



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:00 am BST

PDB ID : 5A5K
Title : AtGSTF2 from Arabidopsis thaliana in complex with camalexin
Authors : Ahmad, L.; Rylott, E.; Bruce, N.C.; Edwards, R.; Grogan, G.
Deposited on : 2015-06-18
Resolution : 2.77 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

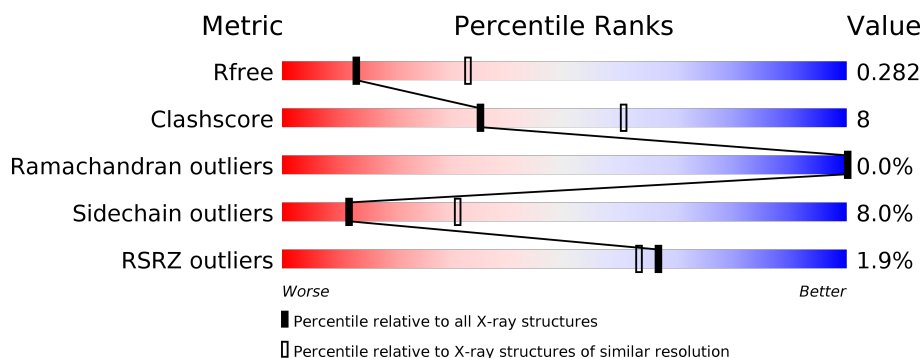
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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.



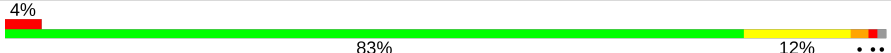
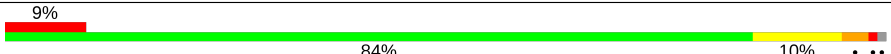
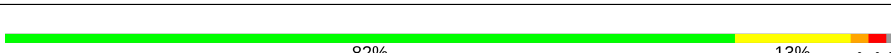
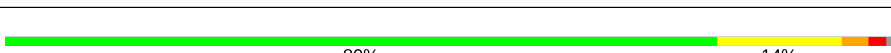
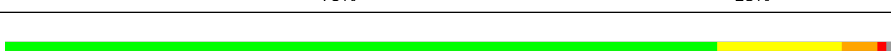

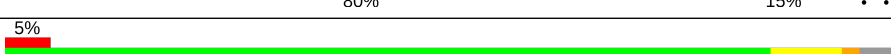
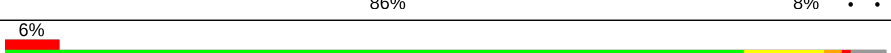
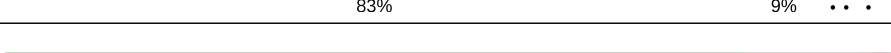
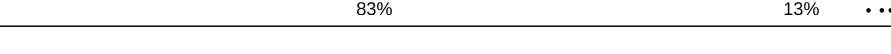
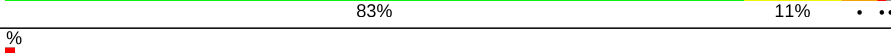





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	212	<div> <div>79%</div> <div>17%</div> <div>• •</div> </div>
1	B	212	<div> <div>79%</div> <div>17%</div> <div>• •</div> </div>
1	C	212	<div> <div>83%</div> <div>14%</div> <div>• •</div> </div>
1	D	212	<div> <div>2%</div> <div>78%</div> <div>16%</div> <div>• • •</div> </div>
1	E	212	<div> <div>5%</div> <div>82%</div> <div>12%</div> <div>• • •</div> </div>
1	F	212	<div> <div>84%</div> <div>10%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	212	
1	H	212	
1	I	212	
1	J	212	
1	K	212	
1	L	212	
1	M	212	
1	N	212	
1	O	212	
1	P	212	
1	Q	212	
1	R	212	
1	S	212	
1	T	212	
1	U	212	
1	V	212	
1	W	212	
1	X	212	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39024 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 GLUTATHIONE S-TRANSFERASE F2.

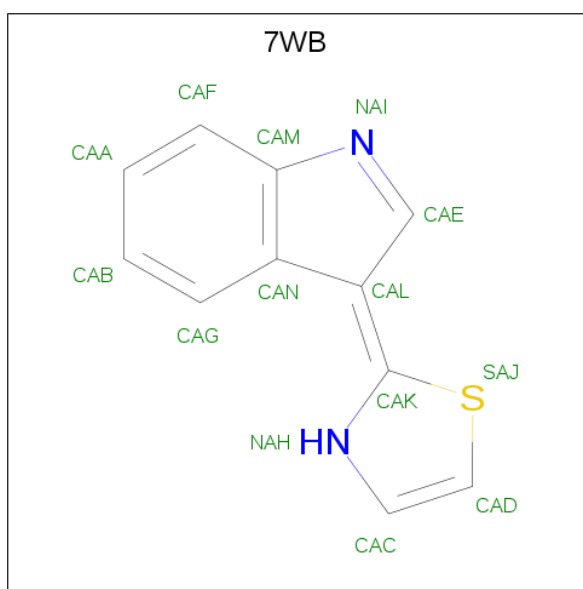
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1602	1035	272	293	2			
1	B	210	Total	C	N	O	S	0	1	0
			1650	1058	280	310	2			
1	C	210	Total	C	N	O	S	0	0	0
			1610	1038	271	299	2			
1	D	209	Total	C	N	O	S	0	0	0
			1589	1021	268	298	2			
1	E	210	Total	C	N	O	S	0	0	0
			1553	999	266	286	2			
1	F	210	Total	C	N	O	S	0	0	0
			1609	1037	274	296	2			
1	G	210	Total	C	N	O	S	0	1	0
			1543	991	266	284	2			
1	H	210	Total	C	N	O	S	0	0	0
			1515	962	260	291	2			
1	I	210	Total	C	N	O	S	0	0	0
			1644	1056	278	308	2			
1	J	210	Total	C	N	O	S	0	0	0
			1640	1054	276	308	2			
1	K	210	Total	C	N	O	S	0	0	0
			1635	1052	276	305	2			
1	L	210	Total	C	N	O	S	0	0	0
			1645	1058	277	308	2			
1	M	210	Total	C	N	O	S	0	0	0
			1642	1057	275	308	2			
1	N	204	Total	C	N	O	S	0	0	0
			1501	968	255	276	2			
1	O	203	Total	C	N	O	S	0	0	0
			1461	944	249	266	2			
1	P	210	Total	C	N	O	S	0	0	0
			1615	1037	272	304	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	210	Total	C	N	O	S	0	0	0
			1619	1041	272	304	2			
1	R	210	Total	C	N	O	S	0	0	0
			1625	1047	277	299	2			
1	S	210	Total	C	N	O	S	0	0	0
			1653	1060	280	311	2			
1	T	206	Total	C	N	O	S	0	0	0
			1473	943	249	279	2			
1	U	210	Total	C	N	O	S	0	0	0
			1644	1057	281	304	2			
1	V	210	Total	C	N	O	S	0	0	0
			1632	1047	277	306	2			
1	W	210	Total	C	N	O	S	0	0	0
			1639	1051	278	308	2			
1	X	210	Total	C	N	O	S	0	0	0
			1645	1059	277	307	2			

- Molecule 2 is (2Z)-2-indol-3-ylidene-3H-1,3-thiazole (three-letter code: 7WB) (formula: $C_{11}H_8N_2S_1$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			14	11	2	1		
2	B	1	Total	C	N	S	0	0
			14	11	2	1		
2	C	1	Total	C	N	S	0	0
			14	11	2	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	S	0	0
			14	11	2	1		
2	E	1	Total	C	N	S	0	0
			14	11	2	1		
2	F	1	Total	C	N	S	0	0
			14	11	2	1		
2	G	1	Total	C	N	S	0	0
			14	11	2	1		
2	H	1	Total	C	N	S	0	0
			14	11	2	1		
2	I	1	Total	C	N	S	0	0
			14	11	2	1		
2	J	1	Total	C	N	S	0	0
			14	11	2	1		
2	K	1	Total	C	N	S	0	0
			14	11	2	1		
2	L	1	Total	C	N	S	0	0
			14	11	2	1		
2	M	1	Total	C	N	S	0	0
			14	11	2	1		
2	N	1	Total	C	N	S	0	0
			14	11	2	1		
2	O	1	Total	C	N	S	0	0
			14	11	2	1		
2	P	1	Total	C	N	S	0	0
			14	11	2	1		
2	Q	1	Total	C	N	S	0	0
			14	11	2	1		
2	R	1	Total	C	N	S	0	0
			14	11	2	1		
2	S	1	Total	C	N	S	0	0
			14	11	2	1		
2	T	1	Total	C	N	S	0	0
			14	11	2	1		
2	U	1	Total	C	N	S	0	0
			14	11	2	1		
2	V	1	Total	C	N	S	0	0
			14	11	2	1		
2	W	1	Total	C	N	S	0	0
			14	11	2	1		
2	X	1	Total	C	N	S	0	0
			14	11	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	18	Total O 18 18	0	0
3	B	15	Total O 15 15	0	0
3	C	13	Total O 13 13	0	0
3	D	15	Total O 15 15	0	0
3	E	19	Total O 19 19	0	0
3	F	10	Total O 10 10	0	0
3	G	13	Total O 13 13	0	0
3	H	6	Total O 6 6	0	0
3	I	15	Total O 15 15	0	0
3	J	22	Total O 22 22	0	0
3	K	13	Total O 13 13	0	0
3	L	13	Total O 13 13	0	0
3	M	15	Total O 15 15	0	0
3	N	9	Total O 9 9	0	0
3	O	7	Total O 7 7	0	0
3	P	9	Total O 9 9	0	0
3	Q	9	Total O 9 9	0	0
3	R	3	Total O 3 3	0	0
3	S	13	Total O 13 13	0	0
3	T	4	Total O 4 4	0	0
3	U	20	Total O 20 20	0	0

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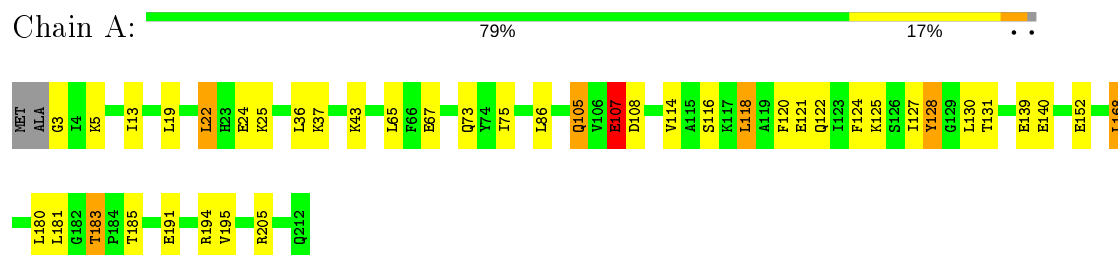
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	V	17	Total	O	0	0
			17	17		
3	W	13	Total	O	0	0
			13	13		
3	X	13	Total	O	0	0
			13	13		

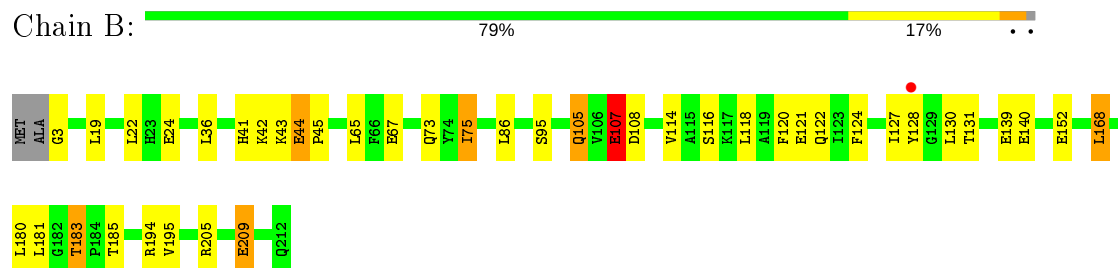
3 Residue-property plots [i](#)

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.

