



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:20 PM UTC

PDB ID : 6IQV / pdb_00006iqv
Title : Crystal Structure of Cell Surface Glyceraldehyde-3-Phosphate Dehydrogenase
Complexed with Hg²⁺ from *Lactobacillus plantarum*
Authors : Yoneda, K.; Kinoshita, H.
Deposited on : 2018-11-09
Resolution : 2.13 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

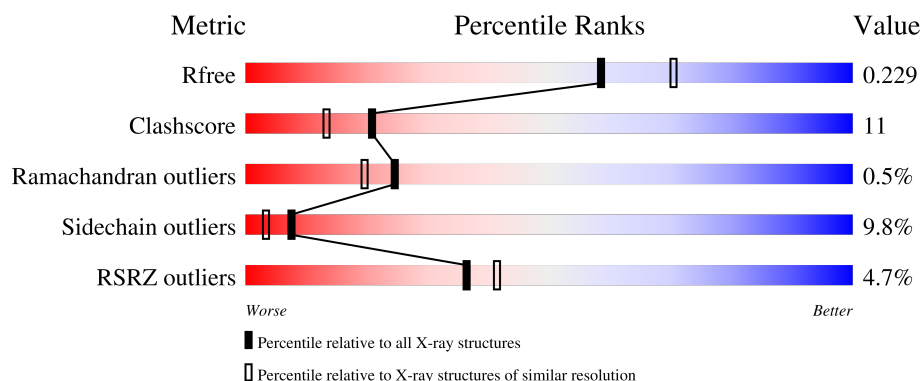
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

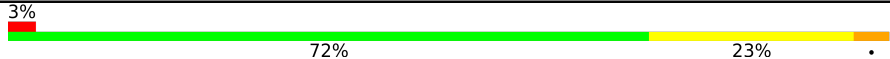
The reported resolution of this entry is 2.13 Å.

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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	340	 3% 72% 23% .
1	B	340	 3% 70% 22% 6% .
1	C	340	 6% 62% 25% 8% .
1	D	340	 6% 64% 27% 6% .

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	EDO	D	405	-	-	X	-
4	TRS	B	401	-	X	X	-

2 Entry composition [i](#)

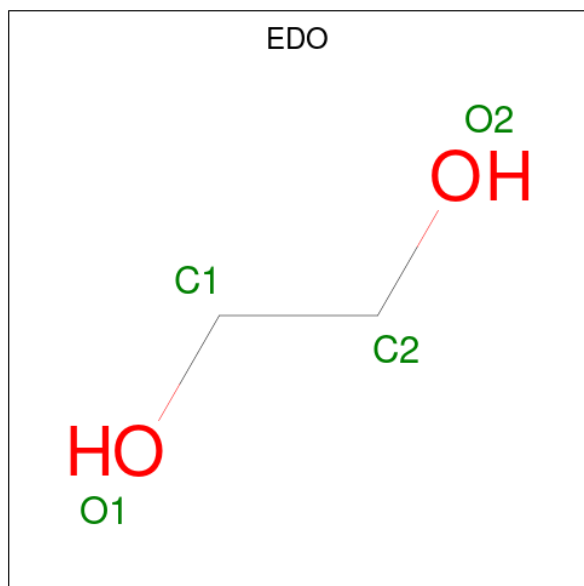
There are 5 unique types of molecules in this entry. The entry contains 10725 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glyceraldehyde-3-phosphate dehydrogenase, type I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2564	1609	439	508	8			
1	B	336	Total	C	N	O	S	0	0	0
			2536	1594	435	500	7			
1	C	326	Total	C	N	O	S	0	0	0
			2463	1550	422	483	8			
1	D	333	Total	C	N	O	S	0	0	0
			2515	1579	431	497	8			

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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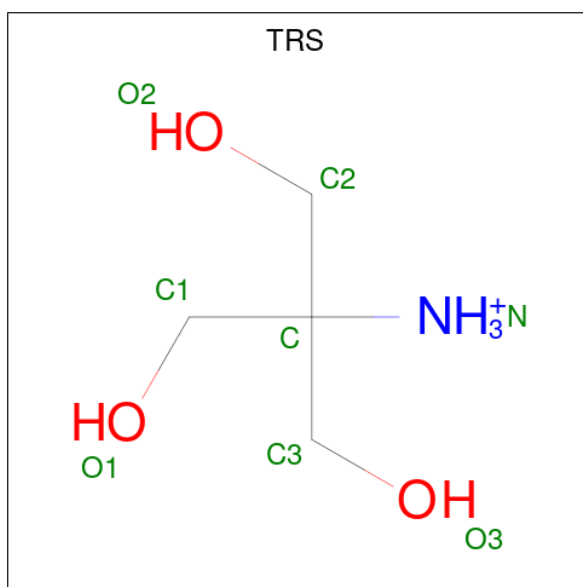
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Hg	0	0
			3	3		
3	B	3	Total	Hg	0	0
			3	3		
3	C	2	Total	Hg	0	0
			2	2		
3	D	3	Total	Hg	0	0
			3	3		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			8	4	1	3		

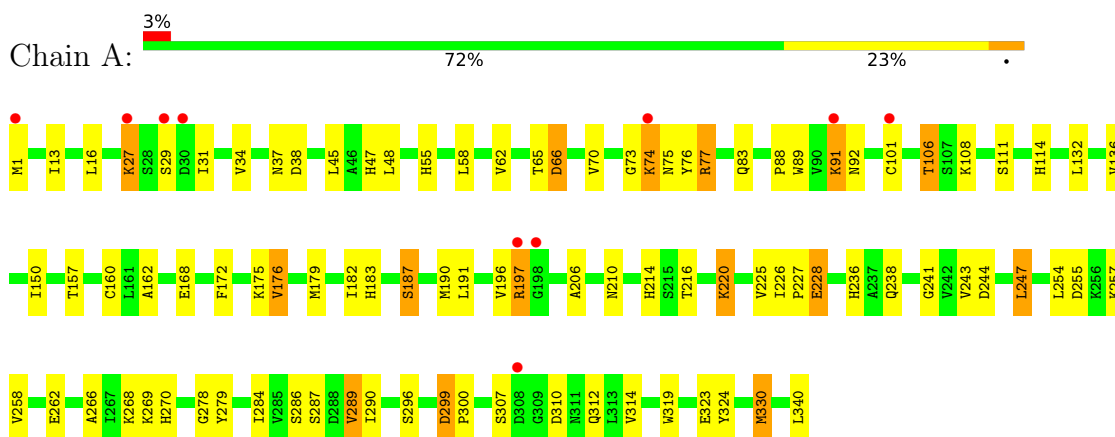
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	169	Total 169	O 169	0	0
5	B	163	Total 163	O 163	0	0
5	C	122	Total 122	O 122	0	0
5	D	150	Total 150	O 150	0	0

