



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:35 am GMT

PDB ID : 2JE5  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

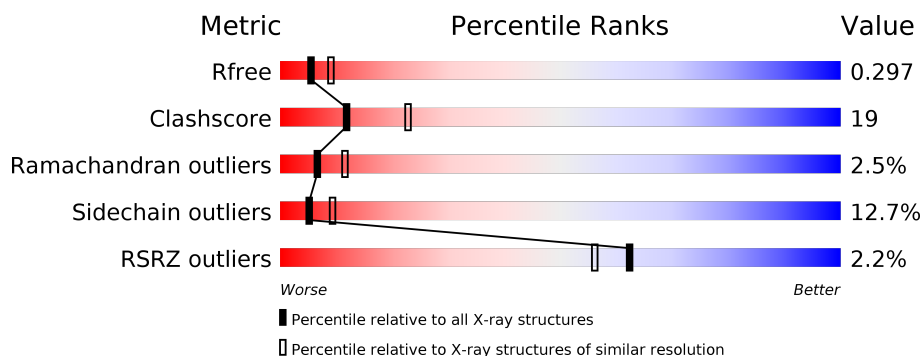
# 1 Overall quality at a glance

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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div></div> <div>31% 25% 6% • 36%</div> </div>
1	B	720	<div> <div></div> <div>32% 23% 6% • 36%</div> </div>

## 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.

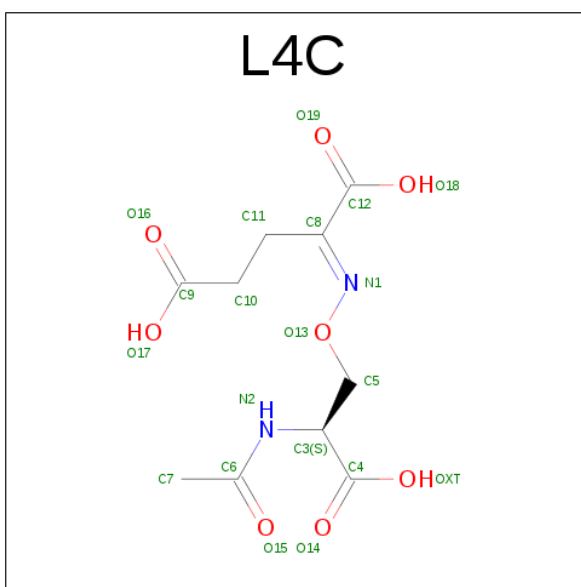
- Molecule 1 is a protein called PENICILLIN-BINDING PROTEIN 1B.

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:

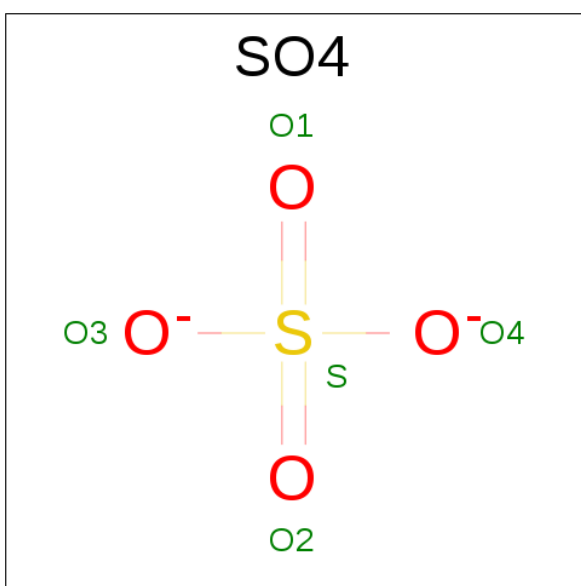
Chain	Residue	Modelled	Actual	Comment	Reference
A	73	SER	ALA	ENGINEERED MUTATION	UNP O70038
A	123	MET	LEU	ENGINEERED MUTATION	UNP O70038
A	158	ASN	LYS	ENGINEERED MUTATION	UNP O70038
A	162	PRO	ARG	ENGINEERED MUTATION	UNP O70038
A	336	GLN	ARG	ENGINEERED MUTATION	UNP O70038
A	686	GLN	ARG	ENGINEERED MUTATION	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 (three-letter code: L4C) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>2</sub>O<sub>8</sub>).



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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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 (three-letter code: CL) (formula: Cl).

