Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 11:13 PM EDT

PDB ID	:	3K9B
Title	:	Crystal structure of human liver carboxylesterase 1 (hCE1) in covalent complex with the nerve agent Cyclosarin (GF)
Authors	:	Hemmert, A.C.; Redinbo, M.R.
Deposited on	:	2009-10-15
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

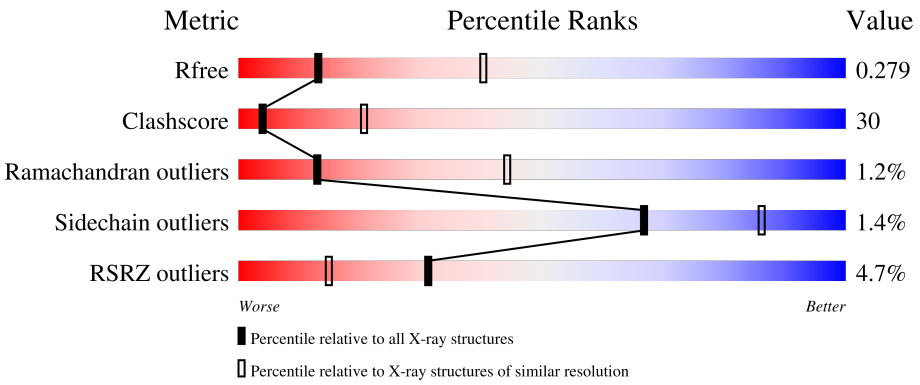
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	529	2%, 54%, 32%, 5%, 8%
1	B	529	5%, 60%, 28%, 5%, • 6%
1	C	529	5%, 54%, 27%, 5%, 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	WW2	B	194	-	-	X	-
2	WW2	C	195	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11251 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.

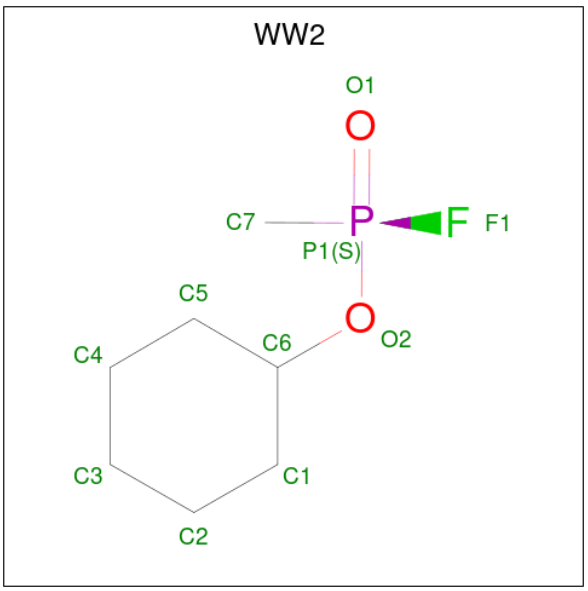
- Molecule 1 is a protein called Liver carboxylesterase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	485	3768	2443	624	681	20	128	0	0
1	B	499	3878	2514	639	706	19	228	0	0
1	C	453	3509	2269	582	642	16	155	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP P23141
B	?	-	GLN	deletion	UNP P23141
C	?	-	GLN	deletion	UNP P23141

- Molecule 2 is cyclohexyl (S)-methylphosphonofluoridoate (three-letter code: WW2) (formula: $C_7H_{14}FO_2P$).



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

- Molecule 3 is water.

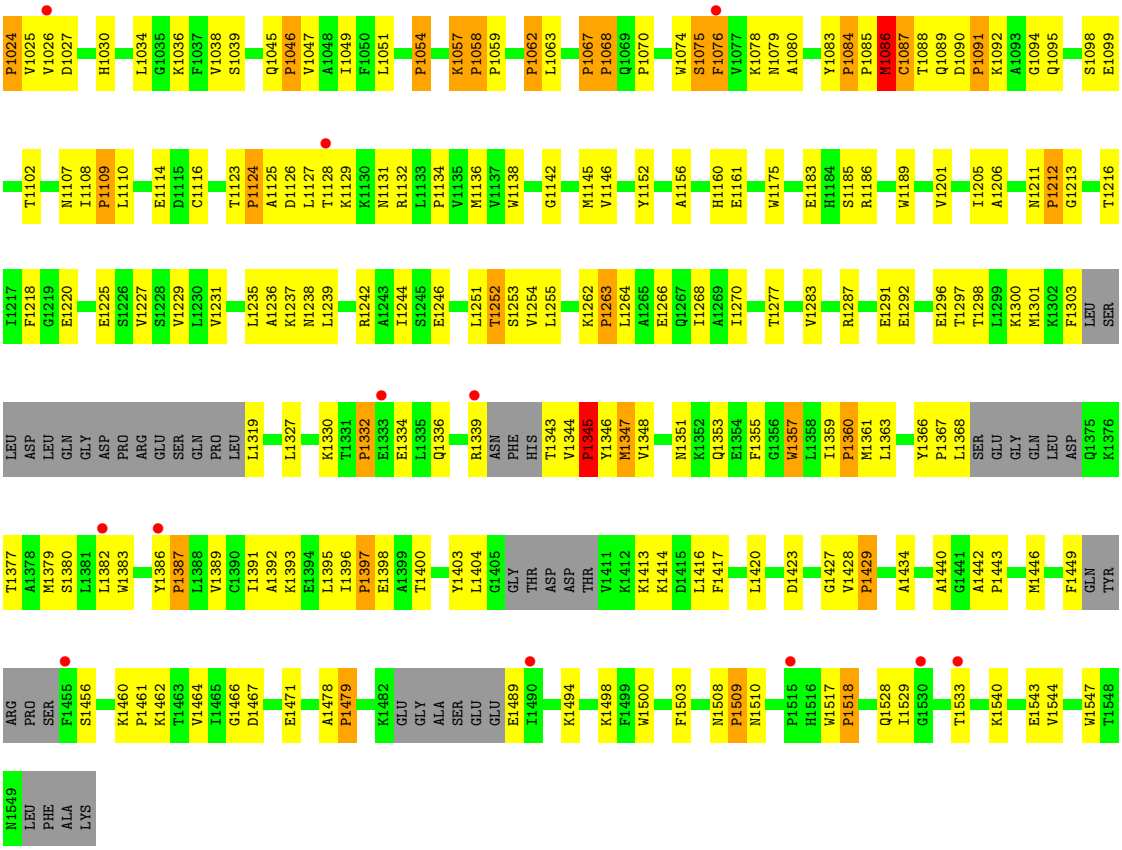
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	23	23	23	0	0
			Total	O		
3	B	19	19	19	0	0
			Total	O		
3	C	24	24	24	0	0

3 Residue-property plots (i)

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.

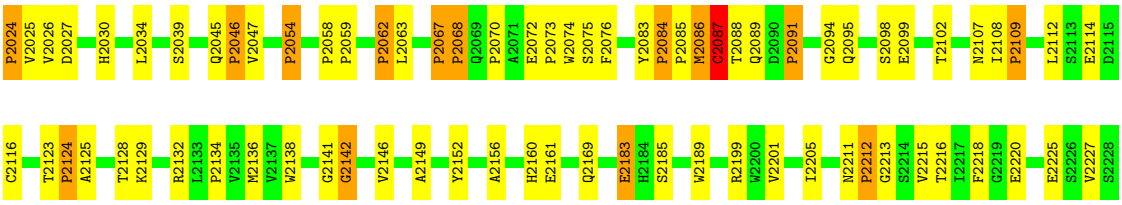
• Molecule 1: Liver carboxylesterase 1

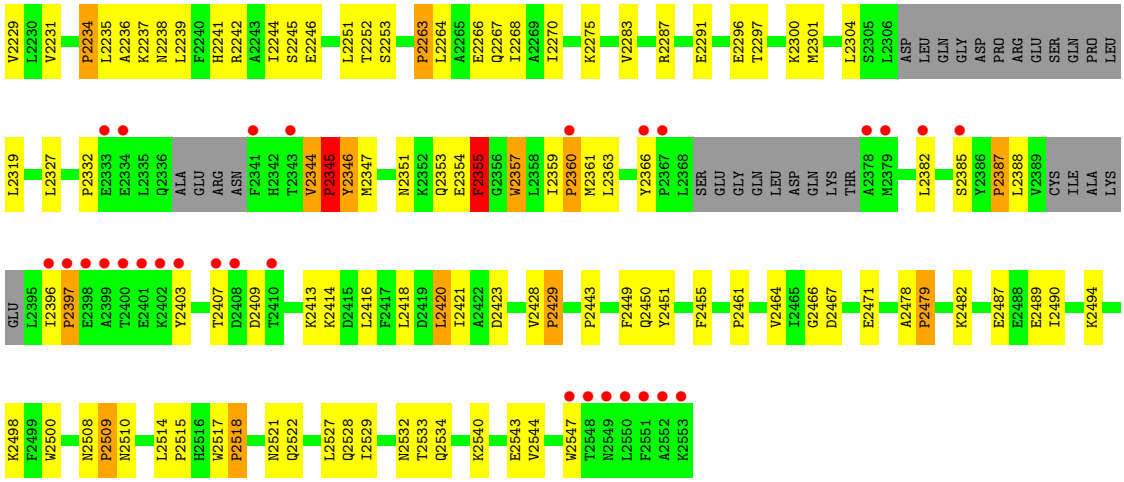
Chain A: 2% 54% 32% 5% 8%



• Molecule 1: Liver carboxylesterase 1

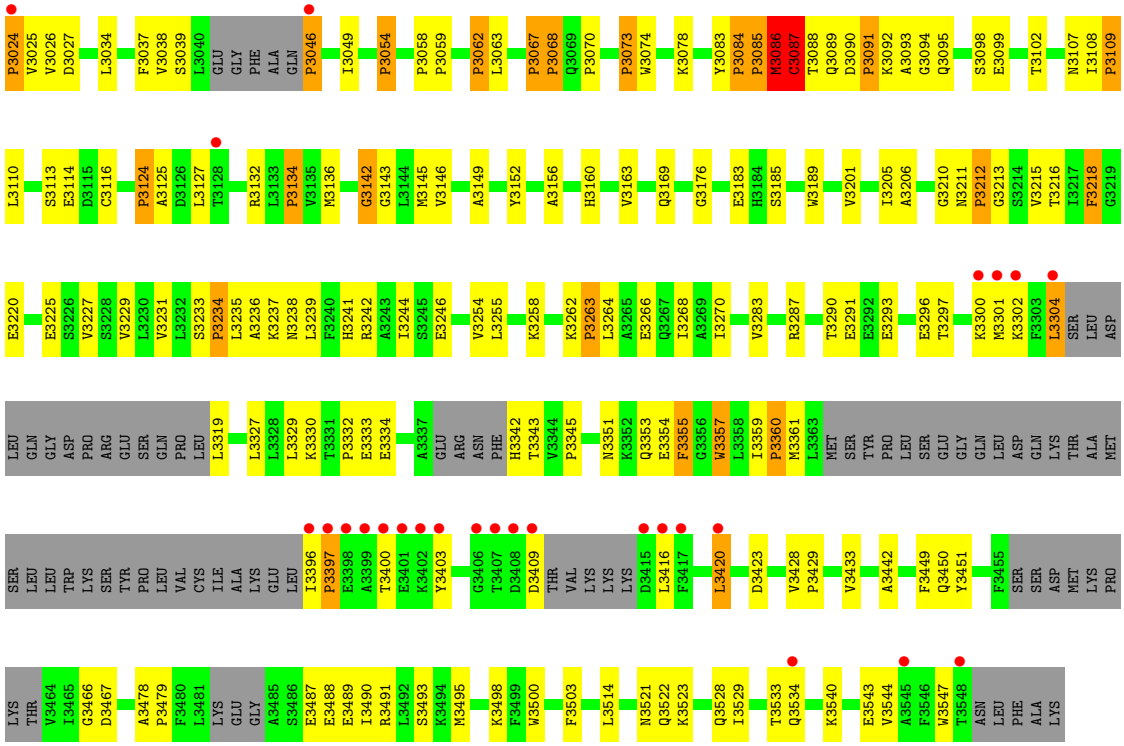
Chain B: 5% 60% 28% 5% • 6%





• Molecule 1: Liver carboxylesterase 1

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.61Å 179.88Å 200.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 3.10 48.60 – 3.12	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.00-3.10) 99.0 (48.60-3.12)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	3.87 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.266 , 0.299 0.248 , 0.279	Depositor DCC
R_{free} test set	3643 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å^2)	61.0	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 79.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	11251	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: WW2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.19	45/3860 (1.2%)	0.99	36/5233 (0.7%)
1	B	1.31	58/3977 (1.5%)	1.03	45/5397 (0.8%)
1	C	0.88	27/3595 (0.8%)	0.93	26/4879 (0.5%)
All	All	1.15	130/11432 (1.1%)	0.99	107/15509 (0.7%)

