



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:26 PM UTC

PDB ID : 4LUS / pdb_00004lus
Title : alanine racemase [Clostridium difficile 630]
Authors : Asojo, O.A.
Deposited on : 2013-07-25
Resolution : 2.10 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

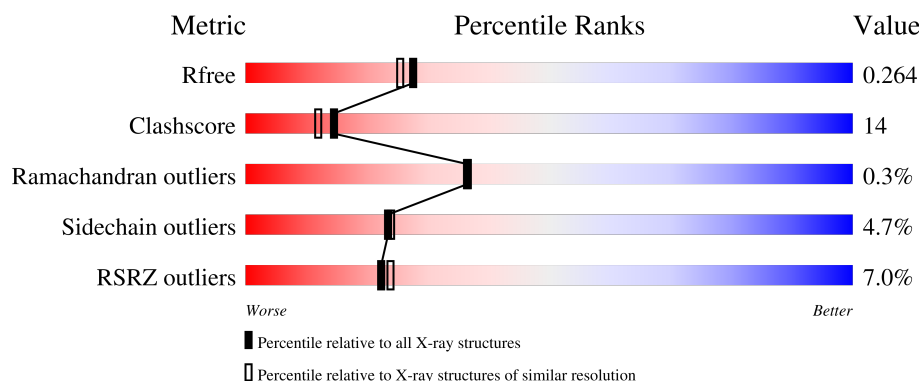
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	385	2% 45% 42% 6% 6%
1	C	385	10% 54% 36% 9% .
1	D	385	11% 55% 36% 7% ..
2	B	385	4% 51% 39% 7% .

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
3	GOL	A	401	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12484 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.

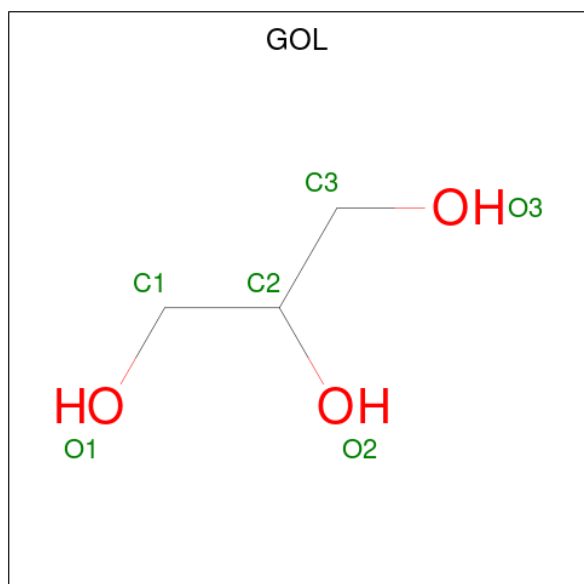
- Molecule 1 is a protein called Alanine racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	P	S	0	0	0
			2880	1828	481	554	1	16			
1	C	382	Total	C	N	O	P	S	0	0	0
			3029	1923	504	585	1	16			
1	D	380	Total	C	N	O	P	S	0	0	0
			3013	1912	501	583	1	16			

- Molecule 2 is a protein called Alanine racemase.

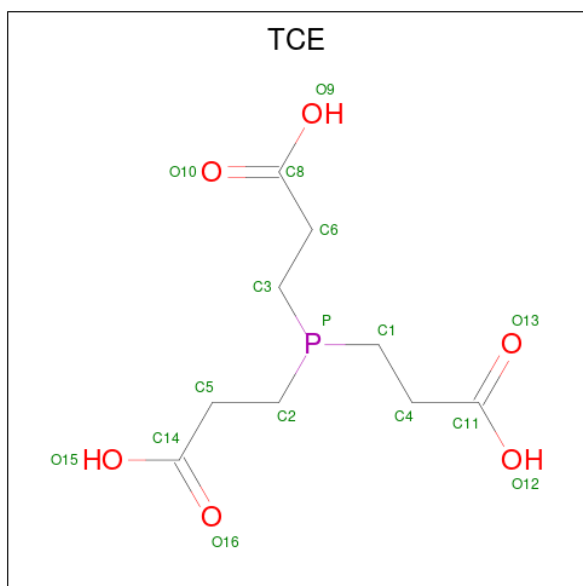
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	374	Total	C	N	O	P	S	0	1	0
			2972	1888	493	575	1	15			

- 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		

- Molecule 4 is 3,3',3''-phosphanetriyltripropanoic acid (CCD ID: TCE) (formula: $C_9H_{15}O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			16	9	6	1		

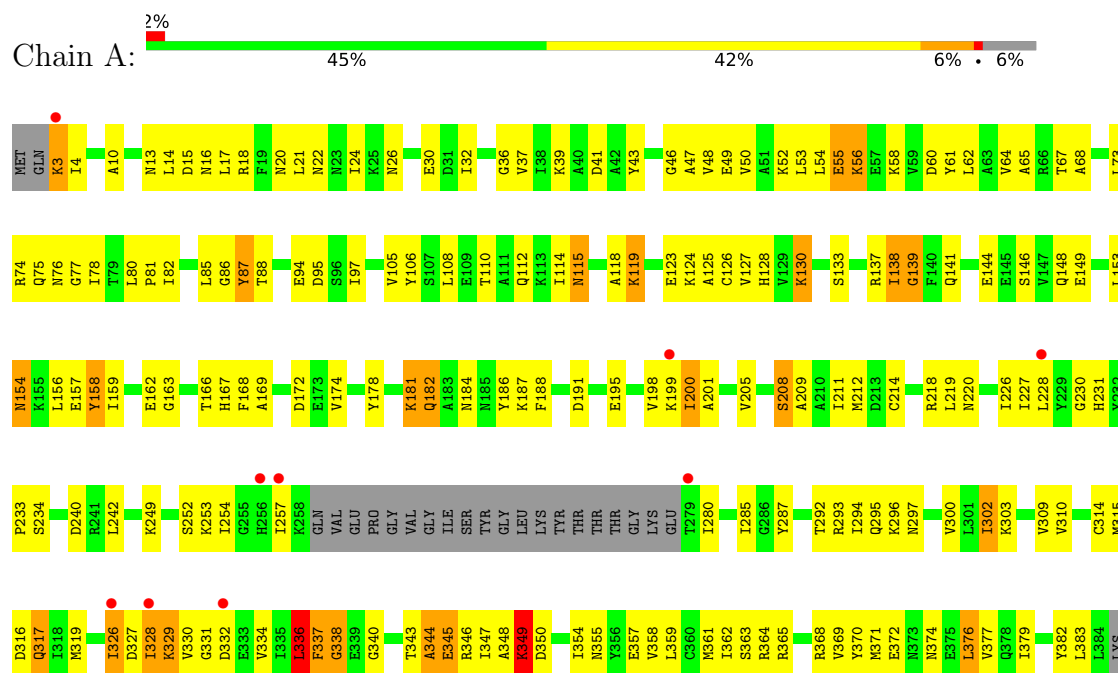
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	186	Total	O	0	0
			186	186		
5	B	150	Total	O	0	0
			150	150		
5	C	125	Total	O	0	0
			125	125		
5	D	107	Total	O	0	0
			107	107		

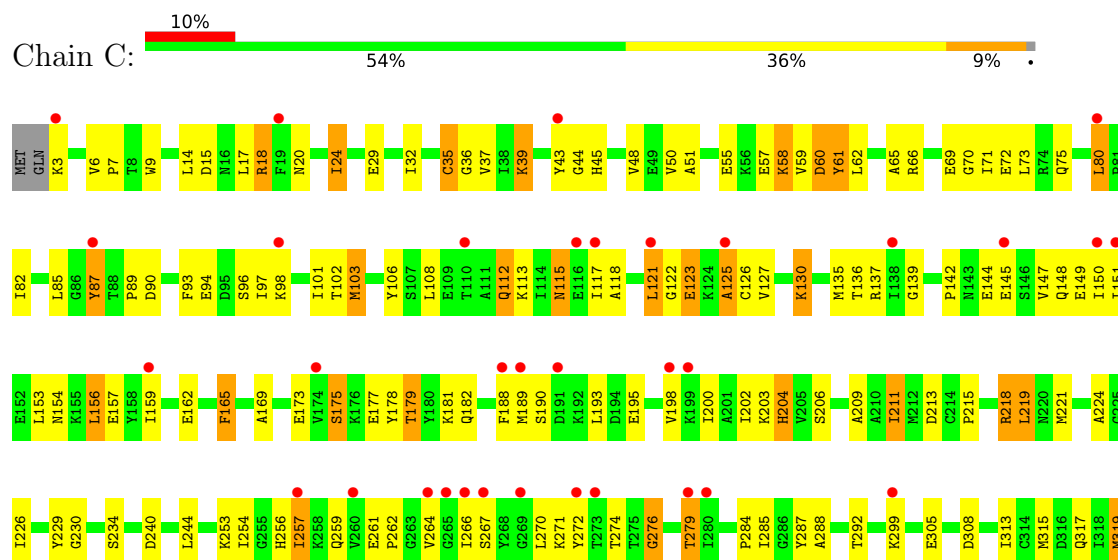
3 Residue-property plots

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: Alanine racemase

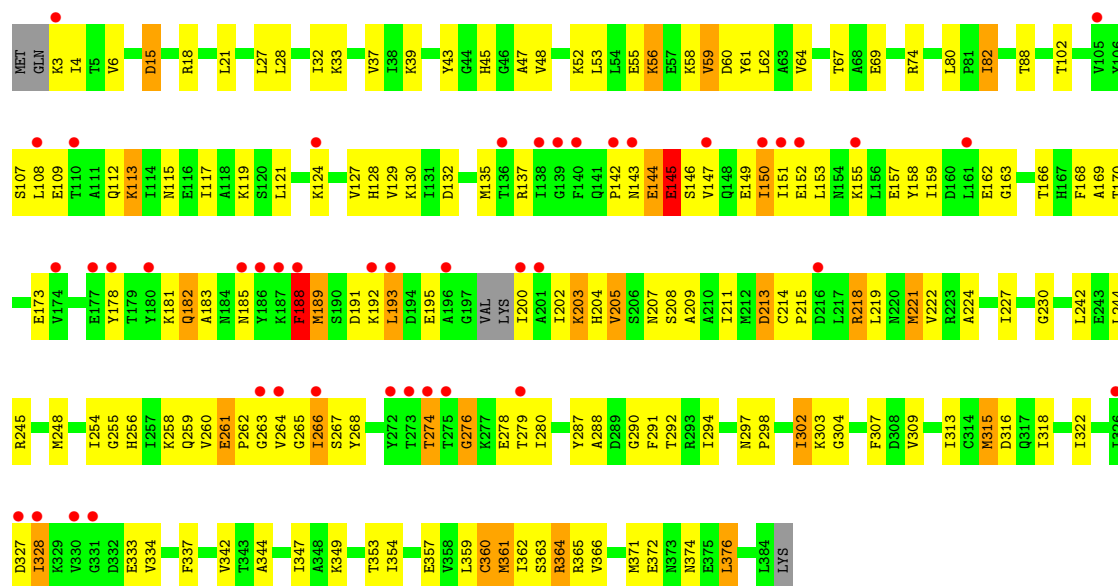


• Molecule 1: Alanine racemase

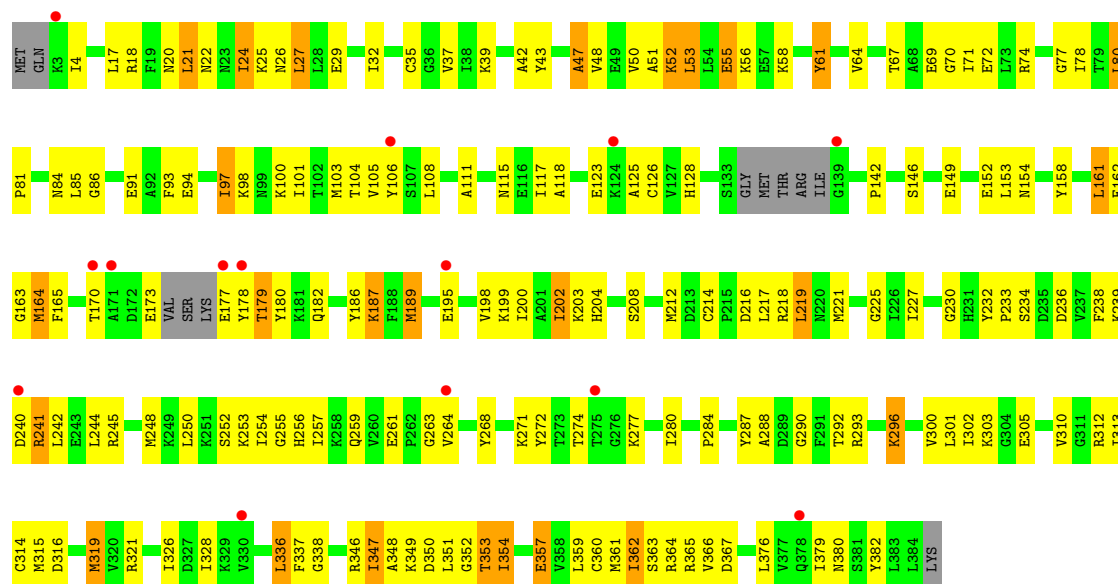




• Molecule 1: Alanine racemase



• Molecule 2: Alanine racemase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.15Å 93.30Å 107.09Å 90.00° 91.00° 90.00°	Depositor
Resolution (Å)	54.54 – 2.10 54.54 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.1 (54.54-2.10) 95.1 (54.54-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.41 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.202 , 0.266 0.215 , 0.264	Depositor DCC
R_{free} test set	4555 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12484	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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: KCX, GOL, TCE, LLP