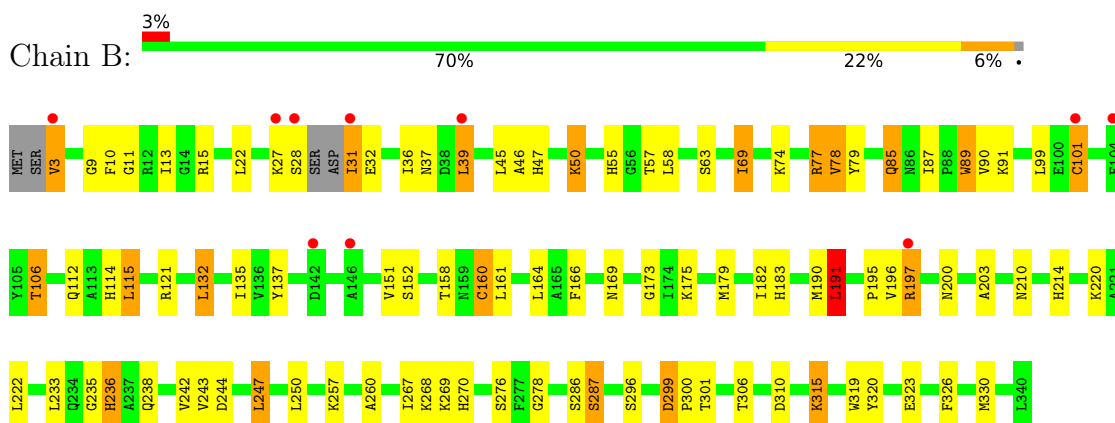
3 Residue-property plots

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.

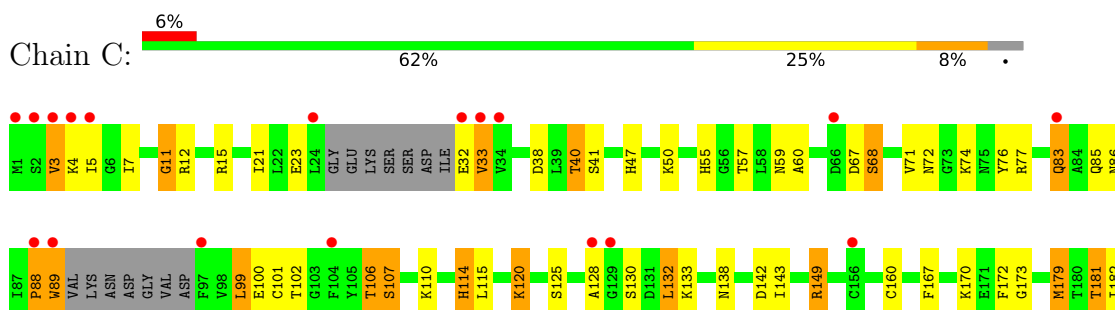
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I

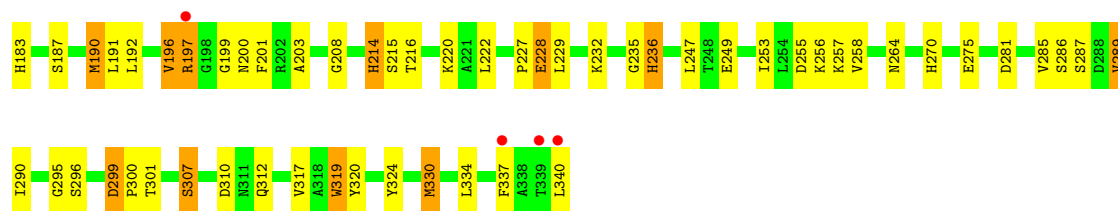


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I

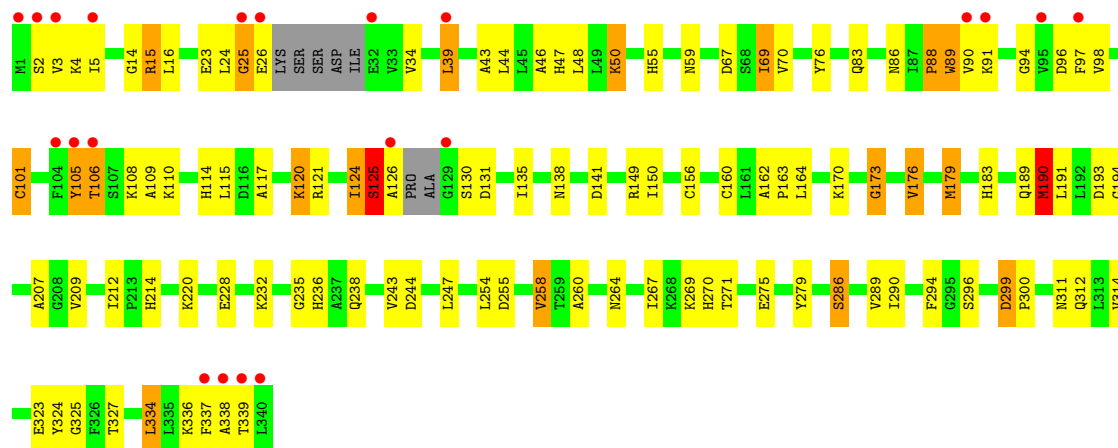


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I





● Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, type I



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	126.04Å 172.95Å 149.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.86 – 2.13 101.86 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.3 (101.86-2.13) 99.7 (101.86-2.13)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.202 , 0.229 0.214 , 0.229	Depositor DCC
R_{free} test set	4550 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10725	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 5.51% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HG, TRS, EDO

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	1.88	45/2605 (1.7%)	1.07	7/3536 (0.2%)
1	B	1.88	44/2576 (1.7%)	1.08	4/3496 (0.1%)
1	C	1.80	32/2502 (1.3%)	1.10	7/3395 (0.2%)
1	D	1.84	48/2553 (1.9%)	1.09	11/3462 (0.3%)
All	All	1.85	169/10236 (1.7%)	1.08	29/13889 (0.2%)