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

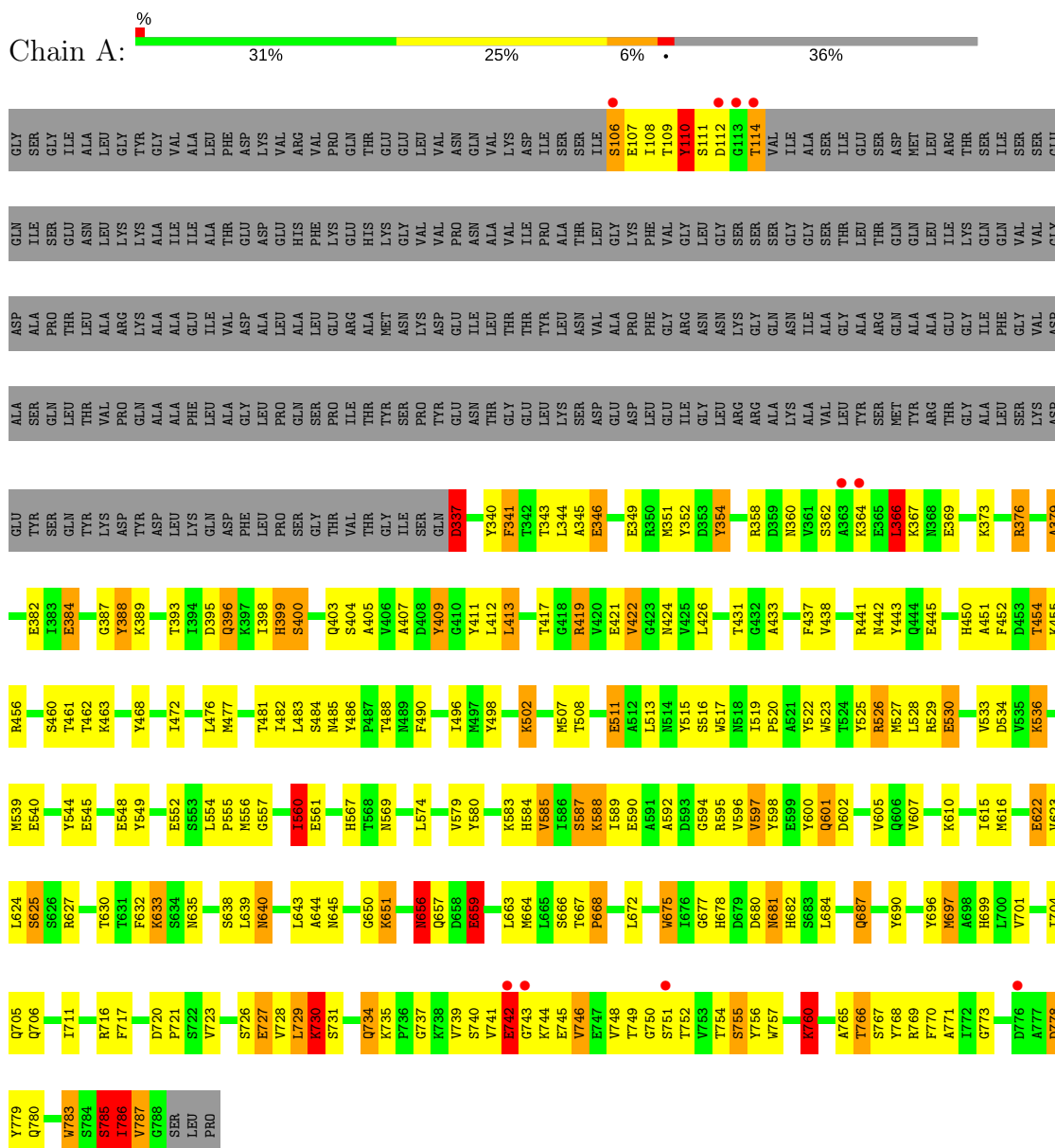
- Molecule 5 is water.

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

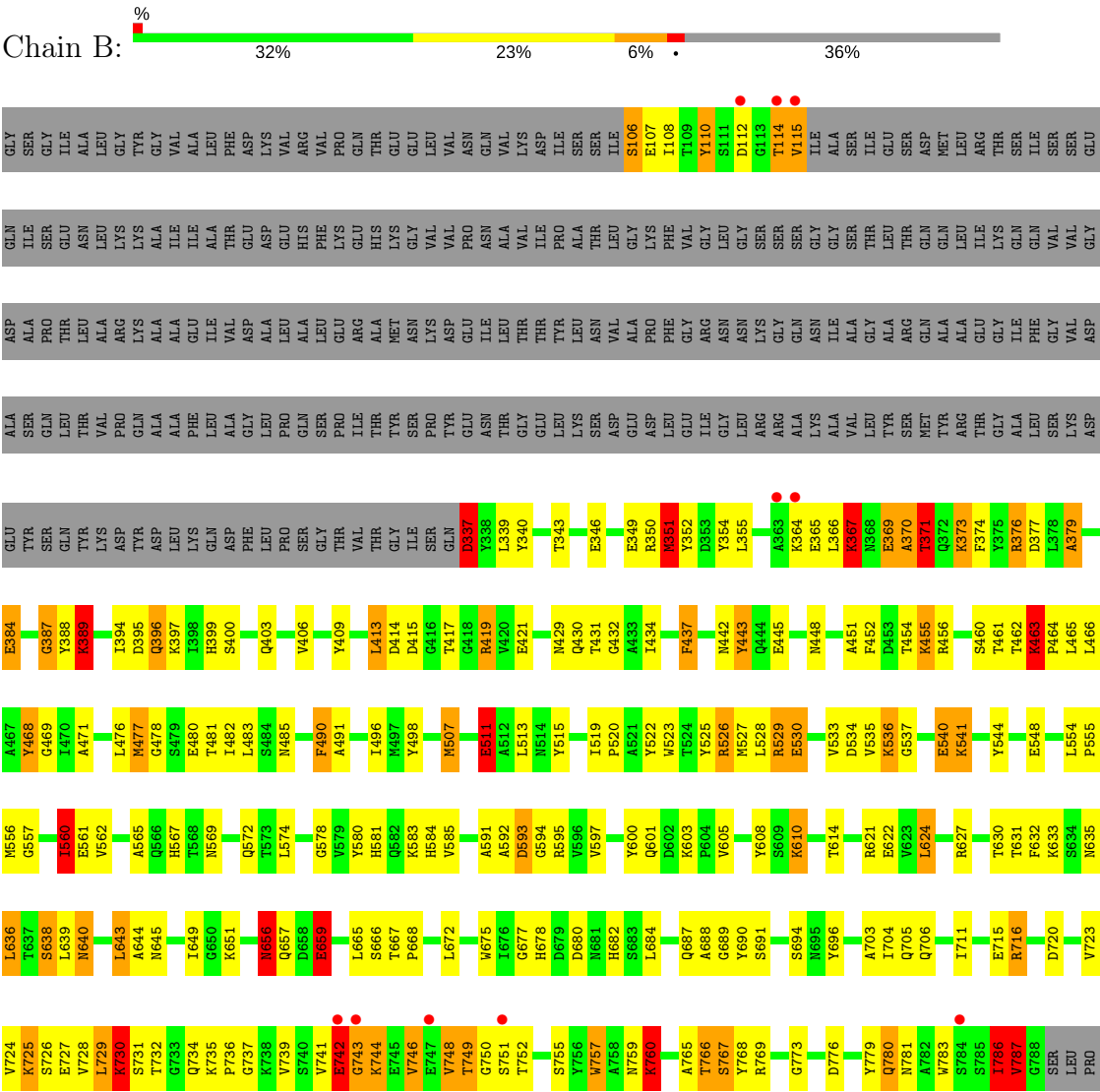
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



