



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:33 PM UTC

PDB ID : 2JE5 / pdb_00002je5
Title : STRUCTURAL AND MECHANISTIC BASIS OF PENICILLIN BINDING
PROTEIN INHIBITION BY LACTIVICINS
Authors : Macheboeuf, P.; Fisher, D.S.; Brown, T.J.; Zervosen, A.; Luxen, A.; Joris, B.;
Dessen, A.; Schofield, C.J.
Deposited on : 2007-01-15
Resolution : 2.60 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

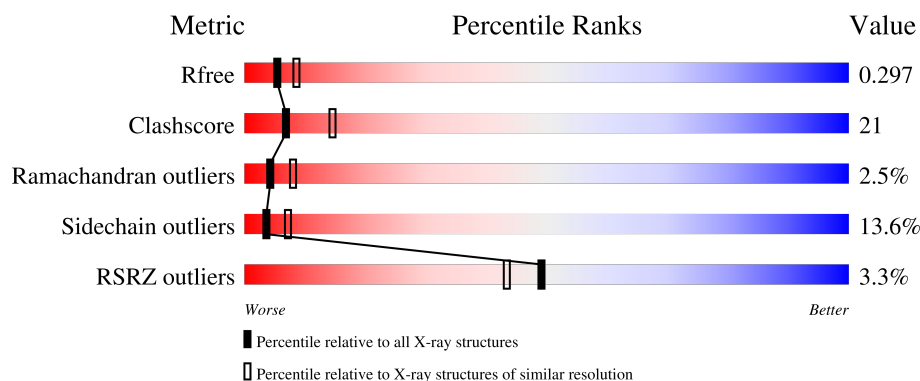
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	720	
1	B	720	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7239 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.

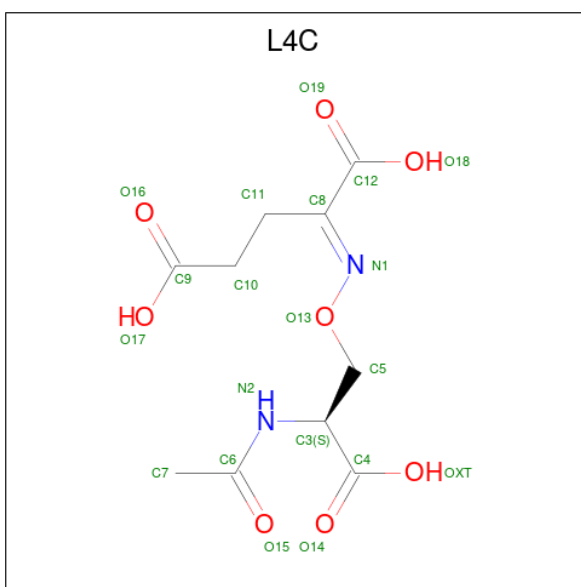
- Molecule 1 is a protein called PENICILLIN-BINDING PROTEIN 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	1	0
			3555	2222	602	716	15			
1	B	462	Total	C	N	O	S	0	0	0
			3553	2222	602	714	15			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	SER	ALA	engineered mutation	UNP O70038
A	123	MET	LEU	engineered mutation	UNP O70038
A	158	ASN	LYS	engineered mutation	UNP O70038
A	162	PRO	ARG	engineered mutation	UNP O70038
A	336	GLN	ARG	engineered mutation	UNP O70038
A	686	GLN	ARG	engineered mutation	UNP O70038
A	687	GLN	ARG	engineered mutation	UNP O70038
B	73	SER	ALA	engineered mutation	UNP O70038
B	123	MET	LEU	engineered mutation	UNP O70038
B	158	ASN	LYS	engineered mutation	UNP O70038
B	162	PRO	ARG	engineered mutation	UNP O70038
B	336	GLN	ARG	engineered mutation	UNP O70038
B	686	GLN	ARG	engineered mutation	UNP O70038
B	687	GLN	ARG	engineered mutation	UNP O70038

- Molecule 2 is (2E)-2-([(2S)-2-(ACETYLAMINO)-2-CARBOXYETHOXY]IMINO}PENTANEDIOIC ACID (CCD ID: L4C) (formula: C₁₀H₁₄N₂O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	10	2	7		
2	B	1	Total	C	N	O	0	0
			19	10	2	7		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Cl 2	0	0
4	B	2	Total 2	Cl 2	0	0

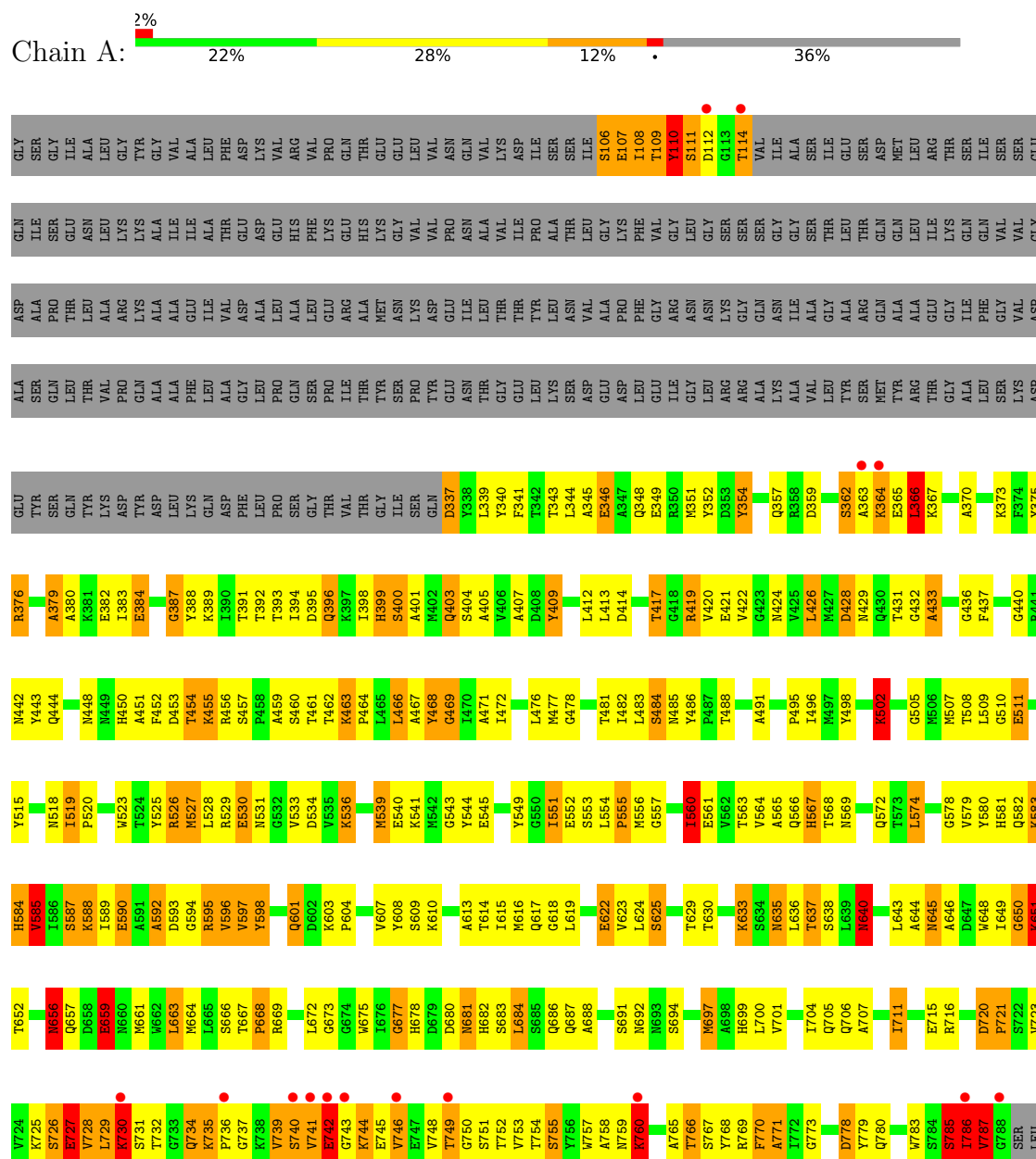
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	36	Total 36	O 36	0	0
5	B	43	Total 43	O 43	0	0

3 Residue-property plots

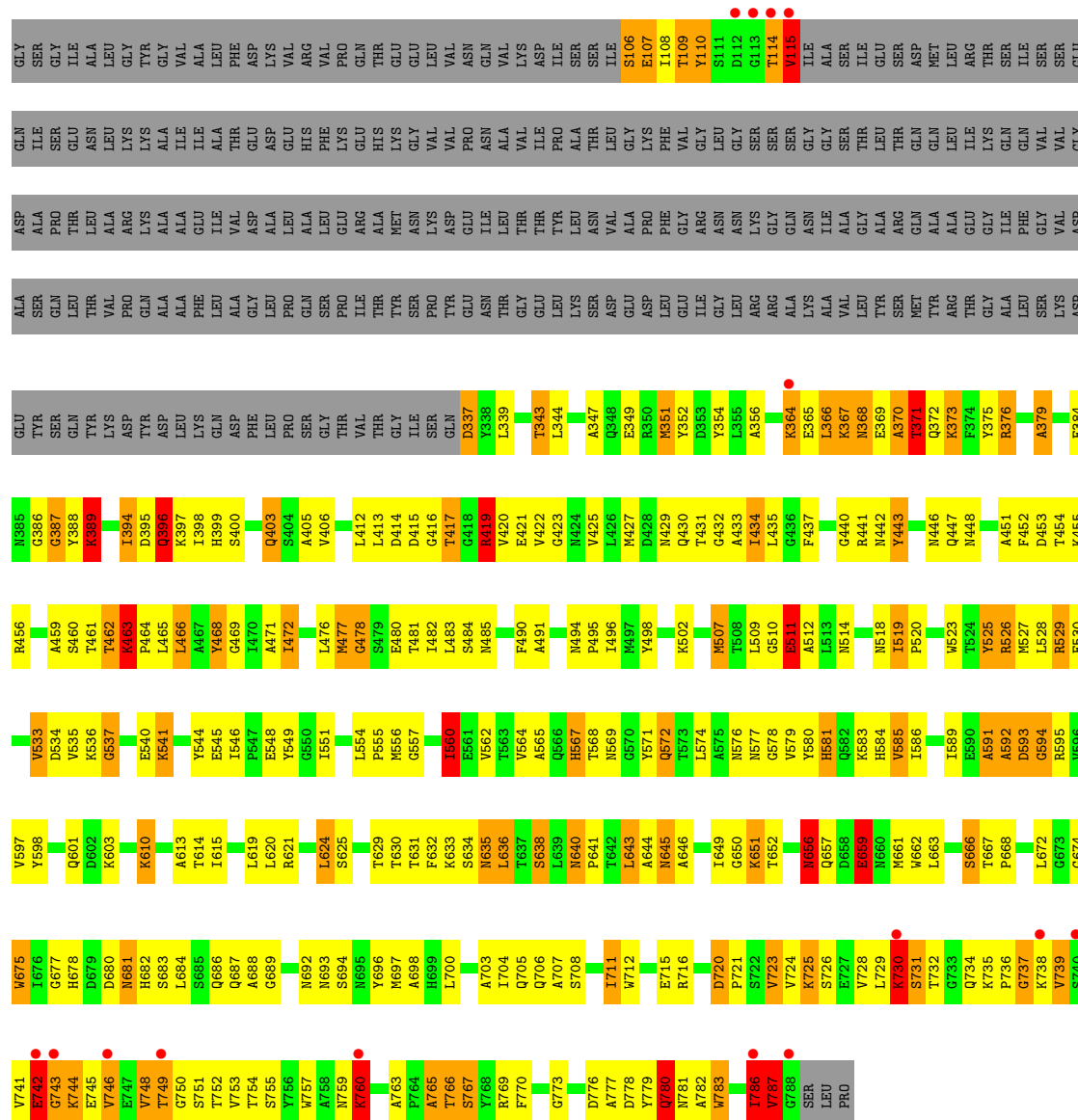
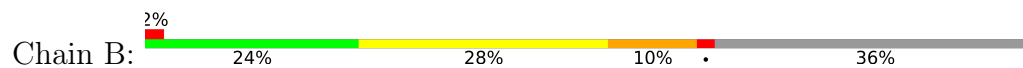
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PENICILLIN-BINDING PROTEIN 1B



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● Molecule 1: PENICILLIN-BINDING PROTEIN 1B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.54Å 99.83Å 152.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.52 – 2.60 83.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (84.52-2.60) 99.3 (83.47-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.260 , 0.298 0.262 , 0.297	Depositor DCC
R_{free} test set	2315 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7239	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 96.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9016e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL, L4C