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	2.24	149/2881 (5.2%)	1.30	19/3883 (0.5%)
1	C	1.98	67/3034 (2.2%)	1.25	21/4092 (0.5%)
1	D	1.93	64/3017 (2.1%)	1.27	23/4068 (0.6%)
2	B	2.04	98/2988 (3.3%)	1.28	29/4029 (0.7%)
All	All	2.05	378/11920 (3.2%)	1.28	92/16072 (0.6%)

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	2
2	B	0	2
All	All	0	4

All (378) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	362	ILE	C-O	-10.06	1.14	1.24
1	A	85	LEU	C-O	-9.61	1.12	1.24
1	A	78	ILE	C-O	-8.24	1.15	1.24
1	A	186	TYR	C-O	-8.19	1.14	1.24
2	B	51	ALA	C-O	-8.14	1.14	1.24
2	B	219	LEU	C-N	-7.99	1.22	1.33
1	A	105	VAL	C-O	-7.76	1.16	1.24
1	A	359	LEU	C-O	-7.69	1.15	1.24
1	C	82	ILE	C-O	-7.64	1.16	1.24
1	A	157	GLU	C-O	-7.50	1.15	1.24
1	D	3	LYS	C-N	-7.49	1.24	1.33
1	A	74	ARG	C-O	-7.37	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	37	VAL	C-O	-7.30	1.15	1.23
1	A	55	GLU	C-O	-7.16	1.15	1.24
2	B	350	ASP	C-O	-7.00	1.16	1.24
1	D	69	GLU	C-O	-6.93	1.16	1.24
1	D	292	THR	C-O	-6.92	1.15	1.23
2	B	314	CYS	C-O	-6.89	1.14	1.23
1	A	167	HIS	C-O	-6.87	1.16	1.24
1	A	226	ILE	C-O	-6.83	1.15	1.24
2	B	105	VAL	C-O	-6.81	1.17	1.24
1	C	50	VAL	C-O	-6.79	1.16	1.24
1	D	334	VAL	C-O	-6.79	1.17	1.24
1	C	363	SER	CA-C	-6.77	1.44	1.53
1	A	315	MET	C-O	-6.75	1.16	1.24
1	A	334	VAL	C-O	-6.74	1.16	1.24
1	A	358	VAL	C-O	-6.74	1.16	1.24
1	A	364	ARG	C-O	-6.72	1.16	1.24
1	A	377	VAL	C-O	-6.71	1.17	1.24
1	A	230	GLY	C-O	-6.66	1.15	1.24
1	A	344	ALA	C-O	-6.66	1.16	1.24
2	B	302	ILE	C-O	-6.66	1.16	1.24
1	A	361	MET	C-O	-6.64	1.15	1.24
2	B	348	ALA	C-O	-6.63	1.16	1.24
1	A	21	LEU	C-O	-6.62	1.16	1.24
1	A	65	ALA	C-O	-6.62	1.15	1.24
1	A	357	GLU	C-O	-6.59	1.16	1.24
2	B	254	ILE	C-O	-6.57	1.17	1.24
1	A	82	ILE	C-O	-6.56	1.17	1.24
1	D	364	ARG	C-O	-6.56	1.16	1.24
1	A	88	THR	C-O	-6.53	1.17	1.24
1	C	359	LEU	C-O	-6.53	1.16	1.24
1	A	249	LYS	C-O	-6.52	1.16	1.24
2	B	85	LEU	C-O	-6.50	1.16	1.24
1	D	362	ILE	C-O	-6.50	1.17	1.24
1	A	17	LEU	C-O	-6.49	1.16	1.24
1	A	296	LYS	C-O	-6.47	1.15	1.24
1	A	15	ASP	C-O	-6.46	1.16	1.24
1	A	209	ALA	C-O	-6.46	1.16	1.24
2	B	233	PRO	C-O	-6.44	1.16	1.24
1	A	64	VAL	C-O	-6.44	1.15	1.23
1	C	287	TYR	C-O	-6.41	1.16	1.24
1	D	102	THR	C-O	-6.39	1.16	1.23
2	B	288	ALA	C-O	-6.37	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	221	MET	C-O	-6.36	1.16	1.23
1	A	128	HIS	C-O	-6.32	1.16	1.24
2	B	104	THR	C-O	-6.32	1.16	1.23
2	B	280	ILE	C-O	-6.31	1.17	1.24
1	C	375	GLU	C-O	-6.30	1.16	1.23
1	D	67	THR	C-O	-6.30	1.16	1.24
1	C	44	GLY	C-O	-6.30	1.15	1.24
1	A	172	ASP	C-O	-6.29	1.15	1.24
2	B	364	ARG	C-O	-6.27	1.16	1.24
1	A	292	THR	C-O	-6.25	1.16	1.23
1	A	349	LYS	C-O	-6.25	1.16	1.24
1	A	4	ILE	C-O	-6.25	1.17	1.24
1	A	345	GLU	C-O	-6.22	1.16	1.24
1	A	212	MET	C-O	-6.20	1.17	1.24
1	D	333	GLU	C-O	-6.18	1.16	1.23
1	A	218	ARG	C-O	-6.17	1.17	1.24
2	B	354	ILE	C-O	-6.17	1.16	1.23
2	B	315	MET	C-O	-6.17	1.16	1.24
1	A	346	ARG	C-O	-6.17	1.17	1.24
1	C	376	LEU	C-O	-6.16	1.16	1.24
2	B	22	ASN	C-O	-6.15	1.17	1.24
2	B	230	GLY	C-O	-6.15	1.15	1.24
1	A	355	ASN	C-O	-6.14	1.16	1.24
2	B	97	ILE	C-O	-6.13	1.17	1.24
2	B	18	ARG	C-O	-6.12	1.17	1.24
1	C	14	LEU	C-O	-6.11	1.17	1.24
1	D	290	GLY	C-O	-6.08	1.16	1.24
2	B	268	TYR	C-O	-6.08	1.16	1.23
1	D	209	ALA	C-O	-6.07	1.17	1.24
2	B	21	LEU	C-O	-6.07	1.17	1.24
2	B	208	SER	C-O	-6.07	1.17	1.24
1	C	362	ILE	C-O	-6.07	1.17	1.24
1	A	337	PHE	C-O	-6.07	1.16	1.23
1	A	181	LYS	C-O	-6.04	1.17	1.24
1	A	242	LEU	C-O	-6.04	1.17	1.24
2	B	50	VAL	C-O	-6.04	1.17	1.24
2	B	103	MET	C-O	-6.03	1.16	1.24
2	B	360	CYS	C-O	-6.03	1.16	1.24
1	A	205	VAL	C-O	-6.00	1.17	1.24
2	B	101	ILE	C-O	-5.99	1.17	1.24
1	A	119	LYS	C-O	-5.98	1.17	1.24
2	B	117	ILE	C-O	-5.98	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	245	ARG	C-O	-5.97	1.18	1.24
1	C	358	VAL	C-O	-5.96	1.17	1.24
1	A	146	SER	C-O	-5.96	1.17	1.24
1	D	287	TYR	C-O	-5.96	1.16	1.24
1	A	114	ILE	C-O	-5.96	1.17	1.24
1	D	291	PHE	C-O	-5.95	1.16	1.23
1	C	226	ILE	C-O	-5.93	1.17	1.24
1	A	126	CYS	C-O	-5.92	1.16	1.24
1	D	344	ALA	C-O	-5.92	1.17	1.24
1	A	118	ALA	C-O	-5.92	1.17	1.24
1	A	97	ILE	C-O	-5.92	1.17	1.24
1	A	18	ARG	C-O	-5.90	1.17	1.24
1	A	48	VAL	C-O	-5.90	1.17	1.24
2	B	252	SER	C-O	-5.90	1.17	1.24
1	C	364	ARG	C-O	-5.90	1.17	1.24
1	A	369	VAL	C-O	-5.89	1.17	1.24
1	A	94	GLU	C-O	-5.89	1.17	1.24
1	C	15	ASP	C-O	-5.88	1.17	1.24
1	A	86	GLY	C-O	-5.87	1.16	1.23
1	C	126	CYS	C-O	-5.87	1.16	1.23
1	A	187	LYS	C-O	-5.86	1.17	1.24
1	A	73	LEU	C-O	-5.85	1.17	1.24
1	C	288	ALA	C-O	-5.84	1.16	1.24
1	D	261	GLU	CA-C	-5.83	1.45	1.53
2	B	248	MET	C-O	-5.82	1.17	1.24
1	A	293	ARG	C-O	-5.81	1.16	1.24
1	D	52	LYS	C-O	-5.81	1.17	1.24
2	B	162	GLU	C-O	-5.81	1.17	1.24
1	D	82	ILE	C-O	-5.80	1.18	1.24
2	B	163	GLY	C-O	-5.80	1.15	1.23
1	A	95	ASP	C-O	-5.79	1.16	1.24
1	D	372	GLU	C-O	-5.79	1.17	1.23
1	C	202	ILE	C-O	-5.78	1.17	1.24
1	A	37	VAL	C-O	-5.77	1.17	1.23
1	D	242	LEU	C-O	-5.77	1.17	1.24
1	C	102	THR	C-O	-5.76	1.16	1.23
1	C	337	PHE	C-O	-5.76	1.17	1.23
1	D	53	LEU	C-O	-5.75	1.17	1.24
1	A	184	ASN	C-O	-5.74	1.17	1.24
1	A	75	GLN	C-O	-5.73	1.16	1.24
1	A	254	ILE	C-O	-5.72	1.18	1.24
1	A	46	GLY	C-O	-5.71	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	48	VAL	C-O	-5.71	1.17	1.24
1	A	383	LEU	C-O	-5.70	1.16	1.24
2	B	204	HIS	C-O	-5.70	1.17	1.23
1	A	22	ASN	C-O	-5.70	1.17	1.24
1	A	252	SER	C-O	-5.70	1.17	1.24
1	C	51	ALA	C-O	-5.69	1.17	1.24
1	A	182	GLN	C-O	-5.69	1.17	1.24
1	A	354	ILE	C-O	-5.68	1.17	1.23
1	D	342	VAL	C-O	-5.68	1.18	1.24
2	B	24	ILE	C-O	-5.68	1.17	1.24
2	B	365	ARG	C-O	-5.68	1.16	1.24
1	A	287	TYR	C-O	-5.67	1.17	1.24
2	B	362	ILE	C-O	-5.66	1.18	1.24
1	C	367	ASP	C-O	-5.66	1.16	1.23
1	A	16	ASN	C-O	-5.66	1.17	1.24
1	A	43	TYR	C-O	-5.65	1.16	1.23
2	B	72	GLU	C-O	-5.64	1.17	1.24
2	B	353	THR	C-O	-5.64	1.18	1.24
2	B	202	ILE	C-O	-5.63	1.17	1.24
1	D	168	PHE	C-O	-5.63	1.16	1.23
1	A	220	ASN	C-O	-5.63	1.17	1.24
2	B	86	GLY	C-O	-5.63	1.18	1.23
2	B	379	ILE	C-O	-5.63	1.18	1.24
1	A	191	ASP	C-O	-5.62	1.17	1.24
1	D	163	GLY	C-O	-5.62	1.18	1.23
1	D	6	VAL	C-O	-5.62	1.17	1.24
1	D	88	THR	C-O	-5.62	1.16	1.24
1	A	50	VAL	C-O	-5.61	1.17	1.24
1	A	234	SER	C-O	-5.61	1.17	1.23
2	B	234	SER	C-O	-5.60	1.17	1.23
1	D	365	ARG	C-O	-5.60	1.16	1.24
2	B	111	ALA	C-O	-5.59	1.17	1.24
1	A	10	ALA	C-O	-5.59	1.17	1.24
1	A	219	LEU	C-O	-5.59	1.17	1.24
1	A	233	PRO	C-O	-5.58	1.17	1.24
1	C	73	LEU	C-O	-5.58	1.17	1.24
1	C	66	ARG	C-O	-5.57	1.16	1.23
1	D	182	GLN	C-O	-5.57	1.17	1.24
1	A	302	ILE	C-O	-5.57	1.18	1.24
2	B	257	ILE	C-O	-5.56	1.18	1.24
2	B	337	PHE	C-O	-5.56	1.17	1.23
1	A	115	ASN	C-O	-5.56	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	313	ILE	C-O	-5.56	1.18	1.24
1	D	62	LEU	C-O	-5.56	1.17	1.23