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

All (169) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	GLU	C-O	-7.52	1.17	1.23
1	A	340	LEU	C-OXT	-7.44	1.08	1.23
1	C	55	HIS	CD2-NE2	-7.39	1.29	1.37
1	D	323	GLU	C-O	-7.25	1.17	1.23
1	A	262	GLU	C-O	-7.18	1.15	1.24
1	A	55	HIS	CG-ND1	-7.16	1.30	1.38
1	A	183	HIS	CG-ND1	-7.11	1.30	1.38
1	A	114	HIS	CG-ND1	-6.87	1.30	1.38
1	A	270	HIS	CD2-NE2	-6.81	1.30	1.37
1	D	47	HIS	CG-ND1	-6.76	1.30	1.38
1	B	323	GLU	C-O	-6.70	1.18	1.23
1	B	270	HIS	CD2-NE2	-6.68	1.30	1.37
1	C	214	HIS	CG-ND1	-6.67	1.30	1.38
1	D	270	HIS	CG-ND1	-6.66	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	HIS	CG-ND1	-6.54	1.31	1.38
1	A	324	TYR	C-O	-6.50	1.16	1.24
1	B	236	HIS	CG-ND1	-6.50	1.31	1.38
1	C	47	HIS	CG-ND1	-6.46	1.31	1.38
1	D	290	ILE	C-O	-6.46	1.17	1.24
1	A	37	ASN	C-O	-6.45	1.16	1.24
1	D	183	HIS	CG-ND1	-6.40	1.31	1.38
1	C	55	HIS	CG-ND1	-6.40	1.31	1.38
1	D	43	ALA	C-O	-6.38	1.16	1.24
1	A	47	HIS	CG-ND1	-6.38	1.31	1.38
1	C	208	GLY	C-O	-6.36	1.17	1.24
1	A	270	HIS	CG-ND1	-6.30	1.31	1.38
1	B	166	PHE	C-O	-6.24	1.16	1.24
1	A	47	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	55	HIS	CD2-NE2	-6.19	1.31	1.37
1	D	55	HIS	CG-ND1	-6.17	1.31	1.38
1	A	70	VAL	C-O	-6.14	1.17	1.24
1	B	50	LYS	C-O	-6.12	1.16	1.24
1	B	301	THR	C-O	-6.09	1.16	1.24
1	D	114	HIS	CG-ND1	-6.08	1.31	1.38
1	D	48	LEU	C-O	-6.06	1.16	1.24
1	B	158	THR	C-O	-6.05	1.17	1.24
1	B	45	LEU	C-O	-6.04	1.17	1.24
1	D	47	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	236	HIS	CG-ND1	-6.00	1.31	1.38
1	A	287	SER	C-O	-6.00	1.16	1.24
1	C	183	HIS	CG-ND1	-5.98	1.31	1.38
1	B	47	HIS	CG-ND1	-5.97	1.31	1.38
1	A	278	GLY	C-O	-5.96	1.18	1.23
1	B	287	SER	C-O	-5.96	1.17	1.24
1	D	270	HIS	CD2-NE2	-5.96	1.31	1.37
1	B	46	ALA	C-O	-5.94	1.17	1.24
1	A	214	HIS	CG-ND1	-5.90	1.31	1.38
1	B	69	ILE	C-O	-5.89	1.18	1.24
1	A	38	ASP	C-O	-5.87	1.17	1.23
1	B	236	HIS	CD2-NE2	-5.87	1.31	1.37
1	D	236	HIS	CG-ND1	-5.86	1.31	1.38
1	A	74	LYS	C-O	-5.85	1.17	1.23
1	D	46	ALA	C-O	-5.82	1.17	1.24
1	C	7	ILE	C-O	-5.80	1.18	1.24
1	C	11	GLY	C-O	-5.80	1.18	1.23
1	B	169	ASN	C-O	-5.79	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	227	PRO	C-O	-5.79	1.17	1.24
1	B	268	LYS	C-O	-5.78	1.17	1.24
1	B	270	HIS	CG-ND1	-5.78	1.31	1.38
1	A	183	HIS	CD2-NE2	-5.77	1.31	1.37
1	A	114	HIS	CD2-NE2	-5.76	1.31	1.37
1	A	243	VAL	C-O	-5.75	1.16	1.24
1	C	299	ASP	C-O	-5.75	1.19	1.24
1	D	156	CYS	C-O	-5.74	1.17	1.24
1	A	241	GLY	C-O	-5.70	1.16	1.23
1	B	244	ASP	C-O	-5.69	1.17	1.23
1	D	191	LEU	C-O	-5.68	1.17	1.24
1	C	289	VAL	C-O	-5.67	1.18	1.24
1	A	16	LEU	C-O	-5.67	1.17	1.24
1	A	284	ILE	C-O	-5.66	1.17	1.24
1	C	183	HIS	CD2-NE2	-5.64	1.31	1.37
1	C	270	HIS	CG-ND1	-5.64	1.32	1.38
1	D	236	HIS	CD2-NE2	-5.64	1.31	1.37
1	C	319	TRP	NE1-CE2	-5.62	1.31	1.37
1	D	59	ASN	C-O	-5.61	1.17	1.23
1	B	214	HIS	CG-ND1	-5.61	1.32	1.38
1	C	200	ASN	C-O	-5.61	1.17	1.23
1	C	290	ILE	C-O	-5.58	1.18	1.24
1	B	47	HIS	CD2-NE2	-5.57	1.31	1.37
1	B	242	VAL	C-O	-5.55	1.18	1.24
1	A	286	SER	C-O	-5.54	1.17	1.24
1	C	199	GLY	C-O	-5.54	1.16	1.24
1	B	164	LEU	C-O	-5.54	1.17	1.24
1	B	137	TYR	C-O	-5.48	1.17	1.23
1	A	150	ILE	C-O	-5.48	1.18	1.24
1	B	135	ILE	C-O	-5.47	1.18	1.24
1	A	45	LEU	C-O	-5.47	1.17	1.24
1	A	299	ASP	C-O	-5.46	1.19	1.24
1	B	183	HIS	CG-ND1	-5.46	1.32	1.38
1	B	58	LEU	C-O	-5.45	1.17	1.24
1	C	236	HIS	CG-ND1	-5.45	1.32	1.38
1	B	55	HIS	CD2-NE2	-5.44	1.31	1.37
1	C	191	LEU	C-O	-5.43	1.17	1.24
1	B	315	LYS	C-O	-5.42	1.17	1.24
1	D	255	ASP	C-O	-5.42	1.17	1.24
1	B	260	ALA	C-O	-5.39	1.17	1.24
1	D	299	ASP	C-O	-5.39	1.19	1.24
1	D	286	SER	C-O	-5.38	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	209	VAL	C-O	-5.35	1.17	1.24
1	D	214	HIS	CD2-NE2	-5.35	1.31	1.37
1	A	168	GLU	C-O	-5.35	1.17	1.24
1	D	44	LEU	C-O	-5.34	1.17	1.24
1	C	287	SER	C-O	-5.34	1.17	1.24
1	D	55	HIS	CD2-NE2	-5.33	1.31	1.37
1	D	271	THR	C-O	-5.31	1.16	1.24
1	A	244	ASP	C-O	-5.30	1.17	1.23
1	A	162	ALA	C-O	-5.30	1.17	1.24
1	B	210	ASN	C-O	-5.30	1.17	1.23
1	A	214	HIS	CD2-NE2	-5.28	1.32	1.37
1	D	114	HIS	CD2-NE2	-5.28	1.32	1.37
1	B	243	VAL	C-O	-5.28	1.17	1.24
1	B	267	ILE	C-O	-5.28	1.17	1.24
1	B	114	HIS	CG-ND1	-5.27	1.32	1.38
1	C	214	HIS	CD2-NE2	-5.26	1.32	1.37
1	B	132	LEU	C-O	-5.25	1.17	1.23
1	D	50	LYS	C-O	-5.24	1.17	1.24
1	A	34	VAL	C-O	-5.24	1.18	1.24
1	C	187	SER	C-O	-5.24	1.17	1.24
1	D	16	LEU	C-O	-5.22	1.17	1.24
1	D	70	VAL	C-O	-5.22	1.18	1.24
1	C	203	ALA	C-O	-5.22	1.17	1.24
1	D	76	TYR	C-O	-5.22	1.18	1.24
1	D	176	VAL	C-O	-5.22	1.18	1.23
1	D	311	ASN	C-O	-5.22	1.17	1.24
1	A	226	ILE	C-O	-5.21	1.17	1.24
1	C	264	ASN	C-O	-5.21	1.18	1.24
1	B	161	LEU	C-O	-5.20	1.18	1.24
1	C	301	THR	C-O	-5.20	1.17	1.24
1	D	193	ASP	C-O	-5.20	1.17	1.23
1	D	324	TYR	C-O	-5.20	1.18	1.24
1	A	216	THR	C-O	-5.18	1.17	1.23
1	D	135	ILE	C-O	-5.18	1.18	1.24
1	D	260	ALA	C-O	-5.18	1.18	1.24
1	A	225	VAL	C-O	-5.17	1.18	1.23
1	D	164	LEU	C-O	-5.17	1.18	1.24
1	D	244	ASP	C-O	-5.15	1.17	1.23
1	B	191	LEU	C-O	-5.15	1.18	1.24
1	B	190	MET	C-O	-5.14	1.17	1.23
1	D	150	ILE	C-O	-5.14	1.18	1.24
1	D	267	ILE	C-O	-5.14	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	114	HIS	CG-ND1	-5.14	1.32	1.38
1	C	181	THR	C-O	-5.12	1.17	1.24
1	B	276	SER	C-O	-5.12	1.17	1.24
1	D	98	VAL	C-O	-5.11	1.18	1.24
1	D	294	PHE	C-O	-5.10	1.17	1.23
1	A	136	VAL	C-O	-5.09	1.18	1.24
1	A	48	LEU	C-O	-5.09	1.17	1.24
1	B	214	HIS	CD2-NE2	-5.09	1.32	1.37
1	B	299	ASP	C-O	-5.09	1.19	1.24
1	B	99	LEU	C-O	-5.09	1.17	1.24
1	C	253	ILE	C-O	-5.07	1.18	1.24
1	D	173	GLY	C-O	-5.07	1.17	1.23
1	A	191	LEU	C-O	-5.06	1.18	1.24
1	D	214	HIS	CG-ND1	-5.06	1.32	1.38
1	A	206	ALA	C-O	-5.06	1.17	1.24
1	A	290	ILE	C-O	-5.06	1.19	1.24
1	D	327	THR	C-O	-5.06	1.18	1.24
1	B	160	CYS	C-O	-5.05	1.18	1.24
1	D	14	GLY	C-O	-5.04	1.17	1.23
1	C	59	ASN	CA-C	-5.03	1.47	1.53
1	C	167	PHE	C-O	-5.03	1.18	1.24
1	D	325	GLY	C-O	-5.03	1.17	1.23
1	D	15	ARG	C-O	-5.02	1.18	1.24
1	A	187	SER	C-O	-5.01	1.17	1.24
1	B	183	HIS	CD2-NE2	-5.01	1.32	1.37
1	A	330	MET	C-O	-5.00	1.18	1.24
1	C	99	LEU	C-O	-5.00	1.17	1.24
1	C	201	PHE	C-O	-5.00	1.17	1.24
1	B	278	GLY	C-O	-5.00	1.19	1.23