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	2.37	167/3628 (4.6%)	2.00	118/4929 (2.4%)
1	B	2.42	160/3626 (4.4%)	2.07	137/4927 (2.8%)
All	All	2.39	327/7254 (4.5%)	2.03	255/9856 (2.6%)

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	4
1	B	0	3
All	All	0	7

All (327) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	601	GLN	CA-CB	14.31	1.75	1.53
1	A	345	ALA	C-O	12.65	1.39	1.24
1	B	601	GLN	CA-CB	12.38	1.72	1.53
1	B	786	ILE	CA-CB	12.29	1.71	1.54
1	A	786	ILE	CA-CB	12.19	1.71	1.54
1	B	371	THR	N-CA	12.17	1.61	1.46
1	B	565	ALA	CA-CB	-11.57	1.35	1.53
1	B	535	VAL	CA-CB	-10.59	1.42	1.54
1	A	754	THR	CA-C	10.55	1.66	1.52
1	B	787	VAL	CA-C	10.41	1.66	1.52
1	B	114	THR	N-CA	10.21	1.59	1.46
1	A	672	LEU	C-O	10.20	1.35	1.24
1	B	379	ALA	N-CA	10.11	1.58	1.46
1	A	422	VAL	CA-CB	10.04	1.68	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	633	LYS	CA-C	9.88	1.66	1.52
1	B	115	VAL	CA-CB	9.74	1.80	1.54
1	A	656	ASN	N-CA	9.52	1.58	1.45
1	A	589	ILE	CA-CB	-9.38	1.42	1.54
1	B	656	ASN	N-CA	9.38	1.58	1.45
1	B	114	THR	CA-CB	9.24	1.67	1.53
1	B	614	THR	C-O	9.10	1.34	1.24
1	A	519	ILE	CA-CB	8.82	1.58	1.54
1	B	703	ALA	CA-CB	-8.79	1.39	1.53
1	A	615	ILE	CA-CB	-8.76	1.43	1.54
1	A	754	THR	CA-CB	8.74	1.67	1.53
1	A	405	ALA	N-CA	-8.65	1.35	1.46
1	A	451	ALA	CA-CB	8.61	1.67	1.53
1	B	603	LYS	CA-CB	8.55	1.67	1.53
1	A	400	SER	N-CA	8.45	1.56	1.46
1	A	379	ALA	N-CA	8.36	1.56	1.46
1	B	704	ILE	C-O	8.34	1.33	1.24
1	B	686	GLN	CA-C	8.27	1.63	1.52
1	A	399	HIS	C-O	8.26	1.34	1.24
1	B	754	THR	CA-C	8.26	1.63	1.52
1	A	659	GLU	C-O	-8.23	1.13	1.24
1	B	649	ILE	N-CA	8.19	1.55	1.46
1	B	615	ILE	CA-CB	-8.17	1.44	1.54
1	B	448	ASN	C-O	8.12	1.33	1.23
1	A	649	ILE	N-CA	8.02	1.54	1.46
1	B	371	THR	CA-CB	7.95	1.66	1.53
1	B	427	MET	N-CA	-7.87	1.36	1.46
1	B	451	ALA	C-O	7.80	1.34	1.23
1	B	541	LYS	CE-NZ	7.73	1.72	1.49
1	A	398	ILE	CA-CB	-7.62	1.46	1.54
1	B	546	ILE	CA-CB	7.62	1.60	1.54
1	B	754	THR	CA-CB	7.59	1.66	1.53
1	B	433	ALA	C-O	-7.59	1.15	1.23
1	A	354	TYR	CA-C	7.56	1.62	1.52
1	A	699	HIS	C-O	7.56	1.32	1.24
1	A	720	ASP	CA-C	7.53	1.60	1.53
1	A	742	GLU	N-CA	7.48	1.55	1.46
1	B	688	ALA	CA-CB	-7.47	1.41	1.53
1	B	753	VAL	N-CA	7.42	1.55	1.46
1	B	692	ASN	N-CA	7.42	1.55	1.46
1	A	598	TYR	C-O	7.36	1.32	1.23
1	A	365	GLU	CA-C	-7.36	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	661	MET	CA-C	-7.34	1.43	1.52
1	B	417	THR	CA-CB	7.34	1.63	1.53
1	B	343	THR	C-O	7.33	1.32	1.24
1	B	387	GLY	N-CA	7.32	1.55	1.45
1	A	758	ALA	CA-C	-7.31	1.43	1.52
1	A	459	ALA	CA-C	-7.29	1.45	1.53
1	A	407	ALA	CA-CB	7.27	1.64	1.53
1	A	419	ARG	C-O	7.26	1.33	1.24
1	A	108	ILE	CA-CB	7.25	1.62	1.54
1	A	464	PRO	C-O	7.23	1.32	1.24
1	B	634	SER	CA-C	-7.23	1.43	1.52
1	A	691	SER	C-O	7.23	1.29	1.23
1	B	484	SER	CA-C	-7.21	1.43	1.52
1	A	753	VAL	N-CA	7.21	1.54	1.46
1	B	589	ILE	CA-CB	-7.18	1.45	1.54
1	B	403	GLN	C-O	7.16	1.32	1.24
1	A	721	PRO	CA-C	7.15	1.62	1.52
1	B	645	ASN	CA-C	-7.11	1.43	1.52
1	A	706	GLN	CB-CG	7.05	1.73	1.52
1	A	396	GLN	CG-CD	7.05	1.69	1.52
1	B	742	GLU	N-CA	7.04	1.55	1.46
1	B	707	ALA	CA-CB	-7.01	1.42	1.53
1	B	519	ILE	CA-CB	7.01	1.58	1.54
1	A	603	LYS	CA-CB	7.00	1.60	1.53
1	A	454	THR	CB-CG2	6.99	1.75	1.52
1	A	624	LEU	N-CA	6.97	1.54	1.46
1	A	677	GLY	N-CA	6.92	1.53	1.45
1	A	455	LYS	C-O	-6.91	1.15	1.24
1	A	443	TYR	CA-CB	-6.90	1.42	1.53
1	B	603	LYS	CA-C	6.87	1.61	1.52
1	B	707	ALA	CA-C	-6.85	1.43	1.52
1	A	491	ALA	CA-CB	-6.81	1.42	1.53
1	A	366	LEU	CG-CD2	6.81	1.75	1.52
1	A	440	GLY	N-CA	6.77	1.53	1.45
1	B	495	PRO	C-O	6.76	1.32	1.23
1	B	491	ALA	CA-CB	-6.73	1.41	1.53
1	B	463	LYS	CE-NZ	6.72	1.69	1.49
1	A	581	HIS	C-O	6.72	1.32	1.23
1	A	649	ILE	C-O	6.72	1.30	1.23
1	A	760	LYS	CB-CG	6.71	1.72	1.52
1	A	567	HIS	C-O	6.67	1.32	1.24
1	A	539	MET	CG-SD	6.65	1.97	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	637	THR	C-O	6.62	1.31	1.24
1	B	700	LEU	C-O	6.61	1.31	1.24
1	A	452	PHE	N-CA	6.61	1.54	1.45
1	B	414	ASP	C-O	-6.61	1.16	1.24
1	A	646	ALA	CA-CB	-6.60	1.42	1.53
1	A	652	THR	CA-C	6.60	1.61	1.53
1	B	405	ALA	N-CA	-6.59	1.38	1.46
1	B	364	LYS	CA-C	6.59	1.61	1.52
1	A	700	LEU	C-O	6.58	1.31	1.24
1	B	704	ILE	CA-C	6.57	1.60	1.52
1	B	659	GLU	C-O	-6.57	1.15	1.24
1	B	427	MET	C-O	-6.56	1.16	1.23
1	B	646	ALA	CA-CB	-6.55	1.42	1.53
1	B	585	VAL	CA-CB	6.55	1.63	1.54
1	B	415	ASP	CG-OD1	6.44	1.37	1.25
1	B	560	ILE	C-O	-6.43	1.17	1.24
1	B	420	VAL	CA-C	-6.43	1.44	1.52
1	B	386	GLY	C-O	-6.42	1.19	1.24
1	A	651	LYS	CA-C	-6.41	1.44	1.52
1	B	115	VAL	N-CA	6.40	1.58	1.46
1	A	495	PRO	C-O	6.39	1.30	1.23
1	B	739	VAL	CA-CB	6.38	1.62	1.54
1	B	625	SER	C-O	-6.37	1.16	1.24
1	A	409	TYR	C-N	6.37	1.42	1.33
1	A	661	MET	CA-C	-6.35	1.44	1.52
1	A	376	ARG	CA-C	-6.33	1.44	1.52
1	B	742	GLU	CA-C	6.33	1.61	1.52
1	A	742	GLU	CA-C	6.31	1.61	1.52
1	B	567	HIS	C-O	6.31	1.31	1.24
1	B	364	LYS	N-CA	6.30	1.53	1.46
1	A	666	SER	C-O	6.27	1.31	1.23
1	A	638	SER	CA-CB	-6.26	1.43	1.53
1	A	668	PRO	N-CA	6.25	1.55	1.47
1	B	114	THR	CA-C	6.25	1.61	1.52
1	B	694	SER	CA-CB	-6.25	1.43	1.53
1	A	560	ILE	N-CA	6.24	1.53	1.46
1	A	572	GLN	C-O	6.23	1.31	1.24
1	B	763	ALA	CA-C	6.23	1.60	1.52
1	B	706	GLN	CG-CD	6.22	1.67	1.52
1	B	689	GLY	N-CA	6.21	1.54	1.45
1	B	339	LEU	N-CA	-6.19	1.39	1.46
1	A	531	ASN	N-CA	6.18	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	354	TYR	CD1-CE1	6.17	1.57	1.38
1	B	562	VAL	N-CA	6.17	1.52	1.46
1	A	681	ASN	CG-ND2	6.16	1.46	1.33
1	A	697	MET	CA-C	6.14	1.60	1.52
1	A	645	ASN	CA-C	-6.13	1.44	1.52
1	B	425	VAL	C-O	6.12	1.30	1.24
1	B	337	ASP	CG-OD1	6.11	1.36	1.25
1	A	401	ALA	CA-CB	6.09	1.62	1.53
1	A	359	ASP	CA-C	6.06	1.61	1.52
1	B	613	ALA	C-O	-6.05	1.17	1.24
1	A	453	ASP	C-O	-6.05	1.15	1.23
1	A	396	GLN	CD-NE2	6.03	1.46	1.33
1	B	556	MET	N-CA	6.03	1.54	1.46
1	A	661	MET	C-O	6.02	1.31	1.23
1	B	529	ARG	CA-C	6.02	1.61	1.52
1	A	582	GLN	N-CA	-6.01	1.38	1.46
1	A	387	GLY	CA-C	6.00	1.59	1.51
1	A	624	LEU	CG-CD1	5.99	1.72	1.52
