B	584	THR	N-CA-C	5.50	117.99	111.33
1	D	604	LEU	N-CA-C	5.50	117.09	111.14
1	B	568	GLY	N-CA-C	-5.50	100.16	113.18
1	C	553	ASN	N-CA-C	5.49	117.61	110.53
1	B	674	LEU	CA-C-N	-5.48	114.95	122.57
1	B	674	LEU	C-N-CA	-5.48	114.95	122.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	667	VAL	N-CA-CB	5.47	120.26	111.23
1	A	582	TRP	CA-C-O	-5.44	114.76	120.63
1	B	809	ILE	N-CA-C	5.42	115.89	107.28
1	A	820	VAL	N-CA-C	-5.42	107.34	111.62
1	C	814	ARG	CG-CD-NE	-5.40	100.13	112.00
1	D	812	ILE	N-CA-C	5.37	115.83	107.99
1	B	485	ARG	CA-C-N	5.34	125.87	119.94
1	B	485	ARG	C-N-CA	5.34	125.87	119.94
1	A	708	ILE	CB-CA-C	-5.33	104.57	111.88
1	C	777	ASN	N-CA-C	5.27	117.19	109.24
1	D	509	LEU	CB-CA-C	-5.27	101.90	110.85
1	D	464	ALA	N-CA-C	-5.26	105.63	111.36
1	C	616	ALA	N-CA-C	-5.21	106.92	113.28
1	C	662	CYS	N-CA-C	5.21	116.77	111.14
1	D	601	VAL	CA-C-N	-5.21	117.12	122.85
1	D	601	VAL	C-N-CA	-5.21	117.12	122.85
1	B	764	ARG	N-CA-C	5.20	116.95	111.28
1	B	462	ASP	N-CA-C	5.18	116.61	111.07
1	C	768	GLU	N-CA-C	-5.18	106.55	112.92
1	C	656	LYS	N-CA-C	5.17	121.81	110.80
1	A	738	ASN	CA-C-N	5.08	124.74	119.56
1	A	738	ASN	C-N-CA	5.08	124.74	119.56
1	D	719	ILE	N-CA-C	-5.05	108.20	113.10
1	C	450	ILE	N-CA-C	-5.04	105.51	111.00
1	A	583	LYS	N-CA-C	5.04	117.89	111.69

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	882	LYS	Peptide
1	D	654	VAL	Peptide

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	3826	0	3807	46	0
1	B	3817	0	3796	34	0
1	C	3806	0	3784	44	0
1	D	3825	0	3802	39	0
2	A	40	0	0	1	0
2	B	35	0	0	2	0
2	C	40	0	0	0	0
2	D	25	0	0	1	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0
3	C	6	0	8	0	0
3	D	6	0	8	1	0
4	A	179	0	0	3	0
4	B	156	0	0	1	0
4	C	179	0	0	1	0
4	D	169	0	0	1	0
All	All	16121	0	15221	155	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 5.

All (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:799:TYR:CE2	1:B:803[B]:GLU:HG3	2.05	0.91
1:C:799:TYR:CE2	1:C:803[A]:GLU:HG3	2.11	0.85
1:D:610:ALA:HB2	1:D:625:ILE:HD12	1.58	0.85
1:A:654:VAL:CB	1:A:655:GLY:HA3	2.07	0.83
1:D:799:TYR:CE2	1:D:803[A]:GLU:HG3	2.15	0.81
1:B:799:TYR:CZ	1:B:803[B]:GLU:HG3	2.16	0.80
1:D:651:SER:OG	1:D:654:VAL:CB	2.30	0.79
1:A:651:SER:O	1:A:654:VAL:CB	2.31	0.79
1:C:687:ASP:OD1	1:C:690:LYS:HD2	1.86	0.76
1:B:843:ILE:HD12	1:C:843:ILE:HD12	1.73	0.69
1:A:799:TYR:CZ	1:A:803[A]:GLU:HG3	2.28	0.68