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	ILE	N-CA-C	-14.31	70.93	111.00
1	D	105	TYR	N-CA-C	-8.15	94.26	108.69
1	C	3	VAL	N-CA-C	6.97	118.61	108.58
1	D	2	SER	N-CA-C	6.45	120.57	110.32
1	C	295	GLY	N-CA-C	-6.31	106.84	114.66
1	D	101	CYS	CB-CA-C	-6.25	100.71	111.45
1	D	25	GLY	N-CA-C	-6.11	98.69	113.18
1	D	264	ASN	N-CA-C	5.99	117.48	111.07
1	C	88	PRO	N-CA-C	-5.88	102.93	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	THR	N-CA-C	-5.79	100.82	109.96
1	A	31	ILE	N-CA-C	-5.78	99.45	108.81
1	B	320	TYR	N-CA-C	5.74	117.13	108.46
1	D	5	ILE	N-CA-C	5.73	116.36	107.99
1	D	124	ILE	CB-CA-C	-5.71	101.92	111.29
1	A	286	SER	N-CA-C	5.67	117.46	111.28
1	B	31	ILE	N-CA-CB	-5.59	102.00	111.50
1	A	62	VAL	N-CA-C	5.48	115.78	108.11
1	A	89	TRP	N-CA-C	5.37	119.09	112.54
1	C	102	THR	N-CA-C	5.35	118.02	111.82
1	C	307	SER	N-CA-C	5.33	117.49	109.23
1	D	258	VAL	N-CA-C	5.32	116.37	108.65
1	D	125	SER	N-CA-C	5.32	117.00	107.80
1	D	101	CYS	N-CA-C	5.30	117.66	110.88
1	D	190	MET	N-CA-C	5.23	118.09	109.72
1	C	320	TYR	N-CA-C	5.20	116.97	108.76
1	A	157	THR	N-CA-C	5.13	116.87	111.28
1	A	73	GLY	N-CA-C	5.11	122.15	115.36
1	C	324	TYR	N-CA-C	5.10	116.92	111.36
1	B	286	SER	N-CA-C	5.08	116.50	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	LYS	Peptide

5.2 Too-close contacts [i](#)

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	2564	0	2549	43	0
1	B	2536	0	2521	45	0
1	C	2463	0	2452	61	0
1	D	2515	0	2497	75	0
2	A	8	0	12	0	0
2	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	4	0	6	0	0
2	D	8	0	12	9	0
3	A	3	0	0	1	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
4	B	8	0	12	6	0
5	A	169	0	0	10	0
5	B	163	0	0	6	0
5	C	122	0	0	11	0
5	D	150	0	0	8	0
All	All	10725	0	10067	224	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 11.