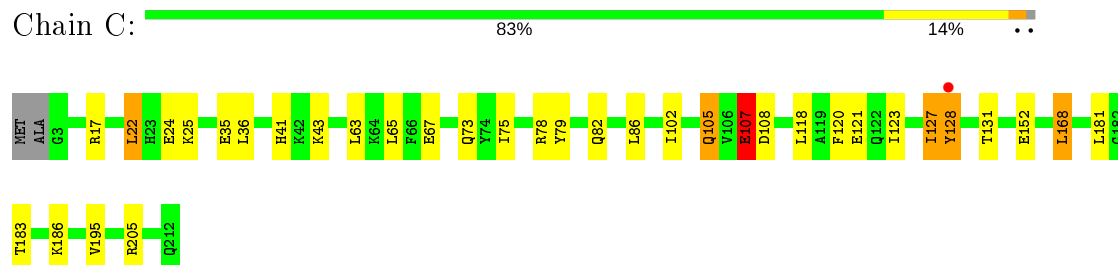
• Molecule 1: GLUTATHIONE S-TRANSFERASE F2



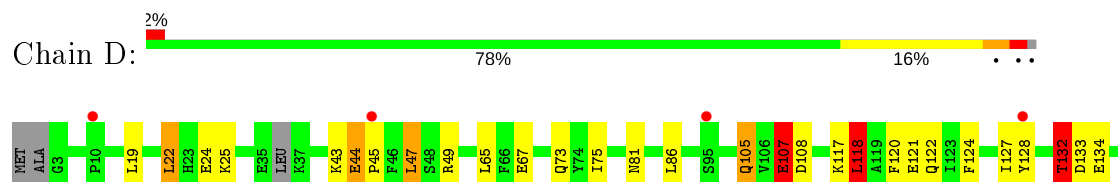
• Molecule 1: GLUTATHIONE S-TRANSFERASE F2



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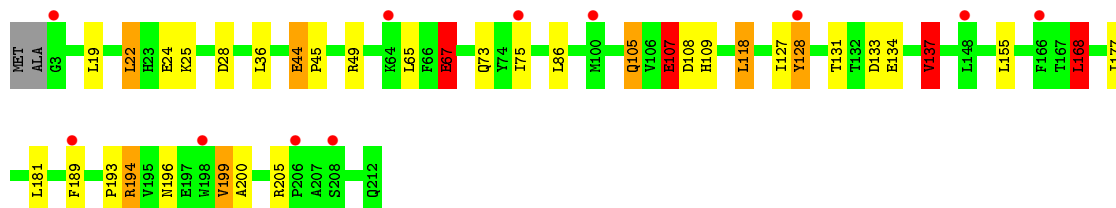
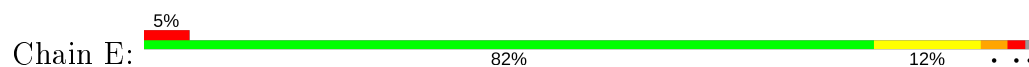


• Molecule 1: GLUTATHIONE S-TRANSFERASE F2

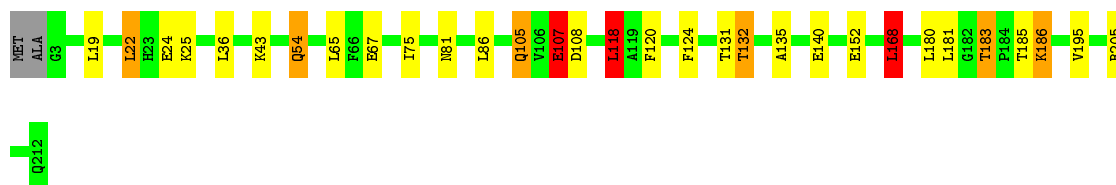
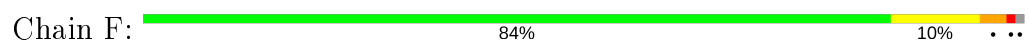




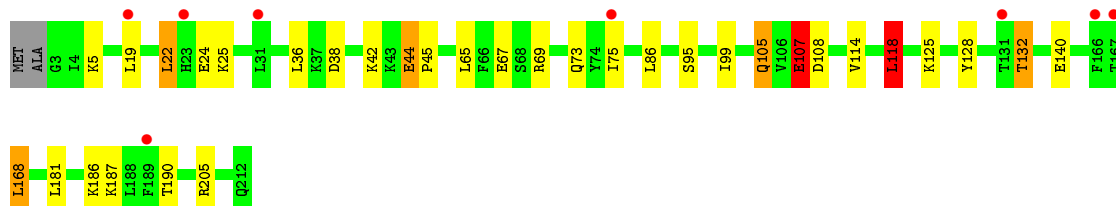
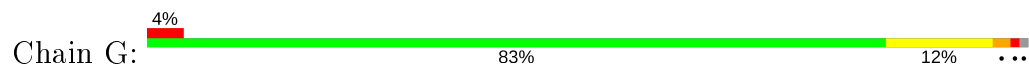
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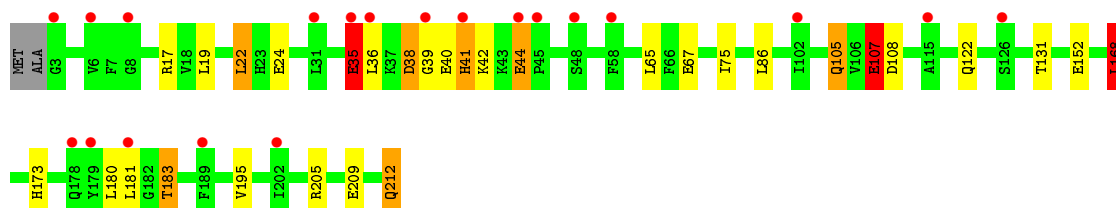
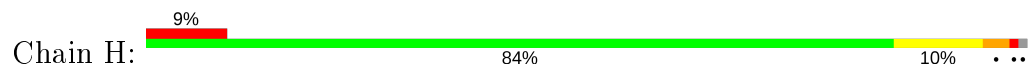
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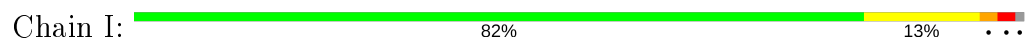
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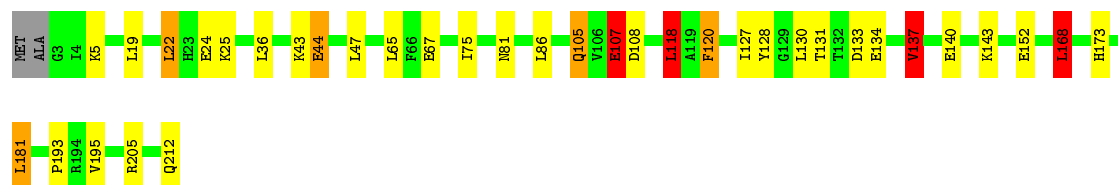


• Molecule 1: GLUTATHIONE S-TRANSFERASE F2



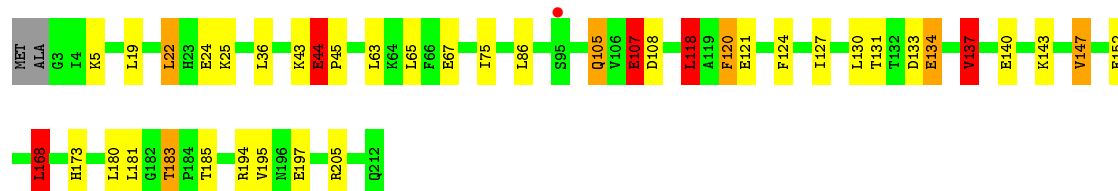
• Molecule 1: GLUTATHIONE S-TRANSFERASE F2





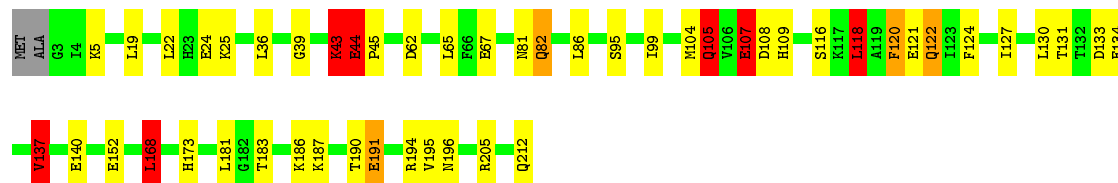
- Molecule 1: GLUTATHIONE S-TRANSFERASE F2

Chain J: 80% 14%



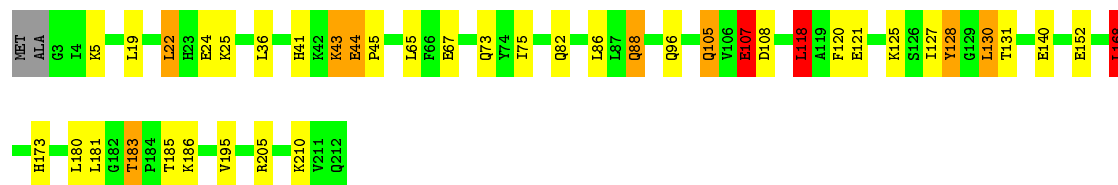
- Molecule 1: GLUTATHIONE S-TRANSFERASE F2