1:A:824:LEU:HD21	1:A:849:VAL:HG13	1.77	0.67
1:C:799:TYR:CZ	1:C:803[A]:GLU:HG3	2.30	0.66
1:B:569:ILE:HD12	1:B:571:ILE:HD11	1.76	0.66
1:B:643:VAL:O	1:B:668:LYS:HE3	1.96	0.66
1:C:799:TYR:CE2	1:C:803[A]:GLU:CG	2.79	0.65
1:A:799:TYR:CE2	1:A:803[A]:GLU:HG3	2.33	0.63
1:B:414:ASN:OD1	1:B:742:ARG:NH2	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:LYS:NZ	2:B:3024:SO4:O3	2.31	0.63
1:B:558:LEU:C	1:B:558:LEU:HD12	2.24	0.61
1:C:651:SER:OG	1:C:654:VAL:CB	2.47	0.61
1:C:702:ASN:O	1:C:703:LYS:HG2	2.01	0.61
1:C:777:ASN:O	1:C:787:GLN:HG3	2.01	0.61
1:C:643:VAL:O	1:C:668:LYS:HE3	2.00	0.60
1:C:717:GLU:OE1	1:C:814:ARG:HD2	2.02	0.60
1:A:654:VAL:CB	1:A:655:GLY:CA	2.77	0.60
1:D:423:GLN:HA	1:D:454:SER:OG	2.02	0.60
1:B:521:THR:O	1:B:522:HIS:C	2.46	0.59
1:A:756:ARG:NH2	4:A:1134:HOH:O	2.35	0.58
1:C:572:PRO:HG2	1:C:579:MET:HG3	1.84	0.58
1:C:425:PHE:CD2	1:C:610:ALA:HB1	2.38	0.58
1:B:694:MET:HE3	1:B:694:MET:HA	1.85	0.58
1:B:708:ILE:HG21	1:B:872:PHE:HE1	1.69	0.58
1:A:694:MET:HE2	1:A:863:TYR:H	1.70	0.57
1:B:651:SER:OG	1:B:654:VAL:CB	2.53	0.56
1:C:654:VAL:N	1:C:655:GLY:HA3	2.20	0.56
1:A:521:THR:O	1:A:522:HIS:C	2.43	0.56
1:A:487:ARG:NH1	1:C:490[B]:TYR:OH	2.33	0.56
1:C:824:LEU:HD21	1:C:849:VAL:HG13	1.86	0.56
1:A:651:SER:C	1:A:654:VAL:CB	2.79	0.56
1:A:799:TYR:CE2	1:A:803[A]:GLU:CG	2.89	0.55
1:D:781[B]:ARG:HD2	1:D:785:PHE:CD2	2.42	0.55
1:A:502:GLU:O	1:A:506:ILE:HG13	2.07	0.54
1:C:521:THR:O	1:C:522:HIS:C	2.49	0.54
1:C:580:LEU:C	1:C:580:LEU:HD23	2.33	0.54
1:C:632:LEU:C	1:C:632:LEU:HD23	2.33	0.53
1:A:738:ASN:HB2	2:A:3020:SO4:O2	2.09	0.53
1:C:654:VAL:N	1:C:655:GLY:CA	2.72	0.53
1:C:819:ASP:C	1:C:819:ASP:OD2	2.52	0.53
1:D:439:TYR:OH	1:D:603:PRO:HG3	2.09	0.53
1:A:651:SER:OG	1:A:654:VAL:CB	2.56	0.52
1:C:779:VAL:HG22	1:C:787:GLN:HG2	1.90	0.52
1:C:877:GLN:NE2	1:D:666:ASN:O	2.41	0.52
1:D:708:ILE:CG2	1:D:872:PHE:HE1	2.23	0.51
1:D:502:GLU:O	1:D:506:ILE:HG13	2.09	0.51
1:A:587:CYS:HB2	1:A:892:TYR:CE1	2.46	0.51
1:A:901:GLU:OE2	4:A:1039:HOH:O	2.19	0.51
1:C:708:ILE:HG21	1:C:872:PHE:HE1	1.75	0.51
1:B:781[A]:ARG:HD2	1:B:785:PHE:CD2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:901:GLU:OE2	4:C:1048:HOH:O	2.19	0.50
1:D:832:PHE:O	1:D:876:LYS:HE3	2.11	0.50
1:D:569:ILE:HD11	1:D:584:THR:OG1	2.12	0.50
1:D:685:ASP:OD2	1:D:845:LYS:NZ	2.45	0.50
1:C:863:TYR:O	1:C:864:ASN:HB2	2.13	0.49
1:A:632:LEU:C	1:A:632:LEU:HD23	2.38	0.49