All (224) 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:196:VAL:HB	5:A:657:HOH:O	1.44	1.18
1:C:125:SER:HB3	5:C:562:HOH:O	1.40	1.16
1:D:15:ARG:HE	2:D:405:EDO:H11	1.07	1.13
5:A:556:HOH:O	4:B:401:TRS:H12	1.47	1.12
1:D:39:LEU:HD23	1:D:39:LEU:H	1.15	1.12
1:A:101:CYS:SG	3:A:404:HG:HG	1.70	1.10
1:D:121:ARG:HD3	1:D:337:PHE:CE1	1.85	1.10
1:C:216:THR:HG23	5:C:566:HOH:O	1.51	1.09
1:B:197:ARG:O	1:B:197:ARG:HD3	1.53	1.05
1:D:39:LEU:HB3	5:D:642:HOH:O	1.55	1.04
4:B:401:TRS:H11	5:B:587:HOH:O	1.60	1.01
1:D:108:LYS:HD3	1:D:131:ASP:OD2	1.59	1.00
1:D:97:PHE:CE1	1:D:121:ARG:HB2	1.98	0.99
1:C:142:ASP:HB2	5:C:618:HOH:O	1.62	0.98
1:B:39:LEU:H	1:B:39:LEU:HD23	1.29	0.95
1:C:88:PRO:O	1:C:89:TRP:HB3	1.65	0.95
1:D:15:ARG:NE	2:D:405:EDO:H11	1.83	0.94
1:C:38:ASP:OD2	1:C:40:THR:HG23	1.71	0.91
1:C:83:GLN:NE2	1:C:86:ASN:HD22	1.70	0.89
1:D:124:ILE:HG22	1:D:125:SER:H	1.39	0.88
1:D:97:PHE:HZ	1:D:337:PHE:CD2	1.92	0.87
1:D:96:ASP:OD2	1:D:120:LYS:HE2	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:LEU:HD23	1:D:39:LEU:N	1.93	0.81
1:D:15:ARG:HH21	2:D:405:EDO:C1	1.93	0.80
1:C:88:PRO:O	1:C:89:TRP:CB	2.30	0.79
1:C:106:THR:O	1:C:106:THR:CG2	2.30	0.79
1:A:190:MET:CG	5:A:657:HOH:O	2.31	0.79
1:A:228:GLU:H	1:A:228:GLU:CD	1.90	0.79
4:B:401:TRS:C2	5:D:526:HOH:O	2.31	0.78
1:B:77:ARG:HD2	5:B:518:HOH:O	1.81	0.78
1:D:121:ARG:CD	1:D:337:PHE:CE1	2.66	0.78
1:D:86:ASN:O	1:D:88:PRO:HD3	1.83	0.77
4:B:401:TRS:H22	5:D:526:HOH:O	1.84	0.77
1:A:190:MET:SD	5:A:657:HOH:O	2.42	0.77
1:D:108:LYS:CD	1:D:131:ASP:OD2	2.32	0.76
1:B:179:MET:HE2	1:B:235:GLY:HA3	1.68	0.76
1:D:39:LEU:H	1:D:39:LEU:CD2	1.87	0.74
1:B:9:GLY:O	1:B:101:CYS:SG	2.46	0.73
1:A:106:THR:HG22	5:A:640:HOH:O	1.89	0.72
1:D:15:ARG:HH21	2:D:405:EDO:H12	1.55	0.72
1:A:197:ARG:NH1	1:A:197:ARG:HG2	2.06	0.71
1:B:197:ARG:O	1:B:197:ARG:CD	2.35	0.71
1:D:24:LEU:O	1:D:25:GLY:C	2.35	0.70
1:D:124:ILE:HG22	1:D:125:SER:N	2.07	0.69
1:D:275:GLU:HG2	5:D:551:HOH:O	1.92	0.69
1:D:121:ARG:HD3	1:D:337:PHE:HE1	1.55	0.68
1:D:258:VAL:H	1:D:312:GLN:HE22	1.39	0.68
1:B:197:ARG:HD3	1:B:197:ARG:C	2.03	0.68
1:C:83:GLN:HE21	1:C:86:ASN:HD22	1.39	0.68
1:A:266:ALA:HA	1:A:269:LYS:HE2	1.77	0.67
1:C:258:VAL:H	1:C:312:GLN:HE22	1.43	0.67
1:B:106:THR:HG23	1:B:106:THR:O	1.94	0.66
1:B:195:PRO:HD2	5:B:535:HOH:O	1.94	0.66
1:C:160:CYS:HA	1:C:296:SER:HB2	1.77	0.66
1:B:39:LEU:H	1:B:39:LEU:CD2	2.01	0.66
1:A:182:ILE:HD12	1:A:247:LEU:HD11	1.77	0.65
1:A:197:ARG:HG2	1:A:197:ARG:HH11	1.60	0.65
1:D:105:TYR:O	1:D:106:THR:HG23	1.97	0.65
1:C:106:THR:O	1:C:106:THR:HG22	1.96	0.64
1:C:100:GLU:OE1	1:C:114:HIS:HE1	1.80	0.64
1:A:160:CYS:HA	1:A:296:SER:HB2	1.80	0.63
1:B:121:ARG:NH1	5:B:504:HOH:O	2.32	0.63
1:D:228:GLU:O	1:D:232:LYS:HE2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ALA:O	1:C:132:LEU:HD11	2.00	0.61
1:C:275:GLU:HG2	5:C:540:HOH:O	2.00	0.61
1:D:3:VAL:HG13	1:D:96:ASP:CB	2.29	0.61
1:D:24:LEU:C	1:D:25:GLY:O	2.39	0.61
1:A:106:THR:CG2	1:A:106:THR:O	2.48	0.61
1:A:106:THR:O	1:A:106:THR:HG23	2.00	0.61
1:D:125:SER:O	1:D:126:ALA:HB3	2.00	0.61
1:A:91:LYS:HG2	1:A:92:ASN:H	1.66	0.61
1:D:125:SER:O	1:D:126:ALA:CB	2.47	0.61
4:B:401:TRS:H21	5:D:526:HOH:O	1.98	0.60
1:D:90:VAL:HG21	1:D:117:ALA:O	2.01	0.60
1:D:97:PHE:CE1	1:D:121:ARG:CB	2.79	0.59
1:D:96:ASP:CG	1:D:120:LYS:HE2	2.27	0.59
5:A:556:HOH:O	4:B:401:TRS:H31	2.03	0.59
1:D:97:PHE:CD1	1:D:121:ARG:HB2	2.38	0.59
1:A:66:ASP:OD2	1:A:66:ASP:N	2.36	0.59
1:C:5:ILE:HG12	1:C:334:LEU:HD13	1.84	0.58
1:D:121:ARG:HD3	1:D:337:PHE:CD1	2.35	0.58
1:B:191:LEU:HD21	1:D:207:ALA:HB3	1.86	0.58
1:C:99:LEU:HD11	5:C:562:HOH:O	2.03	0.58
1:C:214:HIS:CD2	1:C:215:SER:O	2.58	0.57
1:A:197:ARG:HH11	1:A:197:ARG:CG	2.18	0.57
1:B:257:LYS:NZ	1:B:310:ASP:HB3	2.20	0.57
1:C:179:MET:HE3	5:C:566:HOH:O	2.03	0.57
1:C:179:MET:HG3	1:C:235:GLY:HA3	1.87	0.56
1:A:91:LYS:HG2	1:A:92:ASN:N	2.20	0.56
1:A:77:ARG:HH11	1:A:77:ARG:HG3	1.70	0.56
5:A:620:HOH:O	2:D:401:EDO:H12	2.05	0.56
1:A:74:LYS:HG2	1:A:76:TYR:CZ	2.40	0.56
1:C:196:VAL:CG2	1:C:197:ARG:N	2.69	0.55
1:D:15:ARG:CZ	2:D:405:EDO:H11	2.36	0.55
1:C:106:THR:O	1:C:106:THR:HG23	2.05	0.55
1:C:99:LEU:CD1	5:C:562:HOH:O	2.55	0.55
1:D:121:ARG:CD	1:D:337:PHE:CD1	2.90	0.55
1:A:196:VAL:CG2	5:A:657:HOH:O	2.53	0.55
1:C:83:GLN:NE2	1:C:86:ASN:ND2	2.48	0.54
1:B:247:LEU:C	1:B:247:LEU:HD12	2.32	0.54
1:A:106:THR:HB	5:A:630:HOH:O	2.07	0.53
1:A:254:LEU:HD12	1:A:314:VAL:HG21	1.90	0.53
1:A:258:VAL:H	1:A:312:GLN:HE22	1.57	0.53
1:C:67:ASP:OD1	1:C:67:ASP:C	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:VAL:O	1:D:94:GLY:HA2	2.09	0.52
1:D:279:TYR:CE1	1:D:300:PRO:HG3	2.44	0.52
1:B:3:VAL:N	5:B:508:HOH:O	2.42	0.52
1:B:326:PHE:CE2	1:B:330:MET:HE2	2.44	0.52
1:D:97:PHE:CZ	1:D:337:PHE:CD2	2.84	0.52
1:C:256:LYS:CE	5:C:602:HOH:O	2.56	0.52
1:C:286:SER:O	1:C:289:VAL:HG22	2.10	0.52
