



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:03 PM UTC

PDB ID : 3D7E / pdb_00003d7e
Title : Enterococcus casseliflavus glycerol kinase mutant HIS232ALA complexed with glycerol
Authors : Yeh, J.I.; Vahedi-Faridi, A.
Deposited on : 2008-05-21
Resolution : 2.03 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

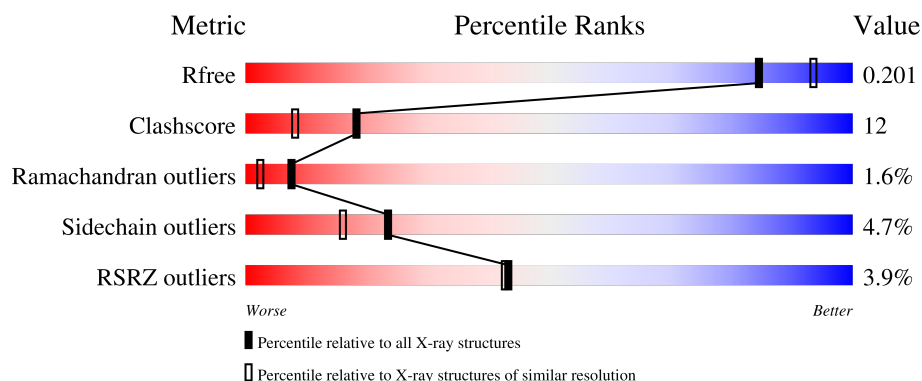
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	O	505	4% 61% 30% 6% ..
1	X	505	4% 64% 28% . ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7995 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 Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	495	Total	C	N	O	S	0	0	0
			3838	2433	638	753	14			
1	X	495	Total	C	N	O	S	0	0	0
			3838	2433	638	753	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	232	ALA	HIS	engineered mutation	UNP O34153
X	232	ALA	HIS	engineered mutation	UNP O34153

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

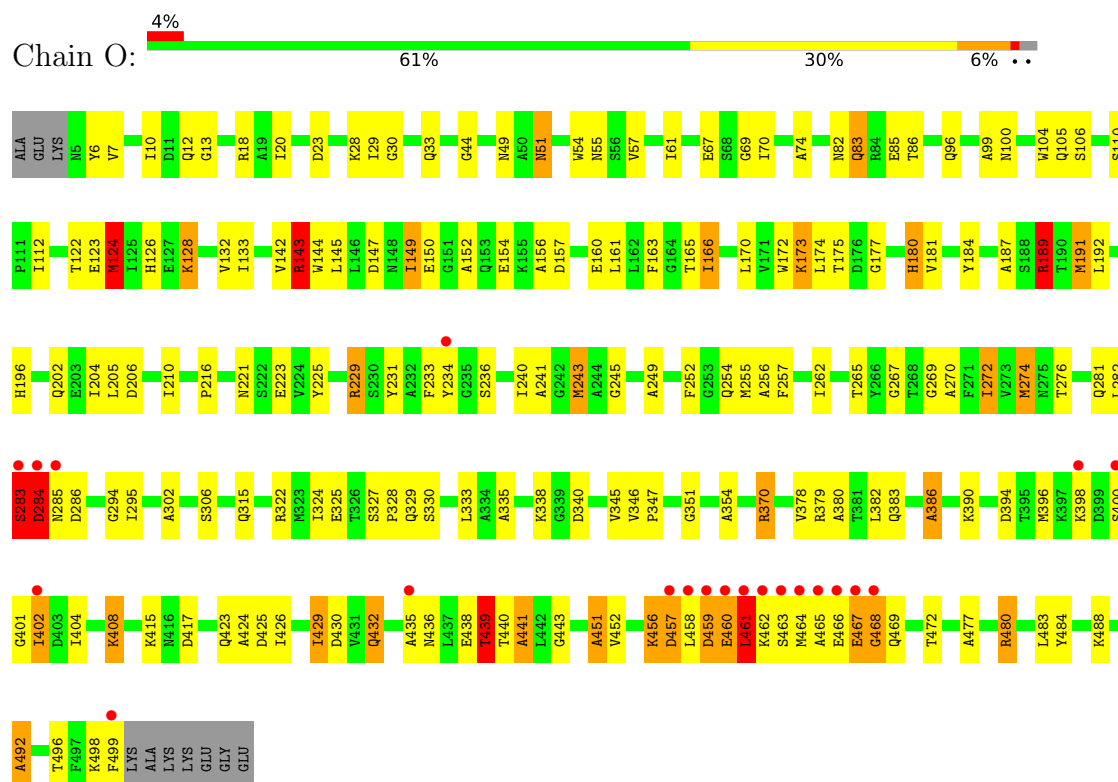
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	165	Total	O	0	0
			165	165		
3	X	142	Total	O	0	0
			142	142		