Chain K: 75% 18%



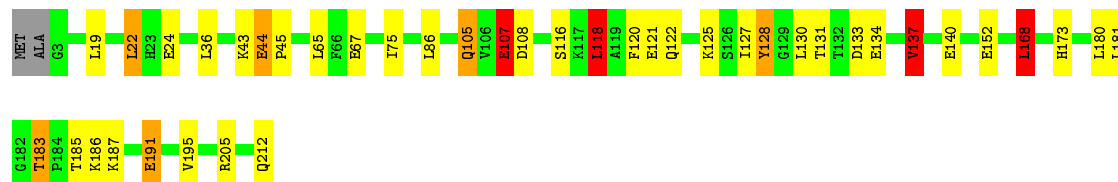
- Molecule 1: GLUTATHIONE S-TRANSFERASE F2

Chain L: 80% 14%



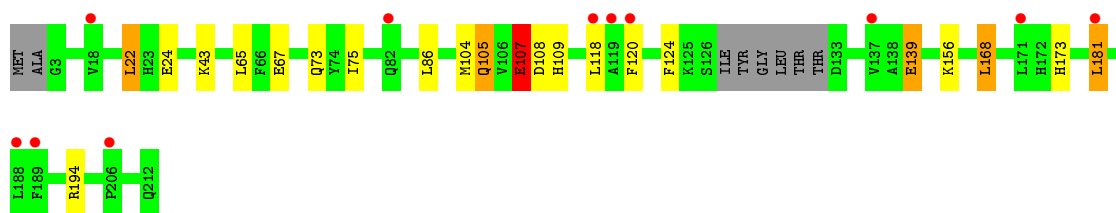
- Molecule 1: GLUTATHIONE S-TRANSFERASE F2

Chain M: 80% 15%

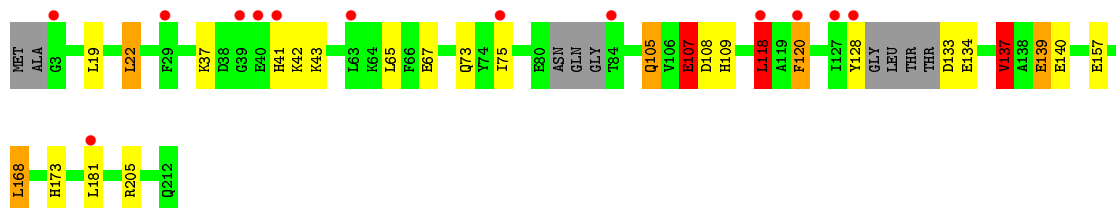
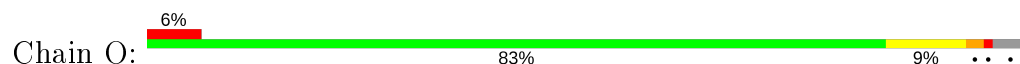


- Molecule 1: GLUTATHIONE S-TRANSFERASE F2

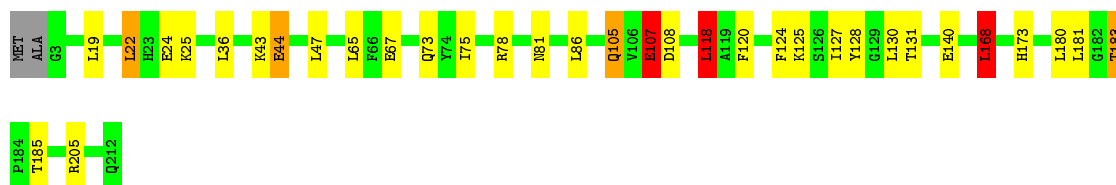
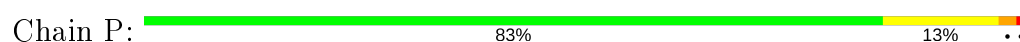
Chain N: 5% 86%



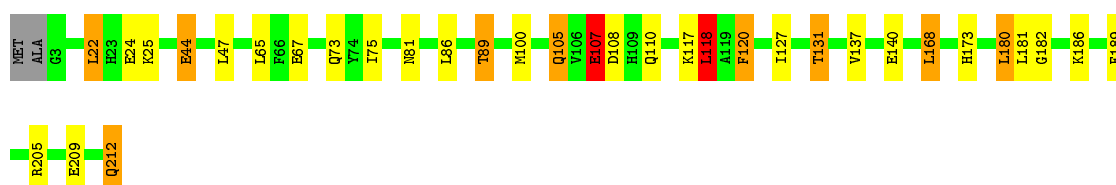
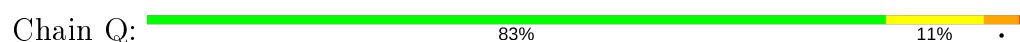
- Molecule 1: GLUTATHIONE S-TRANSFERASE F2



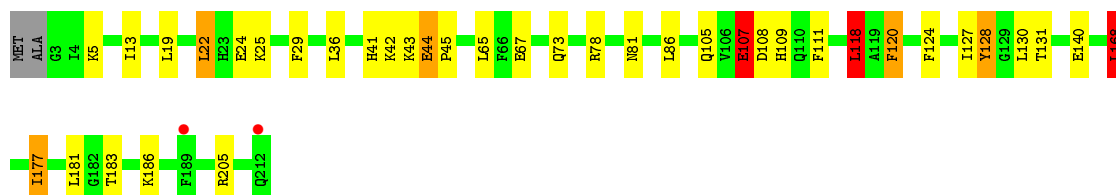
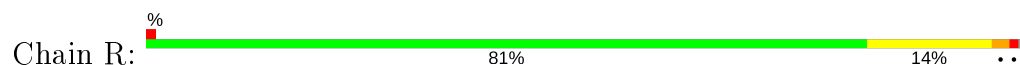
- Molecule 1: GLUTATHIONE S-TRANSFERASE F2




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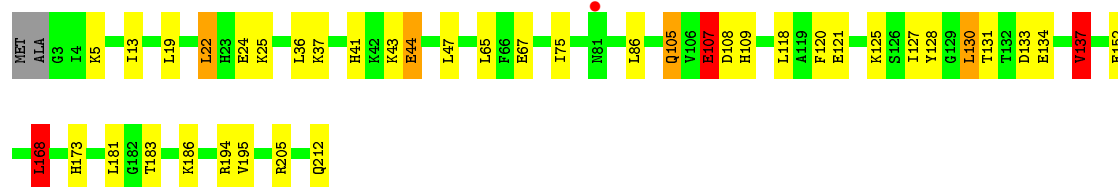


- Molecule 1: GLUTATHIONE S-TRANSFERASE F2




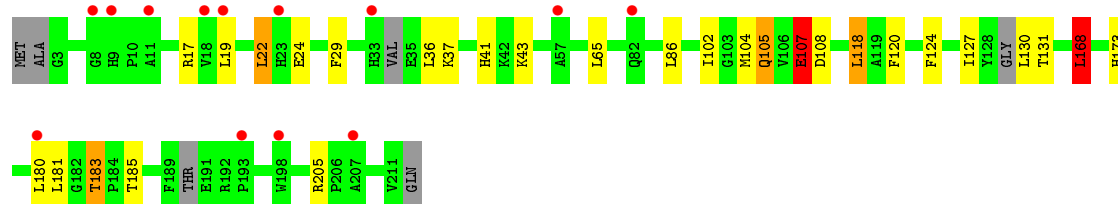
- Molecule 1: GLUTATHIONE S-TRANSFERASE F2

Chain S: 




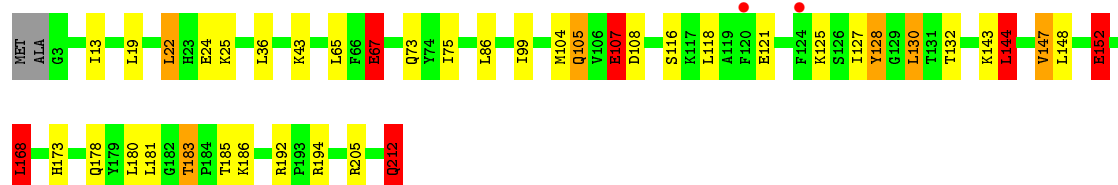
• Molecule 1: GLUTATHIONE S-TRANSFERASE F2

Chain T: 




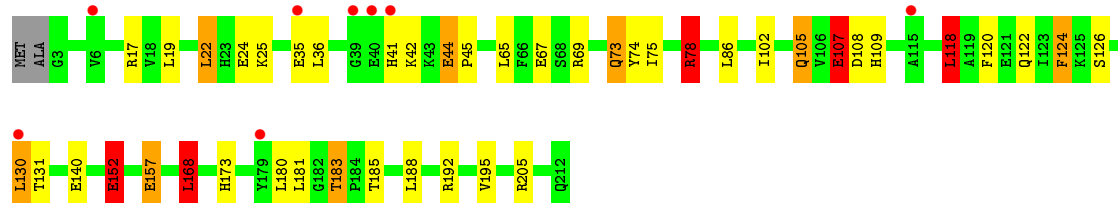
• Molecule 1: GLUTATHIONE S-TRANSFERASE F2

Chain U: 




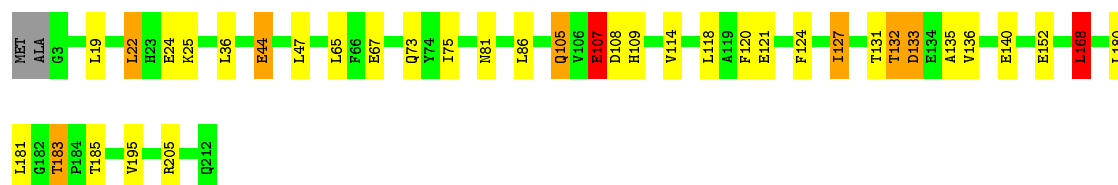
• Molecule 1: GLUTATHIONE S-TRANSFERASE F2

Chain V: 



• Molecule 1: GLUTATHIONE S-TRANSFERASE F2

Chain W: 