1:B:247:LEU:HD12	1:B:247:LEU:O	2.10	0.52
1:C:100:GLU:OE1	1:C:114:HIS:CE1	2.62	0.52
1:D:3:VAL:HG13	1:D:96:ASP:HB3	1.92	0.51
1:B:151:VAL:HG12	1:B:152:SER:N	2.25	0.51
1:B:106:THR:O	1:B:106:THR:CG2	2.56	0.51
1:C:11:GLY:O	1:C:15:ARG:HG3	2.09	0.51
1:D:254:LEU:HD12	1:D:314:VAL:HG21	1.93	0.51
1:C:229:LEU:HA	1:C:232:LYS:HD2	1.92	0.51
1:C:249:GLU:HG2	1:C:317:VAL:HG22	1.92	0.51
1:C:334:LEU:O	1:C:337:PHE:HB2	2.11	0.51
1:D:15:ARG:HH21	2:D:405:EDO:H11	1.73	0.51
1:B:197:ARG:HD3	1:B:197:ARG:N	2.24	0.51
1:D:141:ASP:O	1:D:336:LYS:NZ	2.41	0.51
1:B:250:LEU:O	1:B:315:LYS:HA	2.11	0.50
1:C:125:SER:HB2	1:C:330:MET:SD	2.51	0.50
1:D:15:ARG:NH2	2:D:405:EDO:H11	2.27	0.50
1:D:24:LEU:O	1:D:25:GLY:O	2.30	0.50
1:A:227:PRO:HD2	1:A:228:GLU:OE1	2.12	0.50
1:C:125:SER:CB	1:C:330:MET:SD	2.99	0.50
1:A:190:MET:HG3	5:A:657:HOH:O	2.05	0.50
1:B:36:ILE:HG22	1:B:37:ASN:N	2.27	0.50
1:D:337:PHE:O	1:D:338:ALA:C	2.55	0.50
1:D:15:ARG:NH2	2:D:405:EDO:C1	2.70	0.49
1:B:112:GLN:O	1:B:115:LEU:N	2.43	0.49
1:A:13:ILE:HB	1:A:101:CYS:SG	2.52	0.49
1:D:189:GLN:HG2	5:D:573:HOH:O	2.12	0.49
1:D:247:LEU:HD12	1:D:247:LEU:C	2.38	0.49
1:D:179:MET:HG3	1:D:235:GLY:HA3	1.95	0.49
1:B:247:LEU:HD23	1:B:319:TRP:CH2	2.48	0.49
1:C:99:LEU:HG	1:C:101:CYS:SG	2.53	0.48
1:B:200:ASN:HB3	1:B:203:ALA:HB3	1.95	0.48
1:C:67:ASP:OD1	1:C:68:SER:HB3	2.14	0.48
1:A:238:GLN:HG3	1:B:182:ILE:CD1	2.43	0.48
1:A:228:GLU:CD	1:A:228:GLU:N	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:VAL:O	1:C:72:ASN:C	2.54	0.48
1:D:97:PHE:CD2	1:D:334:LEU:HD21	2.48	0.48
1:C:256:LYS:HE2	5:C:602:HOH:O	2.13	0.47
1:C:285:VAL:HG11	1:D:212:ILE:HG12	1.96	0.47
1:D:3:VAL:HG13	1:D:96:ASP:HB2	1.96	0.47
1:D:190:MET:HB2	1:D:190:MET:HE2	1.44	0.47
1:C:216:THR:CG2	5:C:566:HOH:O	2.28	0.47
1:C:21:ILE:HG21	1:C:33:VAL:HG12	1.98	0.46
1:C:50:LYS:HE3	1:C:57:THR:CG2	2.44	0.46
1:B:257:LYS:HZ1	1:B:310:ASP:HB3	1.80	0.46
1:B:160:CYS:HA	1:B:296:SER:HB2	1.97	0.46
1:D:89:TRP:H	1:D:89:TRP:CD1	2.34	0.46
1:A:182:ILE:HD13	1:B:238:GLN:HG3	1.96	0.46
1:C:247:LEU:HD23	1:C:319:TRP:CZ3	2.51	0.46
1:B:11:GLY:O	1:B:15:ARG:HG3	2.16	0.46
1:B:85:GLN:H	1:B:85:GLN:HG3	1.32	0.46
1:C:12:ARG:HH11	1:C:12:ARG:HG2	1.80	0.46
1:C:67:ASP:HB2	1:C:77:ARG:NH1	2.30	0.46
1:A:268:LYS:HE3	1:A:279:TYR:CZ	2.50	0.46
1:B:90:VAL:HB	5:B:536:HOH:O	2.15	0.46
1:A:74:LYS:HG3	1:A:75:ASN:N	2.31	0.45
1:C:182:ILE:CD1	1:D:238:GLN:HG3	2.46	0.45
1:A:175:LYS:HE3	1:A:255:ASP:HA	1.97	0.45
1:B:222:LEU:HD23	1:B:233:LEU:HD11	1.97	0.45
1:B:299:ASP:HA	1:B:300:PRO:HD2	1.85	0.45
1:A:289:VAL:HG11	1:A:319:TRP:HB3	1.99	0.45
1:C:228:GLU:H	1:C:228:GLU:CD	2.23	0.45
1:D:254:LEU:CD1	1:D:314:VAL:HG21	2.46	0.45
1:B:247:LEU:C	1:B:247:LEU:CD1	2.90	0.45
1:C:120:LYS:O	1:C:149:ARG:HD2	2.17	0.44
1:A:172:PHE:O	1:A:255:ASP:HB2	2.17	0.44
1:D:258:VAL:H	1:D:312:GLN:NE2	2.12	0.44
1:D:90:VAL:O	1:D:94:GLY:CA	2.65	0.44
1:D:160:CYS:HA	1:D:296:SER:HB2	1.99	0.44
1:D:39:LEU:N	1:D:39:LEU:CD2	2.62	0.44
1:B:196:VAL:HG22	1:B:197:ARG:N	2.32	0.44
1:C:196:VAL:HG23	1:C:197:ARG:H	1.82	0.43
1:B:77:ARG:HG2	1:B:79:TYR:CZ	2.54	0.43
1:D:50:LYS:HE2	5:D:627:HOH:O	2.17	0.43
1:A:220:LYS:HE2	1:A:220:LYS:HB3	1.52	0.43
1:B:151:VAL:CG1	1:B:152:SER:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:LEU:HD22	1:C:149:ARG:NH1	2.33	0.43
1:D:108:LYS:O	1:D:109:ALA:C	2.62	0.43
1:A:210:ASN:OD1	1:B:287:SER:HB2	2.18	0.43
1:C:107:SER:HB2	1:C:110:LYS:HB2	2.00	0.43
1:A:182:ILE:HD12	1:A:247:LEU:CD1	2.45	0.43
1:B:87:ILE:HG21	1:B:89:TRP:CD2	2.53	0.43
1:B:77:ARG:HG3	1:B:78:VAL:N	2.32	0.43
1:D:190:MET:HE1	1:D:194:GLY:O	2.19	0.43
1:C:50:LYS:NZ	1:C:60:ALA:O	2.51	0.43
1:C:190:MET:HE3	1:C:192:LEU:O	2.19	0.43
1:C:172:PHE:O	1:C:255:ASP:HB2	2.19	0.42
1:C:247:LEU:C	1:C:247:LEU:HD12	2.44	0.42
1:D:286:SER:O	1:D:289:VAL:HG22	2.18	0.42
1:C:222:LEU:HA	1:C:222:LEU:HD12	1.83	0.42
1:D:162:ALA:HB3	1:D:163:PRO:HD3	2.01	0.42
1:A:247:LEU:HD23	1:A:319:TRP:CZ3	2.55	0.42
1:D:67:ASP:OD1	1:D:67:ASP:C	2.62	0.42
1:A:74:LYS:HG2	1:A:76:TYR:CE1	2.55	0.42
1:C:133:LYS:HD3	1:C:143:ILE:HG13	2.01	0.42
1:A:176:VAL:HG22	1:B:306:THR:HG22	2.02	0.42
1:C:76:TYR:CD1	1:C:76:TYR:N	2.87	0.41
1:D:97:PHE:HE1	1:D:121:ARG:HD2	1.85	0.41
1:B:236:HIS:CD2	1:B:236:HIS:C	2.98	0.41
1:D:120:LYS:HZ3	1:D:120:LYS:HG3	1.55	0.41
1:D:299:ASP:HA	1:D:300:PRO:HD2	1.82	0.41
1:A:13:ILE:HG21	1:A:330:MET:HE1	2.02	0.41
1:B:50:LYS:HE3	1:B:57:THR:CG2	2.51	0.41
1:D:232:LYS:NZ	5:D:511:HOH:O	2.52	0.41
1:D:69:ILE:HD12	1:D:69:ILE:HG21	1.59	0.41
1:D:69:ILE:HG23	1:D:69:ILE:HD13	1.62	0.40
1:C:12:ARG:HG2	1:C:12:ARG:NH1	2.36	0.40
1:C:299:ASP:HA	1:C:300:PRO:HD2	1.89	0.40
1:D:4:LYS:HD3	1:D:34:VAL:HG11	2.03	0.40
1:D:121:ARG:HD2	1:D:337:PHE:CD1	2.56	0.40
1:A:88:PRO:O	1:A:91:LYS:HG2	2.22	0.40
1:B:132:LEU:C	1:B:132:LEU:HD12	2.46	0.40
1:C:101:CYS:HB3	5:C:591:HOH:O	2.22	0.40
1:A:299:ASP:HA	1:A:300:PRO:HD2	1.93	0.40