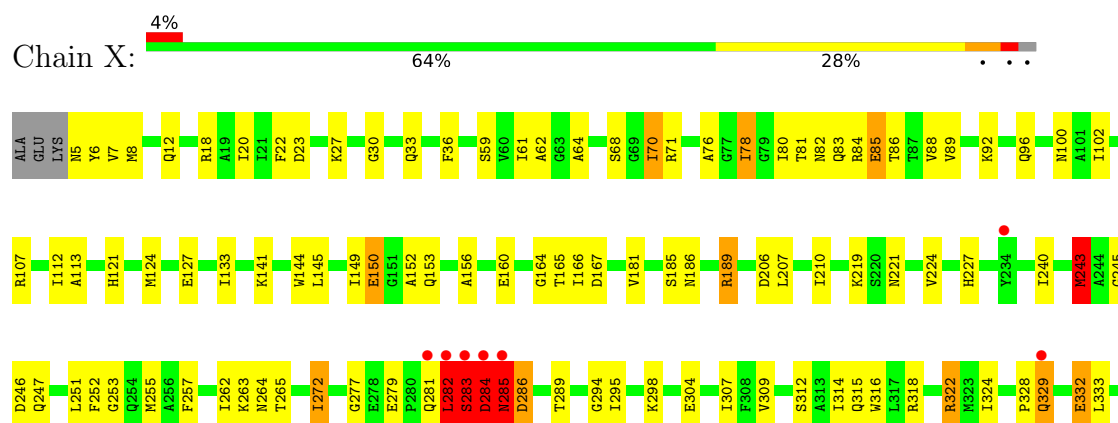
3 Residue-property plots

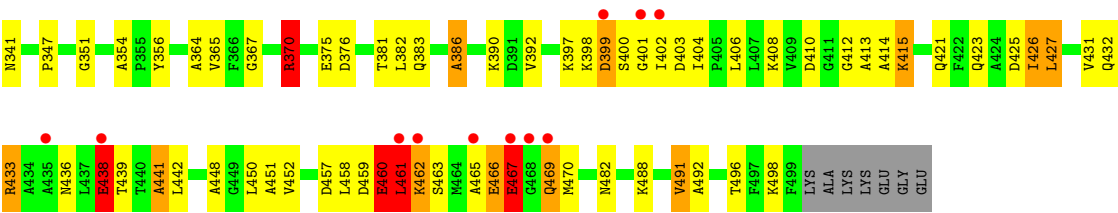
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glycerol kinase



• Molecule 1: Glycerol kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.57Å 200.02Å 56.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.28 – 2.03 39.28 – 2.03	Depositor EDS
% Data completeness (in resolution range)	88.9 (39.28-2.03) 89.1 (39.28-2.03)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.191 , 0.249 0.194 , 0.201	Depositor DCC
R_{free} test set	3224 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.3	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	0.94	EDS
Total number of atoms	7995	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% 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: 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	O	2.10	91/3918 (2.3%)	1.62	57/5314 (1.1%)
1	X	2.12	93/3918 (2.4%)	1.60	34/5314 (0.6%)
All	All	2.11	184/7836 (2.3%)	1.61	91/10628 (0.9%)