2	B	17	LEU	C-O	-5.55	1.17	1.24
2	B	55	GLU	C-O	-5.54	1.17	1.24
2	B	126	CYS	C-O	-5.54	1.17	1.24
1	D	224	ALA	C-O	-5.54	1.17	1.24
1	A	68	ALA	C-O	-5.54	1.17	1.24
1	A	87	TYR	C-O	-5.54	1.17	1.23
1	A	294	ILE	C-O	-5.54	1.16	1.24
1	C	65	ALA	C-O	-5.54	1.17	1.24
2	B	287	TYR	C-O	-5.53	1.17	1.24
1	A	124	LYS	C-O	-5.53	1.17	1.23
1	C	224	ALA	C-O	-5.53	1.17	1.24
1	D	21	LEU	C-O	-5.52	1.17	1.24
1	A	67	THR	C-O	-5.52	1.17	1.24
1	A	49	GLU	C-O	-5.52	1.17	1.24
2	B	256	HIS	C-O	-5.52	1.17	1.23
1	D	43	TYR	C-O	-5.52	1.16	1.23
1	A	163	GLY	C-O	-5.51	1.17	1.24
1	D	45	HIS	C-O	-5.51	1.16	1.24
2	B	67	THR	C-O	-5.51	1.17	1.24
1	A	365	ARG	C-O	-5.51	1.17	1.24
1	C	372	GLU	C-O	-5.51	1.17	1.23
1	D	48	VAL	C-O	-5.51	1.18	1.24
1	D	366	VAL	C-O	-5.50	1.16	1.23
1	A	211	ILE	C-O	-5.50	1.18	1.24
1	A	127	VAL	C-O	-5.49	1.18	1.24
2	B	78	ILE	C-O	-5.49	1.18	1.24
1	C	209	ALA	C-O	-5.49	1.17	1.24
1	A	125	ALA	C-O	-5.48	1.17	1.24
1	A	149	GLU	C-O	-5.48	1.17	1.24
2	B	357	GLU	C-O	-5.48	1.17	1.24
1	C	353	THR	C-O	-5.48	1.17	1.24
1	A	200	ILE	C-O	-5.47	1.17	1.24
2	B	376	LEU	C-O	-5.47	1.17	1.24
1	C	48	VAL	N-CA	-5.47	1.40	1.46
1	A	36	GLY	C-O	-5.47	1.16	1.23
1	C	204	HIS	C-O	-5.46	1.17	1.23
1	A	240	ASP	C-O	-5.46	1.17	1.24
1	C	80	LEU	C-N	5.45	1.40	1.33
1	D	203	LYS	C-O	-5.45	1.17	1.24
1	C	371	MET	C-O	-5.44	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	347	ILE	C-O	-5.43	1.17	1.24
1	A	348	ALA	C-O	-5.43	1.17	1.24
1	A	54	LEU	C-O	-5.43	1.17	1.24
1	A	328	ILE	CA-C	-5.42	1.47	1.53
2	B	165	PHE	C-O	-5.42	1.16	1.23
1	C	211	ILE	C-O	-5.42	1.18	1.24
1	C	344	ALA	C-O	-5.41	1.17	1.24
2	B	366	VAL	C-O	-5.41	1.15	1.23
1	D	315	MET	C-O	-5.40	1.17	1.24
2	B	347	ILE	C-O	-5.40	1.17	1.24
1	C	101	ILE	C-O	-5.40	1.18	1.24
1	A	153	LEU	C-O	-5.39	1.17	1.24
2	B	250	LEU	C-O	-5.38	1.17	1.24
2	B	77	GLY	C-O	-5.38	1.17	1.24
2	B	380	ASN	C-O	-5.38	1.17	1.24
1	A	208	SER	C-O	-5.37	1.17	1.24
1	C	59	VAL	C-O	-5.37	1.18	1.23
1	D	313	ILE	C-O	-5.37	1.18	1.24
1	C	175	SER	C-O	-5.36	1.17	1.23
1	A	41	ASP	C-O	-5.36	1.16	1.23
1	C	360	CYS	C-O	-5.36	1.17	1.24
1	D	64	VAL	C-O	-5.36	1.17	1.23
2	B	70	GLY	C-O	-5.35	1.17	1.23
1	A	368	ARG	C-O	-5.34	1.17	1.24
1	D	128	HIS	C-O	-5.34	1.17	1.24
1	D	202	ILE	C-O	-5.33	1.18	1.24
1	A	372	GLU	C-O	-5.33	1.17	1.23
2	B	293	ARG	C-O	-5.33	1.17	1.24
1	A	316	ASP	C-O	-5.32	1.17	1.24
1	A	178	TYR	C-O	-5.32	1.17	1.24
1	C	165	PHE	C-O	-5.32	1.17	1.23
1	A	56	LYS	C-O	-5.32	1.18	1.24
2	B	125	ALA	C-O	-5.32	1.17	1.24
1	C	292	THR	C-O	-5.32	1.17	1.23
1	D	361	MET	C-O	-5.31	1.17	1.24
2	B	4	ILE	C-O	-5.31	1.17	1.23
1	C	45	HIS	C-O	-5.31	1.17	1.24
1	D	18	ARG	C-O	-5.31	1.18	1.24
2	B	26	ASN	C-O	-5.30	1.17	1.24
1	A	24	ILE	C-O	-5.30	1.17	1.24
1	A	228	LEU	C-O	-5.30	1.18	1.24
2	B	81	PRO	N-CD	5.30	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	36	GLY	C-O	-5.30	1.16	1.23
1	A	81	PRO	C-O	-5.30	1.17	1.23
2	B	349	LYS	C-O	-5.30	1.18	1.24
1	A	62	LEU	C-O	-5.30	1.17	1.24
1	C	313	ILE	C-O	-5.29	1.18	1.24
1	D	337	PHE	C-O	-5.29	1.17	1.23
1	A	297	ASN	C-O	-5.29	1.18	1.23
1	C	9	TRP	C-O	-5.28	1.17	1.23
1	D	113	LYS	C-O	-5.28	1.18	1.24
1	A	285	ILE	C-O	-5.28	1.18	1.24
2	B	56	LYS	C-O	-5.28	1.18	1.24
1	A	376	LEU	C-O	-5.27	1.17	1.24
1	A	148	GLN	C-O	-5.27	1.18	1.24
1	A	363	SER	C-O	-5.27	1.16	1.23
1	A	382	TYR	C-O	-5.26	1.17	1.24
1	C	339	GLU	C-O	-5.25	1.18	1.23
1	A	20	ASN	C-O	-5.25	1.18	1.24
2	B	20	ASN	C-O	-5.24	1.18	1.24
1	D	244	LEU	C-O	-5.24	1.17	1.23
1	A	141	GLN	C-O	-5.24	1.17	1.24
1	A	112	GLN	C-O	-5.24	1.18	1.24
1	A	340	GLY	C-O	-5.23	1.17	1.24
1	D	288	ALA	C-O	-5.23	1.17	1.24
1	D	359	LEU	C-O	-5.23	1.18	1.24
1	A	76	ASN	C-O	-5.23	1.17	1.24
1	A	144	GLU	C-O	-5.23	1.18	1.24
1	A	26	ASN	C-O	-5.22	1.17	1.24
1	D	230	GLY	C-O	-5.21	1.17	1.24
1	A	214	CYS	C-O	-5.21	1.18	1.24
1	C	18	ARG	C-O	-5.21	1.18	1.24
2	B	52	LYS	C-O	-5.20	1.18	1.24
2	B	255	GLY	C-O	-5.20	1.17	1.23
2	B	352	GLY	C-O	-5.20	1.17	1.23
1	A	138	ILE	C-O	-5.19	1.16	1.23
1	C	285	ILE	C-O	-5.19	1.18	1.24
1	A	159	ILE	C-O	-5.19	1.18	1.24
1	A	156	LEU	C-O	-5.19	1.17	1.23
1	C	24	ILE	C-O	-5.19	1.18	1.24
2	B	74	ARG	C-O	-5.18	1.18	1.24
1	A	154	ASN	C-O	-5.18	1.17	1.24
1	C	336	LEU	C-O	-5.17	1.18	1.24
1	D	208	SER	C-O	-5.17	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	69	GLU	C-O	-5.17	1.18	1.24
1	D	37	VAL	C-O	-5.17	1.17	1.23
2	B	346	ARG	C-O	-5.17	1.18	1.24
1	A	370	TYR	C-O	-5.16	1.17	1.24
2	B	292	THR	C-O	-5.16	1.17	1.23
1	D	222	VAL	C-O	-5.16	1.18	1.24
2	B	225	GLY	C-O	-5.16	1.17	1.23
1	C	72	GLU	C-O	-5.16	1.18	1.24
2	B	37	VAL	C-O	-5.15	1.17	1.23
1	C	230	GLY	C-O	-5.15	1.17	1.23
2	B	290	GLY	C-O	-5.15	1.17	1.24
1	C	35	CYS	C-O	-5.15	1.18	1.24
1	A	309	VAL	C-O	-5.14	1.18	1.24
1	A	338	GLY	C-O	-5.14	1.17	1.24
2	B	71	ILE	C-O	-5.14	1.17	1.24
2	B	382	TYR	C-O	-5.14	1.17	1.24
1	C	125	ALA	C-O	-5.14	1.17	1.24
1	A	13	ASN	C-O	-5.14	1.17	1.24
1	C	345	GLU	C-O	-5.14	1.18	1.24
2	B	367	ASP	C-O	-5.14	1.17	1.23
1	C	244	LEU	C-O	-5.13	1.17	1.23
1	D	318	ILE	C-O	-5.13	1.18	1.23
1	D	27	LEU	C-O	-5.13	1.17	1.24
1	D	245	ARG	C-O	-5.13	1.19	1.24
1	C	115	ASN	C-O	-5.13	1.18	1.24
1	D	349	LYS	C-O	-5.13	1.18	1.24
2	B	64	VAL	C-O	-5.13	1.17	1.23
2	B	303	LYS	C-O	-5.13	1.17	1.23
1	C	103	MET	CA-C	-5.13	1.46	1.52
1	A	52	LYS	C-O	-5.12	1.18	1.24
2	B	214	CYS	C-O	-5.12	1.18	1.24
1	D	150	ILE	N-CA	-5.10	1.40	1.46
1	A	168	PHE	C-O	-5.10	1.17	1.24
1	D	59	VAL	C-O	-5.10	1.17	1.24
1	C	69	GLU	C-O	-5.10	1.18	1.24
1	A	188	PHE	C-O	-5.10	1.18	1.24
2	B	128	HIS	C-O	-5.10	1.17	1.24
1	D	227	ILE	C-O	-5.10	1.17	1.24
2	B	296	LYS	C-O	-5.10	1.18	1.24
1	C	179	THR	C-O	-5.09	1.18	1.24
2	B	161	LEU	C-O	-5.09	1.18	1.23
1	D	376	LEU	C-O	-5.09	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	ILE	C-O	-5.08	1.18	1.24
1	C	70	GLY	C-O	-5.08	1.17	1.23
1	D	15	ASP	C-O	-5.08	1.17	1.24
2	B	47	ALA	C-O	-5.08	1.18	1.24
1	C	254	ILE	C-O	-5.08	1.18	1.24
2	B	43	TYR	C-O	-5.08	1.17	1.23
1	A	317	GLN	C-O	-5.07	1.17	1.23
1	A	14	LEU	C-O	-5.06	1.17	1.24
1	C	87	TYR	C-O	-5.06	1.17	1.23
1	D	248	MET	C-O	-5.06	1.17	1.24
1	C	200	ILE	C-O	-5.06	1.18	1.24
1	D	360	CYS	C-O	-5.06	1.17	1.24
1	A	169	ALA	C-O	-5.05	1.17	1.24
1	A	310	VAL	C-O	-5.05	1.18	1.24
2	B	242	LEU	C-O	-5.05	1.18	1.23
1	A	347	ILE	C-O	-5.05	1.18	1.24
1	A	295	GLN	C-O	-5.04	1.17	1.23
2	B	359	LEU	C-O	-5.04	1.18	1.24
1	C	234	SER	C-O	-5.04	1.17	1.23
1	A	364	ARG	CD-NE	-5.04	1.39	1.46
2	B	53	LEU	C-O	-5.03	1.18	1.24
1	A	108	LEU	C-O	-5.03	1.18	1.24
2	B	212	MET	C-O	-5.03	1.18	1.24
2	B	106	TYR	C-O	-5.03	1.17	1.23
1	C	17	LEU	C-O	-5.03	1.18	1.24
1	C	381	SER	C-O	-5.02	1.18	1.24
1	A	47	ALA	C-O	-5.01	1.18	1.24
1	A	158	TYR	C-O	-5.01	1.17	1.24
1	A	60	ASP	C-O	-5.01	1.17	1.24
1	A	319	MET	C-O	-5.00	1.18	1.24