● Molecule 1: GLUTATHIONE S-TRANSFERASE F2

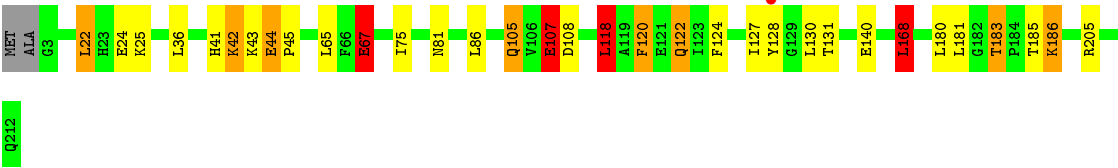
Chain X:

83%

10%

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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	97.10Å 113.72Å 132.02Å 83.65° 79.47° 65.85°	Depositor
Resolution (Å)	87.58 – 2.77 87.58 – 2.77	Depositor EDS
% Data completeness (in resolution range)	98.6 (87.58-2.77) 98.6 (87.58-2.77)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.250 , 0.284 0.250 , 0.282	Depositor DCC
R_{free} test set	6116 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.003 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	39024	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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 78.50 % 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 6.8208e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: 7WB

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	0.68	2/1639 (0.1%)	0.99	13/2233 (0.6%)
1	B	0.71	2/1691 (0.1%)	1.02	14/2298 (0.6%)
1	C	0.71	2/1647 (0.1%)	0.97	11/2246 (0.5%)
1	D	0.70	2/1624 (0.1%)	1.04	18/2213 (0.8%)
1	E	0.77	6/1590 (0.4%)	1.19	17/2175 (0.8%)
1	F	0.67	2/1645 (0.1%)	0.93	8/2240 (0.4%)
1	G	0.70	2/1581 (0.1%)	1.03	12/2159 (0.6%)
1	H	0.64	2/1547 (0.1%)	0.90	8/2119 (0.4%)
1	I	0.59	0/1681	0.92	5/2284 (0.2%)
1	J	0.66	2/1676 (0.1%)	0.93	9/2275 (0.4%)
1	K	0.69	3/1671 (0.2%)	1.00	16/2270 (0.7%)
1	L	0.64	1/1682 (0.1%)	0.95	7/2284 (0.3%)
1	M	0.63	2/1679 (0.1%)	0.95	10/2281 (0.4%)
1	N	0.59	0/1534	0.88	8/2100 (0.4%)
1	O	0.61	0/1494	1.00	11/2048 (0.5%)
1	P	0.60	0/1652	0.98	8/2252 (0.4%)
1	Q	0.69	2/1655 (0.1%)	1.06	13/2252 (0.6%)
1	R	0.67	2/1662 (0.1%)	0.99	11/2260 (0.5%)
1	S	0.64	1/1690 (0.1%)	1.04	13/2295 (0.6%)
1	T	0.56	0/1503	0.91	12/2057 (0.6%)
1	U	0.74	4/1681 (0.2%)	1.00	15/2282 (0.7%)
1	V	0.75	3/1668 (0.2%)	1.01	15/2267 (0.7%)
1	W	0.72	3/1675 (0.2%)	1.09	10/2277 (0.4%)
1	X	0.70	4/1682 (0.2%)	0.95	8/2284 (0.4%)
All	All	0.67	47/39249 (0.1%)	0.99	272/53451 (0.5%)

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	V	0	1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	107	GLU	CD-OE2	-11.13	1.13	1.25
1	B	107	GLU	CD-OE2	-10.54	1.14	1.25
1	R	107	GLU	CD-OE2	-10.35	1.14	1.25
1	X	107	GLU	CD-OE2	-10.33	1.14	1.25
1	V	152	GLU	CD-OE1	-10.26	1.14	1.25
1	A	107	GLU	CD-OE2	-10.23	1.14	1.25
1	U	152	GLU	CD-OE2	-10.11	1.14	1.25
1	W	107	GLU	CD-OE2	-10.03	1.14	1.25
1	W	107	GLU	CD-OE1	-9.97	1.14	1.25
1	C	107	GLU	CD-OE1	-9.88	1.14	1.25
1	F	107	GLU	CD-OE1	-9.86	1.14	1.25
1	C	107	GLU	CD-OE2	-9.85	1.14	1.25
1	E	107	GLU	CD-OE1	-9.72	1.15	1.25
1	F	107	GLU	CD-OE2	-9.62	1.15	1.25
1	E	107	GLU	CD-OE2	-9.62	1.15	1.25
1	V	152	GLU	CD-OE2	-9.54	1.15	1.25
1	G	107	GLU	CD-OE1	-9.50	1.15	1.25
1	B	107	GLU	CD-OE1	-9.48	1.15	1.25
1	R	107	GLU	CD-OE1	-9.39	1.15	1.25
1	X	107	GLU	CD-OE1	-9.38	1.15	1.25
1	A	107	GLU	CD-OE1	-8.79	1.16	1.25
1	U	152	GLU	CD-OE1	-8.54	1.16	1.25
1	D	191	GLU	CD-OE1	-7.30	1.17	1.25
1	H	35	GLU	CD-OE1	-7.17	1.17	1.25
1	Q	89	THR	CA-CB	7.03	1.71	1.53
1	K	105	GLN	CD-OE1	6.76	1.38	1.24
1	X	67	GLU	CB-CG	6.45	1.64	1.52
1	Q	212	GLN	CA-CB	6.37	1.68	1.53
1	J	44	GLU	CD-OE1	-6.29	1.18	1.25
1	U	67	GLU	CB-CG	6.27	1.64	1.52
1	K	44	GLU	CD-OE1	-6.17	1.18	1.25
1	E	67	GLU	CB-CG	6.12	1.63	1.52
1	L	88	GLN	CG-CD	-6.10	1.37	1.51
1	W	133	ASP	CG-OD1	-5.86	1.11	1.25
1	X	67	GLU	CD-OE2	-5.71	1.19	1.25
1	D	197	GLU	CD-OE2	-5.65	1.19	1.25
1	V	157	GLU	CB-CG	5.57	1.62	1.52
1	M	122	GLN	CA-CB	5.54	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	189	PHE	CG-CD1	-5.37	1.30	1.38
1	M	122	GLN	CA-C	5.36	1.66	1.52
1	S	212	GLN	CD-OE1	5.36	1.35	1.24
1	E	189	PHE	CG-CD2	5.32	1.46	1.38
1	H	44	GLU	CD-OE1	-5.29	1.19	1.25
1	K	122	GLN	CD-OE1	-5.25	1.12	1.24
1	U	212	GLN	CD-OE1	5.22	1.35	1.24
1	J	134	GLU	CD-OE2	5.17	1.31	1.25
1	E	67	GLU	CD-OE2	-5.13	1.20	1.25