1:B:832:PHE:O	1:B:876:LYS:HE2	2.13	0.48
1:B:708:ILE:CG2	1:B:872:PHE:HE1	2.26	0.48
1:C:688:LEU:O	1:C:692:VAL:HG23	2.14	0.48
1:C:882:LYS:HE3	1:D:895:ILE:HB	1.96	0.48
1:D:572:PRO:HD3	1:D:649:THR:HB	1.95	0.48
1:D:580:LEU:C	1:D:580:LEU:HD23	2.38	0.48
1:A:666:ASN:O	1:B:877:GLN:NE2	2.43	0.48
1:D:824:LEU:HD21	1:D:849:VAL:HG13	1.95	0.48
1:D:521:THR:O	1:D:522:HIS:C	2.56	0.48
1:C:569:ILE:HD11	1:C:584:THR:OG1	2.14	0.47
1:D:643:VAL:O	1:D:668:LYS:HE3	2.14	0.47
1:C:653:GLU:CA	1:C:654:VAL:CB	2.92	0.47
1:D:554:ARG:NE	2:D:3016:SO4:O4	2.34	0.47
1:B:424:LEU:HD23	1:B:627:PRO:HD2	1.95	0.47
1:C:673:GLN:NE2	1:C:872:PHE:HE2	2.12	0.47
1:D:428:GLY:HA3	1:D:620:LYS:HG2	1.97	0.47
1:A:483:ARG:HB3	1:D:548:ASN:HD21	1.79	0.47
1:A:708:ILE:HG21	1:A:872:PHE:HE1	1.79	0.47
1:C:583:LYS:HE2	1:C:649:THR:OG1	2.15	0.47
1:A:653:GLU:CB	1:A:654:VAL:HA	2.45	0.46
1:D:708:ILE:CG2	1:D:872:PHE:CE1	2.98	0.46
1:A:666:ASN:O	1:A:667:VAL:HG22	2.16	0.46
1:B:423:GLN:HA	1:B:454:SER:OG	2.16	0.46
1:D:692:VAL:O	1:D:696:MET:HG2	2.16	0.46
1:C:658:ILE:O	1:C:660:LYS:N	2.49	0.46
1:D:423:GLN:HB3	1:D:431:VAL:O	2.15	0.45
1:D:610:ALA:HB2	1:D:625:ILE:CD1	2.40	0.45
1:B:654:VAL:N	1:B:655:GLY:HA3	2.30	0.45
1:D:666:ASN:O	1:D:667:VAL:HG13	2.16	0.45
1:B:703:LYS:NZ	1:B:705:GLU:OE1	2.49	0.45
1:D:688:LEU:HD23	1:D:726:LYS:HE3	1.98	0.45
1:C:428:GLY:HA3	1:C:620:LYS:HG2	1.98	0.45
1:C:645:LYS:NZ	1:C:671:SER:HB3	2.32	0.45
1:A:580:LEU:C	1:A:580:LEU:HD23	2.42	0.45
1:B:883:ASP:O	1:B:884:LEU:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:578:MET:HE1	3:D:2004:GOL:H11	1.98	0.45
1:A:745:ASN:C	1:A:745:ASN:HD22	2.24	0.45
1:D:517:LEU:HD11	1:D:701:PHE:CZ	2.51	0.45
1:A:644:ARG:O	1:A:644:ARG:HD2	2.17	0.45
1:B:738:ASN:HB2	2:B:3021:SO4:O1	2.17	0.45
1:B:696:MET:SD	1:B:730:GLU:HB2	2.57	0.45
1:D:465:VAL:HG11	1:D:640:HIS:CE1	2.52	0.44
1:C:574:ASN:HB2	1:C:705:GLU:O	2.17	0.44
1:A:661:SER:HA	4:A:1119:HOH:O	2.17	0.44
1:D:799:TYR:CZ	1:D:803[A]:GLU:HG3	2.52	0.44
1:B:465:VAL:HG11	1:B:640:HIS:CE1	2.52	0.44
1:D:735:LYS:H	1:D:745:ASN:HD21	1.66	0.44
1:A:891:GLU:H	1:A:891:GLU:HG2	1.67	0.43
1:B:477:TRP:CH2	1:B:485:ARG:HG3	2.52	0.43
1:B:600:GLN:HA	4:B:1104:HOH:O	2.17	0.43
1:A:416:LEU:HD12	1:A:416:LEU:C	2.44	0.43
1:D:742:ARG:HD3	1:D:742:ARG:HA	1.90	0.43
1:A:574:ASN:HB2	1:A:705:GLU:O	2.18	0.43
1:C:518:ALA:HA	1:C:522:HIS:HB2	2.00	0.43
1:A:643:VAL:O	1:A:668:LYS:HE3	2.19	0.43