#### • 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, $\alpha$ , $\beta$ , $\gamma$	98.54Å 99.83Å 152.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.52 – 2.60 19.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (84.52-2.60) 99.5 (19.92-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: L4C, SO4, CL

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	2.06	105/3628 (2.9%)	1.62	41/4929 (0.8%)
1	B	2.02	99/3626 (2.7%)	1.63	57/4927 (1.2%)
All	All	2.04	204/7254 (2.8%)	1.63	98/9856 (1.0%)

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 (204) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346[A]	GLU	CB-CG	15.94	1.82	1.52
1	A	346[B]	GLU	CB-CG	15.94	1.82	1.52
1	A	346[A]	GLU	CG-CD	14.33	1.73	1.51
1	A	346[B]	GLU	CG-CD	14.33	1.73	1.51
1	B	115	VAL	CA-CB	12.38	1.80	1.54
1	A	354	TYR	CD1-CE1	11.88	1.57	1.39
1	A	601	GLN	CA-CB	9.53	1.75	1.53
1	B	541	LYS	CE-NZ	9.40	1.72	1.49
1	A	346[A]	GLU	CD-OE1	-9.07	1.15	1.25
1	A	346[B]	GLU	CD-OE1	-9.07	1.15	1.25
1	B	548	GLU	CD-OE1	8.71	1.35	1.25
1	B	468	TYR	CD1-CE1	8.69	1.52	1.39
1	B	696	TYR	CG-CD2	8.54	1.50	1.39
1	B	511	GLU	CD-OE2	8.52	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	GLU	CG-CD	8.32	1.64	1.51
1	A	345	ALA	C-O	8.25	1.39	1.23
1	B	601	GLN	CA-CB	8.24	1.72	1.53
1	B	463	LYS	CE-NZ	8.19	1.69	1.49
1	B	565	ALA	CA-CB	-8.11	1.35	1.52
1	A	396	GLN	CG-CD	8.10	1.69	1.51
1	A	445	GLU	CG-CD	8.06	1.64	1.51
1	B	374	PHE	CE1-CZ	8.01	1.52	1.37
1	A	696	TYR	CG-CD2	7.98	1.49	1.39
1	B	742	GLU	CG-CD	7.91	1.63	1.51
1	B	580	TYR	CD2-CE2	7.89	1.51	1.39
1	A	706	GLN	CB-CG	7.80	1.73	1.52
1	B	371	THR	N-CA	7.77	1.61	1.46
1	A	742	GLU	CG-CD	7.49	1.63	1.51
1	B	452	PHE	CE2-CZ	7.44	1.51	1.37
1	A	760	LYS	CB-CG	7.42	1.72	1.52
1	A	384	GLU	CD-OE2	7.41	1.33	1.25
1	B	632	PHE	CD1-CE1	7.36	1.53	1.39
1	A	675	TRP	CB-CG	7.30	1.63	1.50
1	B	706	GLN	CG-CD	7.19	1.67	1.51
1	B	786	ILE	CA-CB	7.10	1.71	1.54
1	A	454	THR	CB-CG2	7.05	1.75	1.52
1	A	633	LYS	CE-NZ	7.05	1.66	1.49
1	A	786	ILE	CA-CB	7.04	1.71	1.54
1	A	451	ALA	CA-CB	7.03	1.67	1.52
1	A	548	GLU	CD-OE1	7.03	1.33	1.25
1	B	369	GLU	CG-CD	7.03	1.62	1.51
1	A	411	TYR	CE1-CZ	7.02	1.47	1.38
1	A	341	PHE	CE1-CZ	6.91	1.50	1.37
1	B	115	VAL	CB-CG2	6.88	1.67	1.52
1	A	690	TYR	CD1-CE1	6.86	1.49	1.39
1	B	600	TYR	CG-CD2	6.83	1.48	1.39
1	A	421	GLU	CD-OE1	6.79	1.33	1.25
1	B	585	VAL	CB-CG1	-6.77	1.38	1.52
1	B	724	VAL	CB-CG1	6.74	1.67	1.52
1	A	588	LYS	CD-CE	6.74	1.68	1.51
1	A	600	TYR	CG-CD2	6.73	1.48	1.39
1	A	511	GLU	CD-OE2	6.73	1.33	1.25
1	A	638	SER	CA-CB	-6.70	1.43	1.52
1	B	562	VAL	CB-CG2	-6.67	1.38	1.52
1	A	580	TYR	CG-CD2	6.64	1.47	1.39