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	276	GLY	N-CA-C	-11.44	100.52	112.08
1	A	199	LYS	N-CA-C	11.07	123.09	111.14
2	B	362	ILE	O-C-N	-10.87	111.59	122.67
1	A	3	LYS	O-C-N	-10.32	106.49	123.00
1	C	162	GLU	N-CA-C	9.58	121.80	111.36
1	A	58	LYS	N-CA-C	9.16	123.64	111.28
1	A	336	LEU	N-CA-C	8.78	120.93	111.36
2	B	199	LYS	N-CA-C	8.67	120.66	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3	LYS	CA-C-N	-8.52	111.70	122.43
1	D	3	LYS	C-N-CA	-8.52	111.70	122.43
1	D	162	GLU	N-CA-C	8.36	120.47	111.36
1	A	3	LYS	CA-C-N	8.00	132.37	122.37
1	A	3	LYS	C-N-CA	8.00	132.37	122.37
1	A	220	ASN	N-CA-C	7.81	119.87	111.36
1	D	266	ILE	N-CA-C	7.65	118.82	108.11
2	B	162	GLU	N-CA-C	7.54	119.58	111.36
1	A	363	SER	N-CA-C	7.53	119.67	110.41
2	B	165	PHE	N-CA-C	7.32	120.05	109.14
1	C	276	GLY	CA-C-O	-7.22	117.10	122.37
1	A	331	GLY	N-CA-C	7.15	130.12	113.18
2	B	179	THR	N-CA-C	-7.10	103.47	111.07
1	A	200	ILE	N-CA-C	6.98	123.86	109.34
1	D	363	SER	N-CA-C	6.98	119.53	110.53
2	B	58	LYS	N-CA-C	6.95	121.12	111.74
1	A	328	ILE	N-CA-C	-6.94	102.48	110.05
1	C	144	GLU	N-CA-C	6.94	118.84	111.28
2	B	363[A]	SER	CA-C-N	6.92	130.12	120.29
2	B	363[A]	SER	C-N-CA	6.92	130.12	120.29
2	B	363[B]	SER	CA-C-N	6.92	130.12	120.29
2	B	363[B]	SER	C-N-CA	6.92	130.12	120.29
2	B	189	MET	N-CA-C	6.92	118.62	111.14
1	C	218	ARG	N-CA-C	-6.73	101.01	110.50
2	B	236	ASP	N-CA-C	6.68	119.57	111.82
1	A	201	ALA	N-CA-C	6.59	118.54	111.36
1	D	121	LEU	N-CA-C	6.44	119.29	111.82
1	A	169	ALA	N-CA-C	6.42	119.27	111.82
2	B	254	ILE	CA-C-N	6.41	127.05	120.00
2	B	254	ILE	C-N-CA	6.41	127.05	120.00
1	A	162	GLU	N-CA-C	6.38	118.32	111.36
2	B	241	ARG	N-CA-C	6.34	118.19	111.28
2	B	310	VAL	N-CA-C	6.26	117.61	108.53
1	D	60	ASP	N-CA-C	6.23	121.07	112.90
1	C	157	GLU	N-CA-C	6.13	120.76	113.28
1	C	3	LYS	CA-C-N	6.07	129.95	122.37
1	C	3	LYS	C-N-CA	6.07	129.95	122.37
1	C	3	LYS	O-C-N	-6.05	113.32	123.00
1	D	188	PHE	N-CA-CB	-6.05	101.24	110.01
2	B	80	LEU	CA-C-N	-6.04	113.53	119.76
2	B	80	LEU	C-N-CA	-6.04	113.53	119.76
1	D	218	ARG	N-CA-C	6.01	117.83	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	255	GLY	N-CA-C	6.01	120.46	112.77
1	C	80	LEU	CA-C-N	-5.99	113.59	119.76
1	C	80	LEU	C-N-CA	-5.99	113.59	119.76
2	B	84	ASN	CA-C-N	5.98	128.89	120.28
2	B	84	ASN	C-N-CA	5.98	128.89	120.28
2	B	195	GLU	N-CA-C	-5.94	104.88	111.71
1	C	211	ILE	N-CA-C	-5.93	104.73	110.42
1	D	205	VAL	N-CA-C	5.91	119.32	113.71
1	C	165	PHE	N-CA-C	5.80	117.60	108.96
2	B	178	TYR	N-CA-C	-5.78	104.97	111.28
1	C	173	GLU	N-CA-C	-5.78	101.18	110.14
1	C	336	LEU	N-CA-C	5.74	117.62	111.36
1	C	324	LYS	CA-C-N	-5.65	115.25	122.77
1	C	324	LYS	C-N-CA	-5.65	115.25	122.77
1	D	276	GLY	N-CA-C	-5.65	101.19	110.56
1	D	183	ALA	N-CA-C	5.59	117.38	111.28
1	D	107	SER	N-CA-C	5.58	117.32	108.79
1	D	213	ASP	N-CA-C	5.53	119.29	112.54
2	B	338	GLY	N-CA-C	5.50	123.03	115.27
1	D	58	LYS	N-CA-C	5.50	119.29	112.58
1	C	213	ASP	N-CA-C	5.47	120.06	113.17
1	A	349	LYS	N-CA-C	-5.46	105.33	111.28
2	B	212	MET	N-CA-C	5.43	117.01	111.14
1	A	139	GLY	N-CA-C	5.43	118.37	112.29
2	B	240	ASP	N-CA-C	-5.40	105.50	111.71
2	B	219	LEU	O-C-N	-5.39	115.43	122.59
1	C	60	ASP	N-CA-C	5.35	119.89	112.45
1	D	144	GLU	N-CA-C	5.34	116.78	111.07
1	D	188	PHE	N-CA-C	-5.32	105.38	111.07
2	B	244	LEU	N-CA-C	5.28	117.85	109.50
1	D	152	GLU	N-CA-C	-5.24	105.57	111.28
2	B	227	ILE	N-CA-C	5.22	117.58	111.05
1	C	308	ASP	N-CA-C	5.20	117.97	110.28
1	D	145	GLU	N-CA-C	-5.17	105.64	111.28
2	B	182	GLN	N-CA-C	-5.17	105.65	111.28
1	D	47	ALA	N-CA-C	5.17	116.91	111.28
1	A	77	GLY	N-CA-C	5.15	123.01	115.08
1	C	219	LEU	N-CA-C	-5.13	99.86	110.80
1	A	168	PHE	N-CA-C	5.09	117.85	109.76
1	D	276	GLY	CA-C-O	-5.08	116.12	121.56
1	A	280	ILE	N-CA-C	5.07	115.15	107.75
1	D	204	HIS	N-CA-C	5.02	117.33	108.75

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	LYS	Peptide,Mainchain
2	B	218	ARG	Mainchain
2	B	362	ILE	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	2880	0	2926	56	0
1	C	3029	0	3076	120	0
1	D	3013	0	3052	101	0
2	B	2972	0	3010	76	0
3	A	6	0	8	17	0
4	B	16	0	12	6	0
5	A	186	0	0	5	0
5	B	150	0	0	2	0
5	C	125	0	0	6	0
5	D	107	0	0	4	0
All	All	12484	0	12084	336	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 14.