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	B	0	1

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1346	TYR	CE1-CZ	-21.89	1.10	1.38
1	A	1346	TYR	CE2-CZ	-19.72	1.12	1.38
1	B	2346	TYR	CE1-CZ	-19.11	1.13	1.38
1	B	2346	TYR	CE2-CZ	-16.08	1.17	1.38
1	A	1346	TYR	CG-CD1	-15.19	1.19	1.39
1	B	2087	CYS	C-O	-14.58	0.95	1.23
1	B	2346	TYR	CG-CD1	-13.83	1.21	1.39
1	A	1046	PRO	N-CD	-13.51	1.28	1.47
1	A	1346	TYR	CD1-CE1	-13.50	1.19	1.39
1	B	2355	PHE	CD1-CE1	-13.08	1.13	1.39
1	A	1346	TYR	CD2-CE2	-13.06	1.19	1.39
1	B	2355	PHE	CD2-CE2	-13.05	1.13	1.39
1	B	2346	TYR	C-O	-12.14	1.00	1.23
1	B	2355	PHE	CE2-CZ	-12.10	1.14	1.37
1	A	1346	TYR	CG-CD2	-12.09	1.23	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2085	PRO	C-O	-12.03	0.99	1.23
1	B	2355	PHE	CE1-CZ	-12.01	1.14	1.37
1	C	3046	PRO	N-CD	-11.82	1.31	1.47
1	B	2046	PRO	N-CD	-11.52	1.31	1.47
1	A	1347	MET	C-O	-11.49	1.01	1.23
1	B	2347	MET	CG-SD	-11.31	1.51	1.81
1	A	1062	PRO	N-CD	-11.21	1.32	1.47
1	C	3062	PRO	N-CD	-11.20	1.32	1.47
1	B	2479	PRO	N-CD	-10.93	1.32	1.47
1	B	2347	MET	C-O	-10.86	1.02	1.23
1	B	2109	PRO	N-CD	-10.62	1.32	1.47
1	B	2355	PHE	CG-CD1	-10.58	1.22	1.38
1	B	2058	PRO	N-CD	-10.53	1.33	1.47
1	A	1059	PRO	N-CD	-10.49	1.33	1.47
1	A	1345	PRO	C-O	-10.43	1.02	1.23
1	B	2346	TYR	CG-CD2	-10.31	1.25	1.39
1	C	3087	CYS	C-O	-10.18	1.04	1.23
1	C	3058	PRO	N-CD	-10.15	1.33	1.47
1	C	3059	PRO	N-CD	-10.13	1.33	1.47
1	A	1479	PRO	N-CD	-10.06	1.33	1.47
1	A	1109	PRO	N-CD	-10.04	1.33	1.47
1	B	2084	PRO	N-CD	-9.95	1.33	1.47
1	B	2085	PRO	CB-CG	-9.87	1.00	1.50
1	B	2062	PRO	N-CD	-9.86	1.34	1.47
1	C	3332	PRO	N-CD	-9.81	1.34	1.47
1	B	2059	PRO	N-CD	-9.79	1.34	1.47
1	B	2067	PRO	N-CD	-9.78	1.34	1.47
1	A	1058	PRO	N-CD	-9.70	1.34	1.47
1	A	1067	PRO	N-CD	-9.67	1.34	1.47
1	B	2345	PRO	C-O	-9.64	1.03	1.23
1	C	3109	PRO	N-CD	-9.51	1.34	1.47
1	A	1346	TYR	CZ-OH	-9.50	1.21	1.37
1	A	1332	PRO	N-CD	-9.49	1.34	1.47
1	A	1346	TYR	C-O	-9.48	1.05	1.23
1	B	2332	PRO	N-CD	-9.30	1.34	1.47
1	B	2347	MET	CB-CG	-9.23	1.21	1.51
1	B	2355	PHE	CB-CG	-9.19	1.35	1.51
1	B	2397	PRO	N-CD	-9.19	1.34	1.47
1	B	2345	PRO	CB-CG	-9.15	1.04	1.50
1	A	1429	PRO	N-CD	-9.14	1.35	1.47
1	C	3067	PRO	N-CD	-9.13	1.35	1.47
1	C	3084	PRO	N-CD	-9.06	1.35	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3124	PRO	N-CD	-9.05	1.35	1.47
1	B	2355	PHE	CG-CD2	-8.98	1.25	1.38
1	B	2124	PRO	N-CD	-8.82	1.35	1.47
1	A	1263	PRO	N-CD	-8.80	1.35	1.47
1	C	3263	PRO	N-CD	-8.78	1.35	1.47
1	A	1509	PRO	N-CD	-8.73	1.35	1.47
1	A	1084	PRO	N-CD	-8.73	1.35	1.47
1	B	2070	PRO	N-CD	-8.61	1.35	1.47
1	B	2091	PRO	N-CD	-8.56	1.35	1.47
1	C	3086	MET	C-O	-8.52	1.07	1.23
1	B	2345	PRO	CG-CD	-8.50	1.22	1.50
1	C	3070	PRO	N-CD	-8.50	1.35	1.47
1	B	2085	PRO	CG-CD	-8.47	1.22	1.50
1	B	2263	PRO	N-CD	-8.47	1.35	1.47
1	B	2429	PRO	N-CD	-8.47	1.35	1.47
1	C	3345	PRO	N-CD	-8.45	1.36	1.47
1	C	3397	PRO	N-CD	-8.45	1.36	1.47
1	A	1124	PRO	N-CD	-8.37	1.36	1.47
1	B	2345	PRO	CA-CB	-8.23	1.37	1.53
1	B	2073	PRO	N-CD	-8.19	1.36	1.47
1	B	2085	PRO	CA-CB	-8.18	1.37	1.53
1	C	3085	PRO	C-O	-8.10	1.07	1.23
1	A	1345	PRO	CB-CG	-8.08	1.09	1.50
1	A	1397	PRO	N-CD	-7.87	1.36	1.47
1	A	1070	PRO	N-CD	-7.82	1.36	1.47
1	B	2347	MET	CA-CB	-7.75	1.36	1.53
1	A	1387	PRO	N-CD	-7.70	1.37	1.47
1	B	2212	PRO	N-CD	-7.62	1.37	1.47
1	A	1085	PRO	C-O	-7.49	1.08	1.23
1	B	2345	PRO	N-CA	-7.49	1.34	1.47
1	B	2024	PRO	N-CD	-7.46	1.37	1.47
1	A	1347	MET	CG-SD	-7.45	1.61	1.81
1	A	1054	PRO	N-CD	-7.32	1.37	1.47
1	B	2509	PRO	N-CD	-7.31	1.37	1.47
1	C	3087	CYS	CA-CB	7.28	1.70	1.53
1	B	2054	PRO	N-CD	-7.23	1.37	1.47
1	A	1068	PRO	N-CD	-7.17	1.37	1.47
1	A	1085	PRO	CB-CG	-7.12	1.14	1.50
1	C	3085	PRO	CB-CG	-7.12	1.14	1.50
1	B	2387	PRO	N-CD	-7.11	1.37	1.47
1	A	1212	PRO	N-CD	-7.08	1.38	1.47
1	B	2068	PRO	N-CD	-7.08	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1024	PRO	N-CD	-7.03	1.38	1.47
1	A	1345	PRO	CG-CD	-7.00	1.27	1.50
1	B	2518	PRO	N-CD	-7.00	1.38	1.47
1	A	1087	CYS	CA-C	6.99	1.71	1.52
1	A	1346	TYR	CB-CG	-6.96	1.41	1.51
1	A	1091	PRO	N-CD	-6.91	1.38	1.47
1	C	3054	PRO	N-CD	-6.86	1.38	1.47
1	B	2346	TYR	CZ-OH	-6.84	1.26	1.37
1	B	2360	PRO	N-CD	-6.71	1.38	1.47
1	B	2355	PHE	C-O	-6.68	1.10	1.23
1	C	3212	PRO	N-CD	-6.62	1.38	1.47
1	B	2355	PHE	CA-C	-6.55	1.35	1.52
1	C	3360	PRO	N-CD	-6.46	1.38	1.47
1	C	3073	PRO	N-CD	-6.30	1.39	1.47
1	C	3085	PRO	CG-CD	-6.28	1.29	1.50
1	A	1087	CYS	C-O	-6.21	1.11	1.23
1	C	3024	PRO	N-CD	-6.14	1.39	1.47
1	B	2344	VAL	C-N	-6.08	1.22	1.34
1	B	2086	MET	C-O	-5.90	1.12	1.23
1	C	3091	PRO	N-CD	-5.88	1.39	1.47
1	A	1345	PRO	N-CA	-5.80	1.37	1.47
1	A	1347	MET	CA-CB	-5.72	1.41	1.53
1	B	2355	PHE	CA-CB	-5.64	1.41	1.53
1	B	2087	CYS	CB-SG	-5.61	1.72	1.81
1	A	1518	PRO	N-CD	-5.52	1.40	1.47
1	A	1086	MET	CB-CG	-5.45	1.33	1.51
1	C	3068	PRO	N-CD	-5.40	1.40	1.47
1	B	2085	PRO	N-CA	-5.32	1.38	1.47
1	C	3086	MET	CA-C	-5.15	1.39	1.52
1	A	1347	MET	SD-CE	-5.13	1.49	1.77
1	A	1347	MET	CA-C	-5.00	1.40	1.52