1:B:624:ASN:C	1:B:625:ILE:HG12	2.43	0.43
1:C:536:TRP:CG	1:C:889:LEU:HD11	2.54	0.43
1:D:478:GLY:HA3	4:D:1112:HOH:O	2.19	0.43
1:A:694:MET:HE2	1:A:863:TYR:N	2.32	0.42
1:B:866:THR:OG1	3:B:2002:GOL:H11	2.19	0.42
1:C:847:LEU:HD23	1:C:847:LEU:HA	1.78	0.42
1:C:687:ASP:HB2	1:C:841:ARG:NH2	2.34	0.42
1:A:536:TRP:O	1:A:537:CYS:C	2.61	0.42
1:A:624:ASN:C	1:A:625:ILE:HG12	2.44	0.42
1:B:839:PHE:HA	1:B:861:ASN:OD1	2.20	0.42
1:C:572:PRO:CG	1:C:579:MET:HG3	2.49	0.42
1:A:517:LEU:CD2	1:A:522:HIS:CE1	3.03	0.42
1:A:685:ASP:OD2	1:A:845:LYS:NZ	2.52	0.41
1:A:476:LEU:O	1:A:477:TRP:C	2.62	0.41
1:A:649:THR:HG23	1:A:673:GLN:HB3	2.02	0.41
1:C:832:PHE:O	1:C:876:LYS:HE2	2.21	0.41
1:A:536:TRP:CG	1:A:889:LEU:HD11	2.56	0.41
1:B:539:LYS:HD3	1:D:536:TRP:CE2	2.55	0.41
1:C:654:VAL:H	1:C:655:GLY:CA	2.34	0.41
1:B:424:LEU:CD2	1:B:627:PRO:HD2	2.51	0.41
1:B:550:ALA:O	1:B:553:ASN:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:610:ALA:HB2	1:C:625:ILE:HD12	2.01	0.41
1:C:780:PRO:O	1:C:781:ARG:HB3	2.21	0.40
1:A:465:VAL:HG11	1:A:640:HIS:CE1	2.56	0.40
1:A:569:ILE:HD12	1:A:583:LYS:HB2	2.02	0.40
1:A:735:LYS:H	1:A:745:ASN:HD21	1.69	0.40
1:A:819:ASP:HB3	1:A:822:ALA:HB3	2.03	0.40
1:B:772:LEU:HD21	1:B:775:GLY:O	2.21	0.40
1:D:569:ILE:CD1	1:D:584:THR:OG1	2.69	0.40
1:A:676:GLY:HA2	1:A:832:PHE:HB3	2.04	0.40
1:D:560[B]:LYS:NZ	1:D:562:GLU:OE2	2.43	0.40
1:D:708:ILE:HG21	1:D:872:PHE:HE1	1.86	0.40
1:A:696:MET:SD	1:A:730:GLU:HB2	2.61	0.40
1:A:862:THR:HB	1:B:901:GLU:HB2	2.03	0.40
1:D:569:ILE:HG21	1:D:569:ILE:HD13	1.84	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	502/517 (97%)	482 (96%)	16 (3%)	4 (1%)	16	23
1	B	501/517 (97%)	472 (94%)	24 (5%)	5 (1%)	12	17
1	C	499/517 (96%)	475 (95%)	19 (4%)	5 (1%)	12	17
1	D	502/517 (97%)	473 (94%)	23 (5%)	6 (1%)	10	14
All	All	2004/2068 (97%)	1902 (95%)	82 (4%)	20 (1%)	12	17

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	663	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	654	VAL
1	B	659	MET
1	B	665	SER
1	C	654	VAL
1	C	656	LYS
1	C	659	MET
1	D	654	VAL
1	D	658	ILE
1	A	659	MET
1	B	656	LYS
1	B	664	LEU
1	A	667	VAL
1	D	659	MET
1	D	667	VAL
1	A	654	VAL
1	D	661	SER
1	C	781	ARG
1	C	658	ILE
1	D	820	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	402/426 (94%)	385 (96%)	17 (4%)	26	42
1	B	401/426 (94%)	387 (96%)	14 (4%)	32	50
1	C	399/426 (94%)	385 (96%)	14 (4%)	32	50