1	B	434	ILE	N-CA	-5.98	1.39	1.46
1	A	587	SER	N-CA	5.96	1.53	1.46
1	A	451	ALA	C-O	5.96	1.31	1.24
1	B	649	ILE	C-O	5.95	1.30	1.23
1	B	697	MET	C-O	5.94	1.31	1.24
1	B	620	LEU	C-O	-5.93	1.16	1.24
1	B	421	GLU	CA-C	5.92	1.61	1.53
1	A	787	VAL	C-O	5.92	1.31	1.24
1	B	652	THR	CA-C	5.87	1.60	1.53
1	B	373	LYS	CA-C	5.87	1.60	1.52
1	B	452	PHE	CA-C	5.86	1.59	1.52
1	A	608	TYR	CA-CB	-5.86	1.44	1.53
1	B	580	TYR	C-O	-5.86	1.16	1.23
1	A	619	LEU	N-CA	5.85	1.53	1.46
1	A	391	THR	CA-C	5.84	1.60	1.52
1	A	730	LYS	CG-CD	5.82	1.70	1.52
1	B	760	LYS	CB-CG	5.82	1.70	1.52
1	B	514	ASN	C-O	-5.82	1.17	1.24
1	A	590	GLU	N-CA	5.81	1.53	1.46
1	A	741	VAL	CA-CB	5.81	1.62	1.54
1	B	432	GLY	C-O	-5.80	1.15	1.24
1	B	621	ARG	CA-C	-5.79	1.45	1.52
1	A	633	LYS	CE-NZ	5.78	1.66	1.49
1	B	598	TYR	CA-C	5.78	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	465	LEU	C-O	5.77	1.31	1.24
1	B	765	ALA	CA-CB	5.77	1.62	1.53
1	A	750	GLY	C-O	5.76	1.31	1.23
1	A	650	GLY	N-CA	5.76	1.51	1.45
1	B	738	LYS	CA-CB	5.75	1.61	1.53
1	A	375	TYR	N-CA	5.75	1.53	1.46
1	A	633	LYS	CB-CG	5.75	1.69	1.52
1	A	661	MET	N-CA	5.74	1.53	1.46
1	B	564	VAL	C-O	-5.74	1.17	1.24
1	A	694	SER	N-CA	5.74	1.52	1.46
1	B	354	TYR	CA-C	5.74	1.60	1.52
1	B	387	GLY	CA-C	5.73	1.59	1.51
1	A	771	ALA	CA-C	-5.73	1.45	1.53
1	A	426	LEU	C-O	5.73	1.30	1.23
1	B	495	PRO	N-CA	5.73	1.52	1.46
1	A	457	SER	C-N	-5.72	1.28	1.34
1	B	422	VAL	CA-CB	5.72	1.63	1.55
1	A	581	HIS	N-CA	5.70	1.53	1.46
1	B	472	ILE	CA-CB	-5.70	1.47	1.54
1	B	730	LYS	CG-CD	5.70	1.69	1.52
1	A	417	THR	CA-CB	5.69	1.60	1.53
1	A	433	ALA	N-CA	5.69	1.53	1.46
1	B	109	THR	N-CA	5.68	1.52	1.46
1	A	652	THR	C-O	5.68	1.31	1.23
1	A	404	SER	CA-C	-5.66	1.45	1.52
1	B	720	ASP	CA-C	5.64	1.58	1.53
1	B	440	GLY	N-CA	5.64	1.52	1.45
1	A	623	VAL	N-CA	-5.63	1.40	1.46
1	B	537	GLY	CA-C	5.63	1.58	1.52
1	B	425	VAL	N-CA	-5.63	1.39	1.46
1	A	625	SER	C-O	-5.63	1.17	1.24
1	A	707	ALA	CA-CB	-5.63	1.45	1.53
1	B	373	LYS	C-O	5.60	1.30	1.24
1	A	429	ASN	C-O	-5.59	1.16	1.24
1	B	625	SER	CA-C	-5.58	1.45	1.52
1	A	566	GLN	N-CA	5.57	1.53	1.46
1	B	427	MET	CA-C	-5.55	1.45	1.52
1	B	753	VAL	CA-CB	5.55	1.62	1.54
1	B	109	THR	CA-C	5.55	1.59	1.52
1	A	565	ALA	CA-CB	-5.55	1.44	1.53
1	A	384	GLU	N-CA	5.54	1.53	1.46
1	A	486	TYR	N-CA	5.54	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	498	TYR	CA-C	-5.52	1.46	1.53
1	B	454	THR	CB-CG2	5.52	1.70	1.52
1	B	742	GLU	CA-CB	5.52	1.62	1.53
1	A	740	SER	CA-C	5.51	1.60	1.52
1	B	423	GLY	C-O	5.50	1.31	1.23
1	B	452	PHE	CA-CB	-5.50	1.46	1.54
1	A	584	HIS	CA-C	-5.49	1.45	1.52
1	A	749	THR	CA-C	5.48	1.59	1.52
1	A	440	GLY	CA-C	5.47	1.58	1.51
1	B	412	LEU	C-O	-5.46	1.17	1.24
1	B	443	TYR	CA-CB	-5.46	1.44	1.53
1	B	619	LEU	C-O	5.46	1.30	1.24
1	B	459	ALA	CA-CB	-5.45	1.44	1.53
1	A	398	ILE	C-O	5.45	1.30	1.24
1	B	624	LEU	C-O	5.44	1.30	1.24
1	B	724	VAL	CA-CB	5.44	1.60	1.54
1	A	387	GLY	N-CA	5.42	1.53	1.45
1	A	592	ALA	C-O	-5.42	1.17	1.24
1	A	787	VAL	N-CA	5.42	1.53	1.46
1	B	592	ALA	N-CA	5.41	1.53	1.46
1	A	787	VAL	CA-C	5.41	1.59	1.52
1	A	363	ALA	CA-CB	5.40	1.62	1.53
1	A	453	ASP	CA-C	5.39	1.57	1.52
1	B	593	ASP	CB-CG	5.39	1.65	1.52
1	A	617	GLN	C-O	5.38	1.30	1.24
1	B	591	ALA	CA-CB	-5.38	1.44	1.53
1	A	541	LYS	CA-CB	-5.37	1.44	1.53
1	A	609	SER	N-CA	5.35	1.53	1.46
1	A	583	LYS	C-O	-5.35	1.17	1.23
1	B	356	ALA	C-O	5.35	1.30	1.24
1	B	581	HIS	N-CA	5.34	1.52	1.46
1	B	518	ASN	C-O	5.34	1.30	1.24
1	A	484	SER	CA-C	-5.33	1.46	1.52
1	A	742	GLU	CA-CB	5.33	1.62	1.53
1	B	636	LEU	C-O	5.33	1.30	1.24
1	A	114	THR	N-CA	5.32	1.56	1.46
1	A	640	ASN	C-O	5.32	1.31	1.24
1	B	343	THR	N-CA	-5.31	1.40	1.46
1	B	415	ASP	C-O	-5.31	1.16	1.24
1	A	426	LEU	CA-C	-5.31	1.46	1.52
1	A	618	GLY	C-O	5.30	1.30	1.23
1	B	397	LYS	CA-C	5.30	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	749	THR	CB-CG2	5.29	1.70	1.52
1	A	392	THR	N-CA	5.29	1.52	1.45
1	A	590	GLU	C-O	5.28	1.30	1.23
1	A	436	GLY	N-CA	5.26	1.52	1.45
1	A	109	THR	CA-CB	5.25	1.60	1.53
1	A	111	SER	N-CA	5.24	1.52	1.46
1	A	663	LEU	N-CA	5.22	1.52	1.46
1	A	403	GLN	N-CA	5.22	1.52	1.46
1	A	760	LYS	CA-C	5.21	1.59	1.52
1	A	588	LYS	CD-CE	5.21	1.68	1.52
1	B	656	ASN	CA-C	-5.20	1.46	1.53
1	B	548	GLU	CD-OE1	5.20	1.35	1.25
1	B	696	TYR	CG-CD2	5.19	1.50	1.39
1	B	578	GLY	N-CA	-5.19	1.37	1.45
1	B	641	PRO	C-O	5.19	1.30	1.24
1	A	383	ILE	CA-CB	-5.18	1.47	1.54
1	A	421	GLU	C-O	5.18	1.30	1.23
1	A	391	THR	C-O	5.18	1.30	1.24
1	B	451	ALA	CA-CB	5.17	1.61	1.53
1	A	686	GLN	CA-C	5.17	1.59	1.52
1	A	640	ASN	N-CA	-5.17	1.38	1.46
1	A	454	THR	C-O	-5.14	1.17	1.23
1	A	778	ASP	CA-CB	5.14	1.61	1.53
1	A	364	LYS	CA-CB	5.14	1.60	1.53
1	B	576	ASN	N-CA	-5.13	1.40	1.46
1	B	646	ALA	N-CA	5.12	1.52	1.46
1	A	543	GLY	N-CA	5.12	1.52	1.45
1	B	477	MET	C-O	5.11	1.29	1.23
1	B	632	PHE	CD1-CE1	5.11	1.53	1.38
1	A	511	GLU	CA-C	5.10	1.59	1.52
1	A	376	ARG	CZ-NH1	5.10	1.39	1.32
1	A	675	TRP	CA-CB	5.09	1.67	1.54
1	A	448	ASN	C-O	5.09	1.30	1.23
1	B	435	LEU	N-CA	-5.09	1.39	1.46
1	B	511	GLU	CD-OE2	5.09	1.35	1.25
1	B	711	ILE	CG1-CD1	5.09	1.71	1.51
1	B	613	ALA	CA-CB	5.08	1.61	1.53
1	A	420	VAL	CA-C	-5.08	1.46	1.52
1	A	666	SER	N-CA	5.08	1.52	1.45
1	A	726	SER	CA-C	-5.08	1.46	1.52
1	B	674	GLY	N-CA	5.08	1.52	1.45
1	A	707	ALA	CA-C	-5.07	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	467	ALA	N-CA	-5.07	1.39	1.46
1	A	735	LYS	C-N	5.07	1.40	1.33
1	A	736	PRO	CA-C	5.06	1.59	1.52
1	B	446	ASN	N-CA	5.06	1.52	1.46
1	B	643	LEU	N-CA	5.06	1.52	1.46
1	A	624	LEU	C-O	-5.06	1.18	1.24
1	B	675	TRP	CA-C	-5.06	1.46	1.52
1	A	711	ILE	C-O	-5.06	1.18	1.24
1	A	370	ALA	CA-CB	5.04	1.61	1.53
1	B	502	LYS	CA-C	-5.03	1.45	1.52
1	B	739	VAL	N-CA	5.03	1.52	1.46
1	A	744	LYS	CA-CB	5.02	1.61	1.53
1	B	698	ALA	CA-CB	5.02	1.61	1.53
1	B	706	GLN	CB-CG	5.02	1.67	1.52
1	B	525	TYR	CA-C	5.01	1.59	1.52
1	B	693	ASN	C-O	5.01	1.30	1.24
1	A	527	MET	N-CA	-5.01	1.40	1.46
1	A	786	ILE	CG1-CD1	5.01	1.71	1.51
1	B	721	PRO	CA-C	5.00	1.60	1.52