1	B	387	GLY	N-CA	6.63	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346[A]	GLU	N-CA	6.63	1.59	1.46
1	A	346[B]	GLU	N-CA	6.63	1.59	1.46
1	B	340	TYR	CD2-CE2	6.62	1.49	1.39
1	B	742	GLU	CB-CG	6.59	1.64	1.52
1	B	593	ASP	CB-CG	6.56	1.65	1.51
1	B	540	GLU	CG-CD	6.56	1.61	1.51
1	A	696	TYR	CE1-CZ	6.55	1.47	1.38
1	B	114	THR	N-CA	6.54	1.59	1.46
1	B	580	TYR	CG-CD2	6.50	1.47	1.39
1	A	411	TYR	CB-CG	-6.48	1.42	1.51
1	B	541	LYS	CD-CE	6.47	1.67	1.51
1	A	742	GLU	CB-CG	6.44	1.64	1.52
1	B	760	LYS	CB-CG	6.43	1.70	1.52
1	B	421	GLU	CG-CD	6.42	1.61	1.51
1	A	605	VAL	CB-CG2	6.42	1.66	1.52
1	B	694	SER	CA-CB	-6.40	1.43	1.52
1	A	422	VAL	CA-CB	6.36	1.68	1.54
1	A	633	LYS	CB-CG	6.35	1.69	1.52
1	A	672	LEU	C-O	6.35	1.35	1.23
1	B	445	GLU	CG-CD	6.29	1.61	1.51
1	A	366	LEU	CG-CD2	6.26	1.75	1.51
1	A	539	MET	CG-SD	6.24	1.97	1.81
1	B	388	TYR	CE1-CZ	6.24	1.46	1.38
1	B	379	ALA	N-CA	6.19	1.58	1.46
1	B	703	ALA	CA-CB	-6.17	1.39	1.52
1	A	517	TRP	CB-CG	6.17	1.61	1.50
1	B	364	LYS	CD-CE	6.12	1.66	1.51
1	B	515	TYR	CG-CD1	6.10	1.47	1.39
1	B	614	THR	C-O	6.10	1.34	1.23
1	A	369	GLU	CD-OE1	6.08	1.32	1.25
1	B	354	TYR	CD1-CE1	6.06	1.48	1.39
1	B	451	ALA	C-O	6.05	1.34	1.23
1	A	515	TYR	CG-CD1	6.04	1.47	1.39
1	B	115	VAL	N-CA	6.03	1.58	1.46
1	B	578	GLY	N-CA	-5.99	1.37	1.46
1	A	580	TYR	CD2-CE2	5.95	1.48	1.39
1	A	656	ASN	N-CA	5.92	1.58	1.46
1	A	346[A]	GLU	CA-CB	5.92	1.67	1.53
1	A	346[B]	GLU	CA-CB	5.92	1.67	1.53
1	A	623	VAL	CB-CG2	5.91	1.65	1.52
1	A	349	GLU	CB-CG	5.91	1.63	1.52
1	A	600	TYR	CE2-CZ	5.91	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	603	LYS	CA-CB	5.91	1.67	1.53
1	B	535	VAL	CA-CB	-5.89	1.42	1.54
1	A	675	TRP	CA-CB	5.89	1.67	1.53
1	B	443	TYR	CD2-CE2	5.89	1.48	1.39
1	A	561	GLU	CD-OE1	5.88	1.32	1.25
1	A	717	PHE	CE1-CZ	5.88	1.48	1.37
1	B	112	ASP	CB-CG	5.88	1.64	1.51
1	B	585	VAL	CB-CG2	-5.88	1.40	1.52
1	A	399	HIS	C-O	5.86	1.34	1.23
1	A	452	PHE	CE1-CZ	5.85	1.48	1.37
1	A	441	ARG	CG-CD	5.85	1.66	1.51
1	B	388	TYR	CG-CD1	5.84	1.46	1.39
1	B	659	GLU	CD-OE2	5.84	1.32	1.25
1	B	622	GLU	CB-CG	5.83	1.63	1.52
1	B	656	ASN	N-CA	5.83	1.58	1.46
1	B	397	LYS	CE-NZ	5.81	1.63	1.49
1	A	388	TYR	CE1-CZ	5.81	1.46	1.38
1	A	407	ALA	CA-CB	5.80	1.64	1.52
1	A	659	GLU	CB-CG	-5.80	1.41	1.52
1	A	530	GLU	CG-CD	5.79	1.60	1.51
1	A	579	VAL	CB-CG2	5.77	1.65	1.52
1	B	536	LYS	CD-CE	5.74	1.65	1.51
1	B	690	TYR	CD1-CE1	5.69	1.47	1.39
1	B	605	VAL	CB-CG2	5.69	1.64	1.52
1	B	621	ARG	CG-CD	5.68	1.66	1.51
1	B	367	LYS	CE-NZ	5.64	1.63	1.49
1	B	384	GLU	CD-OE2	5.62	1.31	1.25
1	A	727	GLU	CG-CD	5.60	1.60	1.51
1	B	454	THR	CB-CG2	5.58	1.70	1.52
1	A	490	PHE	CE1-CZ	5.57	1.48	1.37
1	B	561	GLU	CD-OE2	5.56	1.31	1.25
1	A	754	THR	CA-CB	5.56	1.67	1.53