1	D	402/426 (94%)	386 (96%)	16 (4%)	28	44
All	All	1604/1704 (94%)	1543 (96%)	61 (4%)	28	46

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405	VAL
1	A	507	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	547	ILE
1	A	583	LYS
1	A	625	ILE
1	A	644	ARG
1	A	667	VAL
1	A	668	LYS
1	A	693	GLN
1	A	703	LYS
1	A	717	GLU
1	A	735	LYS
1	A	742	ARG
1	A	745	ASN
1	A	806	PHE
1	A	831	GLU
1	A	891	GLU
1	B	413	VAL
1	B	418	LEU
1	B	517	LEU
1	B	547	ILE
1	B	579	MET
1	B	583	LYS
1	B	625	ILE
1	B	645	LYS
1	B	668	LYS
1	B	694	MET
1	B	697	SER
1	B	703	LYS
1	B	738	ASN
1	B	757	LYS
1	C	405	VAL
1	C	473	GLU
1	C	509	LEU
1	C	517	LEU
1	C	547	ILE
1	C	629	SER
1	C	635	GLN
1	C	644	ARG
1	C	668	LYS
1	C	697	SER
1	C	703	LYS
1	C	725	GLN
1	C	819	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	843	ILE
1	D	405	VAL
1	D	418	LEU
1	D	437	LYS
1	D	473	GLU
1	D	525	MET
1	D	547	ILE
1	D	667	VAL
1	D	668	LYS
1	D	703	LYS
1	D	735	LYS
1	D	741	GLU
1	D	742	ARG
1	D	745	ASN
1	D	819	ASP
1	D	831	GLU
1	D	845	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	457	GLN
1	A	474	ASN
1	A	693	GLN
1	A	745	ASN
1	A	749	GLN
1	A	844	ASN
1	A	877	GLN
1	B	407	ASN
1	B	423	GLN
1	B	600	GLN
1	B	673	GLN
1	B	725	GLN
1	B	750	ASN
1	C	407	ASN
1	C	600	GLN
1	C	673	GLN
1	C	749	GLN
1	C	797	HIS
1	D	407	ASN
1	D	548	ASN
1	D	673	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	745	ASN
1	D	844	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 ⓘ

32 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	3022	-	4,4,4	0.37	0	6,6,6	1.24	1 (16%)
2	SO4	B	3005	-	4,4,4	0.42	0	6,6,6	0.32	0
2	SO4	C	3028	-	4,4,4	0.47	0	6,6,6	0.96	0
2	SO4	C	3007	-	4,4,4	0.34	0	6,6,6	0.82	0
2	SO4	D	3026	-	4,4,4	0.39	0	6,6,6	1.28	1 (16%)
2	SO4	A	3017	-	4,4,4	0.38	0	6,6,6	0.68	0
2	SO4	B	3024	-	4,4,4	0.37	0	6,6,6	1.37	1 (16%)
2	SO4	D	3012	-	4,4,4	0.37	0	6,6,6	0.36	0
2	SO4	A	3011	-	4,4,4	0.33	0	6,6,6	0.53	0
2	SO4	A	3025	-	4,4,4	0.41	0	6,6,6	1.55	1 (16%)
3	GOL	B	2002	-	5,5,5	0.38	0	5,5,5	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	3001	-	4,4,4	0.39	0	6,6,6	0.76	0
2	SO4	A	3014	-	4,4,4	0.24	0	6,6,6	0.55	0
2	SO4	D	3023	-	4,4,4	0.43	0	6,6,6	0.83	0
2	SO4	B	3003	-	4,4,4	0.30	0	6,6,6	0.73	0
2	SO4	D	3008	-	4,4,4	0.60	0	6,6,6	0.38	0
2	SO4	C	3019	-	4,4,4	0.42	0	6,6,6	0.57	0
2	SO4	A	3018	-	4,4,4	0.62	0	6,6,6	0.50	0
2	SO4	C	3010	-	4,4,4	0.37	0	6,6,6	0.49	0
2	SO4	C	3027	-	4,4,4	0.47	0	6,6,6	1.13	0