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2087	CYS	CB-CA-C	10.82	132.04	110.40
1	C	3068	PRO	CA-N-CD	-10.50	96.80	111.50
1	C	3059	PRO	CA-N-CD	-10.47	96.84	111.50
1	B	2509	PRO	CA-N-CD	-10.37	96.98	111.50
1	A	1518	PRO	CA-N-CD	-10.31	97.06	111.50
1	A	1068	PRO	CA-N-CD	-10.05	97.43	111.50
1	A	1059	PRO	CA-N-CD	-9.88	97.68	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2068	PRO	CA-N-CD	-9.87	97.68	111.50
1	B	2387	PRO	CA-N-CD	-9.86	97.70	111.50
1	B	2212	PRO	CA-N-CD	-9.84	97.73	111.50
1	B	2518	PRO	CA-N-CD	-9.83	97.74	111.50
1	A	1054	PRO	CA-N-CD	-9.83	97.74	111.50
1	B	2234	PRO	CA-N-CD	-9.79	97.79	111.50
1	C	3212	PRO	CA-N-CD	-9.78	97.82	111.50
1	C	3073	PRO	CA-N-CD	-9.74	97.86	111.50
1	B	2479	PRO	CA-N-CD	-9.71	97.90	111.50
1	A	1058	PRO	CA-N-CD	-9.71	97.91	111.50
1	A	1091	PRO	CA-N-CD	-9.70	97.92	111.50
1	A	1062	PRO	CA-N-CD	-9.69	97.93	111.50
1	C	3054	PRO	CA-N-CD	-9.69	97.93	111.50
1	B	2054	PRO	CA-N-CD	-9.66	97.98	111.50
1	A	1509	PRO	CA-N-CD	-9.62	98.03	111.50
1	B	2084	PRO	CA-N-CD	-9.61	98.05	111.50
1	A	1212	PRO	CA-N-CD	-9.59	98.07	111.50
1	C	3134	PRO	CA-N-CD	-9.58	98.09	111.50
1	B	2059	PRO	CA-N-CD	-9.55	98.14	111.50
1	C	3091	PRO	CA-N-CD	-9.54	98.14	111.50
1	A	1360	PRO	CA-N-CD	-9.54	98.14	111.50
1	C	3084	PRO	CA-N-CD	-9.53	98.16	111.50
1	A	1397	PRO	CA-N-CD	-9.52	98.18	111.50
1	C	3062	PRO	CA-N-CD	-9.51	98.18	111.50
1	C	3234	PRO	CA-N-CD	-9.50	98.20	111.50
1	A	1479	PRO	CA-N-CD	-9.49	98.21	111.50
1	A	1084	PRO	CA-N-CD	-9.46	98.26	111.50
1	B	2109	PRO	CA-N-CD	-9.45	98.27	111.50
1	B	2024	PRO	CA-N-CD	-9.44	98.29	111.50
1	B	2058	PRO	CA-N-CD	-9.40	98.33	111.50
1	C	3067	PRO	CA-N-CD	-9.40	98.35	111.50
1	B	2062	PRO	CA-N-CD	-9.36	98.39	111.50
1	A	1429	PRO	CA-N-CD	-9.35	98.41	111.50
1	B	2046	PRO	CA-N-CD	-9.35	98.41	111.50
1	A	1067	PRO	CA-N-CD	-9.34	98.42	111.50
1	C	3332	PRO	CA-N-CD	-9.28	98.50	111.50
1	A	1124	PRO	CA-N-CD	-9.26	98.53	111.50
1	B	2067	PRO	CA-N-CD	-9.25	98.55	111.50
1	C	3109	PRO	CA-N-CD	-9.25	98.55	111.50
1	C	3124	PRO	CA-N-CD	-9.25	98.55	111.50
1	B	2091	PRO	CA-N-CD	-9.23	98.58	111.50
1	C	3058	PRO	CA-N-CD	-9.23	98.58	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2332	PRO	CA-N-CD	-9.22	98.59	111.50
1	B	2429	PRO	CA-N-CD	-9.22	98.59	111.50
1	A	1332	PRO	CA-N-CD	-9.20	98.62	111.50
1	A	1109	PRO	CA-N-CD	-9.19	98.63	111.50
1	B	2263	PRO	CA-N-CD	-9.19	98.63	111.50
1	B	2073	PRO	CA-N-CD	-9.17	98.66	111.50
1	A	1046	PRO	CA-N-CD	-9.16	98.67	111.50
1	C	3263	PRO	CA-N-CD	-9.16	98.67	111.50
1	A	1263	PRO	CA-N-CD	-9.15	98.68	111.50
1	A	1024	PRO	CA-N-CD	-9.14	98.70	111.50
1	C	3360	PRO	CA-N-CD	-9.12	98.74	111.50
1	B	2086	MET	CA-CB-CG	9.08	128.74	113.30
1	A	1387	PRO	CA-N-CD	-8.99	98.91	111.50
1	C	3070	PRO	CA-N-CD	-8.98	98.93	111.50
1	B	2134	PRO	CA-N-CD	-8.97	98.94	111.50
1	B	2124	PRO	CA-N-CD	-8.96	98.95	111.50
1	B	2360	PRO	CA-N-CD	-8.96	98.96	111.50
1	C	3397	PRO	CA-N-CD	-8.95	98.97	111.50
1	A	1134	PRO	CA-N-CD	-8.94	98.99	111.50
1	C	3024	PRO	CA-N-CD	-8.93	98.99	111.50
1	B	2443	PRO	CA-N-CD	-8.91	99.02	111.50
1	A	1070	PRO	CA-N-CD	-8.88	99.06	111.50
1	C	3046	PRO	CA-N-CD	-8.87	99.08	111.50
1	A	1443	PRO	CA-N-CD	-8.86	99.10	111.50
1	B	2070	PRO	CA-N-CD	-8.83	99.14	111.50
1	B	2397	PRO	CA-N-CD	-8.78	99.21	111.50
1	A	1345	PRO	CA-C-O	-8.72	99.27	120.20
1	C	3345	PRO	CA-N-CD	-8.69	99.33	111.50
1	A	1087	CYS	CB-CA-C	8.31	127.02	110.40
1	C	3087	CYS	CA-CB-SG	8.05	128.48	114.00
1	A	1347	MET	CB-CA-C	-7.84	94.73	110.40
1	B	2345	PRO	N-CA-CB	-7.64	94.14	103.30
1	B	2346	TYR	CD1-CE1-CZ	7.37	126.43	119.80
1	A	1345	PRO	CA-C-N	7.21	133.05	117.20
1	A	1087	CYS	O-C-N	-7.19	111.20	122.70
1	B	2347	MET	CG-SD-CE	7.09	111.55	100.20
1	A	1345	PRO	N-CA-CB	-6.93	94.98	102.60
1	B	2085	PRO	CA-N-CD	-6.65	102.19	111.50
1	C	3087	CYS	CB-CA-C	6.62	123.64	110.40
1	B	2085	PRO	CA-C-N	6.58	131.67	117.20
1	B	2087	CYS	O-C-N	-6.57	112.19	122.70
1	B	2085	PRO	N-CA-CB	-6.29	95.68	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2085	PRO	N-CD-CG	-6.17	93.94	103.20
1	B	2345	PRO	N-CD-CG	-6.15	93.97	103.20
1	B	2087	CYS	CA-C-N	6.09	130.60	117.20
1	A	1345	PRO	CA-N-CD	-6.01	103.08	111.50
1	B	2347	MET	CB-CA-C	-5.97	98.46	110.40
1	B	2072	GLU	C-N-CD	-5.84	107.75	120.60
1	A	1085	PRO	CA-C-O	-5.64	106.66	120.20
1	A	1085	PRO	CA-N-CD	-5.61	103.65	111.50
1	C	3087	CYS	O-C-N	-5.55	113.82	122.70
1	B	2346	TYR	CD1-CG-CD2	-5.48	111.88	117.90
1	B	2345	PRO	CA-C-O	-5.44	107.15	120.20
1	B	2346	TYR	CB-CG-CD2	5.37	124.22	121.00
1	A	1086	MET	CA-CB-CG	5.34	122.38	113.30
1	A	1057	LYS	C-N-CD	-5.12	109.34	120.60
1	B	2085	PRO	CA-C-O	-5.06	108.06	120.20
1	C	3085	PRO	N-CA-C	5.03	125.18	112.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2087	CYS	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3768	0	3802	243	4
1	B	3878	0	3891	208	2
1	C	3509	0	3496	193	2
2	A	10	0	11	1	0
2	B	10	0	11	12	0
2	C	10	0	11	2	0
3	A	23	0	0	22	0
3	B	19	0	0	8	0
3	C	24	0	0	12	1
All	All	11251	0	11222	641	5

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 30.