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	O	0	5
1	X	0	6
All	All	0	11

All (184) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	432	GLN	C-O	16.66	1.43	1.24
1	O	152	ALA	CA-CB	12.34	1.72	1.53
1	O	256	ALA	CA-CB	11.92	1.68	1.52
1	O	402	ILE	CA-CB	11.32	1.65	1.53
1	X	152	ALA	CA-CB	11.20	1.70	1.53
1	O	351	GLY	N-CA	10.39	1.55	1.45
1	O	99	ALA	CA-CB	10.34	1.69	1.53
1	O	210	ILE	CA-C	-10.31	1.44	1.53
1	X	469	GLN	C-O	10.01	1.36	1.24
1	O	370	ARG	CG-CD	9.78	1.81	1.52
1	X	284	ASP	CA-C	9.77	1.65	1.52
1	O	272	ILE	CA-CB	9.52	1.65	1.54
1	X	370	ARG	CZ-NH1	9.22	1.45	1.32
1	O	189	ARG	CD-NE	-9.17	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	189	ARG	CD-NE	-8.96	1.33	1.46
1	X	149	ILE	CA-CB	8.92	1.64	1.54
1	X	245	GLY	CA-C	-8.82	1.44	1.52
1	X	376	ASP	C-O	-8.78	1.13	1.24
1	X	286	ASP	N-CA	8.69	1.57	1.46
1	O	210	ILE	CA-CB	8.67	1.64	1.54
1	O	206	ASP	N-CA	8.58	1.56	1.46
1	X	392	VAL	CA-CB	8.45	1.64	1.54
1	X	243	MET	CB-CG	8.26	1.77	1.52
1	X	153	GLN	C-O	8.07	1.33	1.24
1	X	365	VAL	C-O	7.96	1.32	1.24
1	X	448	ALA	CA-C	7.86	1.62	1.52
1	X	285	ASN	C-O	7.81	1.33	1.24
1	X	285	ASN	CA-C	7.80	1.63	1.52
1	O	483	LEU	C-O	7.72	1.32	1.24
1	O	124	MET	C-O	-7.71	1.15	1.24
1	X	100	ASN	N-CA	7.68	1.55	1.46
1	X	282	LEU	CA-C	7.56	1.62	1.52
1	X	78	ILE	C-O	-7.51	1.15	1.24
1	O	302	ALA	CA-CB	7.49	1.66	1.53
1	O	306	SER	N-CA	7.44	1.55	1.46
1	X	36	PHE	CA-C	7.43	1.59	1.52
1	X	414	ALA	CA-CB	7.40	1.66	1.53
1	O	122	THR	CA-C	-7.31	1.43	1.52
1	X	307	ILE	CA-CB	7.31	1.63	1.53
1	O	166	ILE	CA-CB	7.29	1.64	1.54
1	X	247	GLN	CA-C	7.27	1.62	1.52
1	O	441	ALA	N-CA	-7.25	1.37	1.46
1	X	351	GLY	C-O	7.23	1.33	1.23
1	X	102	ILE	CA-CB	7.23	1.62	1.54
1	X	85	GLU	C-O	7.21	1.33	1.24
1	O	181	VAL	C-O	7.20	1.31	1.23
1	O	100	ASN	C-O	7.18	1.32	1.23
1	X	89	VAL	CA-C	7.16	1.61	1.52
1	O	55	ASN	N-CA	7.14	1.55	1.46
1	O	347	PRO	C-O	-7.07	1.14	1.24
1	X	88	VAL	N-CA	7.05	1.54	1.46
1	X	421	GLN	N-CA	7.03	1.55	1.46
1	O	216	PRO	CA-C	-7.02	1.44	1.52
1	O	404	ILE	CA-CB	6.99	1.63	1.54
1	X	386	ALA	CA-CB	6.87	1.64	1.53
1	X	390	LYS	C-O	6.65	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	156	ALA	CA-CB	6.62	1.63	1.53
1	X	347	PRO	N-CA	-6.62	1.42	1.47
1	X	413	ALA	CA-CB	6.62	1.65	1.53
1	O	161	LEU	CA-C	-6.59	1.44	1.52
1	X	113	ALA	CA-C	6.53	1.61	1.52
1	X	491	VAL	CA-CB	6.50	1.62	1.54
1	O	175	THR	N-CA	6.47	1.54	1.46
1	X	399	ASP	CB-CG	6.45	1.68	1.52
1	X	354	ALA	CA-CB	6.40	1.63	1.53
1	O	492	ALA	CA-CB	6.39	1.63	1.53
1	O	206	ASP	C-O	-6.29	1.16	1.24
1	X	425	ASP	N-CA	6.19	1.53	1.46
1	O	55	ASN	C-O	-6.16	1.17	1.24
1	O	51	ASN	CA-CB	6.16	1.63	1.53
1	O	110	SER	C-O	-6.16	1.18	1.24
1	X	145	LEU	N-CA	6.13	1.53	1.46
1	X	133	ILE	CA-CB	6.09	1.61	1.54
1	X	64	ALA	CA-CB	6.08	1.62	1.53
1	O	106	SER	N-CA	-6.08	1.38	1.46
1	X	262	ILE	N-CA	6.06	1.53	1.46
1	X	144	TRP	C-O	6.05	1.31	1.24
1	X	322	ARG	CD-NE	-6.04	1.37	1.46
1	O	49	ASN	C-O	6.03	1.31	1.24
1	O	335	ALA	N-CA	6.01	1.54	1.46
1	O	173	LYS	C-O	-6.00	1.17	1.24
1	O	338	LYS	CA-C	6.00	1.60	1.52
1	X	285	ASN	CG-OD1	6.00	1.34	1.23
1	O	295	ILE	CB-CG2	5.96	1.72	1.52
1	O	380	ALA	CA-CB	5.94	1.62	1.53
1	O	149	ILE	CA-CB	5.91	1.61	1.54
1	X	107	ARG	CB-CG	5.87	1.70	1.52
1	X	370	ARG	N-CA	5.87	1.53	1.46
1	X	7	VAL	C-O	-5.86	1.18	1.24
1	O	143	ARG	N-CA	5.84	1.53	1.46