All (336) 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:C:43:TYR:CE1	1:D:315:MET:HE1	1.57	1.40
1:D:259:GLN:OE1	1:D:279:THR:HG22	1.49	1.12
2:B:264:VAL:H	2:B:274:THR:HG22	1.01	1.12
2:B:264:VAL:H	2:B:274:THR:CG2	1.61	1.11
1:C:96:SER:CB	1:C:103:MET:HE2	1.85	1.05
2:B:100:LYS:HB3	4:B:401:TCE:H2	1.38	1.05
1:A:326:ILE:HD12	1:A:327:ASP:H	1.20	1.03
1:A:343:THR:HA	3:A:401:GOL:H31	1.39	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:VAL:H	1:C:274:THR:HG22	1.19	1.02
1:D:264:VAL:H	1:D:274:THR:HG22	1.23	1.02
2:B:61:TYR:HB2	2:B:221:MET:HE1	1.40	1.01
2:B:264:VAL:N	2:B:274:THR:HG22	1.77	1.00
1:C:261:GLU:O	1:C:274:THR:HG21	1.62	0.99
2:B:347:ILE:O	2:B:351:LEU:HD23	1.60	0.99
2:B:100:LYS:HB3	4:B:401:TCE:C2	1.92	0.98
1:D:55:GLU:HG3	1:D:80:LEU:HD13	1.43	0.97
1:D:115:ASN:OD1	1:D:158:TYR:HB2	1.68	0.94
2:B:326:ILE:HD12	2:B:328:ILE:CG2	1.96	0.94
1:C:96:SER:HB2	1:C:103:MET:HE2	1.50	0.93
2:B:238:PHE:CD2	2:B:241:ARG:NH2	2.37	0.92
1:A:253:LYS:HB2	5:A:668:HOH:O	1.70	0.92
1:C:96:SER:HB2	1:C:103:MET:CE	1.98	0.91
1:C:135:MET:HG3	1:C:169:ALA:HB2	1.54	0.89
2:B:142:PRO:HA	2:B:189:MET:HE2	1.53	0.89
1:C:43:TYR:CD1	1:D:315:MET:HE1	2.06	0.89
1:D:189:MET:O	1:D:193:LEU:HD13	1.72	0.89
1:C:43:TYR:CE1	1:D:315:MET:CE	2.52	0.89
2:B:170:THR:HB	2:B:173:GLU:OE1	1.73	0.89
1:C:259:GLN:OE1	1:C:279:THR:HB	1.74	0.88
1:D:32:ILE:HD13	1:D:218:ARG:HB3	1.57	0.86
1:D:264:VAL:N	1:D:274:THR:HG22	1.93	0.84
1:C:190:SER:OG	1:C:203:LYS:NZ	2.11	0.84
1:C:153:LEU:HA	1:C:156:LEU:HD12	1.58	0.84
1:C:154:ASN:ND2	1:C:198:VAL:HG13	1.92	0.84
2:B:216:ASP:OD1	2:B:217:LEU:HG	1.79	0.83
1:A:343:THR:CA	3:A:401:GOL:H31	2.08	0.83
1:A:130:KCX:HD3	1:A:138:ILE:HG13	1.61	0.83
1:A:326:ILE:HD12	1:A:327:ASP:N	1.94	0.82
1:D:200:ILE:O	1:D:203:LYS:HE3	1.76	0.82
1:D:108:LEU:O	1:D:112:GLN:HG3	1.79	0.82
1:D:207:ASN:O	1:D:211:ILE:HG13	1.80	0.81
1:C:178:TYR:HA	1:C:181:LYS:HD2	1.62	0.81
2:B:326:ILE:HD12	2:B:328:ILE:HG23	1.64	0.79
1:A:338:GLY:HA2	3:A:401:GOL:H32	1.63	0.78
1:C:264:VAL:N	1:C:274:THR:HG22	1.97	0.78
1:C:43:TYR:HE1	1:D:315:MET:HE1	1.03	0.78
1:C:43:TYR:HE1	1:D:315:MET:CE	1.90	0.78
1:D:261:GLU:HB3	1:D:262:PRO:HD2	1.64	0.78
1:D:262:PRO:HA	1:D:274:THR:HG23	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347:ILE:O	2:B:351:LEU:CD2	2.32	0.77
1:C:96:SER:CB	1:C:103:MET:CE	2.59	0.77
1:A:110:THR:HG22	5:A:586:HOH:O	1.84	0.77
1:A:328:ILE:HD12	1:A:328:ILE:O	1.83	0.77
1:C:43:TYR:CD2	1:C:229:TYR:CE2	2.73	0.77
2:B:118:ALA:HB1	2:B:123:GLU:O	1.85	0.76
1:A:343:THR:HA	3:A:401:GOL:C3	2.16	0.76
1:C:106:TYR:HB3	1:C:139:GLY:HA2	1.68	0.75
2:B:61:TYR:HB2	2:B:221:MET:CE	2.16	0.75
1:D:302:ILE:HG13	1:D:307:PHE:HD2	1.51	0.74
1:D:55:GLU:HG3	1:D:80:LEU:CD1	2.18	0.73
1:C:43:TYR:HD2	1:C:229:TYR:CE2	2.05	0.73
1:C:113:LYS:O	1:C:117:ILE:HD13	1.88	0.73
1:A:337:PHE:HD1	3:A:401:GOL:H11	1.54	0.73
1:C:18:ARG:NH2	1:C:372:GLU:OE2	2.19	0.72
1:C:62:LEU:HD11	1:C:80:LEU:HD12	1.71	0.72
1:C:270:LEU:HD11	1:D:178:TYR:CE2	2.23	0.72
1:D:264:VAL:H	1:D:274:THR:CG2	2.00	0.71
1:C:261:GLU:O	1:C:274:THR:CG2	2.38	0.71
1:C:266:ILE:HD12	1:C:272:TYR:CD2	2.26	0.71
1:C:326:ILE:HG13	1:C:327:ASP:H	1.54	0.71
1:C:305:GLU:OE1	1:C:324:LYS:HE3	1.91	0.70
1:A:338:GLY:HA2	3:A:401:GOL:H12	1.72	0.69
1:C:106:TYR:CB	1:C:139:GLY:HA2	2.23	0.69
1:C:319:MET:CE	1:D:137:ARG:HG3	2.22	0.69
1:D:117:ILE:N	1:D:117:ILE:HD12	2.08	0.69
1:D:205:VAL:HG22	1:D:219:LEU:HD12	1.74	0.69
1:A:328:ILE:HD12	1:A:328:ILE:C	2.18	0.69
2:B:261:GLU:O	2:B:274:THR:HG21	1.93	0.68
1:D:327:ASP:OD1	1:D:328:ILE:N	2.27	0.68
2:B:100:LYS:HB3	4:B:401:TCE:H2A	1.74	0.67
1:A:30:GLU:HG3	5:A:638:HOH:O	1.95	0.67
2:B:263:GLY:N	2:B:274:THR:HG23	2.09	0.67
1:D:108:LEU:HD13	1:D:149:GLU:HB3	1.76	0.67
1:A:32:ILE:CD1	5:A:607:HOH:O	2.42	0.66
1:C:55:GLU:HG2	1:C:80:LEU:HG	1.77	0.66
1:D:261:GLU:O	1:D:274:THR:HG21	1.95	0.66
2:B:108:LEU:HB2	2:B:149:GLU:HG2	1.77	0.66
1:C:264:VAL:H	1:C:274:THR:CG2	2.02	0.66
1:C:319:MET:HE1	1:D:137:ARG:HG3	1.77	0.66
1:C:115:ASN:HD22	1:C:156:LEU:HB3	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:GLY:CA	3:A:401:GOL:H32	2.25	0.65
1:C:118:ALA:HB1	1:C:123:GLU:O	1.96	0.65
1:D:185:ASN:O	1:D:188:PHE:HB3	1.96	0.65
2:B:326:ILE:HD12	2:B:328:ILE:HG21	1.77	0.65
1:C:279:THR:HG23	1:C:322:ILE:O	1.97	0.65
1:C:315:MET:HE2	1:D:360:CYS:SG	2.37	0.65
1:D:135:MET:HG3	1:D:169:ALA:HB2	1.79	0.65
2:B:326:ILE:CD1	2:B:328:ILE:CG2	2.72	0.64
2:B:100:LYS:HD3	4:B:401:TCE:H2A	1.79	0.64
1:D:327:ASP:O	1:D:328:ILE:HG23	1.97	0.64
1:D:149:GLU:O	1:D:153:LEU:HB2	1.98	0.63
1:A:329:LYS:HG3	1:A:330:VAL:O	1.99	0.62
1:C:165:PHE:HB2	1:C:204:HIS:O	1.99	0.62
1:D:200:ILE:HB	1:D:203:LYS:HE2	1.79	0.62
1:C:262:PRO:HA	1:C:274:THR:HG23	1.81	0.62
2:B:326:ILE:CD1	2:B:328:ILE:HG21	2.30	0.62
1:D:149:GLU:O	1:D:153:LEU:N	2.33	0.62
1:A:343:THR:CB	3:A:401:GOL:H31	2.29	0.61
1:D:276:GLY:O	1:D:278:GLU:HG3	2.00	0.61
1:A:326:ILE:CD1	1:A:327:ASP:H	2.06	0.60
1:C:20:ASN:O	1:C:24:ILE:HD12	2.01	0.60
1:D:193:LEU:N	1:D:193:LEU:HD12	2.17	0.60
1:A:338:GLY:HA2	3:A:401:GOL:C1	2.31	0.60
1:D:33:LYS:HB2	1:D:221:MET:HB2	1.84	0.60
1:D:193:LEU:N	1:D:193:LEU:CD1	2.65	0.59
1:D:170:THR:O	1:D:173:GLU:HB2	2.02	0.59
2:B:238:PHE:O	2:B:241:ARG:HB2	2.03	0.59
2:B:21:LEU:HG	2:B:25:LYS:HE3	1.85	0.58
2:B:29:GLU:O	2:B:32:ILE:HD12	2.02	0.58
1:C:71:ILE:O	1:C:75:GLN:HG3	2.01	0.58
1:A:106:TYR:HB3	1:A:139:GLY:HA2	1.86	0.58
1:C:203:LYS:HB3	1:C:219:LEU:HD23	1.85	0.58
2:B:264:VAL:N	2:B:274:THR:CG2	2.46	0.58
1:D:302:ILE:HG13	1:D:307:PHE:CD2	2.37	0.58
1:C:115:ASN:HD22	1:C:159:ILE:HG12	1.68	0.57
1:A:137:ARG:HA	2:B:319:MET:HE3	1.85	0.57
1:C:87:TYR:OH	1:C:89:PRO:HB3	2.04	0.57
1:D:191:ASP:HA	5:D:503:HOH:O	2.03	0.57
1:D:113:LYS:O	1:D:117:ILE:HD13	2.04	0.57
1:D:192:LYS:O	1:D:195:GLU:HB2	2.04	0.57
1:D:371:MET:SD	1:D:376:LEU:HA	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:GLY:HA2	3:A:401:GOL:C3	2.33	0.57
1:D:279:THR:OG1	1:D:322:ILE:HB	2.05	0.57
1:D:200:ILE:HB	1:D:203:LYS:CE	2.35	0.57
2:B:177:GLU:HG2	2:B:179:THR:HB	1.87	0.56
1:C:266:ILE:HD12	1:C:272:TYR:HD2	1.69	0.56
1:C:369:VAL:HG12	1:C:371:MET:HE3	1.86	0.56
2:B:238:PHE:CE2	2:B:241:ARG:NH2	2.74	0.56
1:C:94:GLU:HG3	1:C:98:LYS:HE3	1.88	0.56
1:C:61:TYR:HB2	1:C:221:MET:HE1	1.88	0.55
1:C:87:TYR:CZ	1:C:89:PRO:HB3	2.41	0.55
1:C:90:ASP:HA	1:C:93:PHE:CE2	2.41	0.55
1:C:253:LYS:HE3	5:C:457:HOH:O	2.05	0.55
1:A:231:HIS:HD2	1:A:345:GLU:OE2	1.89	0.55
1:C:93:PHE:HA	1:C:103:MET:HE1	1.88	0.55
1:D:145:GLU:O	1:D:149:GLU:HG3	2.05	0.55
1:D:188:PHE:HD1	1:D:188:PHE:C	2.14	0.55
2:B:357:GLU:O	2:B:361:MET:HG3	2.07	0.54
1:A:302:ILE:HG23	1:A:332:ASP:OD2	2.07	0.54
1:C:371:MET:HE1	1:C:376:LEU:CB	2.37	0.54
2:B:154:ASN:ND2	2:B:198:VAL:HG13	2.23	0.54
2:B:271:LYS:HE3	2:B:312:ARG:NH1	2.22	0.54
1:D:188:PHE:C	1:D:188:PHE:CD1	2.85	0.54
1:C:61:TYR:HB2	1:C:221:MET:CE	2.38	0.54
1:C:371:MET:CE	1:C:376:LEU:HA	2.38	0.53
1:C:43:TYR:CD2	1:C:229:TYR:HE2	2.27	0.53
1:C:169:ALA:H	1:C:182:GLN:HE22	1.56	0.53
1:C:61:TYR:CD2	1:C:221:MET:HE1	2.44	0.53
1:C:94:GLU:OE1	1:C:98:LYS:NZ	2.32	0.53
1:A:344:ALA:H	3:A:401:GOL:C2	2.22	0.52
1:D:259:GLN:OE1	1:D:279:THR:CG2	2.41	0.52
1:C:96:SER:HB3	1:C:103:MET:HE2	1.85	0.52
1:D:15:ASP:HB2	5:D:457:HOH:O	2.09	0.52
1:D:117:ILE:N	1:D:117:ILE:CD1	2.73	0.52
1:D:264:VAL:HG12	1:D:265:GLY:N	2.24	0.52
2:B:238:PHE:CD2	2:B:241:ARG:CZ	2.93	0.52
1:A:231:HIS:HE1	5:A:513:HOH:O	1.93	0.52
1:A:343:THR:HB	3:A:401:GOL:H31	1.90	0.52
1:C:39:LLP:HD2	1:C:85:LEU:HD12	1.92	0.52
1:C:136:THR:HG21	1:D:266:ILE:HG12	1.92	0.52
2:B:100:LYS:CB	4:B:401:TCE:H2	2.26	0.51
1:C:190:SER:HG	1:C:203:LYS:HZ3	1.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ILE:CD1	1:A:327:ASP:N	2.71	0.51
1:D:151:ILE:O	1:D:155:LYS:HG3	2.10	0.51