All (641) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3087:CYS:SG	1:C:3116:CYS:CB	2.06	1.41
1:A:1087:CYS:SG	1:A:1116:CYS:CB	2.09	1.40
1:B:2087:CYS:SG	1:B:2116:CYS:CB	2.10	1.35
1:C:3088:THR:CG2	1:C:3291:GLU:OE2	1.87	1.23
1:B:2088:THR:CG2	1:B:2291:GLU:OE2	1.91	1.17
1:B:2234:PRO:HD2	1:B:2235:LEU:H	1.12	1.15
1:A:1054:PRO:HG3	1:A:1078:LYS:NZ	1.61	1.14
1:C:3054:PRO:HG3	1:C:3078:LYS:NZ	1.62	1.13
1:B:2087:CYS:CB	1:B:2116:CYS:SG	2.35	1.12
1:A:1110:LEU:HB3	3:A:75:HOH:O	1.50	1.11
1:A:1088:THR:HG22	3:A:94:HOH:O	1.51	1.11
1:A:1423:ASP:HA	3:A:12:HOH:O	1.52	1.08
1:C:3234:PRO:HD2	1:C:3235:LEU:H	1.13	1.08
1:C:3237:LYS:HA	1:C:3342:HIS:CE1	1.88	1.07
1:C:3396:ILE:HG22	3:C:21:HOH:O	1.52	1.07
1:A:1360:PRO:HD2	1:A:1361:MET:H	0.99	1.07
1:A:1136:MET:HB3	1:A:1218:PHE:HE2	1.17	1.07
1:C:3046:PRO:HD2	1:C:3046:PRO:O	1.56	1.06
1:A:1397:PRO:HD2	1:A:1398:GLU:H	1.16	1.05
1:B:2136:MET:HB3	1:B:2218:PHE:HE2	1.18	1.04
1:A:1046:PRO:HD2	1:A:1046:PRO:O	1.49	1.03
1:B:2509:PRO:HD2	1:B:2510:ASN:H	1.20	1.03
1:A:1509:PRO:HD2	1:A:1510:ASN:H	1.23	1.03
1:B:2046:PRO:HD2	1:B:2046:PRO:O	1.57	1.02
1:A:1138:TRP:HE3	1:A:1218:PHE:CD1	1.78	1.02
1:C:3088:THR:HG22	1:C:3291:GLU:OE2	1.56	1.01
1:C:3237:LYS:CB	1:C:3342:HIS:CE1	2.43	1.01
1:C:3493:SER:HB2	3:C:16:HOH:O	1.59	1.01
1:B:2088:THR:HG22	1:B:2291:GLU:OE2	1.58	1.00
1:B:2138:TRP:HE3	1:B:2218:PHE:CD1	1.78	1.00
1:C:3145:MET:HG3	1:C:3304:LEU:HD21	1.43	1.00
1:A:1386:TYR:HA	3:A:62:HOH:O	1.60	1.00
1:A:1091:PRO:HD2	1:A:1092:LYS:H	1.25	0.99
1:C:3329:LEU:HD23	1:C:3330:LYS:HG3	1.43	0.99
1:C:3091:PRO:HD2	1:C:3092:LYS:H	1.25	0.98
1:C:3237:LYS:CB	1:C:3342:HIS:HE1	1.76	0.98
2:B:194:WW2:C7	2:B:194:WW2:C5	2.42	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1136:MET:HB3	1:A:1218:PHE:CE2	1.99	0.97
1:B:2355:PHE:CD2	1:B:2360:PRO:HG3	1.99	0.96
1:B:2136:MET:HB3	1:B:2218:PHE:CE2	2.00	0.96
1:A:1382:LEU:HD23	1:A:1396:ILE:HG23	1.47	0.95
1:C:3087:CYS:CB	1:C:3116:CYS:SG	2.54	0.95
1:B:2156:ALA:HB3	3:B:84:HOH:O	1.66	0.95
1:C:3534:GLN:HB3	3:C:44:HOH:O	1.66	0.94
1:A:1124:PRO:HD2	1:A:1125:ALA:H	1.32	0.94
1:C:3124:PRO:HD2	1:C:3125:ALA:H	1.32	0.94
1:A:1086:MET:HE1	1:A:1089:GLN:NE2	1.82	0.94
1:C:3088:THR:HG21	1:C:3291:GLU:OE2	1.68	0.94
1:C:3237:LYS:CA	1:C:3342:HIS:CE1	2.50	0.93
1:A:1088:THR:HG21	1:A:1175:TRP:CE2	2.04	0.93
1:A:1397:PRO:HD2	1:A:1398:GLU:N	1.82	0.93
1:B:2382:LEU:HD23	1:B:2396:ILE:HG23	1.51	0.93
1:C:3124:PRO:HD2	1:C:3125:ALA:N	1.84	0.93
1:B:2455:PHE:CE1	1:B:2482:LYS:HB2	2.04	0.92
1:B:2124:PRO:HD2	1:B:2125:ALA:H	1.30	0.92
1:A:1087:CYS:SG	1:A:1116:CYS:HB2	2.11	0.91
1:A:1395:LEU:O	1:A:1397:PRO:HD2	1.69	0.91
1:C:3234:PRO:HD2	1:C:3235:LEU:N	1.85	0.91
1:A:1360:PRO:HD2	1:A:1361:MET:N	1.75	0.91
1:B:2124:PRO:HD2	1:B:2125:ALA:N	1.83	0.90
1:A:1124:PRO:HD2	1:A:1125:ALA:N	1.84	0.90
1:A:1212:PRO:HD2	1:A:1213:GLY:H	1.36	0.90
2:B:194:WW2:C7	2:B:194:WW2:H5A	2.01	0.89
1:B:2396:ILE:HB	1:B:2397:PRO:HD2	1.55	0.89
1:A:1357:TRP:O	1:A:1360:PRO:HD2	1.71	0.89
1:B:2455:PHE:CE1	1:B:2482:LYS:CB	2.55	0.89
1:A:1138:TRP:CE3	1:A:1218:PHE:CD1	2.60	0.89
1:A:1212:PRO:HD2	1:A:1213:GLY:N	1.87	0.88
1:A:1088:THR:HG21	1:A:1175:TRP:CD2	2.08	0.88
1:B:2138:TRP:CE3	1:B:2218:PHE:CD1	2.60	0.87
1:A:1220:GLU:HG2	1:A:1246:GLU:O	1.74	0.87
1:C:3237:LYS:HB2	1:C:3342:HIS:HE1	1.39	0.87
1:A:1138:TRP:HE3	1:A:1218:PHE:CE1	1.94	0.86
1:B:2088:THR:HG21	1:B:2291:GLU:OE2	1.72	0.86
1:A:1088:THR:CG2	1:A:1175:TRP:CE3	2.59	0.86
1:C:3054:PRO:CG	1:C:3078:LYS:NZ	2.37	0.86
1:A:1088:THR:HG23	1:A:1175:TRP:CE3	2.11	0.86
1:A:1427:GLY:HA3	3:A:12:HOH:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3212:PRO:HD2	1:C:3213:GLY:N	1.91	0.85
1:A:1054:PRO:CG	1:A:1078:LYS:NZ	2.39	0.85
1:A:1509:PRO:HD2	1:A:1510:ASN:N	1.90	0.85
1:B:2212:PRO:HD2	1:B:2213:GLY:H	1.42	0.85
1:C:3212:PRO:HD2	1:C:3213:GLY:H	1.41	0.85
1:C:3220:GLU:HG2	1:C:3246:GLU:O	1.75	0.85
1:C:3396:ILE:HB	1:C:3397:PRO:HD2	1.59	0.84
1:B:2357:TRP:CZ2	1:B:2361:MET:SD	2.70	0.84
1:C:3216:THR:HG23	1:C:3242:ARG:HB2	1.60	0.84
1:B:2234:PRO:HD2	1:B:2235:LEU:N	1.83	0.84
1:B:2212:PRO:HD2	1:B:2213:GLY:N	1.90	0.84
1:B:2245:SER:HG	1:B:2346:TYR:HH	1.13	0.83
1:B:2509:PRO:HD2	1:B:2510:ASN:N	1.86	0.83
1:C:3498:LYS:HG2	1:C:3514:LEU:HD11	1.60	0.83
1:A:1360:PRO:CD	1:A:1361:MET:H	1.89	0.83
1:B:2138:TRP:HE3	1:B:2218:PHE:CE1	1.95	0.83
1:A:1395:LEU:O	1:A:1397:PRO:CD	2.26	0.83
1:C:3054:PRO:HG3	1:C:3078:LYS:HZ1	1.43	0.83
1:A:1087:CYS:CB	1:A:1116:CYS:SG	2.66	0.82
1:B:2220:GLU:HG2	1:B:2246:GLU:O	1.78	0.82
1:A:1216:THR:HG23	1:A:1242:ARG:HB2	1.60	0.82
2:B:194:WW2:C7	2:B:194:WW2:H5	2.10	0.82
1:B:2084:PRO:HD2	1:B:2084:PRO:O	1.79	0.82
1:A:1357:TRP:O	1:A:1360:PRO:CD	2.27	0.81
1:B:2455:PHE:CD1	1:B:2482:LYS:HD3	2.16	0.81
1:C:3068:PRO:HD2	1:C:3068:PRO:O	1.78	0.81
1:C:3084:PRO:HD2	1:C:3084:PRO:O	1.80	0.81
1:A:1091:PRO:HD2	1:A:1092:LYS:N	1.95	0.81
1:C:3091:PRO:HD2	1:C:3092:LYS:N	1.96	0.81
1:B:2216:THR:HG23	1:B:2242:ARG:HB2	1.61	0.80
1:C:3109:PRO:HD2	1:C:3109:PRO:O	1.81	0.80
1:C:3262:LYS:HB3	1:C:3263:PRO:HD2	1.63	0.80
1:A:1395:LEU:C	1:A:1397:PRO:HD3	2.00	0.80
1:B:2109:PRO:HD2	1:B:2109:PRO:O	1.81	0.80
1:B:2030:HIS:N	3:B:28:HOH:O	2.11	0.80
1:A:1057:LYS:CG	1:A:1058:PRO:HD3	2.12	0.79
1:A:1389:VAL:HG23	3:A:62:HOH:O	1.81	0.79
1:A:1109:PRO:HD2	1:A:1109:PRO:O	1.82	0.79
1:A:1262:LYS:HB3	1:A:1263:PRO:HD2	1.65	0.79
1:A:1062:PRO:HD2	1:A:1063:LEU:N	1.96	0.78
1:A:1088:THR:HG23	1:A:1175:TRP:CZ3	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1368:LEU:HD22	1:A:1414:LYS:HE3	1.66	0.78
1:B:2455:PHE:CZ	1:B:2482:LYS:HB2	2.19	0.78
1:B:2068:PRO:HD2	1:B:2068:PRO:O	1.82	0.77
1:B:2387:PRO:HD2	1:B:2388:LEU:N	1.98	0.77
1:A:1030:HIS:CD2	3:A:25:HOH:O	2.38	0.77
1:B:2359:ILE:HB	1:B:2360:PRO:HD2	1.66	0.77
1:C:3087:CYS:SG	1:C:3116:CYS:HB2	2.23	0.77
1:A:1054:PRO:HG3	1:A:1078:LYS:HZ3	1.47	0.77
1:A:1339:ARG:HD2	1:A:1440:ALA:HA	1.67	0.77
1:B:2091:PRO:HD3	1:B:2112:LEU:HD11	1.66	0.77
1:C:3054:PRO:HG3	1:C:3078:LYS:HZ3	1.49	0.77
1:C:3062:PRO:HD2	1:C:3063:LEU:N	1.98	0.77
1:B:2089:GLN:O	1:B:2091:PRO:CD	2.32	0.77
1:B:2030:HIS:ND1	3:B:28:HOH:O	2.17	0.77
1:B:2062:PRO:HD2	1:B:2063:LEU:N	2.00	0.77
1:A:1420:LEU:CD1	1:A:1547:TRP:HZ2	1.97	0.77
1:B:2215:VAL:H	1:B:2241:HIS:HD2	1.34	0.76
1:C:3329:LEU:CD2	1:C:3330:LYS:HG3	2.16	0.76
1:A:1054:PRO:HG3	1:A:1078:LYS:HZ1	1.49	0.76
1:A:1386:TYR:HB3	1:A:1387:PRO:HD2	1.66	0.76
1:A:1084:PRO:HD2	1:A:1084:PRO:O	1.85	0.76
1:A:1068:PRO:HD2	1:A:1068:PRO:O	1.84	0.76
1:A:1132:ARG:HB3	1:A:1211:ASN:HB2	1.66	0.76
1:A:1138:TRP:CE3	1:A:1218:PHE:CE1	2.74	0.76
1:A:1420:LEU:HD12	1:A:1547:TRP:HZ2	1.50	0.76
1:A:1086:MET:CE	1:A:1089:GLN:NE2	2.49	0.76
1:A:1088:THR:CG2	1:A:1175:TRP:CD2	2.68	0.76
1:B:2024:PRO:HD2	1:B:2024:PRO:O	1.85	0.75
1:C:3132:ARG:HB3	1:C:3211:ASN:HB2	1.69	0.75
1:A:1024:PRO:HD2	1:A:1024:PRO:O	1.87	0.75
1:A:1420:LEU:CD1	1:A:1547:TRP:CZ2	2.69	0.75
1:C:3134:PRO:HG2	1:C:3163:VAL:HG12	1.67	0.75
1:C:3359:ILE:HB	1:C:3360:PRO:HD2	1.67	0.75
1:C:3487:GLU:HA	1:C:3490:ILE:HD12	1.69	0.75
1:B:2087:CYS:SG	1:B:2116:CYS:HB2	2.25	0.75
1:A:1359:ILE:N	1:A:1360:PRO:HD3	2.02	0.75
1:C:3397:PRO:HD3	3:C:21:HOH:O	1.87	0.74
1:C:3242:ARG:HG2	1:C:3242:ARG:HH11	1.52	0.74
1:B:2242:ARG:HG2	1:B:2242:ARG:HH11	1.50	0.74
1:C:3215:VAL:H	1:C:3241:HIS:HD2	1.33	0.74
1:C:3409:ASP:OD1	1:C:3409:ASP:O	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1529:ILE:HA	1:A:1533:THR:HG23	1.70	0.73
1:B:2455:PHE:CE1	1:B:2482:LYS:HB3	2.24	0.73
1:B:2138:TRP:CE3	1:B:2218:PHE:CE1	2.76	0.73
1:A:1242:ARG:HG2	1:A:1242:ARG:HH11	1.53	0.73
1:A:1348:VAL:HB	1:A:1446:MET:SD	2.29	0.73
1:B:2355:PHE:CE2	1:B:2360:PRO:HG3	2.24	0.73
1:A:1428:VAL:HB	1:A:1429:PRO:HD2	1.71	0.73
1:A:1126:ASP:OD1	1:A:1126:ASP:O	2.07	0.73
1:C:3237:LYS:HB3	1:C:3342:HIS:CE1	2.21	0.73
1:A:1252:THR:HG22	1:A:1254:VAL:HG12	1.70	0.72
1:B:2132:ARG:HB3	1:B:2211:ASN:HB2	1.71	0.72
1:C:3073:PRO:HD2	1:C:3073:PRO:O	1.88	0.72
1:A:1075:SER:O	1:A:1076:PHE:HB2	1.88	0.72
1:C:3024:PRO:HD2	1:C:3024:PRO:O	1.88	0.72
1:B:2089:GLN:O	1:B:2091:PRO:HD3	1.90	0.72
1:B:2062:PRO:HD2	1:B:2063:LEU:H	1.55	0.72
1:B:2387:PRO:HD2	1:B:2388:LEU:H	1.54	0.72
1:B:2487:GLU:HA	1:B:2490:ILE:HD12	1.71	0.72
1:A:1062:PRO:HD2	1:A:1063:LEU:H	1.52	0.72
1:B:2518:PRO:HD2	1:B:2518:PRO:O	1.89	0.72
1:B:2529:ILE:HA	1:B:2533:THR:HG23	1.71	0.72
1:C:3093:ALA:N	3:C:71:HOH:O	2.22	0.72
1:C:3357:TRP:CZ2	1:C:3361:MET:SD	2.82	0.71
1:B:2234:PRO:CD	1:B:2235:LEU:H	1.98	0.71
1:A:1110:LEU:CB	3:A:75:HOH:O	2.20	0.71
1:A:1420:LEU:HD11	1:A:1547:TRP:CH2	2.25	0.71
1:B:2385:SER:C	1:B:2387:PRO:HD3	2.11	0.71
1:A:1058:PRO:HD2	1:A:1058:PRO:O	1.89	0.71
1:B:2428:VAL:HB	1:B:2429:PRO:HD2	1.72	0.71
1:C:3234:PRO:CD	1:C:3235:LEU:H	1.99	0.71
1:A:1036:LYS:NZ	3:A:91:HOH:O	2.20	0.70
1:A:1086:MET:HG2	1:A:1110:LEU:HB3	1.70	0.70
1:C:3529:ILE:HA	1:C:3533:THR:HG23	1.73	0.70
1:A:1461:PRO:HB2	3:A:59:HOH:O	1.90	0.70
1:A:1057:LYS:HG2	1:A:1058:PRO:CD	2.21	0.70
1:A:1518:PRO:HD2	1:A:1518:PRO:O	1.89	0.70
1:C:3134:PRO:HD2	1:C:3134:PRO:O	1.91	0.70
1:A:1086:MET:HE1	1:A:1089:GLN:HE22	1.56	0.70
1:C:3062:PRO:HD2	1:C:3063:LEU:H	1.54	0.69
1:B:2532:ASN:O	1:B:2534:GLN:OE1	2.09	0.69
1:A:1357:TRP:CZ2	1:A:1361:MET:SD	2.86	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2355:PHE:CE2	1:B:2360:PRO:HD3	2.27	0.69
1:C:3227:VAL:O	1:C:3231:VAL:HG23	1.94	0.68
1:A:1054:PRO:HD2	1:A:1054:PRO:O	1.94	0.68
1:B:2138:TRP:CE3	1:B:2218:PHE:HD1	2.11	0.68
1:B:2455:PHE:HE1	1:B:2482:LYS:HB3	1.57	0.67
1:A:1236:ALA:HA	1:A:1239:LEU:HD12	1.76	0.67
1:B:2268:ILE:HD11	1:B:2319:LEU:HD21	1.75	0.67
1:A:1212:PRO:CD	1:A:1213:GLY:N	2.58	0.67
1:C:3268:ILE:HD11	1:C:3319:LEU:HD21	1.77	0.67
1:C:3355:PHE:CD1	1:C:3360:PRO:HG3	2.29	0.66
1:B:2236:ALA:HA	1:B:2239:LEU:HD12	1.76	0.66
1:B:2494:LYS:O	1:B:2498:LYS:HG3	1.94	0.66
1:A:1395:LEU:C	1:A:1397:PRO:CD	2.63	0.66
1:C:3086:MET:HG3	1:C:3110:LEU:HB2	1.77	0.66