3	GOL	D	2004	-	5,5,5	0.81	0	5,5,5	1.36	1 (20%)
2	SO4	D	3016	-	4,4,4	0.43	0	6,6,6	0.41	0
2	SO4	A	3006	-	4,4,4	0.47	0	6,6,6	1.01	0
2	SO4	C	3002	-	4,4,4	0.46	0	6,6,6	0.18	0
2	SO4	B	3015	-	4,4,4	0.42	0	6,6,6	0.81	0
2	SO4	B	3004	-	4,4,4	0.20	0	6,6,6	0.78	0
2	SO4	C	3013	-	4,4,4	0.37	0	6,6,6	0.31	0
2	SO4	A	3020	-	4,4,4	0.48	0	6,6,6	0.60	0
2	SO4	B	3009	-	4,4,4	0.42	0	6,6,6	0.32	0
3	GOL	A	2001	-	5,5,5	0.60	0	5,5,5	1.25	0
3	GOL	C	2003	-	5,5,5	0.73	0	5,5,5	0.95	0
2	SO4	B	3021	-	4,4,4	0.38	0	6,6,6	0.40	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	2003	-	-	1/4/4/4	-
3	GOL	A	2001	-	-	4/4/4/4	-
3	GOL	B	2002	-	-	2/4/4/4	-
3	GOL	D	2004	-	-	1/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3025	SO4	O3-S-O1	-2.67	95.61	109.56
2	B	3024	SO4	O3-S-O1	-2.60	95.96	109.56
3	D	2004	GOL	O1-C1-C2	2.49	121.57	110.38
2	C	3022	SO4	O3-S-O2	2.19	120.99	109.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3026	SO4	O2-S-O1	-2.07	94.47	109.06

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	GOL	C1-C2-C3-O3
3	B	2002	GOL	C1-C2-C3-O3
3	A	2001	GOL	O2-C2-C3-O3
3	A	2001	GOL	O1-C1-C2-O2
3	D	2004	GOL	O1-C1-C2-O2
3	B	2002	GOL	O1-C1-C2-O2
3	C	2003	GOL	O1-C1-C2-O2
3	A	2001	GOL	O1-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3024	SO4	1	0
3	B	2002	GOL	1	0
3	D	2004	GOL	1	0
2	D	3016	SO4	1	0
2	A	3020	SO4	1	0
2	B	3021	SO4	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%)	-0.23	23 (4%) 37 37	15, 38, 56, 110	28 (5%)
1	B	498/517 (96%)	-0.13	20 (4%) 42 42	16, 40, 62, 117	30 (6%)
1	C	498/517 (96%)	-0.28	17 (3%) 48 48	14, 36, 52, 112	24 (4%)
1	D	498/517 (96%)	-0.18	21 (4%) 40 40	16, 39, 59, 109	29 (5%)
All	All	1992/2068 (96%)	-0.21	81 (4%) 41 41	14, 38, 59, 117	111 (5%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	663	ALA	12.3
1	C	663	ALA	10.0
1	A	663	ALA	9.9
1	B	661	SER	9.8
1	D	663	ALA	9.3
1	D	661	SER	8.3
1	A	662	CYS	7.7
1	C	661	SER	7.6
1	B	665	SER	7.4
1	B	659	MET	7.3
1	B	662	CYS	7.1
1	B	656	LYS	6.9
1	B	658	ILE	6.7
1	C	662	CYS	6.5
1	B	660	LYS	6.5
1	D	665	SER	6.4
1	D	662	CYS	6.3
1	C	665	SER	6.2
1	A	664	LEU	6.1
1	A	659	MET	6.1
1	B	664	LEU	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	664	LEU	5.8
1	B	666	ASN	5.8
1	A	652	THR	5.7
1	A	661	SER	5.5
1	A	660	LYS	5.4
1	A	665	SER	5.4
1	D	666	ASN	5.4
1	D	659	MET	5.0
1	C	659	MET	5.0
1	A	658	ILE	5.0
1	A	653	GLU	4.9