All (272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	133	ASP	CB-CG-OD2	18.94	135.35	118.30
1	E	194	ARG	NE-CZ-NH1	15.61	128.10	120.30
1	S	205	ARG	NE-CZ-NH1	15.03	127.81	120.30
1	G	205	ARG	NE-CZ-NH1	14.74	127.67	120.30
1	O	205	ARG	NE-CZ-NH1	14.27	127.44	120.30
1	F	107	GLU	OE1-CD-OE2	-14.03	106.47	123.30
1	G	107	GLU	OE1-CD-OE2	-13.96	106.55	123.30
1	A	107	GLU	OE1-CD-OE2	-13.90	106.62	123.30
1	E	107	GLU	OE1-CD-OE2	-13.90	106.62	123.30
1	X	107	GLU	OE1-CD-OE2	-13.83	106.70	123.30
1	R	107	GLU	OE1-CD-OE2	-13.77	106.78	123.30
1	P	205	ARG	NE-CZ-NH1	13.76	127.18	120.30
1	W	107	GLU	OE1-CD-OE2	-13.70	106.86	123.30
1	C	107	GLU	OE1-CD-OE2	-13.68	106.88	123.30
1	Q	137	VAL	CA-CB-CG1	13.67	131.40	110.90
1	E	189	PHE	CB-CG-CD1	-13.66	111.24	120.80
1	B	107	GLU	OE1-CD-OE2	-13.57	107.02	123.30
1	E	28	ASP	CB-CG-OD2	13.17	130.15	118.30
1	E	189	PHE	CB-CG-CD2	13.09	129.96	120.80
1	M	122	GLN	CB-CA-C	12.44	135.28	110.40
1	E	194	ARG	NE-CZ-NH2	-12.37	114.11	120.30
1	U	144	LEU	CB-CG-CD1	12.10	131.57	111.00
1	G	205	ARG	NE-CZ-NH2	-11.92	114.34	120.30
1	S	205	ARG	NE-CZ-NH2	-11.91	114.34	120.30
1	W	127	ILE	CA-CB-CG1	11.77	133.37	111.00
1	O	205	ARG	NE-CZ-NH2	-11.75	114.42	120.30
1	L	88	GLN	CA-CB-CG	11.73	139.20	113.40
1	O	205	ARG	CD-NE-CZ	11.48	139.67	123.60
1	P	205	ARG	NE-CZ-NH2	-11.32	114.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	177	ILE	CA-CB-CG1	11.19	132.26	111.00
1	G	205	ARG	CD-NE-CZ	11.02	139.03	123.60
1	S	205	ARG	CD-NE-CZ	10.88	138.83	123.60
1	P	205	ARG	CD-NE-CZ	10.76	138.67	123.60
1	V	152	GLU	OE1-CD-OE2	-10.19	111.08	123.30
1	E	199	VAL	CA-CB-CG1	-10.17	95.64	110.90
1	H	212	GLN	CA-CB-CG	9.96	135.30	113.40
1	W	133	ASP	CB-CG-OD1	-9.83	109.46	118.30
1	Q	117	LYS	CD-CE-NZ	-9.82	89.12	111.70
1	H	168	LEU	CB-CG-CD2	9.69	127.47	111.00
1	V	168	LEU	CB-CG-CD2	9.65	127.40	111.00
1	U	152	GLU	OE1-CD-OE2	-9.64	111.73	123.30
1	V	17	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	T	17	ARG	NE-CZ-NH1	9.55	125.07	120.30
1	J	168	LEU	CB-CG-CD2	9.47	127.10	111.00
1	E	168	LEU	CB-CG-CD2	9.46	127.08	111.00
1	D	194	ARG	CA-CB-CG	9.46	134.20	113.40
1	D	168	LEU	CB-CG-CD2	9.38	126.95	111.00
1	U	168	LEU	CB-CG-CD2	9.36	126.92	111.00
1	Q	180	LEU	CB-CG-CD2	9.35	126.89	111.00
1	K	168	LEU	CB-CG-CD2	9.32	126.85	111.00
1	F	168	LEU	CB-CG-CD2	9.31	126.82	111.00
1	P	168	LEU	CB-CG-CD2	9.30	126.81	111.00
1	W	168	LEU	CB-CG-CD2	9.30	126.81	111.00
1	M	168	LEU	CB-CG-CD2	9.29	126.79	111.00
1	H	17	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	X	168	LEU	CB-CG-CD2	9.22	126.67	111.00
1	L	168	LEU	CB-CG-CD2	9.22	126.67	111.00
1	D	191	GLU	CG-CD-OE2	9.21	136.72	118.30
1	I	168	LEU	CB-CG-CD2	9.20	126.64	111.00
1	R	168	LEU	CB-CG-CD2	9.16	126.57	111.00
1	T	168	LEU	CB-CG-CD2	9.14	126.53	111.00
1	S	168	LEU	CB-CG-CD2	9.06	126.41	111.00
1	D	47	LEU	CB-CG-CD1	8.90	126.13	111.00
1	S	181	LEU	CB-CG-CD1	8.90	126.13	111.00
1	Q	180	LEU	CB-CG-CD1	-8.87	95.93	111.00
1	Q	181	LEU	CB-CG-CD1	8.85	126.05	111.00
1	A	181	LEU	CB-CG-CD1	8.82	126.00	111.00
1	K	82	GLN	N-CA-CB	-8.65	95.03	110.60
1	F	181	LEU	CB-CG-CD1	8.64	125.68	111.00
1	A	168	LEU	CB-CG-CD2	-8.52	96.51	111.00
1	C	181	LEU	CB-CG-CD1	8.51	125.47	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	181	LEU	CB-CG-CD1	8.50	125.45	111.00
1	R	181	LEU	CB-CG-CD1	8.50	125.44	111.00
1	J	147	VAL	CB-CA-C	8.45	127.45	111.40
1	C	168	LEU	CB-CG-CD2	-8.37	96.77	111.00
1	G	168	LEU	CB-CG-CD2	-8.34	96.83	111.00
1	U	147	VAL	CB-CA-C	8.25	127.08	111.40
1	L	88	GLN	CG-CD-OE1	-8.25	105.10	121.60
1	O	168	LEU	CB-CG-CD2	-8.17	97.11	111.00
1	B	168	LEU	CB-CG-CD2	-8.14	97.16	111.00
1	Q	168	LEU	CB-CG-CD2	-8.13	97.19	111.00
1	K	43	LYS	CA-CB-CG	8.08	131.17	113.40
1	N	168	LEU	CB-CG-CD2	-8.05	97.31	111.00
1	Q	180	LEU	CA-CB-CG	8.05	133.82	115.30
1	D	191	GLU	CG-CD-OE1	-7.91	102.49	118.30
1	D	47	LEU	CA-CB-CG	7.88	133.43	115.30
1	D	212	GLN	CA-CB-CG	7.81	130.59	113.40
1	D	118	LEU	CA-CB-CG	7.69	132.99	115.30
1	V	188	LEU	CB-CG-CD2	-7.68	97.94	111.00
1	G	118	LEU	CA-CB-CG	7.68	132.96	115.30
1	R	118	LEU	CA-CB-CG	7.66	132.92	115.30
1	L	118	LEU	CA-CB-CG	7.66	132.91	115.30
1	G	107	GLU	CG-CD-OE1	7.62	133.55	118.30
1	M	118	LEU	CA-CB-CG	7.57	132.70	115.30
1	F	107	GLU	CG-CD-OE1	7.56	133.43	118.30
1	V	118	LEU	CA-CB-CG	7.54	132.65	115.30
1	I	118	LEU	CA-CB-CG	7.53	132.61	115.30
1	K	82	GLN	CB-CA-C	7.51	125.42	110.40
1	T	104	MET	CG-SD-CE	7.51	112.21	100.20
1	X	118	LEU	CA-CB-CG	7.50	132.54	115.30
1	P	118	LEU	CA-CB-CG	7.48	132.51	115.30
1	O	118	LEU	CA-CB-CG	7.47	132.48	115.30
1	J	118	LEU	CA-CB-CG	7.45	132.43	115.30
1	Q	118	LEU	CA-CB-CG	7.45	132.43	115.30
1	X	67	GLU	OE1-CD-OE2	-7.44	114.37	123.30
1	X	107	GLU	CG-CD-OE1	7.40	133.11	118.30
1	W	107	GLU	CG-CD-OE1	7.39	133.08	118.30
1	K	118	LEU	CA-CB-CG	7.38	132.27	115.30
1	A	107	GLU	CG-CD-OE1	7.37	133.04	118.30
1	E	107	GLU	CG-CD-OE1	7.37	133.03	118.30
1	B	139	GLU	CA-CB-CG	7.33	129.53	113.40
1	C	107	GLU	CG-CD-OE1	7.33	132.96	118.30
1	B	122	GLN	CB-CA-C	7.32	125.05	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	GLU	CG-CD-OE1	7.32	132.94	118.30
1	F	118	LEU	CA-CB-CG	7.30	132.09	115.30
1	R	107	GLU	CG-CD-OE1	7.29	132.88	118.30
1	A	122	GLN	CB-CA-C	7.28	124.95	110.40
1	E	67	GLU	OE1-CD-OE2	-7.18	114.69	123.30
1	N	104	MET	CG-SD-CE	7.14	111.63	100.20
1	Q	186	LYS	CA-CB-CG	7.04	128.89	113.40
1	V	17	ARG	CG-CD-NE	7.04	126.58	111.80
1	H	17	ARG	CG-CD-NE	6.99	126.47	111.80
1	K	191	GLU	CA-CB-CG	6.94	128.67	113.40
1	M	191	GLU	CA-CB-CG	6.94	128.67	113.40
1	D	137	VAL	CA-CB-CG1	6.92	121.29	110.90
1	K	104	MET	CG-SD-CE	6.92	111.28	100.20
1	A	191	GLU	CA-CB-CG	6.89	128.57	113.40
1	T	17	ARG	CG-CD-NE	6.88	126.24	111.80
1	U	104	MET	CG-SD-CE	6.85	111.16	100.20
1	T	17	ARG	CD-NE-CZ	6.83	133.17	123.60
1	J	134	GLU	CG-CD-OE2	6.74	131.79	118.30
1	U	168	LEU	CA-CB-CG	6.66	130.62	115.30
1	P	168	LEU	CA-CB-CG	6.59	130.47	115.30
1	W	168	LEU	CA-CB-CG	6.57	130.41	115.30
1	L	168	LEU	CA-CB-CG	6.55	130.37	115.30
1	I	168	LEU	CA-CB-CG	6.55	130.36	115.30
1	F	168	LEU	CA-CB-CG	6.51	130.28	115.30
1	E	168	LEU	CA-CB-CG	6.50	130.25	115.30
1	X	168	LEU	CA-CB-CG	6.50	130.24	115.30
1	K	196	ASN	CB-CG-OD1	-6.49	108.62	121.60
1	A	118	LEU	CA-CB-CG	-6.49	100.38	115.30
1	V	168	LEU	CA-CB-CG	6.49	130.22	115.30
1	B	209	GLU	OE1-CD-OE2	6.46	131.06	123.30
1	R	168	LEU	CA-CB-CG	6.46	130.16	115.30
1	T	168	LEU	CA-CB-CG	6.42	130.07	115.30
1	U	67	GLU	OE1-CD-OE2	-6.41	115.61	123.30
1	B	139	GLU	N-CA-CB	6.40	122.12	110.60
1	H	17	ARG	CD-NE-CZ	6.39	132.55	123.60
1	H	168	LEU	CA-CB-CG	6.39	129.99	115.30
1	E	118	LEU	CA-CB-CG	-6.38	100.63	115.30
1	J	168	LEU	CA-CB-CG	6.37	129.94	115.30
1	D	168	LEU	CA-CB-CG	6.35	129.90	115.30
1	M	168	LEU	CA-CB-CG	6.33	129.87	115.30
1	N	118	LEU	CA-CB-CG	-6.33	100.73	115.30
1	T	205	ARG	N-CA-CB	-6.33	99.20	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	118	LEU	CA-CB-CG	-6.32	100.75	115.30
1	H	107	GLU	OE1-CD-OE2	6.31	130.87	123.30
1	K	122	GLN	CG-CD-OE1	-6.29	109.02	121.60
1	W	118	LEU	CA-CB-CG	-6.29	100.84	115.30
1	B	118	LEU	CA-CB-CG	-6.28	100.85	115.30
1	K	105	GLN	CB-CG-CD	6.27	127.90	111.60
1	K	168	LEU	CA-CB-CG	6.23	129.63	115.30
1	S	168	LEU	CA-CB-CG	6.21	129.59	115.30
1	F	54	GLN	CG-CD-OE1	-6.19	109.23	121.60
1	N	139	GLU	CA-CB-CG	6.18	126.99	113.40
1	T	22	LEU	CB-CG-CD1	6.17	121.48	111.00
1	V	17	ARG	CD-NE-CZ	6.16	132.23	123.60
1	S	118	LEU	CA-CB-CG	-6.16	101.13	115.30
1	U	118	LEU	CA-CB-CG	-6.16	101.13	115.30
1	C	118	LEU	CA-CB-CG	-6.09	101.30	115.30
1	O	139	GLU	CA-CB-CG	6.08	126.78	113.40
1	J	44	GLU	OE1-CD-OE2	-6.04	116.05	123.30
1	H	44	GLU	CG-CD-OE1	-6.00	106.30	118.30
1	G	69	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	D	194	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	C	128	TYR	CB-CA-C	5.88	122.16	110.40
1	D	49	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	K	44	GLU	OE1-CD-OE2	-5.88	116.25	123.30
1	V	73	GLN	N-CA-CB	5.87	121.17	110.60
1	U	132	THR	CA-CB-CG2	-5.87	104.19	112.40
1	M	137	VAL	CA-CB-CG2	5.80	119.60	110.90
1	M	122	GLN	CA-CB-CG	-5.79	100.66	113.40
1	C	43	LYS	CB-CA-C	-5.78	98.83	110.40
1	Q	131	THR	N-CA-CB	5.76	121.25	110.30
1	E	49	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	D	107	GLU	OE1-CD-OE2	5.75	130.21	123.30
1	I	137	VAL	CA-CB-CG2	5.75	119.53	110.90
1	J	194	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	V	107	GLU	OE1-CD-OE2	5.73	130.18	123.30
1	B	75	ILE	CG1-CB-CG2	-5.73	98.80	111.40
1	P	107	GLU	OE1-CD-OE2	5.70	130.14	123.30
1	G	19	LEU	CB-CG-CD1	5.67	120.63	111.00
1	B	43	LYS	CB-CA-C	-5.66	99.08	110.40
1	D	194	ARG	CB-CG-CD	5.63	126.24	111.60
1	R	22	LEU	CB-CG-CD1	5.63	120.58	111.00
1	S	107	GLU	OE1-CD-OE2	5.63	130.06	123.30
1	K	107	GLU	OE1-CD-OE2	5.62	130.05	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	212	GLN	CB-CG-CD	5.62	126.20	111.60
1	O	43	LYS	CB-CA-C	-5.60	99.20	110.40
1	U	43	LYS	CB-CA-C	-5.60	99.20	110.40
1	K	105	GLN	CG-CD-OE1	5.60	132.79	121.60
1	T	107	GLU	OE1-CD-OE2	5.58	129.99	123.30
1	D	128	TYR	CB-CA-C	5.57	121.54	110.40
1	R	128	TYR	CB-CA-C	5.57	121.54	110.40
1	I	107	GLU	OE1-CD-OE2	5.57	129.98	123.30
1	J	137	VAL	CA-CB-CG2	5.56	119.25	110.90
1	D	43	LYS	CB-CA-C	-5.54	99.32	110.40
1	K	137	VAL	CA-CB-CG2	5.53	119.19	110.90
1	X	122	GLN	CB-CA-C	-5.49	99.41	110.40
1	N	43	LYS	CB-CA-C	-5.49	99.42	110.40
1	O	137	VAL	CA-CB-CG2	5.48	119.12	110.90
1	C	168	LEU	CB-CG-CD1	5.48	120.31	111.00
1	C	127	ILE	CA-CB-CG1	-5.46	100.62	111.00
1	U	107	GLU	OE1-CD-OE2	5.46	129.85	123.30
1	A	43	LYS	CB-CA-C	-5.46	99.49	110.40
1	S	137	VAL	CA-CB-CG2	5.44	119.06	110.90
1	M	128	TYR	CB-CA-C	5.43	121.26	110.40
1	V	35	GLU	OE1-CD-OE2	5.42	129.81	123.30
1	M	107	GLU	OE1-CD-OE2	5.41	129.79	123.30
1	U	128	TYR	CB-CA-C	5.40	121.21	110.40
1	E	44	GLU	CB-CA-C	5.39	121.18	110.40
1	V	78	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	T	43	LYS	CB-CA-C	-5.37	99.65	110.40
1	Q	107	GLU	OE1-CD-OE2	5.37	129.74	123.30
1	A	168	LEU	CB-CG-CD1	5.36	120.12	111.00
1	L	128	TYR	CB-CA-C	5.36	121.13	110.40
1	Q	168	LEU	CB-CG-CD1	5.34	120.08	111.00
1	N	107	GLU	OE1-CD-OE2	5.33	129.70	123.30
1	G	168	LEU	CB-CG-CD1	5.33	120.06	111.00
1	S	43	LYS	CB-CA-C	-5.33	99.75	110.40
1	O	107	GLU	OE1-CD-OE2	5.33	129.69	123.30
1	E	137	VAL	CA-CB-CG2	5.32	118.88	110.90
1	D	49	ARG	CG-CD-NE	5.32	122.97	111.80
1	N	194	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	37	LYS	CA-CB-CG	5.31	125.08	113.40
1	V	124	PHE	CB-CA-C	-5.29	99.81	110.40
1	S	128	TYR	CB-CA-C	5.28	120.96	110.40
1	O	120	PHE	CB-CG-CD1	-5.27	117.11	120.80
1	C	78	ARG	NE-CZ-NH2	-5.27	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	144	LEU	CA-CB-CG	5.26	127.40	115.30
1	S	194	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	F	132	THR	CA-CB-OG1	-5.21	98.06	109.00
1	G	132	THR	CA-CB-OG1	-5.20	98.08	109.00
1	E	128	TYR	CB-CA-C	5.20	120.79	110.40
1	P	78	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	N	168	LEU	CB-CG-CD1	5.19	119.82	111.00
1	A	128	TYR	CB-CA-C	5.17	120.75	110.40
1	L	107	GLU	OE1-CD-OE2	5.17	129.51	123.30
1	U	194	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	78	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	W	132	THR	CA-CB-OG1	-5.16	98.16	109.00
1	M	191	GLU	CB-CA-C	-5.15	100.10	110.40
1	D	132	THR	CB-CA-C	5.15	125.49	111.60
1	V	78	ARG	CB-CG-CD	5.14	124.98	111.60
1	W	127	ILE	CG1-CB-CG2	-5.14	100.09	111.40
1	E	199	VAL	CB-CA-C	5.14	121.16	111.40
1	A	194	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	O	168	LEU	CB-CG-CD1	5.13	119.73	111.00
1	V	152	GLU	CB-CG-CD	5.13	128.06	114.20
1	B	75	ILE	CA-CB-CG1	5.13	120.74	111.00
1	G	42	LYS	CD-CE-NZ	5.09	123.40	111.70
1	R	78	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	B	168	LEU	CB-CG-CD1	5.04	119.56	111.00
1	B	194	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	X	42	LYS	CD-CE-NZ	5.04	123.28	111.70
1	A	191	GLU	CB-CA-C	-5.02	100.37	110.40
1	U	99	ILE	CA-CB-CG1	-5.02	101.47	111.00
1	K	194	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	R	177	ILE	CG1-CB-CG2	-5.01	100.37	111.40
1	T	37	LYS	CA-CB-CG	5.01	124.43	113.40
1	Q	137	VAL	CA-CB-CG2	-5.01	103.39	110.90
1	J	107	GLU	OE1-CD-OE2	5.00	129.30	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	V	152	GLU	Sidechain