There are no symmetry-related clashes.

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	338/340 (99%)	321 (95%)	17 (5%)	0	100	100
1	B	332/340 (98%)	311 (94%)	20 (6%)	1 (0%)	36	33
1	C	320/340 (94%)	305 (95%)	14 (4%)	1 (0%)	36	33
1	D	327/340 (96%)	309 (94%)	14 (4%)	4 (1%)	10	5
All	All	1317/1360 (97%)	1246 (95%)	65 (5%)	6 (0%)	24	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	106	THR
1	D	91	LYS
1	D	173	GLY
1	C	173	GLY
1	D	88	PRO
1	B	173	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/277 (100%)	254 (92%)	23 (8%)	10	6
1	B	273/277 (99%)	247 (90%)	26 (10%)	8	4
1	C	265/277 (96%)	231 (87%)	34 (13%)	4	1
1	D	271/277 (98%)	248 (92%)	23 (8%)	10	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1086/1108 (98%)	980 (90%)	106 (10%)	7 3

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	27	LYS
1	A	29	SER
1	A	58	LEU
1	A	66	ASP
1	A	77	ARG
1	A	83	GLN
1	A	91	LYS
1	A	106	THR
1	A	108	LYS
1	A	111	SER
1	A	132	LEU
1	A	176	VAL
1	A	179	MET
1	A	187	SER
1	A	197	ARG
1	A	220	LYS
1	A	228	GLU
1	A	247	LEU
1	A	257	LYS
1	A	289	VAL
1	A	307	SER
1	A	310	ASP
1	B	3	VAL
1	B	10	PHE
1	B	13	ILE
1	B	22	LEU
1	B	27	LYS
1	B	28	SER
1	B	31	ILE
1	B	32	GLU
1	B	39	LEU
1	B	63	SER
1	B	69	ILE
1	B	74	LYS
1	B	77	ARG
1	B	78	VAL

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Mol	Chain	Res	Type
1	B	85	GLN
1	B	89	TRP
1	B	91	LYS
1	B	101	CYS
1	B	106	THR
1	B	115	LEU
1	B	175	LYS
1	B	191	LEU
1	B	197	ARG
1	B	220	LYS
1	B	247	LEU
1	B	269	LYS
1	C	3	VAL
1	C	4	LYS
1	C	23	GLU
1	C	32	GLU
1	C	33	VAL
1	C	40	THR
1	C	41	SER
1	C	68	SER
1	C	74	LYS
1	C	83	GLN
1	C	85	GLN
1	C	89	TRP
1	C	106	THR
1	C	107	SER
1	C	120	LYS
1	C	130	SER
1	C	132	LEU
1	C	138	ASN
1	C	149	ARG
1	C	170	LYS
1	C	179	MET
1	C	181	THR
1	C	190	MET
1	C	196	VAL
1	C	197	ARG
1	C	220	LYS
1	C	228	GLU
1	C	236	HIS
1	C	257	LYS
1	C	281	ASP