1:C:3330:LYS:HB3	1:C:3334:GLU:OE1	1.96	0.66
1:C:3236:ALA:HA	1:C:3239:LEU:HD12	1.77	0.66
1:A:1057:LYS:HG3	1:A:1058:PRO:HD3	1.78	0.66
1:B:2141:GLY:N	3:B:31:HOH:O	2.29	0.66
1:C:3086:MET:HG2	1:C:3110:LEU:CD1	2.26	0.66
1:B:2354:GLU:HG2	3:B:98:HOH:O	1.95	0.65
1:A:1225:GLU:O	1:A:1229:VAL:HG23	1.96	0.65
1:B:2091:PRO:CD	1:B:2112:LEU:HD11	2.25	0.65
1:A:1397:PRO:CD	1:A:1398:GLU:N	2.58	0.65
1:B:2218:PHE:HB3	1:B:2244:ILE:HB	1.77	0.65
1:B:2355:PHE:HD2	1:B:2360:PRO:HG3	1.55	0.65
1:B:2423:ASP:OD2	1:B:2543:GLU:HG2	1.97	0.65
1:A:1420:LEU:HD12	1:A:1547:TRP:CZ2	2.28	0.65
1:B:2355:PHE:CD2	1:B:2360:PRO:CG	2.78	0.65
1:A:1517:TRP:HD1	1:A:1518:PRO:HD2	1.62	0.65
1:A:1088:THR:CG2	1:A:1175:TRP:CZ3	2.79	0.64
1:A:1392:ALA:HB3	1:A:1395:LEU:HG	1.80	0.64
1:C:3225:GLU:O	1:C:3229:VAL:HG23	1.97	0.64
1:A:1088:THR:HG21	1:A:1175:TRP:CZ2	2.31	0.64
1:B:2225:GLU:O	1:B:2229:VAL:HG23	1.98	0.64
1:B:2363:LEU:HD13	2:B:194:WW2:H3	1.79	0.64
1:C:3054:PRO:HD2	1:C:3054:PRO:O	1.97	0.64
1:B:2054:PRO:HD2	1:B:2054:PRO:O	1.97	0.64
1:C:3329:LEU:HD23	1:C:3330:LYS:CG	2.25	0.64
1:A:1218:PHE:HB3	1:A:1244:ILE:HB	1.79	0.64
1:A:1138:TRP:CE3	1:A:1218:PHE:HD1	2.12	0.64
1:B:2089:GLN:O	1:B:2091:PRO:HD2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2045:GLN:HE21	1:B:2046:PRO:HD2	1.61	0.63
1:B:2086:MET:O	1:B:2087:CYS:C	2.28	0.63
1:B:2517:TRP:HD1	1:B:2518:PRO:HD2	1.62	0.63
1:C:3132:ARG:HH12	1:C:3206:ALA:HB1	1.62	0.63
1:A:1423:ASP:OD2	1:A:1543:GLU:HG2	1.98	0.63
1:A:1456:SER:HB3	1:A:1460:LYS:HD3	1.80	0.63
1:A:1132:ARG:HH12	1:A:1206:ALA:HB1	1.63	0.63
1:A:1227:VAL:O	1:A:1231:VAL:HG23	1.99	0.63
1:A:1420:LEU:HD11	1:A:1547:TRP:CZ2	2.32	0.63
1:C:3095:GLN:O	1:C:3099:GLU:HG3	1.99	0.62
1:A:1330:LYS:HB3	1:A:1334:GLU:OE1	1.98	0.62
1:B:2478:ALA:HB3	1:B:2479:PRO:HD2	1.81	0.62
1:A:1086:MET:HG2	1:A:1110:LEU:CB	2.25	0.62
1:A:1268:ILE:HD11	1:A:1319:LEU:HD21	1.79	0.62
1:C:3237:LYS:HB3	1:C:3342:HIS:NE2	2.15	0.62
1:C:3089:GLN:OE1	1:C:3146:VAL:HA	1.99	0.62
1:B:2227:VAL:O	1:B:2231:VAL:HG23	2.00	0.62
1:A:1057:LYS:HG2	1:A:1058:PRO:HD2	1.82	0.61
1:C:3218:PHE:CB	1:C:3244:ILE:HB	2.31	0.61
1:B:2509:PRO:CD	1:B:2510:ASN:N	2.62	0.61
1:C:3301:MET:O	1:C:3302:LYS:HG2	2.01	0.61
1:A:1126:ASP:OD1	1:A:1131:ASN:ND2	2.34	0.61
1:A:1074:TRP:HB3	1:B:2183:GLU:OE1	2.01	0.61
1:C:3218:PHE:HB3	1:C:3244:ILE:HB	1.82	0.61
1:A:1397:PRO:CD	1:A:1398:GLU:H	2.02	0.60
1:A:1030:HIS:CG	3:A:25:HOH:O	2.54	0.60
1:A:1083:TYR:CE2	1:A:1108:ILE:HD13	2.36	0.60
1:C:3420:LEU:HD12	1:C:3420:LEU:C	2.22	0.60
1:B:2363:LEU:HD12	2:B:194:WW2:C4	2.31	0.60
1:C:3450:GLN:HG3	1:C:3450:GLN:O	2.02	0.60
1:C:3156:ALA:O	1:C:3160:HIS:HD2	1.85	0.60
1:B:2142:GLY:N	2:B:194:WW2:O1	2.35	0.60
1:C:3085:PRO:C	1:C:3086:MET:O	2.32	0.60
1:A:1090:ASP:OD1	1:A:1091:PRO:HD2	2.02	0.59
1:A:1095:GLN:O	1:A:1099:GLU:HG3	2.01	0.59
1:B:2363:LEU:HD12	2:B:194:WW2:H4A	1.84	0.59
1:A:1348:VAL:O	1:A:1446:MET:SD	2.59	0.59
1:A:1379:MET:HG2	1:A:1400:THR:HG21	1.85	0.59
1:B:2095:GLN:O	1:B:2099:GLU:HG3	2.03	0.59
1:B:2156:ALA:O	1:B:2160:HIS:HD2	1.85	0.59
1:B:2455:PHE:CE1	1:B:2482:LYS:HD3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3423:ASP:OD2	1:C:3543:GLU:HG2	2.03	0.59
1:A:1087:CYS:O	1:A:1088:THR:C	2.32	0.59
1:B:2385:SER:C	1:B:2387:PRO:CD	2.71	0.59
1:C:3090:ASP:OD1	1:C:3091:PRO:HD2	2.03	0.59
1:C:3258:LYS:HE2	1:C:3333:GLU:OE1	2.03	0.59
1:A:1478:ALA:HB3	1:A:1479:PRO:HD2	1.85	0.59
1:C:3521:ASN:HB2	1:C:3522:GLN:OE1	2.02	0.59
1:A:1509:PRO:CD	1:A:1510:ASN:N	2.65	0.59
1:B:2083:TYR:CE2	1:B:2108:ILE:HD13	2.37	0.59
1:C:3086:MET:HG3	1:C:3110:LEU:CB	2.33	0.59
1:A:1057:LYS:HG2	1:A:1058:PRO:HD3	1.82	0.59
1:A:1089:GLN:OE1	1:A:1146:VAL:HA	2.03	0.59
1:B:2218:PHE:CB	1:B:2244:ILE:HB	2.33	0.58
1:B:2420:LEU:HD12	1:B:2420:LEU:C	2.24	0.58
1:A:1386:TYR:HB3	1:A:1387:PRO:CD	2.34	0.58
1:A:1413:LYS:HA	1:A:1416:LEU:HD12	1.86	0.58
1:A:1479:PRO:HG3	1:A:1489:GLU:HG2	1.85	0.58
1:B:2091:PRO:HG3	1:B:2112:LEU:HD11	1.85	0.58
1:C:3145:MET:HG3	1:C:3304:LEU:CD2	2.27	0.58
1:C:3354:GLU:HG2	3:C:58:HOH:O	2.04	0.58
1:A:1054:PRO:CG	1:A:1078:LYS:HZ2	2.16	0.58
1:B:2414:LYS:O	1:B:2418:LEU:HD13	2.03	0.58
1:A:1086:MET:O	1:A:1087:CYS:C	2.41	0.58
1:A:1218:PHE:CB	1:A:1244:ILE:HB	2.33	0.58
1:A:1396:ILE:N	1:A:1397:PRO:HD3	2.19	0.58
1:A:1462:LYS:N	3:A:59:HOH:O	2.37	0.58
1:C:3025:VAL:HG22	1:C:3034:LEU:HD13	1.85	0.57
1:C:3067:PRO:HD3	1:C:3189:TRP:CZ3	2.39	0.57
1:C:3083:TYR:CE2	1:C:3108:ILE:HD13	2.39	0.57
1:B:2363:LEU:CD1	2:B:194:WW2:H4A	2.33	0.57
1:A:1156:ALA:O	1:A:1160:HIS:HD2	1.86	0.57
1:A:1298:THR:CG2	3:A:67:HOH:O	2.52	0.57
1:B:2521:ASN:HB2	1:B:2522:GLN:OE1	2.03	0.57
1:C:3124:PRO:CD	1:C:3125:ALA:H	2.07	0.57
1:A:1090:ASP:OD1	1:A:1091:PRO:CD	2.53	0.57
1:B:2351:ASN:ND2	1:B:2471:GLU:OE1	2.35	0.57
1:B:2413:LYS:HA	1:B:2416:LEU:HD12	1.85	0.57
1:C:3143:GLY:N	2:C:195:WW2:O1	2.37	0.57
1:A:1067:PRO:HD3	1:A:1189:TRP:CZ3	2.40	0.57
1:C:3086:MET:SD	1:C:3089:GLN:NE2	2.78	0.56
1:B:2089:GLN:OE1	1:B:2146:VAL:HA	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2355:PHE:CE2	1:B:2360:PRO:CD	2.88	0.56
1:C:3495:MET:HE3	1:C:3533:THR:HG21	1.86	0.56
1:A:1057:LYS:CG	1:A:1058:PRO:CD	2.79	0.56
1:A:1136:MET:CB	1:A:1218:PHE:HE2	2.06	0.56
1:B:2067:PRO:HD3	1:B:2189:TRP:CZ3	2.41	0.56
1:C:3086:MET:HG2	1:C:3110:LEU:HD12	1.86	0.56
1:B:2025:VAL:HG22	1:B:2034:LEU:HD13	1.87	0.56
1:A:1360:PRO:CD	1:A:1361:MET:N	2.50	0.56
1:B:2451:TYR:HD1	3:B:63:HOH:O	1.89	0.56
1:A:1025:VAL:HG22	1:A:1034:LEU:HD13	1.88	0.56
1:B:2479:PRO:HG3	1:B:2489:GLU:HG2	1.87	0.56
1:A:1292:GLU:OE2	1:B:2275:LYS:NZ	2.38	0.55
1:C:3132:ARG:NH1	1:C:3206:ALA:HB1	2.21	0.55
1:B:2363:LEU:HD13	2:B:194:WW2:C3	2.35	0.55
1:A:1461:PRO:CB	3:A:59:HOH:O	2.52	0.55
1:C:3037:PHE:HD1	3:C:87:HOH:O	1.89	0.55
1:C:3296:GLU:O	1:C:3300:LYS:HG3	2.07	0.55
1:A:1046:PRO:O	1:A:1046:PRO:CD	2.28	0.55
1:B:2359:ILE:HB	1:B:2360:PRO:CD	2.34	0.55
1:B:2450:GLN:O	1:B:2450:GLN:HG3	2.05	0.55
1:C:3090:ASP:OD1	1:C:3091:PRO:CD	2.54	0.55
1:B:2353:GLN:O	1:B:2467:ASP:HA	2.06	0.55
1:C:3086:MET:HG2	1:C:3110:LEU:HD13	1.89	0.55
1:B:2396:ILE:HB	1:B:2397:PRO:CD	2.31	0.55
1:A:1359:ILE:N	1:A:1360:PRO:CD	2.70	0.55
1:B:2242:ARG:HG2	1:B:2242:ARG:NH1	2.21	0.55
1:B:2420:LEU:HD13	1:B:2547:TRP:CZ2	2.42	0.55
1:A:1332:PRO:O	1:A:1336:GLN:HG3	2.07	0.55
1:C:3237:LYS:HB2	1:C:3342:HIS:CE1	2.26	0.55
1:A:1132:ARG:NH1	1:A:1206:ALA:HB1	2.22	0.54
1:B:2062:PRO:CD	1:B:2063:LEU:N	2.70	0.54
1:C:3088:THR:HG21	1:C:3291:GLU:CD	2.26	0.54
1:C:3234:PRO:CD	1:C:3235:LEU:N	2.58	0.54
1:B:2087:CYS:N	3:B:76:HOH:O	2.15	0.54
1:C:3054:PRO:CG	1:C:3078:LYS:HZ2	2.20	0.54
1:C:3495:MET:CE	1:C:3533:THR:HG21	2.37	0.54
1:C:3142:GLY:N	2:C:195:WW2:O1	2.41	0.54
1:C:3301:MET:O	1:C:3302:LYS:CG	2.55	0.54
1:A:1420:LEU:HD11	1:A:1547:TRP:HH2	1.71	0.54
1:A:1030:HIS:HB2	3:A:25:HOH:O	2.06	0.54
1:A:1351:ASN:ND2	1:A:1471:GLU:OE1	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3359:ILE:HB	1:C:3360:PRO:CD	2.35	0.54
1:C:3420:LEU:HD13	1:C:3547:TRP:CZ2	2.42	0.54
1:B:2045:GLN:NE2	1:B:2046:PRO:CD	2.70	0.54
1:B:2387:PRO:CD	1:B:2388:LEU:N	2.68	0.54
1:C:3355:PHE:CE1	1:C:3360:PRO:HD3	2.42	0.54
1:C:3124:PRO:CD	1:C:3125:ALA:N	2.57	0.54
1:B:2099:GLU:HG2	1:B:2107:ASN:HD22	1.72	0.54
1:B:2045:GLN:NE2	1:B:2046:PRO:HD3	2.23	0.53
1:B:2124:PRO:CD	1:B:2125:ALA:H	2.06	0.53
1:B:2199:ARG:HG2	1:B:2239:LEU:HD21	1.89	0.53
1:B:2297:THR:O	1:B:2301:MET:HG2	2.07	0.53
1:C:3099:GLU:HG2	1:C:3107:ASN:HD22	1.73	0.53
1:B:2091:PRO:HG3	1:B:2112:LEU:CD1	2.39	0.53
1:C:3237:LYS:CA	1:C:3342:HIS:HE1	2.05	0.53
1:B:2407:THR:HG22	1:B:2409:ASP:H	1.73	0.53
1:C:3085:PRO:O	1:C:3086:MET:O	2.26	0.53
1:A:1428:VAL:HB	1:A:1429:PRO:CD	2.38	0.53
1:A:1353:GLN:O	1:A:1467:ASP:HA	2.09	0.53
1:A:1296:GLU:O	1:A:1300:LYS:HG3	2.08	0.53
1:A:1298:THR:HG23	3:A:67:HOH:O	2.08	0.53
1:B:2128:THR:O	1:B:2129:LYS:HG3	2.09	0.53
1:C:3297:THR:O	1:C:3301:MET:HG2	2.09	0.53
1:C:3145:MET:CG	1:C:3304:LEU:HD21	2.27	0.53
1:C:3037:PHE:HB2	3:C:87:HOH:O	2.08	0.52
1:C:3353:GLN:O	1:C:3467:ASP:HA	2.09	0.52
1:A:1242:ARG:HG2	1:A:1242:ARG:NH1	2.24	0.52
1:A:1051:LEU:O	1:A:1080:ALA:HB1	2.08	0.52
1:B:2091:PRO:CG	1:B:2112:LEU:HD11	2.39	0.52
1:B:2234:PRO:CD	1:B:2235:LEU:N	2.57	0.52
1:A:1266:GLU:O	1:A:1270:ILE:HG13	2.10	0.52
1:C:3132:ARG:HH12	1:C:3206:ALA:CB	2.22	0.52
1:B:2517:TRP:HD1	1:B:2518:PRO:CD	2.23	0.52
1:C:3396:ILE:HB	1:C:3397:PRO:CD	2.34	0.52
1:A:1262:LYS:HB3	1:A:1263:PRO:CD	2.36	0.52
1:A:1034:LEU:HD23	1:A:1079:ASN:ND2	2.25	0.52
1:B:2296:GLU:O	1:B:2300:LYS:HG3	2.10	0.51
1:C:3109:PRO:O	1:C:3109:PRO:CD	2.56	0.51
1:B:2355:PHE:CE2	1:B:2360:PRO:CG	2.91	0.51
1:B:2212:PRO:CD	1:B:2213:GLY:H	2.14	0.51
1:C:3262:LYS:HB3	1:C:3263:PRO:CD	2.38	0.51
1:A:1235:LEU:HD12	1:A:1327:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1494:LYS:O	1:A:1498:LYS:HG3	2.11	0.51
1:B:2086:MET:O	1:B:2087:CYS:O	2.28	0.51
1:A:1068:PRO:HA	3:A:60:HOH:O	2.10	0.51
1:A:1088:THR:HG23	1:A:1088:THR:O	2.10	0.51
1:A:1517:TRP:HD1	1:A:1518:PRO:CD	2.22	0.50
1:A:1508:ASN:OD1	1:A:1509:PRO:CD	2.60	0.50
1:B:2030:HIS:CG	3:B:28:HOH:O	2.61	0.50
1:A:1377:THR:O	1:A:1380:SER:HB2	2.10	0.50
1:C:3234:PRO:O	1:C:3237:LYS:HG2	2.11	0.50
1:C:3235:LEU:HD12	1:C:3327:LEU:HD12	1.94	0.50
1:C:3242:ARG:HG2	1:C:3242:ARG:NH1	2.23	0.50
1:A:1099:GLU:HG2	1:A:1107:ASN:HD22	1.77	0.50
1:B:2088:THR:HG21	1:B:2291:GLU:CD	2.30	0.50
1:B:2387:PRO:CD	1:B:2388:LEU:H	2.24	0.50
1:C:3343:THR:HB	1:C:3442:ALA:HB2	1.93	0.50
1:C:3450:GLN:HG2	1:C:3529:ILE:O	2.11	0.50
1:A:1132:ARG:HH12	1:A:1206:ALA:CB	2.23	0.50
1:A:1297:THR:O	1:A:1301:MET:HG2	2.11	0.50
1:A:1540:LYS:O	1:A:1544:VAL:HG23	2.12	0.50
1:C:3039:SER:OG	1:C:3046:PRO:HB3	2.12	0.50
1:C:3428:VAL:HB	1:C:3429:PRO:HD3	1.94	0.50
1:A:1237:LYS:O	1:A:1238:ASN:HB2	2.12	0.50
1:A:1400:THR:O	1:A:1404:LEU:HG	2.12	0.50
1:B:2455:PHE:CD1	1:B:2482:LYS:CD	2.92	0.50
1:B:2540:LYS:O	1:B:2544:VAL:HG23	2.12	0.50