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	1602	0	1526	38	0
1	B	1650	0	1587	39	0
1	C	1610	0	1528	32	0
1	D	1589	0	1486	35	0
1	E	1553	0	1414	34	0
1	F	1609	0	1546	25	0
1	G	1543	0	1401	23	0
1	H	1515	0	1343	30	0
1	I	1644	0	1589	41	0
1	J	1640	0	1593	39	0
1	K	1635	0	1580	54	0
1	L	1645	0	1598	41	1
1	M	1642	0	1586	40	0
1	N	1501	0	1371	15	0
1	O	1461	0	1303	32	0
1	P	1615	0	1531	33	0
1	Q	1619	0	1548	31	0
1	R	1625	0	1573	33	1
1	S	1653	0	1604	32	0
1	T	1473	0	1293	23	0
1	U	1644	0	1600	42	0
1	V	1632	0	1569	51	0
1	W	1639	0	1584	26	0
1	X	1645	0	1597	38	0
2	A	14	0	0	0	0
2	B	14	0	0	0	0
2	C	14	0	0	0	0
2	D	14	0	0	0	0
2	E	14	0	0	0	0
2	F	14	0	0	0	0
2	G	14	0	0	0	0
2	H	14	0	0	0	0
2	I	14	0	0	0	0
2	J	14	0	0	0	0
2	K	14	0	0	0	0
2	L	14	0	0	0	0
2	M	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	14	0	0	0	0
2	O	14	0	0	0	0
2	P	14	0	0	0	0
2	Q	14	0	0	0	0
2	R	14	0	0	0	0
2	S	14	0	0	0	0
2	T	14	0	0	0	0
2	U	14	0	0	0	0
2	V	14	0	0	0	0
2	W	14	0	0	0	0
2	X	14	0	0	0	0
3	A	18	0	0	1	0
3	B	15	0	0	1	0
3	C	13	0	0	1	0
3	D	15	0	0	0	0
3	E	19	0	0	2	0
3	F	10	0	0	0	0
3	G	13	0	0	0	0
3	H	6	0	0	0	0
3	I	15	0	0	0	0
3	J	22	0	0	0	0
3	K	13	0	0	1	0
3	L	13	0	0	1	0
3	M	15	0	0	1	0
3	N	9	0	0	0	0
3	O	7	0	0	0	0
3	P	9	0	0	0	0
3	Q	9	0	0	0	0
3	R	3	0	0	0	0
3	S	13	0	0	0	0
3	T	4	0	0	0	0
3	U	20	0	0	1	0
3	V	17	0	0	0	0
3	W	13	0	0	0	0
3	X	13	0	0	1	0
All	All	39024	0	36350	612	1

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 8.