1:D:147:VAL:HG13	1:D:193:LEU:HD11	1.93	0.51
1:D:328:ILE:N	1:D:328:ILE:HD12	2.25	0.51
1:C:204:HIS:HB3	1:C:221:MET:HB3	1.93	0.51
1:D:353:THR:OG1	1:D:354:ILE:N	2.44	0.50
1:A:300:VAL:HG12	1:A:336:LEU:HD13	1.94	0.50
2:B:35:CYS:HB2	2:B:221:MET:HE2	1.93	0.50
1:A:349:LYS:HE3	1:A:350:ASP:HB2	1.93	0.50
1:D:147:VAL:HG13	1:D:193:LEU:CD1	2.42	0.50
1:D:74:ARG:CZ	1:D:82:ILE:HD12	2.43	0.49
2:B:326:ILE:CD1	2:B:328:ILE:HG23	2.36	0.49
1:C:61:TYR:HD2	1:C:221:MET:HE1	1.78	0.49
1:C:115:ASN:ND2	1:C:156:LEU:HB3	2.25	0.49
1:D:115:ASN:O	1:D:119:LYS:N	2.37	0.49
2:B:180:TYR:HE1	2:B:216:ASP:OD2	1.95	0.49
1:D:109:GLU:HG2	1:D:113:LYS:HZ1	1.77	0.49
1:D:109:GLU:CG	1:D:113:LYS:NZ	2.76	0.49
1:A:115:ASN:OD1	1:A:158:TYR:HB2	2.12	0.49
2:B:24:ILE:O	2:B:27:LEU:HB2	2.13	0.49
1:D:267:SER:OG	1:D:268:TYR:N	2.39	0.49
1:D:294:ILE:O	1:D:294:ILE:HG22	2.13	0.48
1:A:338:GLY:N	3:A:401:GOL:H32	2.28	0.48
1:C:326:ILE:CG1	1:C:327:ASP:H	2.22	0.48
1:A:328:ILE:C	1:A:328:ILE:CD1	2.87	0.48
1:A:374:ASN:HB2	1:D:374:ASN:HD21	1.77	0.48
1:C:357:GLU:O	1:C:361:MET:HG3	2.13	0.48
1:C:364:ARG:NH2	5:C:469:HOH:O	2.45	0.48
1:A:338:GLY:H	3:A:401:GOL:H32	1.77	0.48
1:A:119:LYS:HA	1:A:158:TYR:CD2	2.49	0.48
2:B:161:LEU:HG	2:B:161:LEU:O	2.12	0.48
1:D:150:ILE:O	1:D:153:LEU:HB3	2.14	0.48
1:D:55:GLU:CG	1:D:80:LEU:HD13	2.31	0.48
1:D:178:TYR:O	1:D:182:GLN:HG3	2.13	0.48
1:A:338:GLY:CA	3:A:401:GOL:C1	2.91	0.48
2:B:180:TYR:CE1	2:B:216:ASP:OD2	2.67	0.48
2:B:153:LEU:C	2:B:153:LEU:HD23	2.38	0.48
1:C:371:MET:HE2	1:C:376:LEU:HA	1.96	0.48
2:B:272:TYR:OH	2:B:321:ARG:NH1	2.44	0.47
2:B:21:LEU:CG	2:B:25:LYS:HE3	2.44	0.47
1:C:256:HIS:C	1:C:257:ILE:HG13	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:LYS:HD2	5:C:475:HOH:O	2.14	0.47
1:A:133:SER:O	1:A:182:GLN:HG2	2.15	0.47
1:C:35:CYS:HA	1:C:61:TYR:O	2.15	0.47
1:C:87:TYR:CE2	1:C:89:PRO:HB3	2.50	0.47
1:C:203:LYS:CB	1:C:219:LEU:HD23	2.43	0.47
1:C:326:ILE:CG1	1:C:327:ASP:N	2.78	0.47
1:A:137:ARG:CA	2:B:319:MET:HE3	2.44	0.47
1:C:190:SER:HG	1:C:203:LYS:NZ	2.08	0.47
1:C:266:ILE:HD12	1:C:272:TYR:CE2	2.50	0.47
1:C:43:TYR:CD1	1:D:315:MET:CE	2.90	0.47
1:A:55:GLU:HG2	1:A:80:LEU:HG	1.97	0.47
1:C:165:PHE:CB	1:C:204:HIS:O	2.62	0.47
1:D:200:ILE:HG22	1:D:203:LYS:HG3	1.97	0.47
1:A:303:LYS:HE2	1:A:332:ASP:OD1	2.15	0.46
1:A:87:TYR:CD2	2:B:284:PRO:HG3	2.51	0.46
1:C:6:VAL:HB	1:C:7:PRO:HD2	1.96	0.46
1:C:371:MET:HE1	1:C:376:LEU:CG	2.45	0.46
1:D:364:ARG:NH1	5:D:474:HOH:O	2.49	0.46
1:A:257:ILE:HD13	1:A:328:ILE:CD1	2.45	0.46
1:C:142:PRO:HA	1:C:189:MET:SD	2.55	0.46
1:C:188:PHE:CD1	1:C:188:PHE:C	2.93	0.46
1:C:55:GLU:HG2	1:C:80:LEU:CG	2.43	0.46
1:C:218:ARG:C	1:C:219:LEU:HD12	2.41	0.46
1:C:253:LYS:O	1:C:284:PRO:HD2	2.15	0.46
1:A:106:TYR:CB	1:A:139:GLY:HA2	2.46	0.46
1:A:154:ASN:ND2	1:A:198:VAL:HG13	2.31	0.46
2:B:55:GLU:HG3	2:B:80:LEU:HG	1.98	0.46
1:C:153:LEU:CA	1:C:156:LEU:HD12	2.38	0.46
1:C:97:ILE:HG12	1:C:125:ALA:HB2	1.98	0.45
1:C:364:ARG:HD2	5:C:485:HOH:O	2.15	0.45
1:A:374:ASN:HB2	1:D:374:ASN:ND2	2.30	0.45
2:B:216:ASP:OD1	2:B:217:LEU:CG	2.60	0.45
2:B:100:LYS:CD	4:B:401:TCE:H2A	2.45	0.45
1:D:124:LYS:HE2	1:D:157:GLU:O	2.16	0.45
1:A:130:KCX:HD2	1:A:139:GLY:HA3	1.97	0.45
2:B:94:GLU:HG2	2:B:98:LYS:HE2	1.99	0.45
1:D:109:GLU:HG2	1:D:113:LYS:NZ	2.32	0.45
2:B:29:GLU:HB2	2:B:32:ILE:CD1	2.47	0.45
1:C:299:LYS:HD2	1:C:346:ARG:CZ	2.46	0.45
1:A:376:LEU:C	1:A:376:LEU:HD23	2.41	0.45
1:C:147:VAL:O	1:C:151:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:ASP:O	1:D:142:PRO:HD3	2.17	0.45
1:A:338:GLY:CA	3:A:401:GOL:H12	2.45	0.45
1:C:117:ILE:O	1:C:121:LEU:HD23	2.17	0.44
2:B:328:ILE:O	2:B:328:ILE:HG13	2.16	0.44
2:B:300:VAL:HG12	2:B:336:LEU:CD1	2.47	0.44
2:B:186:TYR:OH	2:B:203:LYS:HB3	2.18	0.44
2:B:301:LEU:HD12	2:B:305:GLU:O	2.17	0.44
1:C:153:LEU:O	1:C:156:LEU:HB2	2.18	0.44
2:B:146:SER:HB2	2:B:189:MET:HE1	2.00	0.44
2:B:238:PHE:HD2	2:B:241:ARG:CZ	2.30	0.44
1:D:56:LYS:HB2	1:D:56:LYS:HE2	1.65	0.44
1:A:300:VAL:HG12	1:A:336:LEU:CD1	2.47	0.44
2:B:164:MET:HE3	2:B:186:TYR:CE1	2.53	0.44
2:B:264:VAL:CA	2:B:274:THR:HG22	2.48	0.44
1:C:145:GLU:O	1:C:149:GLU:HG3	2.17	0.44
2:B:259:GLN:HB3	2:B:277:LYS:HE3	1.99	0.43
1:C:135:MET:HG3	1:C:169:ALA:CB	2.37	0.43
1:D:143:ASN:O	1:D:146:SER:HB2	2.18	0.43
1:A:53:LEU:O	1:A:53:LEU:HG	2.16	0.43
1:C:150:ILE:HG21	1:C:193:LEU:HD11	2.01	0.43
1:A:208:SER:OG	1:A:227:ILE:HG12	2.19	0.43
1:C:354:ILE:HD12	1:C:356:TYR:CD1	2.53	0.43
1:D:213:ASP:C	1:D:215:PRO:HD3	2.43	0.43
2:B:253:LYS:HE3	5:B:561:HOH:O	2.19	0.43
1:C:154:ASN:HD22	1:C:198:VAL:HG13	1.80	0.43
1:C:326:ILE:HG13	1:C:327:ASP:N	2.24	0.43
1:C:118:ALA:O	1:C:122:GLY:N	2.52	0.43
1:A:344:ALA:H	3:A:401:GOL:H2	1.84	0.43
1:C:55:GLU:CG	1:C:80:LEU:HG	2.46	0.43
1:C:215:PRO:HD2	5:C:476:HOH:O	2.18	0.43
1:C:106:TYR:HB2	1:C:139:GLY:HA2	2.01	0.42
2:B:29:GLU:HB2	2:B:32:ILE:HD11	2.01	0.42
2:B:42:ALA:HB2	2:B:47:ALA:HA	2.02	0.42
1:D:261:GLU:CB	1:D:262:PRO:HD2	2.40	0.42
1:C:57:GLU:O	1:C:58:LYS:HB2	2.18	0.42
1:D:298:PRO:HG2	1:D:309:VAL:HB	2.00	0.42
2:B:177:GLU:HB3	2:B:180:TYR:HB2	2.00	0.42
2:B:80:LEU:HD23	2:B:80:LEU:HA	1.81	0.42
1:C:130:KCX:OQ1	1:C:137:ARG:HB3	2.19	0.42
1:D:327:ASP:C	1:D:328:ILE:HG13	2.44	0.42
1:C:148:GLN:HA	1:C:151:ILE:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:MET:HE3	1:A:371:MET:HB3	1.87	0.42
2:B:353:THR:OG1	2:B:354:ILE:N	2.51	0.42
1:C:29:GLU:H	1:C:32:ILE:HD12	1.84	0.42
1:D:302:ILE:O	1:D:303:LYS:C	2.63	0.42
2:B:52:LYS:HE2	5:B:639:HOH:O	2.19	0.42
2:B:93:PHE:O	2:B:97:ILE:HD12	2.20	0.42
1:D:256:HIS:HE1	1:D:258:LYS:HD3	1.85	0.42
1:D:263:GLY:N	1:D:274:THR:CG2	2.83	0.42
1:D:327:ASP:OD1	1:D:328:ILE:CA	2.67	0.42
2:B:108:LEU:HB2	2:B:149:GLU:CG	2.49	0.42
1:C:96:SER:OG	1:C:103:MET:HE2	2.17	0.42
2:B:115:ASN:OD1	2:B:158:TYR:HB2	2.19	0.41
1:D:144:GLU:O	1:D:145:GLU:C	2.62	0.41
1:D:262:PRO:CA	1:D:274:THR:HG23	2.43	0.41
1:D:357:GLU:HG2	1:D:361:MET:HE3	2.02	0.41
1:C:178:TYR:HA	1:C:181:LYS:CD	2.42	0.41
1:C:153:LEU:HA	1:C:156:LEU:CD1	2.39	0.41
1:D:260:VAL:HG12	1:D:261:GLU:O	2.20	0.41
1:D:371:MET:SD	1:D:376:LEU:CA	3.08	0.41
1:C:370:TYR:O	1:C:371:MET:HE2	2.21	0.41
1:D:166:THR:HG22	1:D:205:VAL:HG12	2.02	0.41
1:C:262:PRO:CA	1:C:274:THR:HG23	2.49	0.41
1:C:262:PRO:HG3	1:C:276:GLY:C	2.45	0.41
1:C:337:PHE:HZ	1:C:362:ILE:HD11	1.85	0.41
1:D:4:ILE:HD13	1:D:4:ILE:HG21	1.87	0.41
1:D:32:ILE:HD13	1:D:218:ARG:CB	2.38	0.41
1:D:178:TYR:O	1:D:181:LYS:HB2	2.21	0.41
1:D:214:CYS:N	1:D:215:PRO:HD3	2.35	0.41
2:B:263:GLY:H	2:B:274:THR:HG23	1.83	0.41
1:D:263:GLY:N	1:D:274:THR:O	2.47	0.41
1:A:314:CYS:HB2	1:A:317:GLN:O	2.20	0.41
2:B:187:LYS:HB3	2:B:187:LYS:HE3	1.87	0.41
2:B:300:VAL:HG12	2:B:336:LEU:HD13	2.03	0.41
1:C:270:LEU:HD11	1:D:178:TYR:CD2	2.56	0.40
2:B:21:LEU:HA	2:B:24:ILE:HD12	2.04	0.40
2:B:232:TYR:CE2	2:B:239:LYS:HD3	2.56	0.40
1:C:179:THR:HA	5:C:432:HOH:O	2.21	0.40
1:D:304:GLY:N	5:D:498:HOH:O	2.52	0.40
1:C:98:LYS:HE2	1:C:121:LEU:HD11	2.02	0.40
1:C:108:LEU:HD21	1:C:112:GLN:HE22	1.87	0.40
1:D:117:ILE:CD1	1:D:117:ILE:H	2.35	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	356/385 (92%)	346 (97%)	9 (2%)	1 (0%)	36	36
1	C	378/385 (98%)	365 (97%)	11 (3%)	2 (0%)	24	22
1	D	374/385 (97%)	365 (98%)	9 (2%)	0	100	100
2	B	368/385 (96%)	360 (98%)	6 (2%)	2 (0%)	24	22
All	All	1476/1540 (96%)	1436 (97%)	35 (2%)	5 (0%)	36	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	219	LEU
1	C	267	SER
1	C	58	LYS
2	B	200	ILE
1	A	200	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/332 (94%)	302 (96%)	11 (4%)	32	35
1	C	329/332 (99%)	309 (94%)	20 (6%)	17	15
1	D	327/332 (98%)	309 (94%)	18 (6%)	19	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	324/333 (97%)	312 (96%)	12 (4%)	30	33
All	All	1293/1329 (97%)	1232 (95%)	61 (5%)	23	24