1	B	340	TYR	CG-CD1	5.55	1.46	1.39
1	B	689	GLY	N-CA	5.55	1.54	1.46
1	A	360	ASN	CB-CG	5.54	1.63	1.51
1	B	400	SER	CB-OG	-5.54	1.35	1.42
1	B	706	GLN	CB-CG	5.54	1.67	1.52
1	B	490	PHE	CE1-CZ	5.54	1.47	1.37
1	A	624	LEU	CG-CD1	5.53	1.72	1.51
1	B	364	LYS	CB-CG	5.52	1.67	1.52
1	A	438	VAL	CB-CG1	-5.50	1.41	1.52
1	A	585	VAL	CB-CG1	-5.50	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	TYR	CB-CG	5.50	1.59	1.51
1	B	367	LYS	CD-CE	5.47	1.65	1.51
1	B	114	THR	CA-CB	5.47	1.67	1.53
1	A	552	GLU	CD-OE1	5.45	1.31	1.25
1	A	419	ARG	CG-CD	-5.45	1.38	1.51
1	B	346	GLU	CD-OE1	5.45	1.31	1.25
1	B	688	ALA	CA-CB	-5.42	1.41	1.52
1	B	448	ASN	C-O	5.42	1.33	1.23
1	A	468	TYR	CD2-CE2	5.39	1.47	1.39
1	A	717	PHE	CB-CG	-5.39	1.42	1.51
1	B	346	GLU	CG-CD	5.38	1.60	1.51
1	A	600	TYR	CE1-CZ	5.37	1.45	1.38
1	B	768	TYR	CD1-CE1	5.36	1.47	1.39
1	B	749	THR	CB-CG2	5.36	1.70	1.52
1	A	659	GLU	C-O	-5.34	1.13	1.23
1	A	589	ILE	CA-CB	-5.33	1.42	1.54
1	A	681	ASN	CG-ND2	5.33	1.46	1.32
1	B	437	PHE	CE2-CZ	5.33	1.47	1.37
1	B	415	ASP	CG-OD1	5.32	1.37	1.25
1	B	704	ILE	C-O	5.32	1.33	1.23
1	B	409	TYR	CB-CG	5.31	1.59	1.51
1	B	522	TYR	CE2-CZ	5.28	1.45	1.38
1	A	632	PHE	CD1-CE1	5.27	1.49	1.39
1	A	376	ARG	CZ-NH1	5.26	1.39	1.33
1	A	607	VAL	CB-CG2	5.25	1.63	1.52
1	A	405	ALA	N-CA	-5.23	1.35	1.46
1	A	396	GLN	CD-NE2	5.23	1.46	1.32
1	A	754	THR	CA-C	5.22	1.66	1.52
1	A	687	GLN	CB-CG	5.22	1.66	1.52
1	B	757	TRP	CZ3-CH2	5.21	1.48	1.40
1	B	371	THR	CA-CB	5.21	1.66	1.53
1	B	409	TYR	CG-CD1	5.21	1.46	1.39
1	A	400	SER	N-CA	5.20	1.56	1.46
1	B	659	GLU	CG-CD	5.19	1.59	1.51
1	A	443	TYR	CA-CB	-5.19	1.42	1.53
1	B	530	GLU	CD-OE1	5.18	1.31	1.25
1	B	354	TYR	CZ-OH	5.18	1.46	1.37
1	B	367	LYS	CB-CG	5.17	1.66	1.52
1	A	419	ARG	C-O	5.15	1.33	1.23
1	A	756	TYR	CE2-CZ	5.15	1.45	1.38
1	B	491	ALA	CA-CB	-5.14	1.41	1.52
1	A	468	TYR	CD1-CE1	5.14	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	730	LYS	CG-CD	5.14	1.70	1.52
1	A	409	TYR	C-N	5.11	1.42	1.33
1	A	522	TYR	CE2-CZ	5.11	1.45	1.38
1	A	666	SER	CB-OG	-5.11	1.35	1.42
1	B	540	GLU	CB-CG	5.11	1.61	1.52
1	A	615	ILE	CA-CB	-5.10	1.43	1.54
1	B	608	TYR	CB-CG	5.09	1.59	1.51
1	B	638	SER	CB-OG	5.08	1.48	1.42
1	B	633	LYS	CA-C	5.07	1.66	1.52
1	A	379	ALA	N-CA	5.06	1.56	1.46
1	A	699	HIS	C-O	5.06	1.32	1.23
1	A	783	TRP	CB-CG	-5.05	1.41	1.50
1	B	337	ASP	CG-OD1	5.04	1.36	1.25
1	A	398	ILE	CB-CG2	-5.04	1.37	1.52
1	A	486	TYR	CE2-CZ	5.03	1.45	1.38
1	A	750	GLY	C-O	5.03	1.31	1.23
1	B	432	GLY	C-O	-5.03	1.15	1.23
1	B	452	PHE	CE1-CZ	5.03	1.47	1.37
1	B	730	LYS	CG-CD	5.03	1.69	1.52
1	A	668	PRO	N-CA	5.01	1.55	1.47
1	B	787	VAL	CA-C	5.01	1.66	1.52
1	A	114	THR	N-CA	5.00	1.56	1.46