All (612) 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:H:180:LEU:O	1:H:183:THR:HG22	1.41	1.20
1:E:44:GLU:CB	1:K:190:THR:HG23	1.77	1.15
1:H:36:LEU:HD23	1:H:41:HIS:CG	2.00	0.97
1:D:67:GLU:OE2	1:N:109:HIS:HD2	1.48	0.96
1:Q:180:LEU:HD23	1:Q:189:PHE:HE2	1.30	0.95
1:U:130:LEU:HD12	1:X:120:PHE:CD2	2.02	0.94
1:O:120:PHE:HE1	1:V:130:LEU:HD13	1.34	0.93
1:D:127:ILE:HA	1:F:36:LEU:HD13	1.48	0.91
1:E:44:GLU:CB	1:K:190:THR:CG2	2.49	0.91
1:H:36:LEU:HD23	1:H:41:HIS:HB3	1.50	0.91
1:H:122:GLN:OE1	1:H:183:THR:OG1	1.88	0.91
1:D:122:GLN:OE1	1:D:183:THR:HG21	1.72	0.88
1:Q:180:LEU:HD23	1:Q:189:PHE:CE2	2.06	0.88
1:C:123:ILE:O	1:C:127:ILE:HD12	1.75	0.87
1:H:36:LEU:HD23	1:H:41:HIS:CB	2.06	0.86
1:I:36:LEU:HD13	1:S:127:ILE:HA	1.58	0.85
1:J:120:PHE:HE1	1:L:120:PHE:CZ	1.95	0.83
1:D:67:GLU:OE2	1:N:109:HIS:CD2	2.31	0.82
1:H:36:LEU:HD23	1:H:41:HIS:ND1	1.95	0.81
1:O:120:PHE:CE1	1:V:130:LEU:HD13	2.16	0.81
1:A:125:LYS:HA	1:B:120:PHE:CZ	2.19	0.78
1:E:127:ILE:HA	1:W:36:LEU:HD13	1.64	0.77
1:K:120:PHE:HE1	1:M:120:PHE:CZ	2.03	0.76
1:U:65:LEU:HD23	1:V:102:ILE:HD11	1.67	0.76
1:H:36:LEU:CD2	1:H:41:HIS:HB3	2.16	0.76
1:L:88:GLN:HG2	1:L:96:GLN:HB3	1.65	0.76
1:U:65:LEU:CD2	1:V:102:ILE:HD11	2.16	0.76
1:E:155:LEU:O	1:E:194:ARG:NH1	2.16	0.75
1:D:183:THR:CG2	1:D:184:PRO:HD2	2.17	0.75
1:A:120:PHE:CE2	1:B:120:PHE:HE1	2.05	0.75
1:U:178:GLN:HG2	1:U:212:GLN:OE1	1.87	0.75
1:I:120:PHE:CD2	1:S:130:LEU:HD12	2.22	0.74
1:H:36:LEU:CD2	1:H:41:HIS:CG	2.70	0.74
1:V:122:GLN:HE22	1:V:183:THR:CG2	1.99	0.74
1:A:125:LYS:HA	1:B:120:PHE:HZ	1.52	0.74
1:R:65:LEU:CD2	1:T:102:ILE:HD11	2.18	0.73
1:I:193:PRO:HB3	1:K:62:ASP:CB	2.18	0.73
1:D:121:GLU:O	1:D:132:THR:HB	1.89	0.72
1:U:130:LEU:CD1	1:X:120:PHE:CD2	2.72	0.72
1:D:67:GLU:HG2	1:N:105:GLN:CG	2.19	0.72
1:A:105:GLN:CG	1:S:67:GLU:HG2	2.20	0.71
1:C:17:ARG:NH2	3:C:2003:HOH:O	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:120:PHE:CD2	1:S:130:LEU:CD1	2.75	0.70
1:U:125:LYS:HA	1:X:120:PHE:HZ	1.54	0.70
1:F:135:ALA:HB2	1:N:139:GLU:HG3	1.72	0.70
1:A:128:TYR:HB3	1:B:124:PHE:CE2	2.27	0.70
1:H:35:GLU:O	1:H:40:GLU:CB	2.39	0.70
1:R:65:LEU:HD22	1:T:102:ILE:HD11	1.72	0.70
1:E:67:GLU:OE1	1:E:67:GLU:HA	1.92	0.70
1:K:127:ILE:HA	1:M:36:LEU:HD13	1.74	0.69
1:G:125:LYS:HA	1:Q:120:PHE:CZ	2.27	0.69
1:J:36:LEU:HD13	1:L:127:ILE:HA	1.75	0.69
1:D:183:THR:HG22	1:D:184:PRO:HD2	1.75	0.69
1:F:183:THR:O	1:F:186:LYS:HG2	1.92	0.68
1:E:67:GLU:HG3	1:O:105:GLN:HB3	1.76	0.68
1:O:139:GLU:HG3	1:W:135:ALA:HB2	1.76	0.68
1:D:105:GLN:CG	1:N:67:GLU:HG2	2.23	0.68
1:U:67:GLU:HA	1:U:67:GLU:OE1	1.94	0.68
1:C:127:ILE:HA	1:T:36:LEU:HD13	1.76	0.68
1:J:120:PHE:CE1	1:L:120:PHE:CZ	2.82	0.67
1:U:125:LYS:HA	1:X:120:PHE:CZ	2.30	0.67
1:X:67:GLU:HA	1:X:67:GLU:OE1	1.93	0.67
1:Q:209:GLU:HA	1:Q:212:GLN:HG3	1.76	0.67
1:W:105:GLN:HB3	1:X:67:GLU:HG3	1.76	0.66
1:O:120:PHE:CE1	1:V:130:LEU:CD1	2.79	0.66
1:M:67:GLU:HG2	1:P:105:GLN:CG	2.26	0.66
1:D:67:GLU:HG2	1:N:105:GLN:HG3	1.77	0.65
1:K:95:SER:O	1:K:99:ILE:HD12	1.96	0.65
1:L:130:LEU:HD23	3:L:2010:HOH:O	1.97	0.65
1:U:105:GLN:CG	1:V:67:GLU:HG2	2.26	0.65
1:B:105:GLN:CG	1:J:67:GLU:HG2	2.26	0.64
1:K:39:GLY:O	1:K:43:LYS:HG3	1.97	0.64
1:A:114:VAL:HG23	1:A:140:GLU:HB3	1.78	0.64
1:I:128:TYR:CZ	1:S:13:ILE:HD12	2.32	0.64
1:G:95:SER:O	1:G:99:ILE:HD12	1.98	0.64
1:G:125:LYS:HA	1:Q:120:PHE:HZ	1.61	0.64
1:E:177:ILE:HG21	1:E:199:VAL:HG23	1.78	0.64
1:W:114:VAL:HG23	1:W:140:GLU:HB3	1.80	0.64
1:P:36:LEU:HD13	1:R:127:ILE:HA	1.79	0.64
1:A:13:ILE:HD12	1:B:128:TYR:CZ	2.33	0.64
1:J:44:GLU:HG3	1:J:45:PRO:HA	1.80	0.64
1:I:120:PHE:HE1	1:S:120:PHE:CZ	2.17	0.63
1:K:44:GLU:HG3	1:K:45:PRO:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:120:PHE:CD2	1:L:130:LEU:HD12	2.33	0.63
1:J:143:LYS:O	1:J:147:VAL:HG13	1.99	0.63
1:K:120:PHE:CZ	1:M:125:LYS:HA	2.33	0.63
1:V:74:TYR:OH	1:V:78:ARG:CD	2.46	0.63
1:O:134:GLU:HA	1:O:137:VAL:CG1	2.28	0.63
1:W:67:GLU:HG2	1:X:105:GLN:CG	2.29	0.63
1:C:25:LYS:HE3	1:C:82:GLN:O	1.99	0.62
1:C:36:LEU:HD13	1:T:127:ILE:HA	1.81	0.62
1:F:105:GLN:CG	1:Q:67:GLU:HG2	2.28	0.62
1:G:114:VAL:HG23	1:G:140:GLU:HB3	1.79	0.62
1:C:128:TYR:HB3	1:T:124:PHE:CE2	2.33	0.62
1:I:105:GLN:CG	1:L:67:GLU:HG2	2.30	0.62
1:U:143:LYS:O	1:U:147:VAL:HG13	2.00	0.62
1:V:74:TYR:OH	1:V:78:ARG:HD3	2.00	0.62
1:B:114:VAL:HG23	1:B:140:GLU:HB3	1.80	0.62
1:D:105:GLN:HG3	1:N:67:GLU:HG2	1.80	0.62
1:A:105:GLN:HG3	1:S:67:GLU:HG2	1.82	0.62
1:M:134:GLU:HA	1:M:137:VAL:CG1	2.30	0.61
1:P:128:TYR:CZ	1:R:13:ILE:HD12	2.34	0.61
1:K:124:PHE:CZ	1:M:128:TYR:CD1	2.87	0.61
1:C:120:PHE:CE2	1:T:120:PHE:CE2	2.88	0.61
1:F:186:LYS:NZ	1:J:197:GLU:OE1	2.29	0.61
1:A:128:TYR:CD1	1:B:124:PHE:CE1	2.89	0.61
1:H:36:LEU:CD2	1:H:41:HIS:ND1	2.64	0.61
1:P:125:LYS:HA	1:R:120:PHE:HZ	1.64	0.61
1:C:120:PHE:HE2	1:T:120:PHE:HE2	1.47	0.60
1:E:107:GLU:HG3	1:E:108:ASP:N	2.16	0.60
1:I:134:GLU:HA	1:I:137:VAL:CG1	2.31	0.60
1:U:178:GLN:CG	1:U:212:GLN:OE1	2.49	0.60
1:V:69:ARG:O	1:V:73:GLN:HG3	2.01	0.60
1:B:3:GLY:N	3:B:2001:HOH:O	2.34	0.60
1:B:67:GLU:HG2	1:J:105:GLN:CG	2.31	0.60
1:K:124:PHE:CE2	1:M:128:TYR:HB3	2.36	0.60
1:I:120:PHE:CE2	1:S:130:LEU:HD12	2.37	0.60
1:P:125:LYS:HA	1:R:120:PHE:CZ	2.37	0.60
1:C:36:LEU:HD23	1:C:41:HIS:CD2	2.37	0.59
1:K:116:SER:HB3	1:M:130:LEU:HD11	1.83	0.59
1:S:134:GLU:HA	1:S:137:VAL:CG1	2.33	0.59
1:E:193:PRO:HD3	3:E:2017:HOH:O	2.01	0.59
1:G:67:GLU:HG2	1:H:105:GLN:CG	2.32	0.59
1:G:105:GLN:CG	1:H:67:GLU:HG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:120:PHE:CD2	1:L:130:LEU:CD1	2.85	0.59
1:E:67:GLU:OE2	1:O:109:HIS:ND1	2.35	0.59
1:M:105:GLN:CG	1:P:67:GLU:HG2	2.33	0.59
1:V:122:GLN:HE22	1:V:183:THR:HG21	1.66	0.59
1:J:120:PHE:HE1	1:L:120:PHE:CE2	2.21	0.59
1:A:127:ILE:HA	1:B:36:LEU:HD13	1.85	0.58
1:E:134:GLU:HA	1:E:137:VAL:CG1	2.32	0.58
1:K:120:PHE:CE1	1:M:120:PHE:CZ	2.88	0.58
1:R:107:GLU:HG3	1:R:108:ASP:N	2.18	0.58
1:D:44:GLU:HG3	1:D:45:PRO:HA	1.86	0.58
1:C:102:ILE:HD11	1:K:65:LEU:CD2	2.34	0.58
1:O:120:PHE:HD1	1:V:130:LEU:HD11	1.68	0.58