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

Mol	Chain	Res	Type
1	A	56	LYS
1	A	61	TYR
1	A	123	GLU
1	A	166	THR
1	A	174	VAL
1	A	181	LYS
1	A	195	GLU
1	A	326	ILE
1	A	329	LYS
1	A	336	LEU
1	A	349	LYS
2	B	27	LEU
2	B	53	LEU
2	B	61	TYR
2	B	91	GLU
2	B	152	GLU
2	B	164	MET
2	B	187	LYS
2	B	202	ILE
2	B	296	LYS
2	B	316	ASP
2	B	319	MET
2	B	336	LEU
1	C	60	ASP
1	C	61	TYR
1	C	112	GLN
1	C	121	LEU
1	C	123	GLU
1	C	127	VAL
1	C	156	LEU
1	C	175	SER
1	C	177	GLU
1	C	195	GLU
1	C	206	SER
1	C	211	ILE
1	C	240	ASP

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Mol	Chain	Res	Type
1	C	257	ILE
1	C	279	THR
1	C	317	GLN
1	C	319	MET
1	C	326	ILE
1	C	329	LYS
1	C	368	ARG
1	D	28	LEU
1	D	56	LYS
1	D	59	VAL
1	D	61	TYR
1	D	127	VAL
1	D	129	VAL
1	D	145	GLU
1	D	159	ILE
1	D	188	PHE
1	D	189	MET
1	D	193	LEU
1	D	254	ILE
1	D	274	THR
1	D	280	ILE
1	D	297	ASN
1	D	302	ILE
1	D	316	ASP
1	D	328	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	148	GLN
1	A	154	ASN
1	A	297	ASN
1	A	317	GLN
2	B	148	GLN
2	B	259	GLN
2	B	380	ASN
1	C	75	GLN
1	C	115	ASN
1	C	154	ASN
1	C	182	GLN
1	C	317	GLN

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Mol	Chain	Res	Type
1	C	378	GLN
1	D	148	GLN
1	D	154	ASN
1	D	256	HIS
1	D	374	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues 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
1	LLP	A	39	1	23,24,25	2.63	9 (39%)	25,32,34	1.50	6 (24%)
1	LLP	D	39	1	23,24,25	2.16	9 (39%)	25,32,34	2.16	10 (40%)
1	KCX	C	130	1	10,11,12	1.28	1 (10%)	6,12,14	0.90	0
1	LLP	C	39	1	23,24,25	2.22	8 (34%)	25,32,34	1.91	8 (32%)
1	KCX	D	130	1	10,11,12	1.26	0	6,12,14	2.14	2 (33%)
1	KCX	A	130	1	10,11,12	1.94	5 (50%)	6,12,14	1.69	1 (16%)
2	LLP	B	39	2	23,24,25	2.44	11 (47%)	25,32,34	1.50	6 (24%)

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
1	LLP	A	39	1	-	5/16/17/19	0/1/1/1
1	LLP	D	39	1	-	3/16/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	C	130	1	-	3/9/10/12	-
1	LLP	C	39	1	-	6/16/17/19	0/1/1/1
1	KCX	D	130	1	-	2/9/10/12	-
1	KCX	A	130	1	-	4/9/10/12	-
2	LLP	B	39	2	-	3/16/17/19	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	LLP	C3-C2	5.99	1.47	1.41
1	D	39	LLP	C4'-NZ	5.44	1.45	1.27
1	A	39	LLP	C4'-NZ	5.41	1.45	1.27
2	B	39	LLP	C3-C2	4.99	1.46	1.41
1	C	39	LLP	C4'-NZ	4.83	1.43	1.27
2	B	39	LLP	C4'-NZ	4.46	1.42	1.27
1	C	39	LLP	C3-C2	4.42	1.45	1.41
2	B	39	LLP	P-OP2	-4.33	1.38	1.54
2	B	39	LLP	C4-C5	4.27	1.47	1.42
1	A	39	LLP	P-OP1	-4.02	1.38	1.50
1	C	39	LLP	C4-C5	3.96	1.47	1.42
1	A	39	LLP	P-OP2	-3.91	1.40	1.54
1	A	130	KCX	CE-NZ	-3.73	1.37	1.46
1	A	39	LLP	P-OP3	-3.69	1.41	1.54
1	C	39	LLP	P-OP2	-3.68	1.41	1.54
1	D	39	LLP	C3-C2	3.67	1.44	1.41
1	D	39	LLP	P-OP2	-3.48	1.41	1.54
2	B	39	LLP	P-OP3	-3.31	1.42	1.54
1	A	39	LLP	O3-C3	-3.11	1.29	1.36
1	D	39	LLP	C4-C5	3.10	1.46	1.42
1	C	39	LLP	P-OP3	-3.00	1.43	1.54
1	D	39	LLP	P-OP3	-2.99	1.43	1.54
1	A	39	LLP	C4-C5	2.91	1.46	1.42
1	C	39	LLP	C4-C3	2.81	1.45	1.41
1	A	39	LLP	C2-N1	-2.73	1.29	1.33
2	B	39	LLP	P-OP1	-2.70	1.42	1.50
1	C	130	KCX	OQ1-CX	-2.63	1.16	1.21
1	A	130	KCX	CX-NZ	-2.63	1.30	1.35
1	C	39	LLP	P-OP1	-2.60	1.42	1.50
2	B	39	LLP	C4-C3	2.59	1.45	1.41
2	B	39	LLP	C4-C4'	2.52	1.52	1.46
1	A	130	KCX	CB-CA	-2.42	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	39	LLP	P-OP1	-2.36	1.43	1.50
1	D	39	LLP	O3-C3	-2.32	1.31	1.36
1	D	39	LLP	CA-N	-2.23	1.41	1.48
2	B	39	LLP	O3-C3	-2.23	1.31	1.36
2	B	39	LLP	CE-NZ	-2.19	1.41	1.46
1	A	130	KCX	OQ1-CX	-2.16	1.17	1.21
2	B	39	LLP	P-OP4	-2.15	1.53	1.60
1	A	39	LLP	P-OP4	-2.10	1.53	1.60
1	A	130	KCX	CA-N	-2.10	1.42	1.48
1	D	39	LLP	C4-C4'	2.04	1.51	1.46
1	C	39	LLP	O3-C3	-2.01	1.32	1.36

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	39	LLP	C4-C4'-NZ	-5.08	100.59	124.04
1	C	39	LLP	CD-CE-NZ	4.10	121.68	110.83
1	D	39	LLP	C5-C4-C4'	3.85	127.41	121.47
1	C	39	LLP	C4-C4'-NZ	-3.84	106.30	124.04
2	B	39	LLP	C4-C3-C2	-3.76	118.03	120.14
1	A	130	KCX	OQ1-CX-NZ	3.75	130.61	124.92
1	D	130	KCX	CE-NZ-CX	3.69	128.25	121.98
1	D	39	LLP	C2'-C2-C3	-3.56	116.63	120.80
1	C	39	LLP	C2'-C2-C3	-3.45	116.76	120.80
1	C	39	LLP	C2'-C2-N1	3.34	123.94	117.64
1	D	39	LLP	CE-NZ-C4'	3.27	129.18	118.72
1	D	39	LLP	C2'-C2-N1	3.19	123.65	117.64
1	A	39	LLP	C4-C4'-NZ	-2.97	110.34	124.04
1	D	130	KCX	OQ1-CX-NZ	2.85	129.26	124.92
1	D	39	LLP	OP3-P-OP2	2.73	118.03	107.80
1	A	39	LLP	O3-C3-C2	2.70	123.18	117.58
1	A	39	LLP	CD-CE-NZ	2.66	117.87	110.83
1	A	39	LLP	C3-C4-C5	-2.56	116.22	118.28
2	B	39	LLP	CD-CE-NZ	2.53	117.53	110.83
1	D	39	LLP	C3-C4-C5	-2.51	116.26	118.28
1	A	39	LLP	C4-C3-C2	-2.44	118.77	120.14
1	D	39	LLP	O3-C3-C2	2.40	122.56	117.58
1	C	39	LLP	C4-C3-C2	-2.39	118.80	120.14
1	C	39	LLP	C6-N1-C2	2.37	123.49	119.20
1	D	39	LLP	C3-C4-C4'	-2.28	116.28	120.40
1	C	39	LLP	OP2-P-OP4	-2.24	100.84	106.67
2	B	39	LLP	C3-C4-C5	-2.22	116.49	118.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	39	LLP	C4-C4'-NZ	-2.20	113.88	124.04
1	D	39	LLP	OP4-P-OP1	-2.17	100.58	106.44
1	A	39	LLP	C6-N1-C2	2.07	122.96	119.20
1	C	39	LLP	C3-C4-C5	-2.06	116.62	118.28
2	B	39	LLP	O3-C3-C2	2.04	121.81	117.58
2	B	39	LLP	C6-N1-C2	2.02	122.86	119.20

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	39	LLP	C4-C4'-NZ-CE
1	A	130	KCX	N-CA-CB-CG
1	A	130	KCX	C-CA-CB-CG
2	B	39	LLP	C4-C4'-NZ-CE
1	C	39	LLP	C4-C4'-NZ-CE
1	C	130	KCX	N-CA-CB-CG
1	C	130	KCX	C-CA-CB-CG
1	C	130	KCX	CG-CD-CE-NZ
1	D	39	LLP	CG-CD-CE-NZ
1	D	39	LLP	C3-C4-C4'-NZ
1	C	39	LLP	CG-CD-CE-NZ
1	D	130	KCX	CA-CB-CG-CD
1	A	39	LLP	C3-C4-C4'-NZ
1	C	39	LLP	C3-C4-C4'-NZ
1	A	39	LLP	C5-C4-C4'-NZ
1	A	130	KCX	CA-CB-CG-CD
1	C	39	LLP	C5-C4-C4'-NZ
1	D	39	LLP	CD-CE-NZ-C4'
1	A	39	LLP	CG-CD-CE-NZ
1	C	39	LLP	CD-CE-NZ-C4'
1	D	130	KCX	N-CA-CB-CG
1	A	130	KCX	CE-CD-CG-CB
2	B	39	LLP	C3-C4-C4'-NZ
1	A	39	LLP	CD-CE-NZ-C4'
2	B	39	LLP	CD-CE-NZ-C4'
1	C	39	LLP	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	130	KCX	1	0
1	C	39	LLP	1	0
1	A	130	KCX	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	TCE	B	401	-	12,15,15	1.25	0	12,18,18	3.16	3 (25%)
3	GOL	A	401	-	5,5,5	1.20	0	5,5,5	2.17	2 (40%)

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
4	TCE	B	401	-	-	12/15/15/15	-
3	GOL	A	401	-	-	3/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	TCE	C1-P-C3	5.99	120.03	100.95
4	B	401	TCE	C1-P-C2	5.98	120.00	100.95
4	B	401	TCE	C3-P-C2	5.97	119.97	100.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	GOL	O1-C1-C2	3.41	125.75	110.38
3	A	401	GOL	O3-C3-C2	2.62	122.17	110.38

There are no chirality outliers.