1	X	304	GLU	CB-CG	5.83	1.70	1.52
1	X	76	ALA	CA-CB	5.80	1.62	1.53
1	X	85	GLU	N-CA	5.78	1.53	1.46
1	O	160	GLU	CA-C	5.77	1.60	1.52
1	X	431	VAL	CA-CB	5.76	1.61	1.54
1	X	262	ILE	CA-C	-5.72	1.45	1.52
1	X	367	GLY	N-CA	5.72	1.53	1.45
1	X	452	VAL	CB-CG1	5.71	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	381	THR	CB-CG2	5.70	1.71	1.52
1	O	143	ARG	CD-NE	-5.70	1.38	1.46
1	O	267	GLY	N-CA	5.70	1.50	1.45
1	X	206	ASP	N-CA	5.70	1.53	1.46
1	X	433	ARG	N-CA	5.69	1.53	1.46
1	X	295	ILE	C-O	-5.69	1.18	1.23
1	O	382	LEU	C-O	-5.68	1.17	1.24
1	O	83	GLN	CA-C	5.67	1.59	1.52
1	X	448	ALA	C-O	-5.66	1.17	1.24
1	O	223	GLU	C-O	-5.65	1.17	1.23
1	X	364	ALA	C-O	5.64	1.30	1.23
1	O	128	LYS	CD-CE	5.63	1.69	1.52
1	O	30	GLY	N-CA	5.62	1.50	1.45
1	O	265	THR	CA-C	5.62	1.59	1.52
1	X	406	LEU	CA-C	5.62	1.58	1.52
1	X	141	LYS	N-CA	5.60	1.53	1.46
1	O	128	LYS	C-O	-5.60	1.17	1.24
1	X	277	GLY	CA-C	-5.60	1.46	1.52
1	X	112	ILE	CA-CB	5.59	1.61	1.54
1	X	370	ARG	CZ-NH2	5.59	1.40	1.33
1	O	274	MET	N-CA	5.58	1.53	1.46
1	O	315	GLN	CG-CD	5.56	1.66	1.52
1	X	23	ASP	N-CA	5.54	1.52	1.45
1	O	472	THR	CA-CB	5.53	1.64	1.53
1	X	160	GLU	CD-OE2	5.52	1.35	1.25
1	O	180	HIS	C-O	5.52	1.30	1.23
1	O	270	ALA	CA-CB	5.51	1.66	1.53
1	O	144	TRP	CA-C	5.50	1.59	1.52
1	O	99	ALA	CA-C	5.48	1.59	1.52
1	X	185	SER	C-O	5.48	1.30	1.24
1	O	346	VAL	CA-CB	5.48	1.61	1.54
1	X	285	ASN	C-N	5.48	1.41	1.33
1	O	13	GLY	N-CA	5.47	1.51	1.45
1	O	191	MET	C-O	5.46	1.32	1.24
1	O	432	GLN	C-O	5.46	1.30	1.24
1	O	354	ALA	CA-CB	5.46	1.61	1.53
1	O	424	ALA	N-CA	5.46	1.52	1.46
1	X	251	LEU	CG-CD1	5.46	1.70	1.52
1	X	370	ARG	NE-CZ	5.45	1.39	1.33
1	X	127	GLU	CA-C	5.43	1.60	1.52
1	X	450	LEU	N-CA	5.38	1.52	1.46
1	O	112	ILE	CA-C	5.36	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	150	GLU	N-CA	5.36	1.52	1.46
1	X	426	ILE	N-CA	5.36	1.53	1.46
1	X	224	VAL	C-O	-5.34	1.17	1.24
1	O	23	ASP	CA-C	5.33	1.60	1.53
1	X	469	GLN	N-CA	5.33	1.53	1.46
1	X	298	LYS	CE-NZ	5.32	1.65	1.49
1	O	150	GLU	CA-C	-5.30	1.45	1.52
1	O	382	LEU	CA-CB	5.29	1.61	1.53
1	X	59	SER	C-O	5.27	1.30	1.24
1	X	442	LEU	N-CA	5.27	1.52	1.46
1	O	345	VAL	CA-C	-5.26	1.46	1.52
1	X	451	ALA	N-CA	-5.25	1.39	1.46
1	O	252	PHE	N-CA	-5.25	1.40	1.46
1	X	309	VAL	N-CA	-5.24	1.39	1.46
1	O	451	ALA	C-O	5.23	1.30	1.24
1	X	264	ASN	CA-C	-5.21	1.46	1.52
1	O	147	ASP	N-CA	-5.20	1.39	1.46
1	O	270	ALA	C-O	-5.17	1.17	1.24
1	X	427	LEU	N-CA	5.17	1.52	1.46
1	O	408	LYS	N-CA	-5.14	1.39	1.45
1	O	110	SER	N-CA	5.13	1.51	1.46
1	O	254	GLN	C-O	-5.13	1.17	1.24
1	O	274	MET	SD-CE	-5.12	1.66	1.79
1	O	157	ASP	N-CA	5.11	1.52	1.46
1	O	205	LEU	N-CA	5.10	1.52	1.46
1	O	10	ILE	CA-C	-5.09	1.46	1.52
1	X	62	ALA	C-O	-5.07	1.18	1.24
1	O	86	THR	CA-C	5.06	1.58	1.52
1	O	57	VAL	C-O	-5.05	1.18	1.24
1	O	82	ASN	CA-CB	5.05	1.61	1.53
1	O	315	GLN	C-O	-5.05	1.18	1.24
1	X	354	ALA	C-O	-5.05	1.17	1.23
1	X	399	ASP	CG-OD1	5.05	1.34	1.25
1	O	187	ALA	C-O	5.04	1.30	1.24
1	O	262	ILE	CB-CG2	5.04	1.69	1.52
1	O	451	ALA	CA-CB	5.04	1.61	1.53
1	X	5	ASN	N-CA	5.04	1.55	1.46
1	X	286	ASP	CA-C	5.04	1.59	1.52
1	X	210	ILE	CA-CB	5.04	1.60	1.54
1	O	370	ARG	N-CA	5.03	1.52	1.46
1	O	7	VAL	CA-CB	5.03	1.61	1.54
1	O	417	ASP	N-CA	5.01	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	67	GLU	CB-CG	5.01	1.67	1.52
1	X	285	ASN	N-CA	5.01	1.52	1.46