1:C:3025:VAL:CG2	1:C:3034:LEU:HD13	2.42	0.50
1:C:3264:LEU:O	1:C:3268:ILE:HG13	2.12	0.50
1:A:1030:HIS:CB	3:A:25:HOH:O	2.60	0.49
1:B:2075:SER:O	1:B:2076:PHE:HB2	2.10	0.49
1:A:1343:THR:HB	1:A:1442:ALA:HB2	1.93	0.49
1:C:3351:ASN:OD1	1:C:3449:PHE:HB3	2.12	0.49
1:A:1084:PRO:O	1:A:1084:PRO:CD	2.60	0.49
1:B:2045:GLN:HE21	1:B:2046:PRO:CD	2.26	0.49
1:B:2283:VAL:O	1:B:2287:ARG:HG3	2.12	0.49
1:B:2363:LEU:CD1	2:B:194:WW2:C4	2.90	0.49
1:C:3084:PRO:O	1:C:3084:PRO:CD	2.55	0.49
1:C:3152:TYR:CD1	1:C:3152:TYR:N	2.81	0.49
1:B:2508:ASN:OD1	1:B:2509:PRO:CD	2.61	0.49
1:C:3487:GLU:N	3:C:23:HOH:O	2.45	0.49
1:A:1212:PRO:CD	1:A:1213:GLY:H	2.09	0.49
1:A:1128:THR:O	1:A:1129:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2161:GLU:OE2	1:B:2498:LYS:HG2	2.13	0.49
1:B:2237:LYS:O	1:B:2238:ASN:HB2	2.13	0.49
1:B:2264:LEU:HD21	1:B:2319:LEU:HD23	1.95	0.49
1:B:2263:PRO:O	1:B:2267:GLN:HG2	2.13	0.49
1:B:2360:PRO:O	1:B:2366:TYR:HB2	2.13	0.49
1:A:1528:GLN:O	1:A:1533:THR:HA	2.13	0.48
1:B:2235:LEU:HD12	1:B:2327:LEU:HD12	1.95	0.48
1:B:2428:VAL:HB	1:B:2429:PRO:CD	2.40	0.48
1:C:3283:VAL:O	1:C:3287:ARG:HG3	2.13	0.48
1:A:1508:ASN:OD1	1:A:1509:PRO:HD2	2.11	0.48
1:C:3088:THR:HG21	1:C:3291:GLU:CG	2.43	0.48
1:A:1360:PRO:O	1:A:1366:TYR:HB2	2.13	0.48
1:B:2138:TRP:CZ3	1:B:2218:PHE:HD1	2.30	0.48
1:A:1138:TRP:CZ3	1:A:1218:PHE:HD1	2.31	0.48
1:B:2450:GLN:HG2	1:B:2529:ILE:O	2.14	0.48
1:C:3201:VAL:HG13	1:C:3205:ILE:HB	1.96	0.48
1:B:2026:VAL:HG12	1:B:2027:ASP:N	2.29	0.48
1:B:2264:LEU:O	1:B:2268:ILE:HG13	2.14	0.48
1:B:2461:PRO:HG2	1:B:2464:VAL:HG23	1.95	0.48
1:B:2461:PRO:HG2	1:B:2464:VAL:CG2	2.44	0.47
1:A:1152:TYR:N	1:A:1152:TYR:CD1	2.81	0.47
1:A:1461:PRO:HG2	1:A:1464:VAL:HG23	1.95	0.47
1:C:3266:GLU:O	1:C:3270:ILE:HG13	2.14	0.47
1:C:3024:PRO:O	1:C:3024:PRO:CD	2.60	0.47
1:C:3134:PRO:CG	1:C:3163:VAL:HG12	2.40	0.47
1:C:3396:ILE:CB	1:C:3397:PRO:HD2	2.39	0.47
1:C:3528:GLN:O	1:C:3533:THR:HA	2.14	0.47
1:A:1124:PRO:CD	1:A:1125:ALA:H	2.07	0.47
1:A:1145:MET:HE1	1:A:1303:PHE:CD1	2.49	0.47
1:B:2396:ILE:CB	1:B:2397:PRO:CD	2.92	0.47
1:A:1201:VAL:HG13	1:A:1205:ILE:HB	1.96	0.47
1:A:1283:VAL:O	1:A:1287:ARG:HG3	2.15	0.47
1:B:2201:VAL:HG13	1:B:2205:ILE:HB	1.97	0.47
1:B:2355:PHE:CZ	1:B:2360:PRO:HD3	2.48	0.47
1:C:3451:TYR:HE2	1:C:3489:GLU:HG3	1.79	0.47
1:A:1039:SER:OG	1:A:1046:PRO:HB3	2.15	0.47
1:A:1357:TRP:C	1:A:1360:PRO:CD	2.83	0.47
1:C:3026:VAL:HG12	1:C:3027:ASP:N	2.30	0.47
1:B:2508:ASN:OD1	1:B:2509:PRO:HD2	2.14	0.47
1:C:3268:ILE:HD11	1:C:3319:LEU:CD2	2.43	0.47
1:A:1363:LEU:HD13	2:A:193:WW2:H3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2025:VAL:CG2	1:B:2034:LEU:HD13	2.45	0.46
1:A:1211:ASN:OD1	1:A:1212:PRO:CD	2.64	0.46
1:B:2088:THR:HG21	1:B:2291:GLU:CG	2.45	0.46
1:C:3067:PRO:HD3	1:C:3189:TRP:HZ3	1.81	0.46
1:A:1024:PRO:O	1:A:1024:PRO:CD	2.60	0.46
1:A:1461:PRO:C	3:A:59:HOH:O	2.54	0.46
1:B:2152:TYR:CD1	1:B:2152:TYR:N	2.83	0.46
1:B:2351:ASN:OD1	1:B:2449:PHE:HB3	2.15	0.46
1:C:3488:GLU:N	3:C:23:HOH:O	2.39	0.46
1:C:3540:LYS:O	1:C:3544:VAL:HG23	2.14	0.46
1:A:1025:VAL:CG2	1:A:1034:LEU:HD13	2.44	0.46
1:A:1351:ASN:OD1	1:A:1449:PHE:HB3	2.16	0.46
1:B:2304:LEU:C	1:B:2304:LEU:HD12	2.35	0.46
1:A:1067:PRO:HD3	1:A:1189:TRP:HZ3	1.81	0.46
1:B:2099:GLU:CG	1:B:2107:ASN:ND2	2.79	0.46
1:C:3329:LEU:HD23	1:C:3329:LEU:O	2.16	0.46
1:A:1126:ASP:O	1:A:1126:ASP:CG	2.54	0.46
1:B:2099:GLU:HG2	1:B:2107:ASN:ND2	2.31	0.46
1:C:3114:GLU:HG3	1:C:3291:GLU:CD	2.36	0.46
1:C:3134:PRO:O	1:C:3134:PRO:CD	2.61	0.46
1:A:1114:GLU:HG3	1:A:1291:GLU:CD	2.37	0.46
1:A:1461:PRO:HG2	1:A:1464:VAL:CG2	2.46	0.46
1:B:2266:GLU:O	1:B:2270:ILE:HG13	2.16	0.46
1:B:2455:PHE:HE1	1:B:2482:LYS:CB	2.14	0.46
1:C:3478:ALA:N	1:C:3479:PRO:CD	2.79	0.45
1:A:1264:LEU:O	1:A:1268:ILE:HG13	2.16	0.45
1:B:2099:GLU:CG	1:B:2107:ASN:HD22	2.29	0.45
1:B:2242:ARG:NH1	1:B:2242:ARG:CG	2.80	0.45
1:C:3068:PRO:O	1:C:3068:PRO:CD	2.54	0.45
1:A:1034:LEU:HD23	1:A:1079:ASN:HD22	1.82	0.45
1:A:1086:MET:HB3	1:A:1086:MET:HE3	1.48	0.45
1:B:2268:ILE:HD11	1:B:2319:LEU:CD2	2.43	0.45
1:C:3099:GLU:HG2	1:C:3107:ASN:ND2	2.32	0.45
1:A:1156:ALA:O	1:A:1160:HIS:CD2	2.69	0.45
1:A:1518:PRO:O	1:A:1518:PRO:CD	2.62	0.45
1:C:3400:THR:HG21	3:C:21:HOH:O	2.16	0.45
1:C:3038:VAL:HG21	1:C:3049:ILE:HD12	1.99	0.45
1:A:1026:VAL:HG12	1:A:1027:ASP:N	2.31	0.45
1:C:3237:LYS:O	1:C:3238:ASN:HB2	2.16	0.45
1:C:3242:ARG:HH11	1:C:3242:ARG:CG	2.25	0.45
1:B:2046:PRO:O	1:B:2046:PRO:CD	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:VAL:HG21	1:A:1049:ILE:HD12	1.99	0.44
1:B:2074:TRP:HB3	1:C:3183:GLU:OE1	2.17	0.44
1:B:2124:PRO:CD	1:B:2125:ALA:N	2.57	0.44
1:B:2156:ALA:O	1:B:2160:HIS:CD2	2.68	0.44
1:B:2220:GLU:HA	1:B:2246:GLU:O	2.17	0.44
1:C:3099:GLU:CG	1:C:3107:ASN:HD22	2.30	0.44
1:B:2245:SER:OG	1:B:2346:TYR:OH	1.97	0.44
1:B:2355:PHE:CE1	1:B:2421:ILE:HG21	2.52	0.44
1:A:1124:PRO:CD	1:A:1125:ALA:N	2.57	0.44
1:B:2136:MET:CB	1:B:2218:PHE:HE2	2.07	0.44
1:C:3351:ASN:HB3	1:C:3466:GLY:O	2.17	0.44
1:B:2098:SER:O	1:B:2102:THR:HB	2.18	0.44
1:C:3099:GLU:CG	1:C:3107:ASN:ND2	2.80	0.44
1:A:1099:GLU:CG	1:A:1107:ASN:ND2	2.81	0.44
1:A:1268:ILE:HD11	1:A:1319:LEU:CD2	2.45	0.44
1:A:1211:ASN:OD1	1:A:1212:PRO:HD2	2.18	0.44
1:B:2355:PHE:CZ	1:B:2421:ILE:HG21	2.53	0.44
1:B:2363:LEU:CD1	2:B:194:WW2:H3	2.46	0.44
1:C:3254:VAL:HG13	1:C:3255:LEU:HG	2.00	0.44
1:B:2344:VAL:O	1:B:2345:PRO:C	2.52	0.43
1:A:1086:MET:SD	1:A:1110:LEU:HB2	2.58	0.43
1:B:2351:ASN:HB3	1:B:2466:GLY:O	2.18	0.43
1:A:1088:THR:HG21	1:A:1175:TRP:CH2	2.54	0.43
1:A:1086:MET:CG	1:A:1110:LEU:CB	2.95	0.43
1:B:2114:GLU:HG3	1:B:2291:GLU:CD	2.39	0.43
1:A:1091:PRO:CD	1:A:1092:LYS:N	2.68	0.43
1:A:1099:GLU:HG2	1:A:1107:ASN:ND2	2.33	0.43
1:A:1389:VAL:CG2	3:A:62:HOH:O	2.51	0.43
1:B:2045:GLN:NE2	1:B:2046:PRO:HD2	2.29	0.43
1:B:2251:LEU:O	1:B:2253:SER:N	2.51	0.43
1:B:2514:LEU:O	1:B:2515:PRO:C	2.57	0.43
1:C:3156:ALA:O	1:C:3160:HIS:CD2	2.68	0.43
1:C:3301:MET:C	1:C:3302:LYS:HG2	2.39	0.43
1:A:1074:TRP:HB3	1:B:2183:GLU:CD	2.39	0.43
1:A:1254:VAL:HG13	1:A:1255:LEU:HG	2.00	0.43
1:B:2089:GLN:NE2	1:B:2094:GLY:HA3	2.34	0.43
1:B:2357:TRP:CE2	1:B:2361:MET:SD	3.11	0.43
1:C:3089:GLN:NE2	1:C:3094:GLY:HA3	2.32	0.43
1:A:1251:LEU:O	3:A:30:HOH:O	2.21	0.43
1:C:3054:PRO:CG	1:C:3078:LYS:HZ3	2.19	0.43
1:A:1382:LEU:HD13	1:A:1417:PHE:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2109:PRO:O	1:B:2109:PRO:CD	2.56	0.43
1:C:3242:ARG:NH1	1:C:3242:ARG:CG	2.81	0.43
1:C:3220:GLU:HA	1:C:3246:GLU:O	2.19	0.43
1:B:2047:VAL:HG13	1:B:2123:THR:O	2.19	0.43
1:A:1083:TYR:CE2	1:A:1108:ILE:CD1	3.02	0.42
1:A:1098:SER:O	1:A:1102:THR:HB	2.18	0.42
1:B:2199:ARG:HG2	1:B:2239:LEU:CD2	2.48	0.42
1:C:3396:ILE:CB	1:C:3397:PRO:CD	2.96	0.42
1:A:1075:SER:O	1:A:1076:PHE:CB	2.61	0.42
1:A:1161:GLU:OE2	1:A:1498:LYS:HG2	2.19	0.42
1:A:1351:ASN:HB3	1:A:1466:GLY:O	2.20	0.42
1:C:3136:MET:HB3	1:C:3218:PHE:CE1	2.54	0.42
1:C:3290:THR:OG1	1:C:3293:GLU:HG3	2.20	0.42
1:C:3493:SER:CA	3:C:16:HOH:O	2.66	0.42
1:A:1089:GLN:NE2	1:A:1094:GLY:HA3	2.35	0.42
1:B:2067:PRO:HD3	1:B:2189:TRP:HZ3	1.83	0.42
1:B:2517:TRP:HA	1:B:2527:LEU:HD13	2.01	0.42
1:A:1086:MET:SD	1:A:1110:LEU:HD12	2.60	0.42
1:A:1367:PRO:HA	3:A:93:HOH:O	2.19	0.42
1:B:2039:SER:OG	1:B:2046:PRO:HB3	2.19	0.42
1:B:2528:GLN:O	1:B:2533:THR:HA	2.19	0.42
1:C:3176:GLY:HA2	1:C:3189:TRP:HB2	2.02	0.42
1:C:3262:LYS:CB	1:C:3263:PRO:CD	2.98	0.42
1:A:1054:PRO:O	1:A:1054:PRO:CD	2.67	0.42
1:A:1277:THR:HG21	1:C:3113:SER:HB2	2.01	0.42
1:A:1252:THR:CG2	1:A:1254:VAL:HG12	2.46	0.42
1:A:1383:TRP:CZ3	1:A:1393:LYS:HB2	2.55	0.42
1:A:1086:MET:HG2	1:A:1110:LEU:HD13	2.01	0.41
1:B:2067:PRO:CD	1:B:2189:TRP:CZ3	3.04	0.41
1:C:3091:PRO:CD	1:C:3092:LYS:N	2.69	0.41
1:C:3211:ASN:OD1	1:C:3212:PRO:CD	2.67	0.41
1:C:3218:PHE:N	1:C:3218:PHE:CD1	2.88	0.41
1:A:1220:GLU:HA	1:A:1246:GLU:O	2.20	0.41
1:A:1391:ILE:CG2	1:A:1396:ILE:HD13	2.51	0.41
1:C:3067:PRO:CD	1:C:3189:TRP:CZ3	3.02	0.41
1:C:3085:PRO:O	1:C:3086:MET:C	2.50	0.41
1:C:3304:LEU:N	1:C:3304:LEU:HD23	2.34	0.41
1:A:1108:ILE:HG23	1:A:1109:PRO:CD	2.51	0.41
1:A:1339:ARG:HD2	1:A:1440:ALA:CA	2.43	0.41
1:B:2211:ASN:OD1	1:B:2212:PRO:CD	2.68	0.41
1:C:3262:LYS:CB	1:C:3263:PRO:HD2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1128:THR:O	1:A:1129:LYS:CG	2.69	0.41
1:A:1434:ALA:HB2	1:A:1446:MET:SD	2.59	0.41
1:C:3149:ALA:H	1:C:3169:GLN:HE21	1.68	0.41
1:C:3403:TYR:O	1:C:3416:LEU:HB3	2.20	0.41
1:A:1099:GLU:CG	1:A:1107:ASN:HD22	2.32	0.41
1:A:1047:VAL:HG13	1:A:1123:THR:O	2.20	0.41
1:A:1344:VAL:O	1:A:1345:PRO:C	2.52	0.41
1:A:1403:TYR:C	1:A:1404:LEU:HD23	2.41	0.41
1:B:2237:LYS:HG2	1:B:2238:ASN:ND2	2.36	0.41
1:C:3206:ALA:HA	1:C:3210:GLY:O	2.21	0.41
1:C:3233:SER:OG	1:C:3234:PRO:CD	2.69	0.41
1:C:3242:ARG:HD3	1:C:3503:PHE:O	2.21	0.41
1:B:2359:ILE:CB	1:B:2360:PRO:CD	2.98	0.41
1:B:2363:LEU:CD1	2:B:194:WW2:C3	2.98	0.41
1:C:3054:PRO:CD	1:C:3078:LYS:NZ	2.83	0.41
1:B:2455:PHE:CD1	1:B:2482:LYS:CE	3.04	0.40
1:B:2088:THR:HG21	1:B:2291:GLU:HG3	2.03	0.40
1:C:3098:SER:O	1:C:3102:THR:HB	2.20	0.40
1:C:3359:ILE:CB	1:C:3360:PRO:CD	2.99	0.40
1:A:1251:LEU:O	1:A:1253:SER:N	2.53	0.40
1:B:2026:VAL:CG1	1:B:2027:ASP:N	2.84	0.40
1:B:2149:ALA:H	1:B:2169:GLN:HE21	1.68	0.40
1:A:1132:ARG:NH1	1:A:1206:ALA:CB	2.84	0.40
1:A:1186:ARG:NH2	1:C:3074:TRP:HA	2.37	0.40
1:A:1403:TYR:O	1:A:1404:LEU:HD23	2.20	0.40
1:A:1242:ARG:HD3	1:A:1503:PHE:O	2.21	0.40
1:B:2403:TYR:O	1:B:2416:LEU:HB3	2.22	0.40
1:C:3087:CYS:O	1:C:3088:THR:C	2.55	0.40
1:C:3429:PRO:O	1:C:3433:VAL:HG23	2.22	0.40
1:C:3451:TYR:CE2	1:C:3489:GLU:HG3	2.56	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1045:GLN:OE1	3:C:23:HOH:O[2_465]	1.42	0.78
1:A:1039:SER:OG	1:C:3491:ARG:NH1[2_465]	1.98	0.22
1:B:2132:ARG:CD	1:B:2275:LYS:CG[1_455]	2.00	0.20
1:A:1095:GLN:NE2	1:B:2238:ASN:ND2[1_655]	2.08	0.12
1:A:1128:THR:CG2	1:C:3487:GLU:OE2[2_465]	2.14	0.06