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Mol	Chain	Res	Type
1	C	307	SER
1	C	310	ASP
1	C	330	MET
1	C	340	LEU
1	D	23	GLU
1	D	26	GLU
1	D	39	LEU
1	D	69	ILE
1	D	83	GLN
1	D	89	TRP
1	D	101	CYS
1	D	110	LYS
1	D	115	LEU
1	D	120	LYS
1	D	125	SER
1	D	130	SER
1	D	138	ASN
1	D	149	ARG
1	D	170	LYS
1	D	176	VAL
1	D	179	MET
1	D	190	MET
1	D	220	LYS
1	D	243	VAL
1	D	269	LYS
1	D	334	LEU
1	D	339	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	312	GLN
1	B	85	GLN
1	B	86	ASN
1	B	112	GLN
1	B	234	GLN
1	C	83	GLN
1	C	114	HIS
1	C	138	ASN
1	C	214	HIS
1	C	311	ASN

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Mol	Chain	Res	Type
1	C	312	GLN
1	D	214	HIS
1	D	234	GLN
1	D	312	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 11 are monoatomic - leaving 7 for Mogul analysis.

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	EDO	D	401	-	3,3,3	0.61	0	2,2,2	0.13	0
4	TRS	B	401	-	7,7,7	1.21	1 (14%)	9,9,9	1.67	2 (22%)
2	EDO	C	401	-	3,3,3	0.63	0	2,2,2	0.33	0
2	EDO	A	405	-	3,3,3	0.35	0	2,2,2	0.61	0
2	EDO	B	402	-	3,3,3	0.54	0	2,2,2	0.42	0
2	EDO	D	405	-	3,3,3	1.10	0	2,2,2	1.25	0
2	EDO	A	401	-	3,3,3	0.78	0	2,2,2	0.46	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
2	EDO	D	401	-	-	0/1/1/1	-
4	TRS	B	401	-	-	9/9/9/9	-
2	EDO	C	401	-	-	1/1/1/1	-
2	EDO	A	405	-	-	0/1/1/1	-
2	EDO	B	402	-	-	1/1/1/1	-
2	EDO	D	405	-	-	0/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	TRS	C1-C	-2.30	1.47	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	TRS	C2-C-C1	-2.38	104.31	110.66
4	B	401	TRS	C2-C-N	2.20	113.79	108.17

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	TRS	C1-C-C2-O2
4	B	401	TRS	C1-C-C3-O3
4	B	401	TRS	C2-C-C3-O3
4	B	401	TRS	N-C-C3-O3
4	B	401	TRS	C2-C-C1-O1
2	C	401	EDO	O1-C1-C2-O2
4	B	401	TRS	N-C-C1-O1
4	B	401	TRS	C3-C-C2-O2
2	B	402	EDO	O1-C1-C2-O2
4	B	401	TRS	C3-C-C1-O1
4	B	401	TRS	N-C-C2-O2

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	EDO	1	0
4	B	401	TRS	6	0
2	D	405	EDO	8	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 ⓘ

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	340/340 (100%)	0.01	10 (2%) 53 57	24, 35, 57, 112	0
1	B	336/340 (98%)	0.23	10 (2%) 52 56	25, 38, 60, 101	0
1	C	326/340 (95%)	0.49	22 (6%) 24 27	25, 42, 71, 105	0
1	D	333/340 (97%)	0.37	21 (6%) 26 30	25, 36, 72, 115	0
All	All	1335/1360 (98%)	0.27	63 (4%) 36 41	24, 37, 68, 115	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	126	ALA	9.1
1	C	3	VAL	6.4
1	B	3	VAL	6.4
1	D	129	GLY	5.9
1	D	338	ALA	5.6
1	D	1	MET	5.3
1	D	25	GLY	5.0
1	B	39	LEU	5.0
1	D	3	VAL	4.9
1	D	39	LEU	4.9
1	D	337	PHE	4.9
1	A	1	MET	4.5
1	D	340	LEU	4.3
1	D	97	PHE	4.2
1	B	28	SER	3.9
1	D	26	GLU	3.7
1	A	101	CYS	3.6
1	C	1	MET	3.5
1	C	89	TRP	3.5
1	C	32	GLU	3.4
1	A	91	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	104	PHE	3.1
1	C	24	LEU	3.1
1	D	32	GLU	3.0
1	C	340	LEU	3.0
1	A	27	LYS	2.8
1	D	339	THR	2.8
1	B	31	ILE	2.8
1	B	101	CYS	2.7
1	D	104	PHE	2.7
1	C	83	GLN	2.7
1	A	74	LYS	2.7
1	C	88	PRO	2.6
1	A	197	ARG	2.6
1	C	337	PHE	2.6
1	A	29	SER	2.6
1	C	34	VAL	2.5
1	D	2	SER	2.5
1	C	5	ILE	2.5
1	C	197	ARG	2.4
1	D	5	ILE	2.4
1	B	197	ARG	2.4
1	C	156	CYS	2.4
1	D	105	TYR	2.4
1	C	97	PHE	2.3
1	D	106	THR	2.3
1	A	308	ASP	2.3
1	B	146	ALA	2.2
1	C	2	SER	2.2
1	B	27	LYS	2.2
1	C	33	VAL	2.2
1	B	142	ASP	2.2
1	D	90	VAL	2.1
1	D	95	VAL	2.1
1	C	4	LYS	2.1
1	B	104	PHE	2.1
1	A	198	GLY	2.1
1	C	129	GLY	2.1
1	A	30	ASP	2.1
1	C	339	THR	2.1
1	D	91	LYS	2.0
1	C	128	ALA	2.0
1	C	66	ASP	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	EDO	D	405	4/4	0.48	0.33	20,20,20,20	0
4	TRS	B	401	8/8	0.75	0.22	24,31,34,39	0
3	HG	B	405	1/1	0.85	0.28	174,174,174,174	0
3	HG	D	402	1/1	0.87	0.18	116,116,116,116	0
3	HG	A	404	1/1	0.89	0.30	165,165,165,165	0
3	HG	D	403	1/1	0.90	0.20	127,127,127,127	0
3	HG	B	403	1/1	0.90	0.42	181,181,181,181	0
2	EDO	A	401	4/4	0.91	0.10	42,43,47,48	0
2	EDO	C	401	4/4	0.91	0.13	47,51,53,53	0
3	HG	C	403	1/1	0.91	0.24	119,119,119,119	0
2	EDO	B	402	4/4	0.92	0.11	47,50,51,54	0
3	HG	A	402	1/1	0.93	0.30	117,117,117,117	0
2	EDO	D	401	4/4	0.94	0.10	38,38,45,47	0
2	EDO	A	405	4/4	0.94	0.19	20,20,20,20	0
3	HG	B	404	1/1	0.95	0.11	74,74,74,74	0
3	HG	D	404	1/1	0.96	0.10	70,70,70,70	0
3	HG	A	403	1/1	0.96	0.10	66,66,66,66	0
3	HG	C	402	1/1	0.98	0.09	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.