All (255) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	THR	N-CA-C	11.59	127.23	109.96
1	B	635	ASN	N-CA-C	-11.00	99.37	111.36
1	A	635	ASN	N-CA-C	-10.69	98.76	112.23
1	B	750	GLY	N-CA-C	-10.43	95.45	110.88
1	B	560	ILE	CB-CA-C	-9.94	95.20	110.50
1	A	560	ILE	CB-CA-C	-9.87	95.92	110.62
1	B	494	ASN	CA-C-N	-9.57	110.22	120.66
1	B	494	ASN	C-N-CA	-9.57	110.22	120.66
1	A	597	VAL	CB-CA-C	-9.36	99.70	112.24
1	B	339	LEU	N-CA-C	-9.13	101.28	111.14
1	B	432	GLY	N-CA-C	-8.89	104.51	115.08
1	B	708	SER	CA-C-N	-8.74	110.78	119.87
1	B	708	SER	C-N-CA	-8.74	110.78	119.87
1	A	603	LYS	CA-C-N	8.72	128.74	119.76
1	A	603	LYS	C-N-CA	8.72	128.74	119.76
1	A	749	THR	N-CA-C	8.69	119.39	108.45
1	B	371	THR	N-CA-CB	8.68	125.15	110.49
1	B	370	ALA	CA-C-N	-8.13	106.01	121.54
1	B	370	ALA	C-N-CA	-8.13	106.01	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	739	VAL	N-CA-C	8.08	119.73	107.77
1	A	376	ARG	N-CA-C	-8.01	102.63	111.36
1	B	518	ASN	N-CA-C	8.00	121.53	111.69
1	B	597	VAL	CB-CA-C	-7.87	100.55	111.65
1	B	568	THR	N-CA-C	-7.73	101.85	111.75
1	A	615	ILE	N-CA-C	-7.53	103.11	110.72
1	A	683	SER	N-CA-C	7.47	121.16	109.96
1	B	686	GLN	N-CA-C	7.43	120.03	111.11
1	A	751	SER	N-CA-CB	7.39	120.51	110.38
1	A	739	VAL	N-CA-C	7.39	118.76	108.12
1	B	107	GLU	N-CA-C	7.37	120.42	108.34
1	B	650	GLY	N-CA-C	7.36	121.86	111.19
1	B	472	ILE	N-CA-C	-7.35	103.13	110.62
1	A	468	TYR	CA-C-N	-7.29	111.03	120.14
1	A	468	TYR	C-N-CA	-7.29	111.03	120.14
1	B	783	TRP	N-CA-C	7.19	122.32	112.90
1	B	468	TYR	CA-C-N	-7.07	111.30	120.14
1	B	468	TYR	C-N-CA	-7.07	111.30	120.14
1	B	656	ASN	CA-C-N	-7.05	108.08	121.54
1	B	656	ASN	C-N-CA	-7.05	108.08	121.54
1	A	451	ALA	N-CA-C	-6.96	102.78	112.45
1	A	432	GLY	N-CA-C	-6.90	106.66	115.42
1	A	404	SER	CB-CA-C	-6.89	99.14	110.85
1	B	370	ALA	O-C-N	-6.88	114.89	123.01
1	A	585	VAL	CB-CA-C	-6.87	105.02	111.06
1	A	384	GLU	N-CA-CB	6.85	122.37	110.39
1	B	376	ARG	N-CA-C	-6.83	103.91	111.36
1	B	688	ALA	N-CA-C	6.83	119.57	111.71
1	B	403	GLN	N-CA-C	6.83	118.72	111.28
1	A	697	MET	CG-SD-CE	-6.81	85.91	100.90
1	A	362	SER	N-CA-C	6.77	119.30	110.43
1	A	727	GLU	CA-C-N	-6.75	114.22	123.46
1	A	727	GLU	C-N-CA	-6.75	114.22	123.46
1	B	594	GLY	CA-C-N	-6.72	111.17	120.71
1	B	594	GLY	C-N-CA	-6.72	111.17	120.71
1	B	672	LEU	N-CA-C	-6.70	97.44	108.76
1	A	551	ILE	CA-C-N	-6.67	110.82	120.29
1	A	551	ILE	C-N-CA	-6.67	110.82	120.29
1	B	512	ALA	N-CA-C	-6.66	103.94	111.07
1	B	603	LYS	CA-C-N	6.66	126.58	119.85
1	B	603	LYS	C-N-CA	6.66	126.58	119.85
1	B	624	LEU	N-CA-C	6.63	118.17	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	604	PRO	CB-CA-C	-6.61	102.93	111.46
1	B	551	ILE	CA-C-N	-6.57	110.32	120.31
1	B	551	ILE	C-N-CA	-6.57	110.32	120.31
1	A	391	THR	N-CA-C	6.57	118.99	108.41
1	B	466	LEU	N-CA-C	-6.57	105.40	113.41
1	B	615	ILE	N-CA-C	-6.51	104.41	110.53
1	B	396	GLN	N-CA-C	6.51	118.17	111.14
1	A	613	ALA	N-CA-C	-6.50	104.28	111.36
1	B	545	GLU	CA-C-N	-6.49	117.68	123.33
1	B	545	GLU	C-N-CA	-6.49	117.68	123.33
1	A	428	ASP	N-CA-C	6.48	119.12	109.59
1	A	375	TYR	N-CA-C	6.39	119.92	111.75
1	A	502	LYS	N-CA-C	-6.38	105.46	113.18
1	B	387	GLY	N-CA-C	6.37	124.10	114.61
1	A	625	SER	CB-CA-C	-6.33	99.92	110.68
1	B	763	ALA	CA-C-N	-6.33	111.93	119.84
1	B	763	ALA	C-N-CA	-6.33	111.93	119.84
1	B	574	LEU	CB-CG-CD1	-6.29	91.82	110.70
1	A	498	TYR	N-CA-C	-6.28	96.94	107.80
1	A	518	ASN	N-CA-C	6.26	119.39	111.69
1	B	462	THR	CA-C-N	-6.26	112.62	120.06
1	B	462	THR	C-N-CA	-6.26	112.62	120.06
1	A	656	ASN	CA-C-N	-6.25	109.60	121.54
1	A	656	ASN	C-N-CA	-6.25	109.60	121.54
1	A	750	GLY	N-CA-C	-6.23	98.42	113.18
1	B	371	THR	CB-CA-C	-6.21	98.07	110.42
1	A	387	GLY	N-CA-C	6.19	123.45	114.10
1	B	419	ARG	CB-CA-C	6.19	119.12	109.84
1	B	786	ILE	CA-C-N	6.17	133.07	121.97
1	B	786	ILE	C-N-CA	6.17	133.07	121.97
1	B	707	ALA	N-CA-C	-6.16	105.92	113.50
1	A	346[A]	GLU	N-CA-C	-6.16	104.47	112.23
1	A	346[B]	GLU	N-CA-C	-6.16	104.47	112.23
1	A	357	GLN	N-CA-C	-6.16	105.89	113.41
1	B	400	SER	CB-CA-C	-6.15	100.40	110.85
1	A	574	LEU	N-CA-C	-6.14	104.67	111.36
1	B	751	SER	CB-CA-C	6.13	122.25	109.68
1	B	533	VAL	CB-CA-C	-6.13	101.94	111.26
1	A	107	GLU	N-CA-C	6.11	119.50	108.69
1	B	347	ALA	N-CA-C	-6.11	104.53	111.07
1	A	457	SER	CA-C-N	-6.10	113.45	120.04
1	A	457	SER	C-N-CA	-6.10	113.45	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	663	LEU	CA-C-O	-6.08	113.76	120.33
1	B	777	ALA	N-CA-C	6.08	118.69	111.33
1	B	692	ASN	CA-C-O	6.07	127.19	120.82
1	B	337	ASP	CB-CG-OD2	-6.05	104.48	118.40
1	B	662	TRP	CA-C-N	-6.01	114.33	122.86
1	B	662	TRP	C-N-CA	-6.01	114.33	122.86
1	A	399	HIS	CA-C-N	-6.01	111.76	120.29
1	A	399	HIS	C-N-CA	-6.01	111.76	120.29
1	B	472	ILE	CB-CA-C	-6.00	104.03	112.14
1	B	683	SER	N-CA-C	6.00	119.17	110.28
1	A	466	LEU	N-CA-C	-5.98	106.52	113.88
1	A	648	TRP	CA-C-O	-5.98	114.23	121.05
1	B	778	ASP	N-CA-C	-5.95	104.37	111.69
1	A	656	ASN	N-CA-C	-5.93	102.87	110.53
1	B	441	ARG	N-CA-C	5.93	118.53	111.71
1	B	576	ASN	N-CA-C	-5.93	103.43	111.55
1	A	414	ASP	CA-C-N	-5.88	113.26	122.73
1	A	414	ASP	C-N-CA	-5.88	113.26	122.73
1	B	666	SER	N-CA-C	5.78	118.19	109.23
1	B	765	ALA	CA-C-O	-5.78	114.99	121.81
1	B	751	SER	N-CA-CB	5.74	118.57	110.36
1	A	614	THR	CA-C-N	-5.73	112.29	120.42
1	A	614	THR	C-N-CA	-5.73	112.29	120.42
1	A	442	ASN	CB-CA-C	-5.71	99.06	110.42
1	A	770	PHE	N-CA-C	-5.71	105.42	112.90
1	A	692	ASN	N-CA-C	5.70	117.95	111.11
1	B	344	LEU	CB-CA-C	-5.70	101.69	110.81
1	B	712	TRP	N-CA-C	-5.66	106.21	113.23
1	B	577	ASN	N-CA-C	5.64	119.22	111.54
1	A	728	VAL	N-CA-C	5.62	115.39	108.53
1	A	110	TYR	CB-CA-C	-5.60	99.28	110.42
1	A	593	ASP	N-CA-C	-5.57	105.80	112.59
1	B	638	SER	CA-C-N	-5.57	111.40	121.14
1	B	638	SER	C-N-CA	-5.57	111.40	121.14
1	A	688	ALA	CA-C-O	-5.56	114.62	120.63
1	A	561	GLU	CB-CG-CD	-5.54	103.18	112.60
1	B	416	GLY	N-CA-C	-5.54	107.02	115.00
1	A	515	TYR	N-CA-C	-5.52	106.71	113.50
1	B	468	TYR	N-CA-C	5.51	117.37	111.36
1	A	354	TYR	N-CA-C	5.51	116.96	111.07
1	B	453	ASP	CA-C-N	-5.51	113.05	120.87
1	B	453	ASP	C-N-CA	-5.51	113.05	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	578	GLY	N-CA-C	5.50	122.68	115.47
1	A	598	TYR	N-CA-C	5.50	118.15	108.75
1	A	638	SER	CB-CA-C	-5.50	100.12	110.67
1	B	629	THR	N-CA-C	-5.50	106.58	113.72
1	B	723	VAL	N-CA-C	-5.50	102.49	109.80
1	A	715	GLU	N-CA-C	5.49	117.62	110.43
1	B	109	THR	N-CA-C	5.49	117.91	109.07
1	A	580	TYR	CA-C-N	-5.49	113.84	122.73
1	A	580	TYR	C-N-CA	-5.49	113.84	122.73
1	A	403	GLN	N-CA-C	5.48	117.33	111.36
1	A	110	TYR	N-CA-CB	-5.47	101.24	110.49
1	A	354	TYR	CA-C-N	5.45	127.53	120.44
1	A	354	TYR	C-N-CA	5.45	127.53	120.44
1	A	673	GLY	CA-C-O	-5.45	116.38	121.18
1	A	444	GLN	N-CA-C	5.44	117.96	111.71
1	A	478	GLY	N-CA-C	-5.44	103.02	111.12
1	A	778	ASP	N-CA-CB	5.43	118.67	110.30
1	A	564	VAL	CB-CA-C	-5.43	104.73	112.22
1	A	394	ILE	N-CA-C	5.43	117.45	109.63
1	B	541	LYS	N-CA-C	-5.42	105.53	111.82
1	B	633	LYS	N-CA-C	-5.42	105.48	111.71
1	B	548	GLU	CG-CD-OE2	-5.40	105.98	118.40
1	B	371	THR	OG1-CB-CG2	-5.38	98.54	109.30
1	A	633	LYS	N-CA-CB	5.37	118.63	110.14
1	B	394	ILE	CB-CA-C	-5.37	103.09	111.26
1	B	498	TYR	N-CA-C	-5.37	96.48	107.70
1	A	111	SER	N-CA-C	5.36	122.23	110.80
1	B	337	ASP	CB-CG-OD1	5.36	130.73	118.40
1	A	348	GLN	N-CA-C	5.36	117.56	111.02
1	B	545	GLU	CA-CB-CG	-5.35	103.40	114.10
1	B	632	PHE	N-CA-C	5.35	116.92	111.14
1	A	568	THR	N-CA-C	-5.35	105.56	111.71
1	B	371	THR	CA-C-N	-5.35	112.80	120.82
1	B	371	THR	C-N-CA	-5.35	112.80	120.82
1	A	629	THR	O-C-N	-5.34	115.78	122.24
1	B	368	ASN	N-CA-C	5.34	117.43	109.59
1	B	447	GLN	N-CA-C	5.33	119.78	113.28
1	A	563	THR	CA-C-O	-5.32	115.67	121.89
1	B	389	LYS	CD-CE-NZ	5.32	128.91	111.90
1	A	720	ASP	N-CA-C	5.31	116.38	109.64
1	B	579	VAL	CB-CA-C	-5.29	103.73	110.98
1	A	564	VAL	CA-C-O	5.29	126.46	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ARG	N-CA-CB	5.28	117.97	110.16
1	B	414	ASP	CA-C-N	-5.28	114.20	122.49
1	B	414	ASP	C-N-CA	-5.28	114.20	122.49
1	B	737	GLY	N-CA-C	5.27	118.28	110.42
1	B	421	GLU	CG-CD-OE1	5.26	130.51	118.40
1	B	629	THR	O-C-N	-5.25	115.89	122.35
1	A	511	GLU	CB-CA-C	5.24	119.75	110.85
1	B	375	TYR	N-CA-C	5.24	117.73	111.71
1	A	556	MET	CG-SD-CE	-5.22	89.41	100.90
1	B	770	PHE	N-CA-C	-5.22	105.65	112.23
1	A	587	SER	N-CA-CB	5.21	118.08	110.47
1	B	776	ASP	CB-CA-C	5.21	119.44	110.79
1	B	389	LYS	N-CA-C	-5.20	100.04	108.52
1	B	614	THR	CA-C-N	-5.20	113.90	120.56
1	B	614	THR	C-N-CA	-5.20	113.90	120.56
1	A	650	GLY	N-CA-C	5.20	117.86	110.74
1	A	337	ASP	N-CA-C	5.20	125.55	111.00
1	B	780	GLN	CB-CA-C	5.19	119.91	110.11
1	A	622	GLU	CB-CA-C	-5.19	99.15	109.99
1	A	646	ALA	CA-C-N	-5.18	114.38	122.16
1	A	646	ALA	C-N-CA	-5.18	114.38	122.16
1	B	398	ILE	CB-CA-C	-5.18	105.07	112.22
1	B	422	VAL	N-CA-C	5.18	115.83	108.42
1	A	339	LEU	CD1-CG-CD2	5.18	122.19	110.80
1	A	778	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	692	ASN	N-CA-C	5.16	116.59	111.07
1	B	405	ALA	CA-C-N	-5.16	113.40	120.46
1	B	405	ALA	C-N-CA	-5.16	113.40	120.46
1	B	572	GLN	N-CA-C	-5.15	104.93	111.11
1	B	349	GLU	CB-CG-CD	-5.14	103.86	112.60
1	B	421	GLU	CA-C-O	-5.14	115.36	121.89
1	A	109	THR	N-CA-C	5.14	117.09	107.99
1	A	505	GLY	CA-C-O	-5.13	116.80	121.72
1	B	782	ALA	CA-C-N	-5.12	112.11	121.52
1	B	782	ALA	C-N-CA	-5.12	112.11	121.52
1	A	463	LYS	CA-C-N	-5.11	113.77	119.19
1	A	463	LYS	C-N-CA	-5.11	113.77	119.19
1	B	451	ALA	N-CA-C	-5.11	106.73	113.12
1	B	478	GLY	N-CA-C	-5.11	103.64	111.10
1	B	681	ASN	CA-C-N	-5.11	112.40	121.29
1	B	681	ASN	C-N-CA	-5.11	112.40	121.29
1	A	530	GLU	N-CA-CB	5.10	117.54	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	LEU	CB-CA-C	-5.09	100.93	109.48
1	B	765	ALA	N-CA-C	-5.09	103.68	110.55
1	A	455	LYS	N-CA-CB	-5.09	102.14	110.68
1	A	349	GLU	CB-CG-CD	-5.08	103.96	112.60
1	A	555	PRO	N-CA-C	-5.08	106.80	113.65
1	A	581	HIS	N-CA-C	-5.07	100.78	109.24
1	A	669	ARG	CB-CG-CD	-5.06	99.66	111.30
1	B	651	LYS	CA-C-N	-5.06	113.92	122.67
1	B	651	LYS	C-N-CA	-5.06	113.92	122.67
1	B	364	LYS	N-CA-C	5.06	117.19	111.02
1	A	595	ARG	CA-C-N	-5.05	116.31	122.93
1	A	595	ARG	C-N-CA	-5.05	116.31	122.93
1	A	607	VAL	N-CA-C	5.05	115.72	110.82
1	B	586	ILE	CB-CA-C	-5.05	104.30	111.21
1	B	579	VAL	N-CA-C	5.04	115.35	107.99
1	B	571	TYR	N-CA-C	-5.04	105.88	112.23
1	A	590	GLU	N-CA-C	-5.04	100.82	109.24
1	A	684	LEU	N-CA-C	-5.04	104.03	110.53
1	A	469	GLY	O-C-N	-5.03	116.90	122.24
1	B	337	ASP	N-CA-C	5.03	125.09	111.00
1	A	699	HIS	CA-C-N	-5.03	113.54	120.28
1	A	699	HIS	C-N-CA	-5.03	113.54	120.28
1	B	731	SER	N-CA-C	5.02	118.67	112.54
1	A	579	VAL	N-CA-C	5.02	115.56	107.73
1	B	541	LYS	CB-CG-CD	5.01	122.83	111.30
1	B	656	ASN	N-CA-C	-5.01	104.07	110.53