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	471/529 (89%)	435 (92%)	29 (6%)	7 (2%)	10	39
1	B	489/529 (92%)	445 (91%)	39 (8%)	5 (1%)	15	49
1	C	437/529 (83%)	399 (91%)	33 (8%)	5 (1%)	14	46
All	All	1397/1587 (88%)	1279 (92%)	101 (7%)	17 (1%)	13	44

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1185	SER
1	B	2185	SER
1	A	1076	PHE
1	C	3086	MET
1	C	3185	SER
1	A	1127	LEU
1	A	1183	GLU
1	B	2183	GLU
1	B	2252	THR
1	C	3357	TRP
1	A	1252	THR
1	A	1357	TRP
1	B	2357	TRP
1	C	3127	LEU
1	B	2142	GLY
1	A	1142	GLY
1	C	3142	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	407/445 (92%)	401 (98%)	6 (2%)	65	85
1	B	419/445 (94%)	415 (99%)	4 (1%)	76	90
1	C	377/445 (85%)	370 (98%)	7 (2%)	57	81
All	All	1203/1335 (90%)	1186 (99%)	17 (1%)	67	86

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1075	SER
1	A	1086	MET
1	A	1345	PRO
1	A	1347	MET
1	A	1355	PHE
1	A	1500	TRP
1	B	2345	PRO
1	B	2355	PHE
1	B	2420	LEU
1	B	2500	TRP
1	C	3087	CYS
1	C	3218	PHE
1	C	3304	LEU
1	C	3355	PHE
1	C	3420	LEU
1	C	3500	TRP
1	C	3523	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1045	GLN
1	A	1079	ASN
1	A	1107	ASN
1	A	1140	HIS
1	A	1160	HIS
1	A	1169	GLN
1	B	2045	GLN
1	B	2107	ASN
1	B	2140	HIS