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	460	GLU	N-CA-C	-11.97	87.70	108.52
1	O	283	SER	N-CA-C	9.81	131.70	110.80
1	O	452	VAL	N-CA-C	-9.25	103.59	112.29
1	X	189	ARG	NE-CZ-NH2	-9.09	111.02	119.20
1	X	460	GLU	N-CA-C	-9.05	91.53	110.80
1	X	467	GLU	N-CA-C	8.94	122.88	108.76
1	O	189	ARG	CB-CG-CD	-8.79	91.07	111.30
1	X	189	ARG	CB-CG-CD	-8.61	91.51	111.30
1	O	457	ASP	N-CA-C	8.47	121.59	108.96
1	O	145	LEU	N-CA-C	-8.23	102.39	111.36
1	O	105	GLN	N-CA-C	8.16	121.28	111.82
1	O	189	ARG	NE-CZ-NH2	-8.15	111.86	119.20
1	O	44	GLY	N-CA-C	-7.99	104.54	114.92
1	O	236	SER	CA-C-N	-7.97	110.97	122.77
1	O	236	SER	C-N-CA	-7.97	110.97	122.77
1	O	142	VAL	N-CA-C	-7.81	103.19	110.53
1	X	279	GLU	CA-C-N	-7.62	111.94	119.78
1	X	279	GLU	C-N-CA	-7.62	111.94	119.78
1	X	370	ARG	NE-CZ-NH2	-7.49	112.46	119.20
1	X	165	THR	N-CA-C	-7.36	101.06	110.19
1	X	243	MET	CA-CB-CG	7.22	128.55	114.10
1	O	386	ALA	N-CA-C	-7.20	103.51	111.36
1	X	283	SER	N-CA-C	7.16	126.06	110.80
1	O	456	LYS	CA-C-N	-7.09	110.25	121.87
1	O	456	LYS	C-N-CA	-7.09	110.25	121.87
1	O	283	SER	CA-C-N	7.08	135.07	121.54
1	O	283	SER	C-N-CA	7.08	135.07	121.54
1	X	252	PHE	CA-C-N	7.02	128.92	120.14
1	X	252	PHE	C-N-CA	7.02	128.92	120.14
1	X	432	GLN	N-CA-C	7.02	120.30	111.24
1	X	96	GLN	CA-C-N	6.98	126.95	119.76
1	X	96	GLN	C-N-CA	6.98	126.95	119.76
1	O	170	LEU	N-CA-C	6.96	118.51	111.07
1	X	441	ALA	N-CA-C	-6.72	103.95	111.28
1	X	322	ARG	NE-CZ-NH2	-6.68	113.19	119.20
1	X	398	LYS	N-CA-C	6.67	119.12	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	367	GLY	N-CA-C	-6.64	105.49	115.32
1	X	164	GLY	O-C-N	6.61	128.29	123.27
1	O	61	ILE	CB-CA-C	-6.32	103.88	111.97
1	X	461	LEU	N-CA-C	6.25	124.11	110.80
1	O	430	ASP	N-CA-C	6.23	119.26	110.23
1	O	404	ILE	CA-C-N	-6.14	113.61	121.04
1	O	404	ILE	C-N-CA	-6.14	113.61	121.04
1	O	189	ARG	NE-CZ-NH1	6.11	127.61	121.50
1	X	452	VAL	CB-CA-C	-6.08	105.20	112.19
1	O	472	THR	CB-CA-C	6.04	116.60	109.47
1	O	61	ILE	N-CA-C	-5.90	104.75	110.42
1	O	243	MET	CG-SD-CE	-5.90	87.92	100.90
1	X	71	ARG	CB-CA-C	5.90	117.75	108.84
1	O	370	ARG	CB-CG-CD	5.87	124.79	111.30
1	O	122	THR	N-CA-C	5.85	118.15	111.02
1	O	477	ALA	N-CA-C	-5.75	105.09	111.36
1	O	143	ARG	NE-CZ-NH2	-5.71	114.06	119.20
1	O	245	GLY	N-CA-C	-5.69	105.39	111.93
1	X	133	ILE	N-CA-C	-5.67	102.22	109.30
1	X	156	ALA	N-CA-C	-5.63	105.22	111.36
1	X	70	ILE	N-CA-C	-5.61	101.65	109.45
1	O	44	GLY	CA-C-N	-5.59	114.31	122.65
1	O	44	GLY	C-N-CA	-5.59	114.31	122.65
1	O	74	ALA	CA-C-N	-5.59	115.89	122.93
1	O	74	ALA	C-N-CA	-5.59	115.89	122.93
1	O	143	ARG	CD-NE-CZ	5.57	132.19	124.40
1	O	429	ILE	CB-CG1-CD1	-5.56	102.11	113.80
1	O	401	GLY	N-CA-C	-5.55	108.27	115.59
1	O	184	TYR	CB-CA-C	-5.52	101.63	110.79
1	X	253	GLY	N-CA-C	-5.46	106.09	113.24
1	O	272	ILE	N-CA-CB	5.34	117.08	111.00
1	X	189	ARG	NE-CZ-NH1	5.34	126.84	121.50
1	X	438	GLU	CA-CB-CG	5.33	124.75	114.10
1	O	149	ILE	CG1-CB-CG2	-5.32	94.73	110.70
1	O	236	SER	O-C-N	-5.32	117.26	123.27
1	O	210	ILE	CA-C-N	-5.31	114.45	119.76
1	O	210	ILE	C-N-CA	-5.31	114.45	119.76
1	O	69	GLY	N-CA-C	-5.24	108.40	115.21
1	O	282	LEU	CA-C-N	5.21	131.50	121.54
1	O	282	LEU	C-N-CA	5.21	131.50	121.54
1	O	460	GLU	N-CA-CB	5.21	118.08	110.58
1	O	202	GLN	N-CA-C	5.21	116.95	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	192	LEU	N-CA-C	-5.21	106.89	114.12
1	X	433	ARG	N-CA-CB	5.20	119.28	110.49
1	O	283	SER	O-C-N	5.20	129.50	122.59
1	X	240	ILE	N-CA-C	-5.17	100.44	107.99
1	O	283	SER	CB-CA-C	-5.16	100.16	110.42
1	O	174	LEU	N-CA-C	-5.14	105.85	111.82
1	O	269	GLY	N-CA-C	-5.13	102.76	112.10
1	O	480	ARG	N-CA-C	-5.11	105.70	111.28
1	O	240	ILE	N-CA-C	-5.07	99.96	107.51
1	X	322	ARG	CB-CG-CD	-5.04	99.71	111.30
1	X	243	MET	CB-CG-SD	-5.04	97.59	112.70
1	O	439	THR	N-CA-C	-5.03	107.10	113.18
1	X	469	GLN	CB-CG-CD	5.01	121.12	112.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	233	PHE	Peptide
1	O	283	SER	Peptide
1	O	459	ASP	Peptide
1	O	461	LEU	Peptide
1	O	468	GLY	Peptide
1	X	282	LEU	Peptide
1	X	283	SER	Peptide
1	X	284	ASP	Peptide
1	X	461	LEU	Peptide
1	X	466	GLU	Peptide
1	X	467	GLU	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	O	3838	0	3735	106	0
1	X	3838	0	3735	83	0
2	O	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	6	0	8	0	0
3	O	165	0	0	5	0
3	X	142	0	0	4	0
All	All	7995	0	7486	184	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 12.