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	THR	Peptide
1	A	112	ASP	Peptide
1	A	337	ASP	Peptide
1	A	760	LYS	Peptide
1	B	666	SER	Peptide
1	B	759	ASN	Peptide
1	B	760	LYS	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	3555	0	3386	163	0
1	B	3553	0	3390	136	0
2	A	19	0	11	0	0
2	B	19	0	11	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	2	0	0	1	0
4	B	2	0	0	0	0
5	A	36	0	0	3	0
5	B	43	0	0	4	0
All	All	7239	0	6798	297	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 21.

All (297) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LEU:CG	1:A:366:LEU:CD2	1.75	1.62
1:B:115:VAL:CB	1:B:115:VAL:CA	1.80	1.59
1:A:601:GLN:CB	1:A:601:GLN:CA	1.74	1.58
1:A:346[A]:GLU:CG	1:A:346[A]:GLU:CB	1.82	1.57
1:A:454:THR:CB	1:A:454:THR:CG2	1.75	1.56
1:B:463:LYS:NZ	1:B:463:LYS:CE	1.69	1.55
1:B:541:LYS:CE	1:B:541:LYS:NZ	1.72	1.52
1:B:471:ALA:HB3	1:B:477:MET:HE3	1.26	1.10
1:A:526:ARG:HH11	1:A:526:ARG:CG	1.69	1.04
1:A:526:ARG:HG3	1:A:526:ARG:NH1	1.60	0.99
1:A:783:TRP:O	1:A:787:VAL:HG23	1.62	0.99
1:B:108:ILE:HG21	1:B:343:THR:HG21	1.47	0.96
1:B:370:ALA:O	1:B:371:THR:CB	2.13	0.94
1:B:680:ASP:OD1	1:B:682:HIS:HD2	1.53	0.91
1:A:526:ARG:HH11	1:A:526:ARG:HG3	0.78	0.91
1:B:766:THR:CG2	1:B:767:SER:N	2.34	0.89
1:B:471:ALA:HB3	1:B:477:MET:CE	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:766:THR:HG22	1:B:767:SER:N	1.91	0.84
1:B:734:GLN:HB3	1:B:766:THR:HA	1.58	0.83
1:B:485:ASN:HD22	1:B:519:ILE:HB	1.42	0.82
1:A:108:ILE:HG21	1:A:343:THR:HG21	1.59	0.82
1:A:366:LEU:CD2	1:A:366:LEU:HG	2.05	0.81
1:B:471:ALA:CB	1:B:477:MET:HE3	2.08	0.81
1:B:656:ASN:O	1:B:657:GLN:HB2	1.81	0.81
1:B:766:THR:CG2	1:B:767:SER:H	1.95	0.80
1:B:337:ASP:HB2	5:B:2002:HOH:O	1.82	0.79
1:B:737:GLY:O	1:B:748:VAL:HG22	1.83	0.78
1:A:680:ASP:OD1	1:A:682:HIS:HD2	1.66	0.78
1:A:108:ILE:CG2	1:A:343:THR:HG21	2.14	0.78
1:A:783:TRP:O	1:A:787:VAL:CG2	2.31	0.78
1:B:108:ILE:CG2	1:B:343:THR:HG21	2.14	0.77
1:A:485:ASN:HD22	1:A:519:ILE:HB	1.49	0.76
1:A:766:THR:HG22	1:A:767:SER:N	1.99	0.76
1:A:635:ASN:HB3	1:B:638:SER:OG	1.85	0.76
1:B:485:ASN:ND2	1:B:519:ILE:HB	2.01	0.76
1:B:729:LEU:HD21	1:B:736:PRO:HB3	1.68	0.76
1:A:110:TYR:CE1	1:A:396:GLN:HA	2.21	0.76
1:A:476:LEU:HD13	1:A:527:MET:HE3	1.67	0.75
1:A:352:TYR:OH	1:A:366:LEU:HD21	1.86	0.75
1:B:417:THR:OG1	1:B:678:HIS:HE1	1.68	0.75
1:B:481:THR:HG22	1:B:482:ILE:N	2.01	0.75
1:A:729:LEU:O	1:A:731:SER:N	2.20	0.74
1:B:728:VAL:O	1:B:752:THR:HB	1.88	0.74
1:A:728:VAL:O	1:A:752:THR:HB	1.86	0.73
1:B:737:GLY:O	1:B:748:VAL:CG2	2.37	0.72
1:B:370:ALA:O	1:B:371:THR:HB	1.87	0.72
1:A:110:TYR:CG	1:A:396:GLN:HG2	2.25	0.72
1:B:766:THR:HG23	1:B:767:SER:H	1.53	0.72
1:B:471:ALA:CB	1:B:477:MET:CE	2.68	0.71
1:B:729:LEU:O	1:B:730:LYS:C	2.32	0.70
1:B:526:ARG:HG3	1:B:526:ARG:HH11	1.57	0.70
1:A:766:THR:CG2	1:A:767:SER:N	2.55	0.70
1:A:481:THR:HG22	1:A:482:ILE:N	2.07	0.70
1:B:544:TYR:OH	1:B:567:HIS:HD2	1.75	0.69
1:B:640:ASN:HD22	1:B:640:ASN:C	2.01	0.69
1:A:729:LEU:O	1:A:730:LYS:C	2.36	0.68
1:B:680:ASP:OD1	1:B:682:HIS:CD2	2.44	0.68
1:A:417:THR:OG1	1:A:678:HIS:HE1	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:THR:OG1	1:A:567:HIS:HE1	1.77	0.67
1:A:734:GLN:HE22	1:A:770:PHE:HA	1.59	0.67
1:A:476:LEU:CD1	1:A:527:MET:HE3	2.25	0.67
1:A:472:ILE:HG13	1:A:477:MET:HG3	1.77	0.66
1:B:779:TYR:O	1:B:783:TRP:HD1	1.78	0.66
1:B:656:ASN:O	1:B:657:GLN:CB	2.34	0.66
1:A:734:GLN:HB3	1:A:766:THR:HA	1.77	0.66
1:B:461:THR:OG1	1:B:567:HIS:HE1	1.78	0.66
1:B:337:ASP:CB	5:B:2002:HOH:O	2.42	0.65
1:B:769:ARG:HA	1:B:779:TYR:CE1	2.31	0.65
1:B:557:GLY:HA2	1:B:560:ILE:HG13	1.79	0.65
1:A:737:GLY:O	1:A:748:VAL:HG23	1.97	0.65
1:A:485:ASN:ND2	1:A:519:ILE:HB	2.11	0.64
1:B:481:THR:CG2	1:B:482:ILE:N	2.61	0.64
1:B:720:ASP:O	1:B:723:VAL:HG23	1.98	0.63
1:B:394:ILE:HD13	1:B:434:ILE:O	1.99	0.63
1:B:480:GLU:HB2	1:B:755:SER:HB2	1.80	0.63
1:B:643:LEU:HD13	1:B:705:GLN:HG3	1.81	0.63
1:A:645:ASN:O	1:A:716:ARG:NH2	2.32	0.63
1:A:544:TYR:OH	1:A:567:HIS:HD2	1.81	0.63
1:B:110:TYR:CD1	1:B:396:GLN:HB2	2.34	0.63
1:A:496:ILE:HG21	1:A:519:ILE:HG13	1.80	0.62
1:B:399:HIS:HD2	1:B:437:PHE:H	1.48	0.61
1:A:786:ILE:O	1:A:786:ILE:CG2	2.48	0.61
1:B:734:GLN:CB	1:B:766:THR:HA	2.30	0.60
1:A:454:THR:CG2	1:A:454:THR:CA	2.72	0.60
1:B:741:VAL:HG21	1:B:746:VAL:HG23	1.82	0.60
1:B:786:ILE:O	1:B:786:ILE:HG22	2.01	0.60
1:A:382:GLU:OE1	1:A:388:TYR:OH	2.17	0.60
1:A:734:GLN:NE2	1:A:770:PHE:HB2	2.17	0.59
1:A:734:GLN:HE22	1:A:770:PHE:CB	2.14	0.59
1:B:554:LEU:HB3	1:B:555:PRO:CD	2.32	0.59
1:B:115:VAL:CA	1:B:115:VAL:HB	2.17	0.59
1:B:569:ASN:ND2	1:B:583:LYS:H	2.01	0.59
1:B:417:THR:O	1:B:682:HIS:HE1	1.85	0.59
1:A:734:GLN:CB	1:A:766:THR:HA	2.32	0.59
1:A:585:VAL:O	1:A:585:VAL:CG1	2.48	0.58
1:A:417:THR:O	1:A:682:HIS:HE1	1.87	0.58
1:A:769:ARG:HA	1:A:779:TYR:CE1	2.38	0.58
1:B:645:ASN:O	1:B:716:ARG:NH2	2.37	0.58
1:A:476:LEU:HB3	1:A:527:MET:CE	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LEU:CB	1:A:527:MET:CE	2.82	0.57
1:A:536:LYS:O	1:A:540:GLU:HG3	2.04	0.57
1:A:651:LYS:HE3	5:A:2023:HOH:O	2.03	0.57
1:B:434:ILE:O	1:B:434:ILE:HG22	2.04	0.57
1:B:779:TYR:O	1:B:783:TRP:CD1	2.56	0.57
1:A:476:LEU:CB	1:A:527:MET:HE1	2.34	0.57
1:B:569:ASN:HD21	1:B:583:LYS:H	1.53	0.57
1:B:735:LYS:HB2	1:B:765:ALA:HA	1.87	0.57
1:B:507:MET:HB2	1:B:511:GLU:HG2	1.87	0.57
1:B:640:ASN:ND2	1:B:643:LEU:H	2.02	0.57
1:A:525:TYR:HB2	1:A:555:PRO:HG3	1.85	0.57
1:A:471:ALA:HB3	1:A:477:MET:HE3	1.86	0.56
1:A:601:GLN:CB	1:A:601:GLN:C	2.72	0.56
1:A:650:GLY:HA3	1:A:664:MET:O	2.05	0.56
1:A:399:HIS:O	1:A:403:GLN:HG2	2.06	0.56
1:A:785:SER:C	1:A:787:VAL:H	2.14	0.56
1:B:667:THR:HB	1:B:668:PRO:CD	2.36	0.56
1:A:640:ASN:C	1:A:640:ASN:HD22	2.14	0.56
1:B:536:LYS:O	1:B:540:GLU:HG3	2.05	0.56
1:A:496:ILE:CG2	1:A:519:ILE:HG13	2.36	0.55
1:A:729:LEU:C	1:A:731:SER:N	2.62	0.55
1:B:729:LEU:O	1:B:731:SER:N	2.39	0.55
1:A:466:LEU:HD12	1:A:539:MET:HE2	1.88	0.55
1:B:526:ARG:NE	1:B:530:GLU:OE2	2.36	0.55
1:B:110:TYR:CG	1:B:396:GLN:HB2	2.42	0.55
1:A:657:GLN:HB2	1:A:659:GLU:OE2	2.07	0.55
1:B:786:ILE:O	1:B:786:ILE:CG2	2.55	0.54
1:A:366:LEU:CD2	1:A:366:LEU:CD1	2.79	0.54
1:A:677:GLY:HA2	1:A:684:LEU:HD11	1.89	0.54
1:A:729:LEU:C	1:A:731:SER:H	2.15	0.54
1:A:481:THR:CG2	1:A:482:ILE:N	2.71	0.54
1:A:585:VAL:O	1:A:585:VAL:HG13	2.07	0.54
1:A:569:ASN:HD21	1:A:583:LYS:H	1.55	0.54
1:B:765:ALA:O	1:B:766:THR:O	2.26	0.54
1:A:533:VAL:HG12	1:A:534:ASP:N	2.21	0.53
1:A:734:GLN:HE22	1:A:770:PHE:CA	2.20	0.53
1:A:680:ASP:OD1	1:A:682:HIS:CD2	2.56	0.53
1:B:526:ARG:HG3	1:B:526:ARG:NH1	2.23	0.53
1:B:554:LEU:N	1:B:555:PRO:HD2	2.23	0.53
1:B:787:VAL:O	1:B:787:VAL:HG13	2.08	0.53
1:A:569:ASN:ND2	1:A:583:LYS:H	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:ASN:C	1:B:640:ASN:ND2	2.65	0.53
1:A:485:ASN:HD22	1:A:520:PRO:HD3	1.74	0.53
1:A:656:ASN:O	1:A:659:GLU:OE2	2.27	0.53