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346[A]	GLU	OE1-CD-OE2	-17.73	102.02	123.30
1	A	346[B]	GLU	OE1-CD-OE2	-17.73	102.02	123.30
1	B	337	ASP	CB-CG-OD2	-15.36	104.48	118.30
1	B	337	ASP	CB-CG-OD1	13.81	130.73	118.30
1	B	377	ASP	CB-CG-OD1	11.91	129.02	118.30
1	B	574	LEU	CB-CG-CD1	-11.28	91.82	111.00
1	B	377	ASP	CB-CG-OD2	-10.07	109.23	118.30
1	A	627	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	697	MET	CG-SD-CE	-8.93	85.91	100.20
1	A	639	LEU	CB-CG-CD1	-8.90	95.87	111.00
1	A	627	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	B	560	ILE	CB-CA-C	-8.20	95.20	111.60
1	A	778	ASP	CB-CG-OD2	7.95	125.45	118.30
1	A	560	ILE	CB-CA-C	-7.84	95.92	111.60
1	B	371	THR	N-CA-CB	7.82	125.15	110.30
1	B	624	LEU	CB-CG-CD2	7.78	124.22	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	TYR	CD1-CE1-CZ	-7.68	112.89	119.80
1	B	643	LEU	CB-CG-CD2	-7.63	98.03	111.00
1	B	389	LYS	CD-CE-NZ	7.48	128.91	111.70
1	B	639	LEU	CB-CG-CD1	-7.46	98.33	111.00
1	A	376	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	750	GLY	N-CA-C	-7.06	95.45	113.10
1	B	627	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	B	776	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	376	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	B	729	LEU	CA-CB-CG	6.80	130.93	115.30
1	B	529	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	556	MET	CG-SD-CE	-6.75	89.41	100.20
1	B	414	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	A	751	SER	N-CA-CB	6.67	120.51	110.50
1	B	665	LEU	CB-CG-CD1	-6.66	99.68	111.00
1	A	384	GLU	N-CA-CB	6.54	122.37	110.60
1	B	751	SER	CB-CA-C	6.39	122.25	110.10
1	B	370	ALA	C-N-CA	-6.28	106.01	121.70
1	A	597	VAL	CB-CA-C	-6.16	99.70	111.40
1	B	548	GLU	CG-CD-OE2	-6.16	105.98	118.30
1	B	421	GLU	CG-CD-OE1	6.10	130.51	118.30
1	B	556	MET	CG-SD-CE	-6.07	90.50	100.20
1	B	351	MET	CG-SD-CE	-6.06	90.51	100.20
1	A	346[A]	GLU	CG-CD-OE2	6.02	130.34	118.30
1	A	346[B]	GLU	CG-CD-OE2	6.02	130.34	118.30
1	B	114	THR	N-CA-C	6.01	127.23	111.00
1	A	346[A]	GLU	N-CA-CB	6.00	121.40	110.60
1	A	346[B]	GLU	N-CA-CB	6.00	121.40	110.60
1	B	624	LEU	CB-CG-CD1	-5.97	100.85	111.00
1	B	413	LEU	CB-CG-CD2	-5.95	100.89	111.00
1	B	477	MET	CG-SD-CE	-5.92	90.72	100.20
1	A	750	GLY	N-CA-C	-5.87	98.42	113.10
1	B	421	GLU	OE1-CD-OE2	-5.86	116.27	123.30
1	A	404	SER	CB-CA-C	-5.77	99.14	110.10
1	A	413	LEU	CA-CB-CG	-5.76	102.04	115.30
1	A	585	VAL	CG1-CB-CG2	-5.72	101.75	110.90
1	B	597	VAL	CB-CA-C	-5.71	100.55	111.40
1	B	465	LEU	CB-CG-CD2	5.68	120.65	111.00
1	A	442	ASN	CB-CA-C	-5.67	99.06	110.40
1	B	691	SER	N-CA-CB	-5.63	102.06	110.50
1	A	622	GLU	CB-CA-C	-5.62	99.15	110.40
1	B	513	LEU	CB-CG-CD2	5.61	120.54	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	TYR	CB-CA-C	-5.56	99.28	110.40
1	A	751	SER	CB-CA-C	5.49	120.53	110.10
1	A	366	LEU	CB-CG-CD2	5.47	120.29	111.00
1	A	513	LEU	CB-CG-CD2	5.46	120.28	111.00
1	A	602	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	B	643	LEU	CB-CG-CD1	5.45	120.27	111.00
1	B	656	ASN	C-N-CA	-5.45	108.08	121.70
1	B	349	GLU	OE1-CD-OE2	5.40	129.78	123.30
1	B	413	LEU	CB-CG-CD1	-5.39	101.84	111.00
1	A	337	ASP	N-CA-C	5.39	125.55	111.00
1	B	376	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	751	SER	N-CA-CB	5.38	118.57	110.50
1	B	498	TYR	N-CA-C	-5.38	96.48	111.00
1	A	468	TYR	C-N-CA	-5.37	111.03	122.30
1	B	468	TYR	CB-CG-CD1	5.36	124.22	121.00
1	A	625	SER	CB-CA-C	-5.36	99.92	110.10
1	B	716	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	364	LYS	CD-CE-NZ	5.31	123.91	111.70
1	A	638	SER	CB-CA-C	-5.25	100.12	110.10
1	B	468	TYR	C-N-CA	-5.24	111.30	122.30
1	B	636	LEU	CB-CG-CD2	5.23	119.89	111.00
1	B	337	ASP	N-CA-C	5.22	125.09	111.00
1	A	498	TYR	N-CA-C	-5.21	96.94	111.00
1	B	355	LEU	CB-CG-CD1	-5.21	102.15	111.00
1	A	110	TYR	N-CA-CB	-5.20	101.24	110.60
1	B	339	LEU	CA-CB-CG	-5.18	103.38	115.30
1	B	112	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	649	ILE	CG1-CB-CG2	-5.15	100.07	111.40
1	A	366	LEU	CA-CB-CG	-5.12	103.52	115.30
1	B	400	SER	CB-CA-C	-5.11	100.40	110.10
1	B	529	ARG	CD-NE-CZ	5.09	130.73	123.60
1	A	354	TYR	CB-CG-CD2	-5.06	117.96	121.00
1	B	373	LYS	CD-CE-NZ	-5.06	100.06	111.70
1	A	587	SER	N-CA-CB	5.05	118.08	110.50
1	B	455	LYS	CD-CE-NZ	5.04	123.29	111.70
1	A	548	GLU	CG-CD-OE2	-5.02	108.26	118.30
1	B	672	LEU	N-CA-C	-5.02	97.44	111.00
1	B	371	THR	CB-CA-C	-5.01	98.07	111.60
1	A	358	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	B	350	ARG	NE-CZ-NH1	-5.01	117.80	120.30