All (184) 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:X:243:MET:CB	1:X:243:MET:CG	1.77	1.56
1:O:370:ARG:CD	1:O:370:ARG:CG	1.81	1.52
1:O:229:ARG:HH11	1:O:229:ARG:HG3	1.09	1.11
1:X:459:ASP:C	1:X:461:LEU:N	2.11	1.02
1:X:466:GLU:O	1:X:466:GLU:HG2	1.60	1.01
1:O:18:ARG:HD2	3:O:600:HOH:O	1.61	0.99
1:O:284:ASP:OD1	1:O:286:ASP:HB2	1.64	0.98
1:O:126:HIS:NE2	1:O:283:SER:HB3	1.80	0.96
1:O:435:ALA:H	1:O:467:GLU:HB2	1.32	0.94
1:X:85:GLU:OE2	1:X:189:ARG:HD2	1.69	0.91
1:X:459:ASP:C	1:X:461:LEU:H	1.70	0.90
1:O:435:ALA:HB2	1:O:467:GLU:HA	1.51	0.90
1:O:133:ILE:HA	1:O:191:MET:HE1	1.55	0.87
1:O:12:GLN:HE22	1:O:83:GLN:HE21	1.21	0.87
1:O:370:ARG:HG2	3:O:627:HOH:O	1.74	0.87
1:X:312:SER:HA	1:X:315:GLN:HG2	1.60	0.82
1:O:124:MET:HE3	1:O:128:LYS:HE3	1.60	0.82
1:O:370:ARG:HG3	1:O:370:ARG:NH1	1.94	0.82
1:X:85:GLU:OE2	1:X:189:ARG:CD	2.29	0.81
1:X:243:MET:CB	1:X:243:MET:SD	2.71	0.79
1:O:322:ARG:NH2	1:X:375:GLU:OE2	2.15	0.79
1:X:221:ASN:HD22	1:X:294:GLY:H	1.27	0.79
1:O:435:ALA:H	1:O:467:GLU:CB	1.97	0.77
1:X:284:ASP:HB3	1:X:286:ASP:H	1.49	0.77
1:O:126:HIS:NE2	1:O:283:SER:CB	2.48	0.76
1:O:229:ARG:HH11	1:O:229:ARG:CG	1.96	0.76
1:O:229:ARG:HG3	1:O:229:ARG:NH1	1.88	0.76
1:O:221:ASN:HD22	1:O:294:GLY:H	1.32	0.75
1:O:370:ARG:CG	3:O:627:HOH:O	2.33	0.74
1:O:132:VAL:O	1:O:191:MET:HE1	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:283:SER:OG	1:O:284:ASP:N	2.21	0.74
1:O:126:HIS:CE1	1:O:283:SER:HB3	2.23	0.73
1:O:12:GLN:HE21	1:O:166:ILE:HG21	1.51	0.73
1:O:457:ASP:H	1:O:460:GLU:HG3	1.54	0.73
1:X:227:HIS:HB2	3:X:519:HOH:O	1.89	0.72
1:O:379:ARG:O	1:O:383:GLN:HG3	1.90	0.71
1:X:12:GLN:HE21	1:X:166:ILE:HG21	1.56	0.71
1:X:466:GLU:O	1:X:466:GLU:CG	2.39	0.70
1:O:370:ARG:CG	1:O:370:ARG:NE	2.54	0.69
1:X:221:ASN:ND2	1:X:294:GLY:H	1.90	0.69
1:O:457:ASP:OD1	1:O:460:GLU:N	2.26	0.68
1:O:459:ASP:C	1:O:461:LEU:N	2.50	0.68
1:X:458:LEU:O	1:X:461:LEU:HA	1.93	0.68
1:X:18:ARG:HD2	1:X:438:GLU:OE1	1.94	0.67
1:O:462:LYS:HB3	1:O:465:ALA:HB2	1.77	0.66
1:O:285:ASN:CG	1:O:285:ASN:O	2.39	0.66
1:O:370:ARG:HG3	1:O:370:ARG:HH11	1.59	0.66
1:X:412:GLY:O	1:X:415:LYS:HG2	1.95	0.66
1:O:133:ILE:CA	1:O:191:MET:HE1	2.26	0.65
1:O:276:THR:HB	1:O:281:GLN:HE21	1.61	0.64
1:O:85:GLU:OE2	1:O:189:ARG:CD	2.46	0.64
1:O:143:ARG:O	1:O:143:ARG:HD3	1.98	0.62
1:X:461:LEU:C	1:X:463:SER:H	2.07	0.62
1:O:438:GLU:HG3	1:O:441:ALA:HB3	1.82	0.62
1:X:12:GLN:HE22	1:X:83:GLN:HE21	1.48	0.61
1:O:492:ALA:O	1:O:496:THR:HG23	2.00	0.61
1:O:370:ARG:HD3	3:X:532:HOH:O	2.01	0.61
1:O:438:GLU:OE1	1:O:440:THR:HB	2.02	0.60
1:O:132:VAL:O	1:O:191:MET:CE	2.50	0.60
1:O:124:MET:HE2	1:O:128:LYS:HD2	1.83	0.60
1:O:124:MET:CE	1:O:204:ILE:HG13	2.32	0.60
1:O:221:ASN:ND2	1:O:294:GLY:H	1.99	0.60
1:X:324:ILE:HG22	1:X:333:LEU:CD1	2.32	0.59
1:O:124:MET:HE3	1:O:128:LYS:CE	2.29	0.59
1:O:436:ASN:O	1:O:439:THR:HG22	2.01	0.59
1:X:426:ILE:C	1:X:426:ILE:HD12	2.28	0.59
1:X:461:LEU:C	1:X:463:SER:N	2.61	0.59
1:O:274:MET:HE1	1:O:400:SER:OG	2.01	0.59
1:O:154:GLU:H	1:O:154:GLU:CD	2.12	0.57
1:O:325:GLU:HB2	1:O:329:GLN:OE1	2.04	0.57
1:O:85:GLU:OE2	1:O:189:ARG:HD3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:370:ARG:CG	1:O:370:ARG:HH11	2.17	0.57
1:O:126:HIS:CE1	1:O:283:SER:CB	2.86	0.57
1:O:400:SER:C	1:O:402:ILE:H	2.14	0.56
1:O:322:ARG:HH21	1:X:375:GLU:CD	2.14	0.56
1:O:370:ARG:HE	1:X:315:GLN:HG3	1.69	0.56
1:O:133:ILE:HA	1:O:191:MET:CE	2.34	0.56
1:X:282:LEU:C	1:X:399:ASP:OD2	2.49	0.56
1:X:436:ASN:O	1:X:439:THR:HG22	2.05	0.56
1:O:18:ARG:HG2	1:O:33:GLN:HG3	1.87	0.56
1:O:124:MET:HE1	1:O:204:ILE:HG13	1.87	0.56
1:X:18:ARG:HG3	1:X:33:GLN:HB3	1.87	0.56
1:X:82:ASN:HD21	1:X:186:ASN:ND2	2.04	0.56
1:O:435:ALA:N	1:O:467:GLU:HB2	2.13	0.56
1:X:82:ASN:HD21	1:X:186:ASN:HD21	1.53	0.55
1:O:85:GLU:OE2	1:O:189:ARG:HD2	2.07	0.55
1:O:370:ARG:CG	1:O:370:ARG:NH1	2.67	0.55
1:O:370:ARG:HG3	1:O:370:ARG:CZ	2.36	0.54
1:X:124:MET:HE1	1:X:207:LEU:HD22	1.89	0.54
1:X:457:ASP:OD1	1:X:460:GLU:N	2.41	0.54
1:X:461:LEU:HB2	1:X:463:SER:H	1.73	0.53
1:O:123:GLU:HG2	3:O:660:HOH:O	2.07	0.53
1:O:386:ALA:HA	1:O:423:GLN:NE2	2.23	0.53
1:X:124:MET:HE1	1:X:207:LEU:CD2	2.39	0.53