1:A:680:ASP:O	1:A:681:ASN:HB2	2.09	0.53
1:A:529:ARG:O	1:A:530:GLU:C	2.52	0.53
1:B:430:GLN:O	1:B:581:HIS:CD2	2.63	0.52
1:A:786:ILE:O	1:A:786:ILE:HG22	2.08	0.52
1:A:399:HIS:HD2	1:A:437:PHE:H	1.58	0.52
1:A:460:SER:HB3	1:A:463:LYS:HD2	1.91	0.52
1:A:476:LEU:HB2	1:A:527:MET:HE1	1.91	0.52
1:A:667:THR:HB	1:A:668:PRO:CD	2.40	0.51
1:B:533:VAL:HG12	1:B:534:ASP:N	2.26	0.51
1:B:106:SER:HB2	1:B:387:GLY:H	1.74	0.51
1:B:667:THR:HB	1:B:668:PRO:HD2	1.92	0.51
1:A:454:THR:CG2	1:A:454:THR:OG1	2.51	0.51
1:A:526:ARG:CG	1:A:526:ARG:NH1	2.44	0.51
1:A:526:ARG:HD3	1:A:530:GLU:CD	2.36	0.51
1:A:596:VAL:O	1:A:596:VAL:HG12	2.11	0.51
1:A:769:ARG:HA	1:A:779:TYR:CZ	2.45	0.51
1:A:110:TYR:CD1	1:A:396:GLN:HG2	2.45	0.51
1:A:766:THR:CG2	1:A:767:SER:H	2.24	0.50
1:A:393:THR:HB	1:A:433:ALA:HB1	1.92	0.50
1:B:442:ASN:HA	5:B:2011:HOH:O	2.11	0.50
1:B:490:PHE:CE2	1:B:496:ILE:HG12	2.47	0.50
1:B:529:ARG:O	1:B:530:GLU:C	2.53	0.50
1:B:399:HIS:CD2	1:B:437:PHE:H	2.30	0.50
1:B:352:TYR:OH	1:B:366:LEU:HD11	2.12	0.50
1:A:735:LYS:HB2	1:A:765:ALA:HA	1.94	0.49
1:B:367:LYS:NZ	1:B:367:LYS:HB2	2.27	0.49
1:A:419:ARG:O	1:A:678:HIS:CD2	2.65	0.49
1:A:741:VAL:HG21	1:A:746:VAL:HG23	1.95	0.49
1:B:351:MET:HE1	1:B:388:TYR:CE1	2.48	0.49
1:B:523:TRP:CG	1:B:773:GLY:HA3	2.47	0.49
1:A:424:ASN:O	1:A:437:PHE:HB2	2.13	0.49
1:A:502:LYS:HE3	1:A:502:LYS:HB2	1.51	0.49
1:B:741:VAL:CG2	1:B:746:VAL:HG23	2.42	0.49
1:A:450:HIS:HA	1:A:454:THR:OG1	2.13	0.49
1:A:554:LEU:N	1:A:555:PRO:CD	2.76	0.49
1:A:588:LYS:HA	1:A:598:TYR:O	2.13	0.48
1:A:640:ASN:ND2	1:A:643:LEU:H	2.10	0.48
1:B:107:GLU:OE2	1:B:115:VAL:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:TYR:OH	1:A:549:TYR:O	2.26	0.48
1:B:525:TYR:OH	1:B:549:TYR:O	2.28	0.48
1:B:466:LEU:HD21	1:B:525:TYR:CD1	2.48	0.48
1:B:656:ASN:O	1:B:659:GLU:OE2	2.31	0.48
1:B:769:ARG:HA	1:B:779:TYR:CZ	2.49	0.48
1:B:594:GLY:O	1:B:595:ARG:C	2.55	0.48
1:A:426:LEU:HD22	1:A:704:ILE:HD13	1.94	0.48
1:A:663:LEU:HB3	1:A:697:MET:SD	2.54	0.47
1:B:525:TYR:O	1:B:528:LEU:N	2.47	0.47
1:A:340:TYR:CD1	1:A:340:TYR:C	2.91	0.47
1:B:780:GLN:HE21	1:B:781:ASN:N	2.12	0.47
1:A:409:TYR:HB3	1:A:412:LEU:HD12	1.96	0.47
1:B:468:TYR:O	1:B:469:GLY:C	2.51	0.47
1:A:399:HIS:CD2	1:A:437:PHE:H	2.32	0.47
1:A:720:ASP:O	1:A:723:VAL:HG23	2.14	0.47
1:B:743:GLY:O	1:B:744:LYS:CB	2.63	0.47
1:A:476:LEU:HB3	1:A:527:MET:HE1	1.94	0.47
1:A:727:GLU:OE2	1:A:727:GLU:HA	2.15	0.47
1:A:656:ASN:O	1:A:657:GLN:CB	2.61	0.47
1:B:460:SER:HB3	1:B:463:LYS:HE3	1.96	0.47
1:B:403:GLN:O	1:B:406:VAL:HG12	2.15	0.46
1:A:536:LYS:HB2	1:A:549:TYR:CZ	2.51	0.46
1:A:557:GLY:HA2	1:A:560:ILE:HG13	1.97	0.46
1:B:108:ILE:HG21	1:B:343:THR:CG2	2.33	0.46
1:A:351:MET:HE1	1:A:388:TYR:CE1	2.51	0.46
1:A:734:GLN:NE2	1:A:770:PHE:CB	2.77	0.46
1:B:370:ALA:O	1:B:371:THR:OG1	2.32	0.46
1:A:354:TYR:CG	1:A:597:VAL:HG13	2.51	0.46
1:A:472:ILE:CG1	1:A:477:MET:HG3	2.45	0.46
1:A:476:LEU:CB	1:A:527:MET:HE3	2.47	0.46
1:A:640:ASN:C	1:A:640:ASN:ND2	2.74	0.46
1:B:715:GLU:CD	1:B:715:GLU:H	2.24	0.45
1:A:419:ARG:HH11	1:A:419:ARG:HD2	1.57	0.45
1:B:478:GLY:HA3	1:B:757:TRP:CE2	2.51	0.45
1:A:106:SER:HB2	1:A:387:GLY:H	1.81	0.45
1:A:462:THR:HB	1:A:555:PRO:O	2.17	0.45
1:A:344:LEU:HD12	1:A:344:LEU:HA	1.77	0.45
1:B:442:ASN:O	1:B:443:TYR:C	2.55	0.45
1:A:431:THR:O	1:A:584:HIS:HE1	1.99	0.45
1:A:601:GLN:CB	1:A:601:GLN:HA	2.18	0.45
1:B:476:LEU:HB3	1:B:527:MET:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:HA	1:A:413:LEU:HD23	1.68	0.45
1:A:594:GLY:O	1:A:595:ARG:C	2.58	0.45
1:A:720:ASP:O	1:A:721:PRO:C	2.60	0.45
1:A:635:ASN:CB	1:B:638:SER:OG	2.60	0.45
1:A:651:LYS:CE	5:A:2023:HOH:O	2.63	0.45
1:B:371:THR:O	1:B:372:GLN:C	2.60	0.45
1:B:471:ALA:O	1:B:472:ILE:C	2.59	0.44
1:B:368:ASN:O	1:B:369:GLU:C	2.56	0.44
1:B:431:THR:O	1:B:584:HIS:HE1	2.01	0.44
1:A:526:ARG:HD3	1:A:530:GLU:OE2	2.17	0.44
1:A:656:ASN:O	1:A:657:GLN:HB2	2.18	0.44
1:A:508:THR:O	1:A:509:LEU:C	2.60	0.44
1:B:462:THR:HB	1:B:555:PRO:O	2.18	0.44
1:A:523:TRP:CG	1:A:773:GLY:HA3	2.53	0.44
1:A:455:LYS:C	1:A:456:ARG:HG2	2.43	0.44
1:A:678:HIS:HD2	5:A:2005:HOH:O	2.00	0.44
1:B:481:THR:CG2	1:B:482:ILE:H	2.30	0.44
1:B:554:LEU:HB3	1:B:555:PRO:HD3	1.99	0.44
1:B:476:LEU:CB	1:B:527:MET:HE3	2.48	0.43
1:A:428:ASP:OD1	1:A:428:ASP:C	2.61	0.43
1:A:574:LEU:HD23	1:A:574:LEU:HA	1.81	0.43
1:A:468:TYR:O	1:A:469:GLY:C	2.59	0.43
1:B:631:THR:OG1	1:B:635:ASN:ND2	2.41	0.43
1:B:483:LEU:HB3	1:B:520:PRO:HB3	2.01	0.43
1:B:725:LYS:H	1:B:725:LYS:HG2	1.49	0.43
1:B:509:LEU:O	1:B:510:GLY:C	2.61	0.43
1:A:379:ALA:O	1:A:380:ALA:C	2.59	0.43
1:B:389:LYS:HB3	1:B:389:LYS:HE2	1.93	0.43
1:A:351:MET:HB3	1:A:379:ALA:HB1	2.01	0.43
1:A:481:THR:HG22	1:A:482:ILE:H	1.83	0.43
1:A:771:ALA:O	1:A:779:TYR:OH	2.36	0.43
1:B:537:GLY:O	1:B:541:LYS:HG3	2.19	0.43
1:A:616:MET:O	1:A:616:MET:HG3	2.17	0.43
1:B:367:LYS:HB2	1:B:367:LYS:HZ2	1.82	0.42
1:B:413:LEU:HD23	1:B:413:LEU:HA	1.79	0.42
1:B:636:LEU:HG	1:B:644:ALA:HB2	2.01	0.42
1:B:765:ALA:C	1:B:766:THR:O	2.62	0.42
1:B:369:GLU:H	1:B:369:GLU:HG3	1.61	0.42
1:B:476:LEU:HB3	1:B:527:MET:HE3	2.02	0.42
1:A:509:LEU:O	1:A:510:GLY:C	2.62	0.42
1:A:536:LYS:HB2	1:A:549:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:SER:O	1:B:463:LYS:HG3	2.20	0.42
1:B:765:ALA:O	1:B:766:THR:C	2.61	0.42
1:A:484:SER:O	1:A:519:ILE:HG22	2.19	0.42
1:A:508:THR:HG21	1:A:730:LYS:HE3	2.02	0.42
1:B:351:MET:HB3	1:B:379:ALA:HB1	2.01	0.42
1:B:455:LYS:C	1:B:456:ARG:HG2	2.44	0.42
1:A:525:TYR:O	1:A:528:LEU:N	2.52	0.42
1:A:551:ILE:O	1:A:552:GLU:C	2.61	0.42
1:A:755:SER:HB3	1:A:757:TRP:HE1	1.85	0.42
1:B:419:ARG:O	1:B:678:HIS:CD2	2.73	0.41
1:B:429:ASN:HA	1:B:572:GLN:HG2	2.02	0.41
1:B:610:LYS:HG2	5:B:2024:HOH:O	2.20	0.41
1:A:554:LEU:HB3	1:A:555:PRO:HD3	2.02	0.41
1:A:455:LYS:O	1:A:456:ARG:HG2	2.21	0.41
1:A:476:LEU:HB2	1:A:527:MET:CE	2.49	0.41
1:B:677:GLY:HA2	1:B:684:LEU:HD11	2.03	0.41
1:A:553:SER:O	1:A:554:LEU:C	2.61	0.41
1:B:455:LYS:O	1:B:456:ARG:HG2	2.21	0.41
1:A:633:LYS:HE3	4:A:1792:CL:CL	2.57	0.41
1:A:526:ARG:O	1:A:527:MET:C	2.61	0.41
1:B:591:ALA:O	1:B:593:ASP:N	2.54	0.41
1:A:697:MET:HE2	1:A:697:MET:HB3	1.62	0.41
1:A:768:TYR:CE2	1:A:783:TRP:CD1	3.09	0.41
1:A:730:LYS:HA	1:A:730:LYS:HD2	1.88	0.40
1:B:109:THR:C	1:B:110:TYR:O	2.64	0.40
1:B:476:LEU:O	1:B:477:MET:HB3	2.21	0.40
1:A:340:TYR:CD1	1:A:341:PHE:N	2.89	0.40
1:A:476:LEU:O	1:A:477:MET:HB3	2.21	0.40
1:A:533:VAL:CG1	1:A:534:ASP:N	2.84	0.40
1:A:759:ASN:OD1	1:A:759:ASN:C	2.65	0.40
1:B:523:TRP:CD2	1:B:773:GLY:HA3	2.57	0.40
1:A:483:LEU:HB3	1:A:520:PRO:HB3	2.02	0.40
1:A:636:LEU:O	1:A:637:THR:C	2.64	0.40
1:A:643:LEU:HD13	1:A:705:GLN:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	458/720 (64%)	404 (88%)	41 (9%)	13 (3%)	4	6
1	B	458/720 (64%)	417 (91%)	31 (7%)	10 (2%)	5	10
All	All	916/1440 (64%)	821 (90%)	72 (8%)	23 (2%)	4	8