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Mol	Chain	Res	Type
1	B	2160	HIS
1	B	2169	GLN
1	B	2238	ASN
1	B	2241	HIS
1	B	2436	ASN
1	C	3107	ASN
1	C	3140	HIS
1	C	3160	HIS
1	C	3169	GLN
1	C	3241	HIS
1	C	3342	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	WW2	B	194	1	7,10,11	2.83	7 (100%)	8,12,15	1.28	2 (25%)
2	WW2	C	195	1	7,10,11	2.73	7 (100%)	8,12,15	1.35	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	WW2	A	193	1	7,10,11	2.65	6 (85%)	8,12,15	1.31	2 (25%)

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	WW2	B	194	1	-	1/2/12/13	0/1/1/1
2	WW2	C	195	1	-	1/2/12/13	0/1/1/1
2	WW2	A	193	1	-	0/2/12/13	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	195	WW2	C5-C6	3.75	1.61	1.51
2	B	194	WW2	C5-C6	3.74	1.61	1.51
2	A	193	WW2	C5-C6	3.62	1.60	1.51
2	A	193	WW2	C1-C6	3.50	1.60	1.51
2	B	194	WW2	C1-C6	3.44	1.60	1.51
2	C	195	WW2	C1-C6	3.41	1.60	1.51
2	B	194	WW2	O2-C6	2.97	1.50	1.45
2	B	194	WW2	C2-C1	2.72	1.60	1.53
2	C	195	WW2	C2-C1	2.68	1.60	1.53
2	A	193	WW2	C2-C1	2.66	1.60	1.53
2	C	195	WW2	C4-C5	2.34	1.59	1.53
2	B	194	WW2	C4-C5	2.30	1.59	1.53
2	C	195	WW2	O2-C6	2.28	1.49	1.45
2	C	195	WW2	C3-C2	2.17	1.60	1.51
2	A	193	WW2	C4-C5	2.14	1.58	1.53
2	A	193	WW2	C3-C2	2.11	1.59	1.51
2	B	194	WW2	C3-C2	2.11	1.59	1.51
2	B	194	WW2	C4-C3	2.06	1.59	1.51
2	A	193	WW2	C4-C3	2.05	1.59	1.51
2	C	195	WW2	C4-C3	2.02	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	195	WW2	O2-C6-C5	2.67	114.26	109.33
2	B	194	WW2	O2-C6-C5	2.57	114.08	109.33
2	A	193	WW2	O2-C6-C5	2.49	113.92	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	193	WW2	C5-C6-C1	-2.31	107.29	111.74
2	C	195	WW2	C5-C6-C1	-2.29	107.31	111.74
2	B	194	WW2	C5-C6-C1	-2.16	107.57	111.74

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	194	WW2	C5-C6-O2-P1
2	C	195	WW2	C5-C6-O2-P1

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	194	WW2	12	0
2	C	195	WW2	2	0
2	A	193	WW2	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	481/529 (90%)	0.15	12 (2%)	57	34	10, 47, 77, 105	21 (4%)
1	B	488/529 (92%)	0.13	29 (5%)	22	10	5, 41, 82, 104	31 (6%)
1	C	448/529 (84%)	0.22	26 (5%)	23	10	13, 51, 82, 115	25 (5%)
All	All	1417/1587 (89%)	0.16	67 (4%)	31	15	5, 47, 81, 115	77 (5%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3403	TYR	5.4
1	B	2367	PRO	5.0
1	C	3407	THR	4.9
1	C	3406	GLY	4.6
1	C	3399	ALA	4.3
1	C	3400	THR	4.0
1	C	3548	THR	3.8
1	B	2385	SER	3.7
1	B	2343	THR	3.6
1	B	2549	ASN	3.6
1	B	2553	LYS	3.6
1	B	2410	THR	3.3
1	C	3046	PRO	3.2
1	B	2408	ASP	3.2
1	C	3408	ASP	3.2
1	B	2378	ALA	3.1
1	B	2396	ILE	3.0
1	A	1455	PHE	3.0
1	B	2399	ALA	3.0
1	C	3302	LYS	3.0
1	B	2401	GLU	2.9
1	B	2397	PRO	2.9
1	B	2548	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1026	VAL	2.8
1	A	1128	THR	2.8
1	C	3401	GLU	2.8
1	B	2366	TYR	2.8
1	C	3415	ASP	2.8
1	C	3545	ALA	2.8
1	C	3397	PRO	2.7
1	A	1533	THR	2.7
1	B	2398	GLU	2.6
1	B	2379	MET	2.6
1	A	1530	GLY	2.6
1	C	3024	PRO	2.6
1	C	3398	GLU	2.5
1	C	3402	LYS	2.5
1	C	3417	PHE	2.5
1	B	2341	PHE	2.5
1	B	2552	ALA	2.5
1	A	1076	PHE	2.5
1	A	1386	TYR	2.4
1	B	2402	LYS	2.4
1	B	2334	GLU	2.4
1	C	3409	ASP	2.4
1	B	2400	THR	2.4
1	C	3301	MET	2.3
1	A	1339	ARG	2.3
1	B	2333	GLU	2.3
1	C	3416	LEU	2.3
1	B	2547	TRP	2.3
1	B	2407	THR	2.3
1	B	2551	PHE	2.3
1	C	3300	LYS	2.2
1	C	3128	THR	2.2
1	C	3420	LEU	2.1
1	A	1490	ILE	2.1
1	B	2382	LEU	2.1
1	C	3534	GLN	2.1
1	B	2360	PRO	2.1
1	B	2550	LEU	2.1
1	C	3304	LEU	2.1
1	A	1515	PRO	2.1
1	A	1382	LEU	2.1
1	A	1333	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	2403	TYR	2.1
1	C	3396	ILE	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	WW2	C	195	10/11	0.69	0.85	47,47,47,47	10
2	WW2	B	194	10/11	0.82	0.32	73,73,73,73	10
2	WW2	A	193	10/11	0.82	0.34	64,64,64,64	10

6.5 Other polymers (i)

There are no such residues in this entry.