1:X:397:LYS:HG2	1:X:404:ILE:HD12	1.90	0.53
1:X:85:GLU:OE2	1:X:189:ARG:HD3	2.09	0.53
1:X:438:GLU:HB3	3:X:587:HOH:O	2.08	0.53
1:X:436:ASN:O	1:X:439:THR:CG2	2.57	0.52
1:X:400:SER:O	1:X:402:ILE:N	2.42	0.52
1:X:121:HIS:HB3	1:X:124:MET:HE2	1.91	0.52
1:X:282:LEU:HD22	1:X:282:LEU:N	2.25	0.52
1:O:196:HIS:HE1	3:O:561:HOH:O	1.92	0.52
1:O:408:LYS:HZ3	1:O:432:GLN:NE2	2.08	0.52
1:O:85:GLU:HB2	1:O:104:TRP:HB3	1.93	0.51
1:O:408:LYS:HZ3	1:O:432:GLN:HE21	1.59	0.51
1:O:124:MET:CE	1:O:128:LYS:HD2	2.41	0.51
1:O:370:ARG:CG	1:O:370:ARG:CZ	2.89	0.50
1:X:282:LEU:N	1:X:282:LEU:CD2	2.74	0.50
1:X:492:ALA:O	1:X:496:THR:HG23	2.12	0.50
1:X:281:GLN:OE1	1:X:400:SER:CB	2.60	0.49
1:X:255:MET:HA	1:X:257:PHE:CZ	2.48	0.49
1:O:154:GLU:CD	1:O:154:GLU:N	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:167:ASP:HB2	1:X:243:MET:HG2	1.95	0.48
1:X:462:LYS:HG2	1:X:465:ALA:CB	2.42	0.48
1:X:386:ALA:HA	1:X:423:GLN:HE22	1.78	0.48
1:O:390:LYS:HE3	1:O:484:TYR:CD2	2.49	0.48
1:O:241:ALA:HB1	1:O:451:ALA:HB3	1.96	0.47
1:O:396:MET:O	1:O:400:SER:HB2	2.14	0.47
1:X:80:ILE:O	1:X:243:MET:HA	2.14	0.47
1:X:341:ASN:HD21	1:X:383:GLN:HE22	1.61	0.47
1:X:272:ILE:HD12	1:X:272:ILE:N	2.29	0.47
1:X:314:ILE:HD11	1:X:382:LEU:HD23	1.97	0.47
1:O:458:LEU:O	1:O:461:LEU:HA	2.14	0.47
1:X:356:TYR:CZ	1:X:491:VAL:HG11	2.50	0.47
1:O:459:ASP:HA	1:O:461:LEU:HA	1.96	0.47
1:X:20:ILE:HD13	1:X:441:ALA:CB	2.45	0.46
1:O:51:ASN:HD21	1:O:96:GLN:NE2	2.13	0.46
1:X:281:GLN:OE1	1:X:400:SER:HB2	2.15	0.46
1:X:498:LYS:HA	1:X:498:LYS:HD3	1.67	0.46
1:X:283:SER:HB3	1:X:289:THR:OG1	2.16	0.46
1:O:249:ALA:O	1:O:443:GLY:HA3	2.16	0.46
1:O:386:ALA:HA	1:O:423:GLN:HE22	1.79	0.46
1:X:284:ASP:HB3	1:X:286:ASP:N	2.24	0.46
1:O:438:GLU:HG3	1:O:438:GLU:O	2.16	0.46
1:O:394:ASP:O	1:O:398:LYS:HG3	2.17	0.45
1:X:457:ASP:O	1:X:460:GLU:HB2	2.16	0.45
1:X:30:GLY:HA3	1:X:68:SER:HB3	1.99	0.45
1:X:81:THR:OG1	1:X:246:ASP:HA	2.17	0.45
1:O:20:ILE:HG23	1:O:28:LYS:HG3	1.98	0.45
1:X:243:MET:SD	1:X:243:MET:HB2	2.55	0.45
1:O:124:MET:HE3	1:O:128:LYS:CD	2.47	0.45
1:O:124:MET:HE1	1:O:204:ILE:CG1	2.47	0.45
1:X:461:LEU:HB2	1:X:463:SER:N	2.30	0.45
1:O:6:TYR:CE2	1:O:70:ILE:HD12	2.52	0.45
1:X:386:ALA:HA	1:X:423:GLN:NE2	2.32	0.45
1:O:124:MET:CE	1:O:128:LYS:CD	2.95	0.45
1:X:22:PHE:HA	1:X:27:LYS:O	2.17	0.45
1:O:370:ARG:HD2	1:X:316:TRP:HB2	1.99	0.44
1:O:132:VAL:C	1:O:191:MET:HE1	2.42	0.44
1:X:263:LYS:HA	1:X:408:LYS:O	2.18	0.44
1:O:400:SER:C	1:O:402:ILE:N	2.72	0.44
1:O:425:ASP:O	1:O:480:ARG:HD3	2.17	0.44
1:X:285:ASN:HD22	1:X:285:ASN:HA	1.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:283:SER:HB2	1:O:284:ASP:O	2.18	0.43
1:O:400:SER:HB3	1:O:402:ILE:HB	2.00	0.43
1:O:231:TYR:O	1:O:234:TYR:HB2	2.19	0.43
1:O:459:ASP:O	1:O:461:LEU:HG	2.18	0.43
1:X:461:LEU:CA	1:X:463:SER:H	2.31	0.43
1:X:8:MET:HB3	1:X:78:ILE:HD13	2.00	0.43
1:X:283:SER:O	1:X:284:ASP:O	2.37	0.43
1:X:181:VAL:CG2	1:X:219:LYS:HG3	2.48	0.43
1:O:330:SER:HA	1:O:378:VAL:HG11	2.01	0.42
1:O:225:TYR:CE1	1:O:243:MET:HG3	2.54	0.42
1:X:263:LYS:HD2	1:X:263:LYS:C	2.44	0.42
1:X:84:ARG:C	1:X:86:THR:H	2.26	0.42
1:X:426:ILE:HD12	1:X:427:LEU:N	2.35	0.42
1:O:54:TRP:CD1	1:O:173:LYS:HE2	2.54	0.42
1:X:329:GLN:OE1	1:X:332:GLU:OE1	2.38	0.42
1:O:172:TRP:CE2	1:O:177:GLY:HA2	2.54	0.42
1:O:498:LYS:HD3	1:O:498:LYS:HA	1.71	0.42
1:O:499:PHE:CZ	1:X:482:ASN:O	2.74	0.41
1:O:438:GLU:CG	1:O:441:ALA:HB3	2.47	0.41
1:O:327:SER:N	1:O:328:PRO:CD	2.83	0.41
1:X:318:ARG:O	1:X:322:ARG:HA	2.21	0.41
1:O:255:MET:HA	1:O:257:PHE:CZ	2.56	0.41
1:X:282:LEU:O	1:X:399:ASP:OD2	2.38	0.41
1:X:265:THR:HG23	1:X:410:ASP:OD2	2.21	0.41
1:O:163:PHE:O	1:O:180:HIS:CE1	2.74	0.41
1:X:370:ARG:NE	3:X:633:HOH:O	2.54	0.41
1:O:124:MET:CE	1:O:204:ILE:CG1	2.97	0.41
1:O:461:LEU:C	1:O:463:SER:N	2.79	0.40
1:O:324:ILE:HG22	1:O:333:LEU:CD1	2.52	0.40
1:X:6:TYR:CE2	1:X:70:ILE:HD12	2.56	0.40
1:X:78:ILE:HG23	1:X:78:ILE:HD12	1.88	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	O	493/505 (98%)	466 (94%)	21 (4%)	6 (1%)	10	4
1	X	493/505 (98%)	466 (94%)	17 (3%)	10 (2%)	6	1
All	All	986/1010 (98%)	932 (94%)	38 (4%)	16 (2%)	7	2