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	TYR
1	A	111	SER
1	A	740	SER
1	A	744	LYS
1	B	110	TYR
1	B	371	THR
1	B	592	ALA
1	B	744	LYS
1	B	766	THR
1	B	787	VAL
1	A	592	ALA
1	A	730	LYS
1	A	742	GLU
1	A	743	GLY
1	A	766	THR
1	A	785	SER
1	B	730	LYS
1	B	743	GLY
1	B	742	GLU
1	A	787	VAL
1	A	786	ILE
1	A	644	ALA
1	B	786	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	375/590 (64%)	321 (86%)	54 (14%)	3	6
1	B	375/590 (64%)	327 (87%)	48 (13%)	4	8
All	All	750/1180 (64%)	648 (86%)	102 (14%)	3	7

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	SER
1	A	107	GLU
1	A	114	THR
1	A	362	SER
1	A	364	LYS
1	A	366	LEU
1	A	367	LYS
1	A	373	LYS
1	A	376	ARG
1	A	384	GLU
1	A	389	LYS
1	A	395	ASP
1	A	400	SER
1	A	488	THR
1	A	502	LYS
1	A	507	MET
1	A	511	GLU
1	A	526	ARG
1	A	536	LYS
1	A	545	GLU
1	A	560	ILE
1	A	585	VAL
1	A	587	SER
1	A	590	GLU
1	A	596	VAL
1	A	610	LYS
1	A	622	GLU

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Mol	Chain	Res	Type
1	A	625	SER
1	A	630	THR
1	A	640	ASN
1	A	651	LYS
1	A	656	ASN
1	A	659	GLU
1	A	687	GLN
1	A	701	VAL
1	A	711	ILE
1	A	725	LYS
1	A	726	SER
1	A	727	GLU
1	A	729	LEU
1	A	730	LYS
1	A	732	THR
1	A	734	GLN
1	A	739	VAL
1	A	742	GLU
1	A	745	GLU
1	A	746	VAL
1	A	749	THR
1	A	755	SER
1	A	760	LYS
1	A	778	ASP
1	A	780	GLN
1	A	785	SER
1	A	786	ILE
1	B	106	SER
1	B	114	THR
1	B	115	VAL
1	B	351	MET
1	B	364	LYS
1	B	365	GLU
1	B	366	LEU
1	B	367	LYS
1	B	373	LYS
1	B	376	ARG
1	B	384	GLU
1	B	389	LYS
1	B	395	ASP
1	B	396	GLN
1	B	419	ARG

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Mol	Chain	Res	Type
1	B	463	LYS
1	B	464	PRO
1	B	507	MET
1	B	511	GLU
1	B	526	ARG
1	B	560	ILE
1	B	585	VAL
1	B	610	LYS
1	B	624	LEU
1	B	630	THR
1	B	640	ASN
1	B	651	LYS
1	B	656	ASN
1	B	659	GLU
1	B	675	TRP
1	B	681	ASN
1	B	687	GLN
1	B	711	ILE
1	B	725	LYS
1	B	726	SER
1	B	730	LYS
1	B	732	THR
1	B	739	VAL
1	B	742	GLU
1	B	745	GLU
1	B	746	VAL
1	B	748	VAL
1	B	749	THR
1	B	760	LYS
1	B	767	SER
1	B	780	GLN
1	B	786	ILE
1	B	787	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	GLN
1	A	357	GLN
1	A	399	HIS
1	A	403	GLN
1	A	424	ASN

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Mol	Chain	Res	Type
1	A	444	GLN
1	A	447	GLN
1	A	448	ASN
1	A	485	ASN
1	A	494	ASN
1	A	567	HIS
1	A	569	ASN
1	A	640	ASN
1	A	656	ASN
1	A	657	GLN
1	A	678	HIS
1	A	682	HIS
1	A	734	GLN
1	B	399	HIS
1	B	403	GLN
1	B	429	ASN
1	B	447	GLN
1	B	448	ASN
1	B	485	ASN
1	B	567	HIS
1	B	569	ASN
1	B	606	GLN
1	B	635	ASN
1	B	640	ASN
1	B	678	HIS
1	B	682	HIS
1	B	686	GLN
1	B	687	GLN
1	B	692	ASN
1	B	705	GLN
1	B	706	GLN
1	B	734	GLN
1	B	780	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	1790	-	4,4,4	0.71	0	6,6,6	0.50	0
2	L4C	A	1789	1	15,18,19	0.97	0	15,22,24	5.50	9 (60%)
2	L4C	B	1789	1	15,18,19	1.23	1 (6%)	15,22,24	3.98	8 (53%)
3	SO4	A	1790	-	4,4,4	0.66	0	6,6,6	0.94	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	L4C	A	1789	1	-	10/20/21/23	-
2	L4C	B	1789	1	-	9/20/21/23	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1789	L4C	C8-N1	2.55	1.31	1.28

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1789	L4C	C5-O13-N1	13.72	123.22	108.33
2	A	1789	L4C	O13-N1-C8	13.05	130.97	111.47
2	B	1789	L4C	O13-N1-C8	12.22	129.73	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1789	L4C	O17-C9-C10	5.22	130.48	114.00
2	B	1789	L4C	C5-O13-N1	4.69	113.43	108.33
2	A	1789	L4C	O16-C9-C10	-4.51	108.78	123.09
2	A	1789	L4C	C4-C3-N2	3.99	117.19	109.50
2	B	1789	L4C	C4-C3-N2	3.85	116.93	109.50
2	B	1789	L4C	C11-C10-C9	-3.47	104.46	113.67
2	B	1789	L4C	O16-C9-C10	-3.12	113.20	123.09
2	A	1789	L4C	C11-C8-N1	-2.91	120.11	125.55
2	B	1789	L4C	C11-C8-N1	-2.80	120.32	125.55
2	A	1789	L4C	C11-C10-C9	-2.53	106.95	113.67
2	A	1789	L4C	C7-C6-N2	2.39	120.08	116.12
2	B	1789	L4C	O18-C12-O19	-2.14	118.81	123.90
2	B	1789	L4C	C7-C6-N2	2.06	119.54	116.12
2	A	1789	L4C	O18-C12-O19	-2.05	119.01	123.90

There are no chirality outliers.

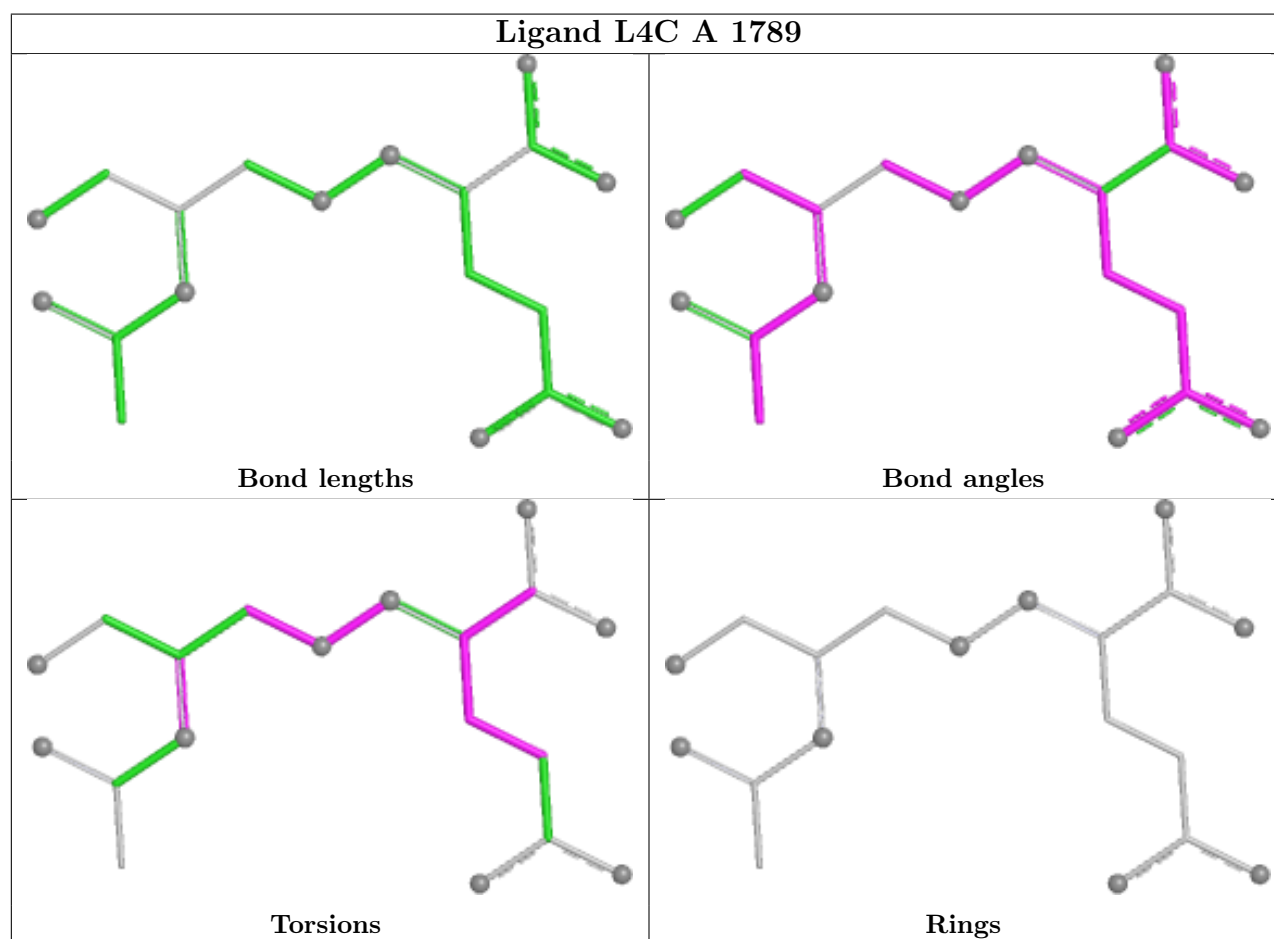
All (19) torsion outliers are listed below:

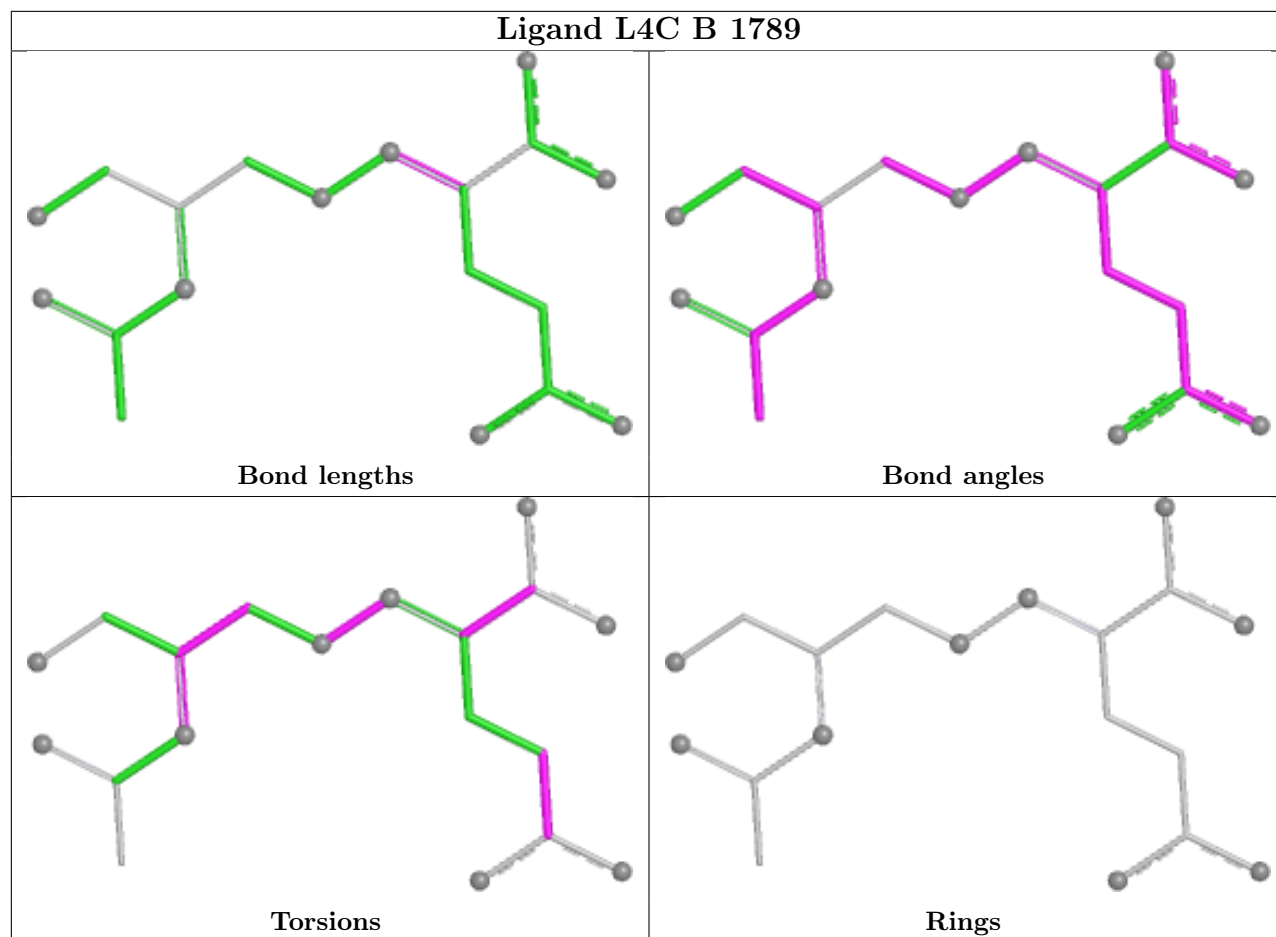
Mol	Chain	Res	Type	Atoms
2	A	1789	L4C	C9-C10-C11-C8
2	A	1789	L4C	C10-C11-C8-C12
2	A	1789	L4C	C10-C11-C8-N1
2	A	1789	L4C	O18-C12-C8-C11
2	A	1789	L4C	O19-C12-C8-N1
2	A	1789	L4C	C5-C3-N2-C6
2	A	1789	L4C	C4-C3-N2-C6
2	B	1789	L4C	O18-C12-C8-C11
2	B	1789	L4C	O19-C12-C8-N1
2	B	1789	L4C	C5-C3-N2-C6
2	B	1789	L4C	C4-C3-N2-C6
2	A	1789	L4C	O18-C12-C8-N1
2	B	1789	L4C	O18-C12-C8-N1
2	A	1789	L4C	C3-C5-O13-N1
2	B	1789	L4C	C4-C3-C5-O13
2	B	1789	L4C	C11-C10-C9-O17
2	B	1789	L4C	C11-C10-C9-O16
2	A	1789	L4C	C8-N1-O13-C5
2	B	1789	L4C	C8-N1-O13-C5

There are no ring outliers.

No monomer is involved in short contacts.

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	461/720 (64%)	-0.34	15 (3%)	49	43	11, 34, 78, 99	1 (0%)
1	B	462/720 (64%)	-0.36	15 (3%)	50	44	13, 34, 77, 99	0
All	All	923/1440 (64%)	-0.35	30 (3%)	49	43	11, 34, 78, 99	1 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	115	VAL	8.8
1	A	786	ILE	4.3
1	B	788	GLY	4.2
1	A	740	SER	4.1
1	B	114	THR	4.1
1	A	363	ALA	4.0
1	B	786	ILE	4.0
1	A	742	GLU	3.8
1	A	114	THR	3.3
1	B	742	GLU	3.1
1	B	743	GLY	3.0
1	B	364	LYS	3.0
1	B	730	LYS	2.9
1	A	112	ASP	2.9
1	B	740	SER	2.7
1	A	746	VAL	2.7
1	A	788	GLY	2.6
1	A	741	VAL	2.6
1	A	364	LYS	2.5
1	A	760	LYS	2.5
1	B	112	ASP	2.4
1	B	749	THR	2.4
1	B	760	LYS	2.3
1	B	113	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	738	LYS	2.2
1	A	743	GLY	2.2
1	B	746	VAL	2.1
1	A	749	THR	2.1
1	A	736	PRO	2.1
1	A	730	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

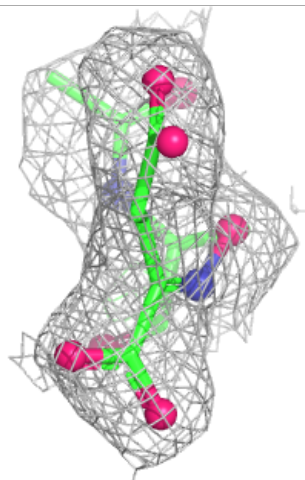
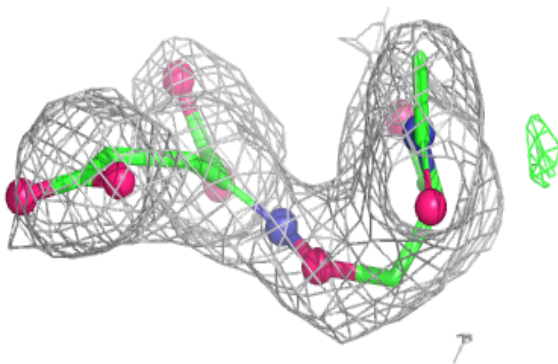
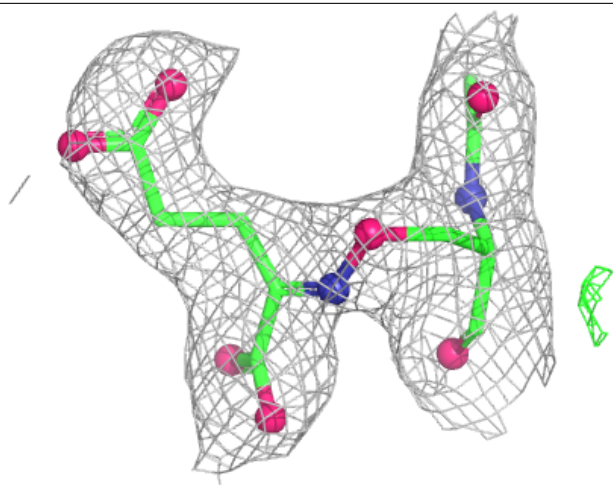
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

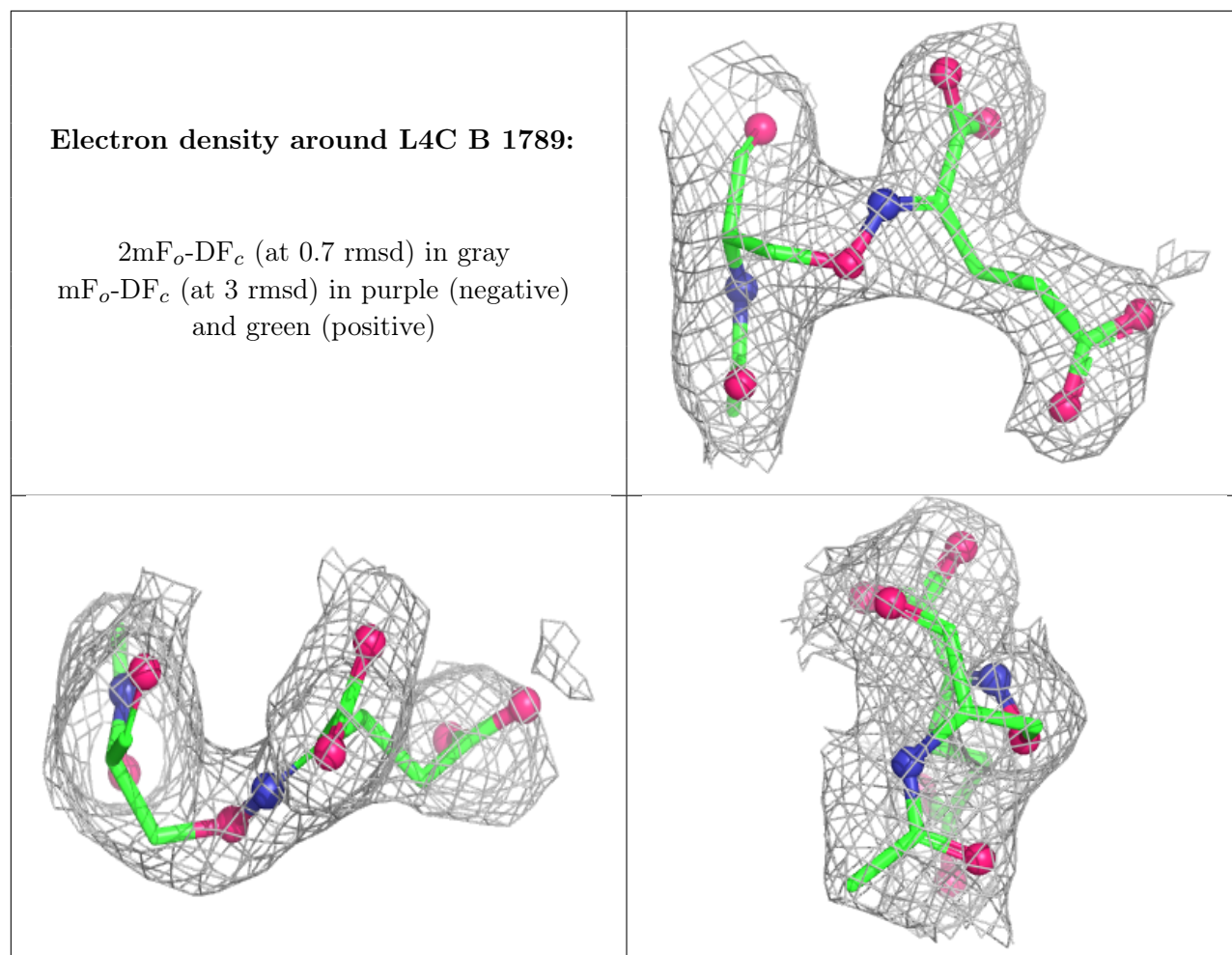
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CL	B	1791	1/1	0.93	0.16	56,56,56,56	0
3	SO4	B	1790	5/5	0.94	0.11	53,57,59,59	0
2	L4C	A	1789	19/20	0.94	0.10	25,47,60,66	0
2	L4C	B	1789	19/20	0.95	0.09	21,45,62,63	0
4	CL	A	1792	1/1	0.95	0.11	48,48,48,48	0
3	SO4	A	1790	5/5	0.95	0.10	50,50,55,57	0
4	CL	B	1792	1/1	0.97	0.09	39,39,39,39	0
4	CL	A	1791	1/1	0.99	0.09	26,26,26,26	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.

Electron density around L4C A 1789:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.