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	147	0
1	B	3553	0	3390	125	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	270	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 19.

All (270) 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:CD2	1:A:366:LEU:CG	1.75	1.62
1:B:115:VAL:CA	1:B:115:VAL:CB	1.80	1.59
1:A:601:GLN:CA	1:A:601:GLN:CB	1.74	1.58
1:A:346[A]:GLU:CB	1:A:346[A]:GLU:CG	1.82	1.57
1:A:454:THR:CG2	1:A:454:THR:CB	1.75	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:LYS:NZ	1:B:463:LYS:CE	1.69	1.55
1:B:541:LYS:NZ	1:B:541:LYS:CE	1.72	1.52
1:A:526:ARG:HH11	1:A:526:ARG:CG	1.69	1.04
1:A:526:ARG:NH1	1:A:526:ARG:HG3	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:471:ALA:HB3	1:B:477:MET:HE3	1.51	0.92
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
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:HG	1:A:366:LEU:CD2	2.05	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: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:A:476:LEU:HD13	1:A:527:MET:HE3	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:476:LEU:CD1	1:A:527:MET:HE3	2.24	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
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: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:729:LEU:O	1:B:730:LYS:C	2.32	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:B:640:ASN:HD22	1:B:640:ASN:C	2.01	0.65
1:A:737:GLY:O	1:A:748:VAL:HG23	1.97	0.65
1:B:471:ALA:CB	1:B:477:MET:HE2	2.28	0.64
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:A:729:LEU:O	1:A:730:LYS:C	2.36	0.63
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:CA	1:A:454:THR:CG2	2.72	0.60
1:B:741:VAL:HG21	1:B:746:VAL:HG23	1.82	0.60
1:B:786:ILE:HG22	1:B:786:ILE:O	2.01	0.60
1:A:382:GLU:OE1	1:A:388:TYR:OH	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG1	1:A:585:VAL:O	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
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: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: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:B:667:THR:HB	1:B:668:PRO:CD	2.36	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:B:729:LEU:O	1:B:731:SER:N	2.39	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:CG2	1:B:786:ILE:O	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:481:THR:CG2	1:A:482:ILE:N	2.71	0.54
1:A:585:VAL:HG13	1:A:585:VAL:O	2.07	0.54
1:B:471:ALA:HB1	1:B:477:MET:HE2	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:ASP:OD1	1:A:682:HIS:CD2	2.56	0.53
1:B:526:ARG:NH1	1:B:526:ARG:HG3	2.23	0.53
1:B:554:LEU:N	1:B:555:PRO:HD2	2.23	0.53
1:B:787:VAL:HG13	1:B:787:VAL:O	2.08	0.53
1:A:569:ASN:ND2	1:A:583:LYS:H	2.06	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:476:LEU:CB	1:A:527:MET:HE3	2.39	0.53
1:B:430:GLN:O	1:B:581:HIS:CD2	2.63	0.52
1:A:729:LEU:C	1:A:731:SER:N	2.62	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:601:GLN:C	1:A:601:GLN:CB	2.72	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:A:785:SER:C	1:A:787:VAL:H	2.14	0.51
1:A:640:ASN:HD22	1:A:640:ASN:C	2.14	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:NH1	1:A:526:ARG:CG	2.44	0.51
1:A:596:VAL:HG12	1:A:596:VAL:O	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:476:LEU:CB	1:A:527:MET:HE1	2.41	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: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:A:729:LEU:C	1:A:731:SER:H	2.15	0.49
1:B:367:LYS:HB2	1:B:367:LYS:NZ	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:523:TRP:CG	1:B:773:GLY:HA3	2.47	0.49
1:B:476:LEU:HB3	1:B:527:MET:HE1	1.94	0.49
1:A:424:ASN:O	1:A:437:PHE:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:640:ASN:ND2	1:B:640:ASN:C	2.65	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:A:426:LEU:HD22	1:A:704:ILE:HD13	1.94	0.48
1:A:529:ARG:O	1:A:530:GLU:C	2.52	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: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:A:399:HIS:CD2	1:A:437:PHE:H	2.32	0.47
1:A:476:LEU:HB2	1:A:527:MET:HE1	1.96	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:727:GLU:HA	1:A:727:GLU:OE2	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:526:ARG:HD3	1:A:530:GLU:CD	2.36	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:B:529:ARG:O	1:B:530:GLU:C	2.53	0.46
1:A:419:ARG:HD2	1:A:419:ARG:HH11	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:A:431:THR:O	1:A:584:HIS:HE1	1.99	0.45
1:A:601:GLN:HA	1:A:601:GLN:CB	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:LEU:HB3	1:B:527:MET:CE	2.46	0.45
1:A:413:LEU:HD23	1:A:413:LEU:HA	1.68	0.45
1:A:651:LYS:CE	5:A:2023:HOH:O	2.63	0.45
1:A:635:ASN:CB	1:B:638:SER:OG	2.60	0.45
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: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: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:A:574:LEU:HA	1:A:574:LEU:HD23	1.81	0.43
1:B:594:GLY:O	1:B:595:ARG:C	2.55	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:442:ASN:O	1:B:443:TYR:C	2.55	0.43
1:B:389:LYS:HB3	1:B:389:LYS:HE2	1.93	0.43
1:A:340:TYR:C	1:A:340:TYR:CD1	2.91	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:468:TYR:O	1:B:469:GLY:C	2.51	0.43
1:B:413:LEU:HA	1:B:413:LEU:HD23	1.79	0.42
1:B:636:LEU:HG	1:B:644:ALA:HB2	2.01	0.42
1:B:369:GLU:H	1:B:369:GLU:HG3	1.61	0.42
1:A:536:LYS:HB2	1:A:549:TYR:CE1	2.54	0.42
1:B:460:SER:O	1:B:463:LYS:HG3	2.20	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:A:525:TYR:O	1:A:528:LEU:N	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:640:ASN:C	1:A:640:ASN:ND2	2.74	0.41
1:B:591:ALA:O	1:B:593:ASP:N	2.54	0.41
1:A:768:TYR:CE2	1:A:783:TRP:CD1	3.09	0.41
1:B:715:GLU:H	1:B:715:GLU:CD	2.24	0.41
1:A:730:LYS:HA	1:A:730:LYS:HD2	1.88	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:422:VAL:HG13	1:A:422:VAL:O	2.20	0.40
1:A:533:VAL:CG1	1:A:534:ASP:N	2.84	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:594:GLY:O	1:A:595:ARG:C	2.58	0.40
1:A:643:LEU:HD13	1:A:705:GLN:HG3	2.03	0.40
1:A:720:ASP:O	1:A:721:PRO:C	2.60	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%)	6	9
1	B	458/720 (64%)	417 (91%)	31 (7%)	10 (2%)	8	14
All	All	916/1440 (64%)	821 (90%)	72 (8%)	23 (2%)	6	11