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	283	SER
1	O	461	LEU
1	X	283	SER
1	X	284	ASP
1	X	461	LEU
1	X	469	GLN
1	O	340	ASP
1	O	468	GLY
1	X	285	ASN
1	X	401	GLY
1	X	462	LYS
1	X	470	MET
1	X	282	LEU
1	O	466	GLU
1	X	433	ARG
1	O	284	ASP

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	O	401/408 (98%)	382 (95%)	19 (5%)	23	16
1	X	401/408 (98%)	382 (95%)	19 (5%)	23	16
All	All	802/816 (98%)	764 (95%)	38 (5%)	23	16

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	29	ILE
1	O	124	MET
1	O	143	ARG
1	O	149	ILE
1	O	165	THR
1	O	189	ARG
1	O	229	ARG
1	O	272	ILE
1	O	284	ASP
1	O	415	LYS
1	O	426	ILE
1	O	429	ILE
1	O	439	THR
1	O	456	LYS
1	O	461	LEU
1	O	464	MET
1	O	467	GLU
1	O	469	GLN
1	O	488	LYS
1	X	61	ILE
1	X	92	LYS
1	X	150	GLU
1	X	243	MET
1	X	272	ILE
1	X	282	LEU
1	X	284	ASP
1	X	285	ASN
1	X	328	PRO
1	X	329	GLN
1	X	332	GLU
1	X	370	ARG
1	X	403	ASP
1	X	415	LYS
1	X	438	GLU
1	X	460	GLU
1	X	461	LEU
1	X	467	GLU
1	X	488	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	12	GLN

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Mol	Chain	Res	Type
1	O	96	GLN
1	O	196	HIS
1	O	221	ASN
1	O	264	ASN
1	O	281	GLN
1	O	285	ASN
1	O	315	GLN
1	O	341	ASN
1	O	423	GLN
1	O	432	GLN
1	X	5	ASN
1	X	12	GLN
1	X	33	GLN
1	X	115	GLN
1	X	180	HIS
1	X	186	ASN
1	X	221	ASN
1	X	264	ASN
1	X	285	ASN
1	X	315	GLN
1	X	329	GLN
1	X	383	GLN
1	X	423	GLN
1	X	432	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	GOL	X	507	-	5,5,5	1.01	0	5,5,5	1.76	1 (20%)
2	GOL	O	507	-	5,5,5	1.01	0	5,5,5	1.77	1 (20%)

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	GOL	X	507	-	-	0/4/4/4	-
2	GOL	O	507	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	O	507	GOL	C3-C2-C1	-3.29	99.75	111.80
2	X	507	GOL	C3-C2-C1	-3.28	99.76	111.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	O	495/505 (98%)	-0.10	21 (4%) 40 40	14, 24, 46, 79	0
1	X	495/505 (98%)	-0.08	18 (3%) 46 45	15, 23, 46, 71	0
All	All	990/1010 (98%)	-0.09	39 (3%) 43 43	14, 23, 46, 79	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	461	LEU	7.5
1	O	461	LEU	7.1
1	O	462	LYS	6.4
1	X	469	GLN	4.9
1	X	285	ASN	4.8
1	O	463	SER	4.7
1	X	399	ASP	4.6
1	X	467	GLU	4.3
1	X	468	GLY	4.2
1	X	282	LEU	4.1
1	O	467	GLU	4.0
1	O	283	SER	3.9
1	O	285	ASN	3.9
1	O	458	LEU	3.9
1	X	284	ASP	3.8
1	X	234	TYR	3.8
1	O	402	ILE	3.6
1	O	465	ALA	3.4
1	O	499	PHE	3.4
1	O	284	ASP	3.4
1	O	464	MET	3.2
1	X	402	ILE	3.2
1	O	400	SER	3.1
1	O	457	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	O	466	GLU	3.0
1	X	435	ALA	2.9
1	X	281	GLN	2.9
1	O	234	TYR	2.9
1	O	459	ASP	2.8
1	O	468	GLY	2.9
1	O	398	LYS	2.8
1	X	401	GLY	2.7
1	O	435	ALA	2.7
1	X	438	GLU	2.5
1	X	462	LYS	2.3
1	X	465	ALA	2.2
1	O	460	GLU	2.2
1	X	283	SER	2.1
1	X	329	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	X	507	6/6	0.93	0.07	15,16,18,18	0
2	GOL	O	507	6/6	0.97	0.06	15,16,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.