All (15) torsion outliers are listed below:

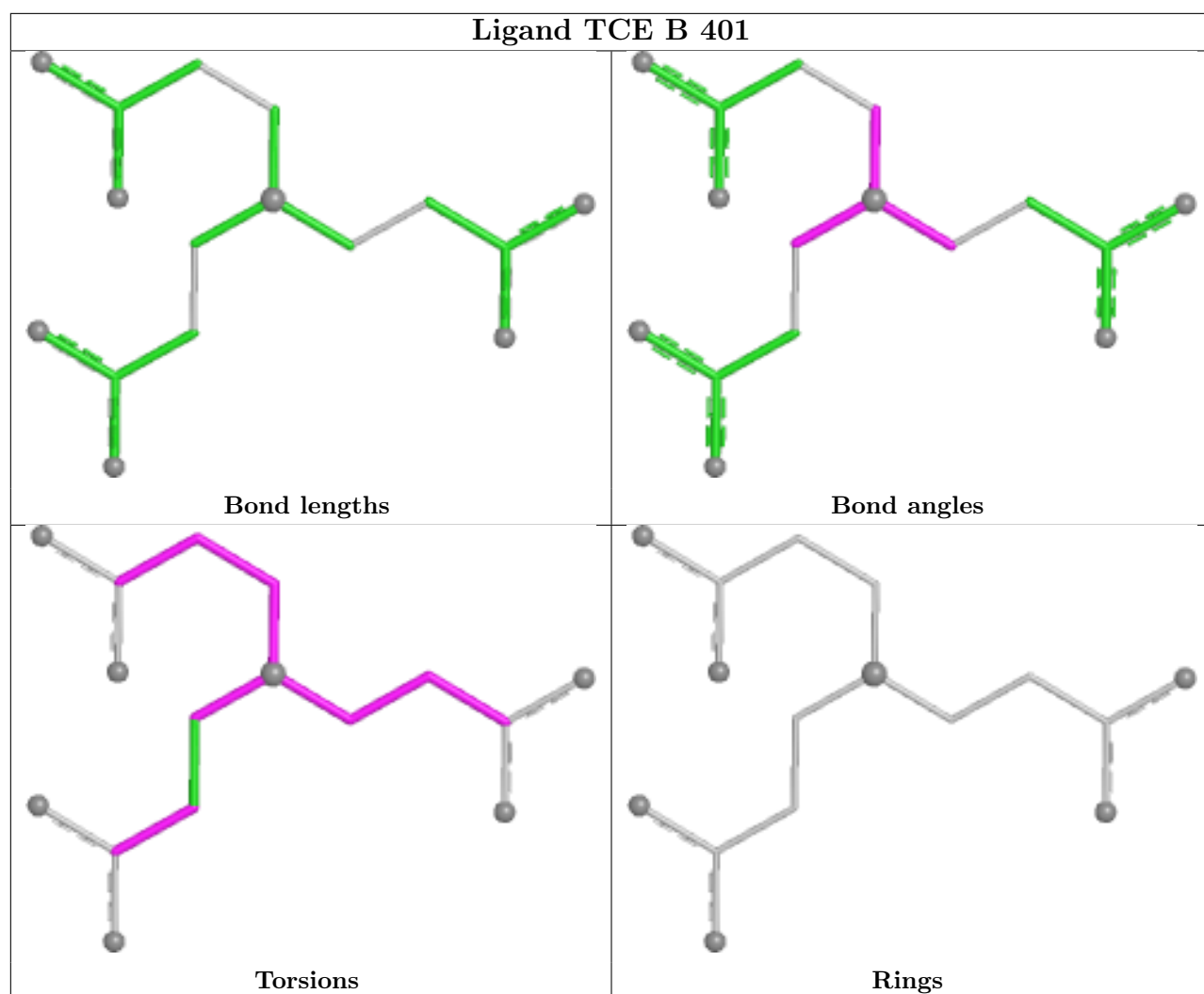
Mol	Chain	Res	Type	Atoms
3	A	401	GOL	O1-C1-C2-C3
4	B	401	TCE	P-C2-C5-C14
4	B	401	TCE	C5-C2-P-C3
4	B	401	TCE	C5-C2-P-C1
4	B	401	TCE	C6-C3-P-C2
4	B	401	TCE	C4-C1-P-C3
4	B	401	TCE	P-C3-C6-C8
4	B	401	TCE	C3-C6-C8-O10
3	A	401	GOL	O1-C1-C2-O2
4	B	401	TCE	O16-C14-C5-C2
4	B	401	TCE	O12-C11-C4-C1
4	B	401	TCE	O15-C14-C5-C2
4	B	401	TCE	O13-C11-C4-C1
4	B	401	TCE	C3-C6-C8-O9
3	A	401	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	TCE	6	0
3	A	401	GOL	17	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	360/385 (93%)	-0.02	9 (2%) 58 61	16, 28, 49, 73	0
1	C	380/385 (98%)	0.69	38 (10%) 12 13	23, 42, 63, 85	0
1	D	378/385 (98%)	0.73	44 (11%) 9 10	21, 43, 72, 92	0
2	B	373/385 (96%)	0.24	14 (3%) 44 46	10, 35, 63, 81	1 (0%)
All	All	1491/1540 (96%)	0.42	105 (7%) 22 24	10, 37, 65, 92	1 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	332	ASP	6.9
1	D	188	PHE	5.2
1	D	273	THR	5.1
1	D	216	ASP	4.3
1	C	266	ILE	4.3
1	C	43	TYR	4.3
1	D	193	LEU	4.1
1	D	200	ILE	3.9
1	D	178	TYR	3.7
1	D	180	TYR	3.5
1	D	142	PRO	3.4
1	D	136	THR	3.4
1	C	328	ILE	3.4
1	D	326	ILE	3.2
2	B	171	ALA	3.2
1	D	266	ILE	3.2
1	C	326	ILE	3.1
1	A	328	ILE	3.1
1	D	275	THR	3.1
1	C	80	LEU	3.0
1	D	328	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	106	TYR	3.0
1	D	263	GLY	2.9
1	A	326	ILE	2.8
1	C	280	ILE	2.8
1	C	257	ILE	2.8
1	D	124	LYS	2.8
1	D	187	LYS	2.8
1	C	191	ASP	2.7
1	C	117	ILE	2.7
1	D	272	TYR	2.7
1	D	138	ILE	2.7
1	D	150	ILE	2.7
1	C	3	LYS	2.7
1	C	116	GLU	2.6
1	D	264	VAL	2.6
1	C	267	SER	2.6
1	D	331	GLY	2.6
1	A	279	THR	2.6
1	C	125	ALA	2.6
1	C	330	VAL	2.5
1	C	159	ILE	2.5
1	D	192	LYS	2.5
1	D	151	ILE	2.5
1	D	174	VAL	2.5
1	C	145	GLU	2.5
1	D	152	GLU	2.5
1	D	274	THR	2.5
1	A	228	LEU	2.5
1	D	177	GLU	2.4
1	D	105	VAL	2.4
1	D	147	VAL	2.4
1	D	330	VAL	2.4
2	B	124	LYS	2.4
1	D	140	PHE	2.4
1	C	273	THR	2.4
1	C	188	PHE	2.4
1	C	198	VAL	2.4
1	D	3	LYS	2.4
1	C	279	THR	2.4
1	C	87	TYR	2.3
2	B	178	TYR	2.3
1	C	384	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	108	LEU	2.3
1	A	3	LYS	2.3
1	C	265	GLY	2.3
2	B	330	VAL	2.3
1	C	98	LYS	2.3
2	B	177	GLU	2.3
2	B	3	LYS	2.3
2	B	240	ASP	2.2
2	B	195	GLU	2.2
1	D	186	TYR	2.2
1	C	151	ILE	2.2
1	D	279	THR	2.2
2	B	264	VAL	2.2
1	C	110	THR	2.2
1	C	19	PHE	2.1
1	C	264	VAL	2.1
1	C	121	LEU	2.1
1	C	199	LYS	2.1
1	C	138	ILE	2.1
1	C	150	ILE	2.1
1	D	139	GLY	2.1
1	D	161	LEU	2.1
2	B	378	GLN	2.1
1	A	256	HIS	2.1
1	C	174	VAL	2.1
1	C	272	TYR	2.1
1	C	269	GLY	2.1
1	A	257	ILE	2.1
1	C	299	LYS	2.1
1	D	196	ALA	2.1
1	D	143	ASN	2.0
2	B	170	THR	2.0
1	C	260	VAL	2.0
1	C	189	MET	2.0
1	D	201	ALA	2.0
1	D	185	ASN	2.0
1	D	327	ASP	2.0
1	A	199	LYS	2.0
1	D	155	LYS	2.0
1	D	110	THR	2.0
2	B	275	THR	2.0
2	B	139	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KCX	D	130	12/13	0.85	0.14	36,45,56,61	0
1	KCX	C	130	12/13	0.88	0.12	40,45,50,56	0
1	KCX	A	130	12/13	0.93	0.10	20,29,37,37	0
1	LLP	C	39	24/25	0.95	0.08	28,33,42,47	0
2	LLP	B	39	24/25	0.96	0.07	16,28,32,34	0
1	LLP	D	39	24/25	0.96	0.07	25,34,42,43	0
1	LLP	A	39	24/25	0.96	0.07	15,23,29,36	0

6.3 Carbohydrates [i](#)

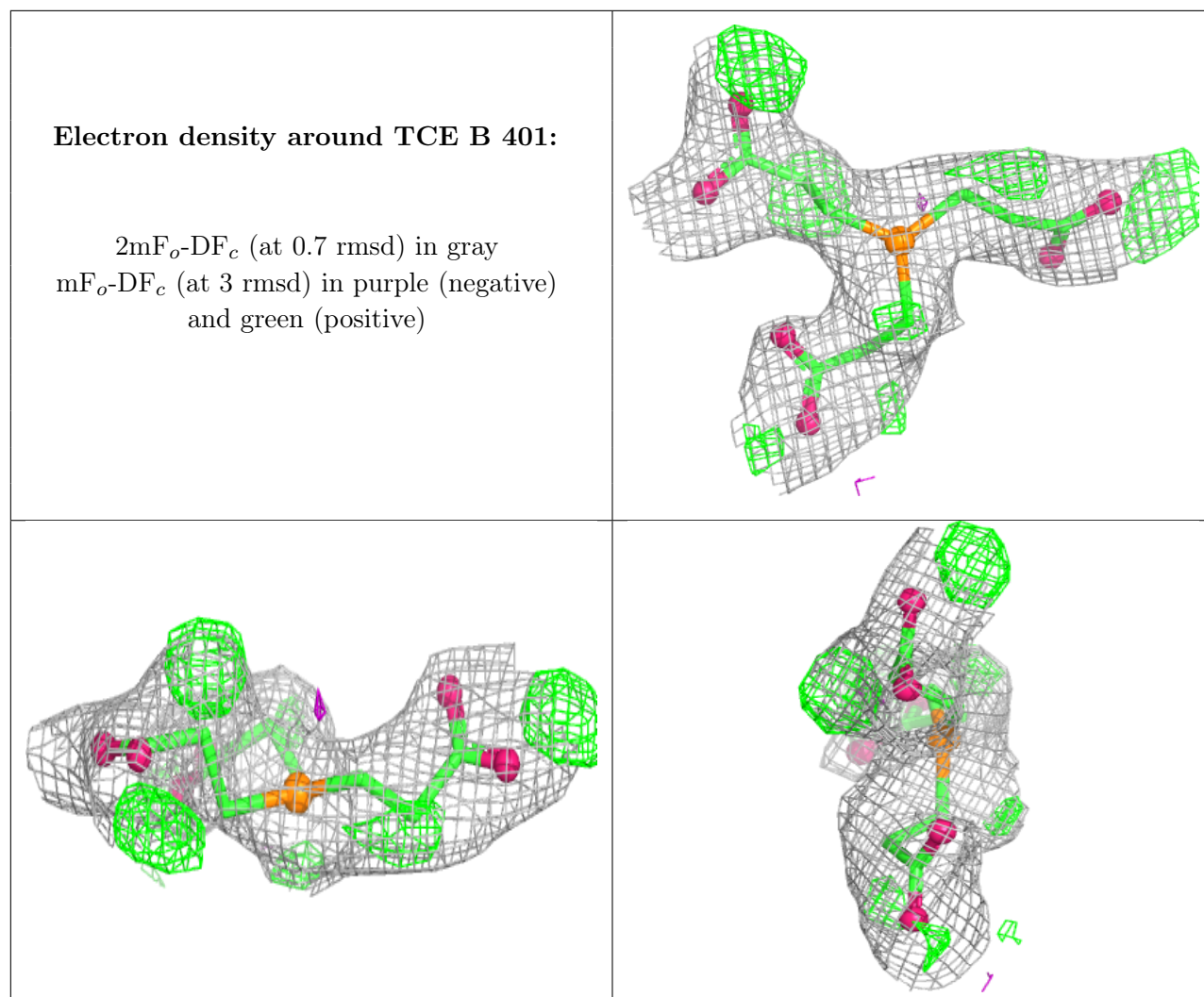
There are no oligosaccharides in this entry.

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
4	TCE	B	401	16/16	0.74	0.17	40,48,58,59	0
3	GOL	A	401	6/6	0.92	0.18	21,29,39,54	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.