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%)	323 (86%)	52 (14%)	4	7
1	B	375/590 (64%)	332 (88%)	43 (12%)	6	12
All	All	750/1180 (64%)	655 (87%)	95 (13%)	5	9

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	SER

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Mol	Chain	Res	Type
1	A	107	GLU
1	A	114	THR
1	A	337	ASP
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	516	SER
1	A	526	ARG
1	A	536	LYS
1	A	545	GLU
1	A	560	ILE
1	A	587	SER
1	A	590	GLU
1	A	610	LYS
1	A	622	GLU
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	675	TRP
1	A	687	GLN
1	A	701	VAL
1	A	711	ILE
1	A	726	SER
1	A	729	LEU
1	A	730	LYS
1	A	734	GLN
1	A	739	VAL
1	A	742	GLU

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Mol	Chain	Res	Type
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	337	ASP
1	B	351	MET
1	B	365	GLU
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
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	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	687	GLN
1	B	711	ILE
1	B	725	LYS
1	B	726	SER
1	B	727	GLU
1	B	730	LYS

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Mol	Chain	Res	Type
1	B	732	THR
1	B	739	VAL
1	B	742	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	787	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	GLN
1	A	399	HIS
1	A	424	ASN
1	A	448	ASN
1	A	485	ASN
1	A	494	ASN
1	A	514	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	348	GLN
1	B	399	HIS
1	B	424	ASN
1	B	429	ASN
1	B	448	ASN
1	B	485	ASN
1	B	567	HIS
1	B	569	ASN
1	B	635	ASN
1	B	640	ASN
1	B	656	ASN
1	B	678	HIS
1	B	682	HIS

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Mol	Chain	Res	Type
1	B	686	GLN
1	B	734	GLN
1	B	780	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z  > 2$
2	L4C	A	1789	1	13,18,19	1.57	2 (15%)	9,22,24	4.72	5 (55%)
3	SO4	A	1790	-	4,4,4	0.68	0	6,6,6	0.91	0
2	L4C	B	1789	1	13,18,19	1.62	3 (23%)	9,22,24	2.77	4 (44%)
3	SO4	B	1790	-	4,4,4	0.71	0	6,6,6	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	L4C	A	1789	1	-	0/11/21/23	0/0/0/0
3	SO4	A	1790	-	-	0/0/0/0	0/0/0/0
2	L4C	B	1789	1	-	0/11/21/23	0/0/0/0
3	SO4	B	1790	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1789	L4C	C12-C8	-2.65	1.47	1.52
2	B	1789	L4C	C12-C8	-2.08	1.48	1.52
2	B	1789	L4C	C3-C4	2.56	1.53	1.50
2	A	1789	L4C	C3-C4	3.26	1.54	1.50
2	B	1789	L4C	C8-N1	3.62	1.31	1.28

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1789	L4C	C11-C10-C9	-4.80	104.46	112.66
2	A	1789	L4C	C11-C10-C9	-3.34	106.95	112.66
2	A	1789	L4C	C11-C8-N1	-2.99	120.11	125.91
2	B	1789	L4C	C11-C8-N1	-2.88	120.32	125.91
2	A	1789	L4C	C7-C6-N2	2.20	120.08	116.11
2	A	1789	L4C	O13-C5-C3	3.24	114.60	108.39
2	B	1789	L4C	O13-C5-C3	3.27	114.66	108.39
2	B	1789	L4C	C5-O13-N1	4.28	113.43	108.47
2	A	1789	L4C	C5-O13-N1	12.74	123.22	108.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	461/720 (64%)	-0.42	10 (2%) 62 56	14, 34, 78, 99	0
1	B	462/720 (64%)	-0.40	10 (2%) 62 56	13, 34, 77, 99	0
All	All	923/1440 (64%)	-0.41	20 (2%) 62 56	13, 34, 78, 99	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	115	VAL	8.2
1	B	114	THR	4.0
1	A	114	THR	4.0
1	A	112	ASP	3.5
1	B	364	LYS	3.4
1	A	364	LYS	3.1
1	A	742	GLU	3.0
1	B	112	ASP	2.9
1	B	363	ALA	2.6
1	B	742	GLU	2.6
1	B	743	GLY	2.6
1	A	743	GLY	2.4
1	A	363	ALA	2.4
1	A	106	SER	2.4
1	A	751	SER	2.3
1	B	751	SER	2.2
1	A	113	GLY	2.1
1	A	776	ASP	2.1
1	B	747	GLU	2.1
1	B	784	SER	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	1790	5/5	0.97	0.17	1.28	50,50,55,57	0
2	L4C	A	1789	19/20	0.95	0.13	-0.05	25,47,60,66	0
2	L4C	B	1789	19/20	0.96	0.12	-0.11	21,45,62,63	0
4	CL	A	1791	1/1	0.99	0.04	-5.01	26,26,26,26	0
4	CL	B	1791	1/1	0.93	0.11	-	56,56,56,56	0
3	SO4	B	1790	5/5	0.96	0.19	-	53,57,59,59	0
4	CL	A	1792	1/1	0.97	0.08	-	48,48,48,48	0
4	CL	B	1792	1/1	0.99	0.16	-	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.