1	A	666	ASN	4.8
1	C	405	VAL	4.8
1	B	653	GLU	4.7
1	C	666	ASN	4.7
1	B	652	THR	4.6
1	D	660	LYS	4.5
1	D	405	VAL	4.5
1	D	664	LEU	4.4
1	A	657	HIS	4.4
1	D	819	ASP	4.4
1	D	657	HIS	4.3
1	A	655	GLY	4.2
1	C	652	THR	4.1
1	B	405	VAL	4.0
1	C	660	LYS	3.8
1	C	657	HIS	3.8
1	B	657	HIS	3.5
1	D	620	LYS	3.4
1	A	819	ASP	3.4
1	C	658	ILE	3.3
1	C	653	GLU	3.2
1	C	656	LYS	3.2
1	A	405	VAL	3.0
1	B	654	VAL	3.0
1	D	653	GLU	2.9
1	D	652	THR	2.8
1	B	452	GLN	2.8
1	C	819	ASP	2.7
1	A	757	LYS	2.7
1	D	725	GLN	2.6
1	D	690	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	742	ARG	2.5
1	D	655	GLY	2.5
1	D	658	ILE	2.5
1	A	742	ARG	2.3
1	A	841	ARG	2.3
1	A	654	VAL	2.3
1	B	819	ASP	2.2
1	A	620[A]	LYS	2.2
1	B	520	LYS	2.2
1	A	690	LYS	2.2
1	C	757	LYS	2.2
1	B	841	ARG	2.1
1	D	841	ARG	2.1
1	B	620	LYS	2.1
1	C	639	ASP	2.1
1	D	818	GLY	2.0
1	A	831	GLU	2.0
1	A	656	LYS	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	3009	5/5	0.75	0.11	101,102,104,105	0
2	SO4	A	3011	5/5	0.77	0.11	92,92,94,94	5
2	SO4	C	3010	5/5	0.78	0.12	80,80,84,87	5
2	SO4	A	3017	5/5	0.79	0.20	52,58,60,63	5
2	SO4	D	3023	5/5	0.80	0.22	54,56,58,60	5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	3012	5/5	0.84	0.10	89,90,90,92	5
2	SO4	B	3021	5/5	0.85	0.20	49,49,52,54	5
2	SO4	D	3016	5/5	0.86	0.19	56,56,57,59	5
2	SO4	C	3019	5/5	0.86	0.16	51,52,55,55	5
2	SO4	D	3008	5/5	0.87	0.11	61,62,64,67	5
2	SO4	B	3005	5/5	0.88	0.12	75,76,78,80	5
2	SO4	A	3006	5/5	0.88	0.11	63,65,67,69	5
2	SO4	A	3018	5/5	0.88	0.14	40,46,48,52	5
2	SO4	C	3007	5/5	0.89	0.10	69,70,73,73	5
2	SO4	A	3020	5/5	0.90	0.14	34,37,39,42	5
2	SO4	C	3022	5/5	0.90	0.13	46,47,50,51	5
2	SO4	A	3025	5/5	0.91	0.15	58,61,64,68	5
2	SO4	C	3013	5/5	0.91	0.12	51,53,55,58	5
2	SO4	A	3014	5/5	0.92	0.17	41,42,47,48	5
2	SO4	C	3027	5/5	0.92	0.15	58,63,66,66	5
2	SO4	B	3024	5/5	0.93	0.14	63,66,70,72	5
3	GOL	C	2003	6/6	0.93	0.18	69,73,73,74	0
2	SO4	D	3026	5/5	0.94	0.10	55,62,65,67	5
3	GOL	A	2001	6/6	0.94	0.15	67,71,71,73	0
2	SO4	B	3015	5/5	0.94	0.10	48,49,52,55	5
3	GOL	D	2004	6/6	0.94	0.18	75,77,80,81	0
2	SO4	B	3003	5/5	0.95	0.13	33,34,37,40	5
2	SO4	B	3004	5/5	0.95	0.10	42,44,48,49	5
3	GOL	B	2002	6/6	0.95	0.15	61,69,72,73	0
2	SO4	A	3001	5/5	0.95	0.10	44,46,49,53	5
2	SO4	C	3028	5/5	0.95	0.08	42,51,55,57	5
2	SO4	C	3002	5/5	0.97	0.07	42,42,47,48	5

6.5 Other polymers [i](#)

There are no such residues in this entry.