1:V:44:GLU:HG3	1:V:45:PRO:HA	1.86	0.58
1:A:67:GLU:HG2	1:S:105:GLN:CG	2.34	0.58
1:D:122:GLN:CD	1:D:183:THR:CG2	2.71	0.57
1:E:105:GLN:HG3	1:O:67:GLU:HG2	1.85	0.57
1:F:67:GLU:HG2	1:Q:105:GLN:CG	2.33	0.57
1:K:134:GLU:HA	1:K:137:VAL:CG1	2.34	0.57
1:W:109:HIS:ND1	1:X:67:GLU:OE2	2.36	0.57
1:A:107:GLU:HG3	1:A:108:ASP:N	2.18	0.57
1:A:130:LEU:HD11	1:B:116:SER:HB3	1.85	0.57
1:J:134:GLU:HA	1:J:137:VAL:CG1	2.35	0.57
1:S:44:GLU:OE1	1:S:44:GLU:HA	2.04	0.57
1:H:40:GLU:C	1:H:42:LYS:H	2.07	0.57
1:M:44:GLU:HG3	1:M:45:PRO:HA	1.85	0.57
1:K:122:GLN:OE1	1:K:183:THR:HB	2.05	0.57
1:O:120:PHE:CD1	1:V:130:LEU:HD11	2.39	0.57
1:G:36:LEU:HD13	1:Q:127:ILE:HA	1.87	0.57
1:U:67:GLU:HG3	1:V:105:GLN:HB3	1.86	0.57
1:U:130:LEU:HD12	1:X:120:PHE:CE2	2.40	0.57
1:F:107:GLU:HG3	1:F:108:ASP:N	2.19	0.57
1:A:67:GLU:HG2	1:S:105:GLN:HG3	1.86	0.56
1:I:44:GLU:OE1	1:I:44:GLU:HA	2.05	0.56
1:E:45:PRO:CA	1:K:190:THR:HG22	2.35	0.56
1:G:107:GLU:HG3	1:G:108:ASP:N	2.19	0.56
1:G:44:GLU:HG3	1:G:45:PRO:HA	1.86	0.56
1:C:105:GLN:CG	1:K:67:GLU:HG2	2.35	0.56
1:L:44:GLU:HG3	1:L:45:PRO:HA	1.86	0.56
1:M:107:GLU:HB2	1:M:173:HIS:CE1	2.40	0.56
1:R:22:LEU:HD13	1:R:29:PHE:CG	2.41	0.56
1:D:122:GLN:CD	1:D:183:THR:HG21	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:GLN:CG	1:O:67:GLU:HG2	2.35	0.56
1:W:44:GLU:OE1	1:W:44:GLU:HA	2.06	0.56
1:Q:209:GLU:O	1:Q:212:GLN:HG3	2.06	0.56
1:S:86:LEU:HB3	1:S:168:LEU:HD13	1.87	0.56
1:J:107:GLU:HB2	1:J:173:HIS:CE1	2.41	0.56
1:B:44:GLU:HG3	1:B:45:PRO:HA	1.87	0.56
1:E:86:LEU:HB3	1:E:168:LEU:HD13	1.87	0.55
1:V:107:GLU:HB2	1:V:173:HIS:CE1	2.41	0.55
1:K:86:LEU:HB3	1:K:168:LEU:HD13	1.88	0.55
1:C:120:PHE:HE2	1:T:120:PHE:CE2	2.25	0.55
1:P:44:GLU:OE1	1:P:44:GLU:HA	2.06	0.55
1:P:127:ILE:HA	1:R:36:LEU:HD13	1.89	0.55
1:R:86:LEU:HB3	1:R:168:LEU:HD13	1.88	0.55
1:X:44:GLU:HG3	1:X:45:PRO:HA	1.88	0.55
1:O:107:GLU:HB2	1:O:173:HIS:CE1	2.42	0.55
1:W:107:GLU:HG3	1:W:108:ASP:N	2.21	0.55
1:K:124:PHE:CE1	1:M:128:TYR:CD1	2.94	0.55
1:V:122:GLN:HE22	1:V:183:THR:HG23	1.70	0.55
1:H:86:LEU:HB3	1:H:168:LEU:HD13	1.87	0.55
1:U:105:GLN:HG3	1:V:67:GLU:HG2	1.87	0.55
1:U:86:LEU:HB3	1:U:168:LEU:HD13	1.89	0.55
1:X:86:LEU:HB3	1:X:168:LEU:HD13	1.88	0.55
1:A:13:ILE:CD1	1:B:128:TYR:CZ	2.89	0.55
1:K:107:GLU:HB2	1:K:173:HIS:CE1	2.42	0.55
1:Q:44:GLU:OE1	1:Q:44:GLU:HA	2.06	0.55
1:L:86:LEU:HB3	1:L:168:LEU:HD13	1.88	0.54
1:T:22:LEU:HD13	1:T:29:PHE:CG	2.41	0.54
1:P:86:LEU:HB3	1:P:168:LEU:HD13	1.88	0.54
1:V:86:LEU:HB3	1:V:168:LEU:HD13	1.88	0.54
1:H:107:GLU:HB2	1:H:173:HIS:CE1	2.42	0.54
1:U:107:GLU:HB2	1:U:173:HIS:CE1	2.41	0.54
1:X:107:GLU:HG3	1:X:108:ASP:N	2.20	0.54
1:U:128:TYR:HB3	1:X:124:PHE:CE2	2.43	0.54
1:B:107:GLU:HG3	1:B:108:ASP:N	2.22	0.54
1:M:86:LEU:HB3	1:M:168:LEU:HD13	1.88	0.54
1:A:13:ILE:CD1	1:B:128:TYR:OH	2.55	0.54
1:I:193:PRO:CB	1:K:62:ASP:CB	2.86	0.54
1:I:86:LEU:HB3	1:I:168:LEU:HD13	1.88	0.54
1:J:86:LEU:HB3	1:J:168:LEU:HD13	1.89	0.54
1:F:86:LEU:HB3	1:F:168:LEU:HD13	1.88	0.54
1:K:120:PHE:HZ	1:M:125:LYS:HA	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:124:PHE:CE1	1:R:128:TYR:CD1	2.96	0.54
1:U:65:LEU:HD22	1:V:102:ILE:HD11	1.90	0.54
1:D:86:LEU:HB3	1:D:168:LEU:HD13	1.89	0.54
1:D:107:GLU:HB2	1:D:173:HIS:CE1	2.43	0.54
1:N:107:GLU:HB2	1:N:173:HIS:CE1	2.42	0.54
1:I:67:GLU:HG2	1:L:105:GLN:CG	2.38	0.54
1:Q:107:GLU:HB2	1:Q:173:HIS:CE1	2.43	0.54
1:P:128:TYR:OH	1:R:13:ILE:HD12	2.08	0.54
1:S:107:GLU:HB2	1:S:173:HIS:CE1	2.43	0.54
1:T:86:LEU:HB3	1:T:168:LEU:HD13	1.89	0.54
1:C:25:LYS:HE2	1:C:79:TYR:O	2.07	0.53
1:G:67:GLU:HG2	1:H:105:GLN:HG3	1.90	0.53
1:I:107:GLU:HB2	1:I:173:HIS:CE1	2.43	0.53
1:O:120:PHE:CE1	1:V:130:LEU:HD22	2.43	0.53
1:M:67:GLU:HG2	1:P:105:GLN:HG3	1.88	0.53
1:A:116:SER:HB3	1:B:130:LEU:HD11	1.89	0.53
1:V:122:GLN:NE2	1:V:183:THR:HG21	2.23	0.53
1:W:86:LEU:HB3	1:W:168:LEU:HD13	1.89	0.53
1:E:199:VAL:HG13	1:E:200:ALA:N	2.23	0.53
1:V:74:TYR:OH	1:V:78:ARG:HD2	2.09	0.53
1:D:183:THR:HG23	1:D:184:PRO:HD2	1.90	0.53
1:O:107:GLU:OE1	1:O:108:ASP:N	2.42	0.53
1:Q:209:GLU:HA	1:Q:212:GLN:CG	2.39	0.53
1:R:65:LEU:HD23	1:T:102:ILE:HD11	1.88	0.53
1:D:107:GLU:OE1	1:D:108:ASP:N	2.41	0.53
1:L:107:GLU:HB2	1:L:173:HIS:CE1	2.43	0.53
1:U:144:LEU:HD22	1:U:148:LEU:HG	1.90	0.53
1:C:102:ILE:HD11	1:K:65:LEU:HD23	1.91	0.53
1:C:63:LEU:HD11	1:K:99:ILE:HD11	1.90	0.53
1:F:105:GLN:HG3	1:Q:67:GLU:HG2	1.91	0.52
1:E:45:PRO:N	1:K:190:THR:HG22	2.24	0.52
1:K:124:PHE:CE1	1:M:128:TYR:CE1	2.97	0.52
1:P:124:PHE:CE2	1:R:128:TYR:HB3	2.43	0.52
1:V:107:GLU:OE1	1:V:108:ASP:N	2.42	0.52
1:W:67:GLU:HG2	1:X:105:GLN:HG3	1.91	0.52
1:O:41:HIS:CD2	1:O:42:LYS:N	2.78	0.52
1:G:128:TYR:CB	1:Q:120:PHE:CE2	2.93	0.52
1:U:183:THR:HG23	1:U:185:THR:H	1.75	0.52
1:X:183:THR:HG23	1:X:185:THR:H	1.75	0.52
1:A:120:PHE:CE2	1:B:120:PHE:CE1	2.94	0.51
1:P:183:THR:HG23	1:P:185:THR:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:GLU:OE2	1:E:205:ARG:NH1	2.44	0.51
1:J:107:GLU:OE1	1:J:108:ASP:N	2.43	0.51
1:Q:24:GLU:OE2	1:Q:205:ARG:NH1	2.43	0.51
1:V:24:GLU:OE2	1:V:205:ARG:NH1	2.44	0.51
1:H:24:GLU:OE2	1:H:205:ARG:NH1	2.44	0.51
1:J:183:THR:HG23	1:J:185:THR:H	1.75	0.51
1:W:183:THR:HG23	1:W:185:THR:H	1.74	0.51
1:C:107:GLU:HG3	1:C:108:ASP:N	2.24	0.51
1:B:67:GLU:HG2	1:J:105:GLN:HG3	1.91	0.51
1:J:127:ILE:HA	1:L:36:LEU:HD13	1.93	0.51
1:U:24:GLU:OE2	1:U:205:ARG:NH1	2.44	0.51
1:O:120:PHE:CD1	1:V:130:LEU:CD1	2.93	0.51
1:X:24:GLU:OE2	1:X:205:ARG:NH1	2.43	0.51
1:C:25:LYS:CE	1:C:79:TYR:O	2.58	0.51
1:V:122:GLN:NE2	1:V:183:THR:CG2	2.71	0.51
1:D:81:ASN:CB	1:K:81:ASN:HA	2.41	0.51
1:M:183:THR:HG23	1:M:185:THR:H	1.75	0.51
1:T:107:GLU:HB2	1:T:173:HIS:CE1	2.45	0.51
1:B:24:GLU:OE2	1:B:205:ARG:NH1	2.43	0.51
1:K:24:GLU:OE2	1:K:205:ARG:NH1	2.43	0.51
1:K:120:PHE:HE1	1:M:120:PHE:CE2	2.29	0.51
1:C:24:GLU:OE2	1:C:205:ARG:NH1	2.44	0.51
1:H:107:GLU:OE1	1:H:108:ASP:N	2.44	0.51
1:M:24:GLU:OE2	1:M:205:ARG:NH1	2.44	0.51
1:A:24:GLU:OE2	1:A:205:ARG:NH1	2.44	0.50
1:D:24:GLU:HG2	1:D:86:LEU:HD21	1.94	0.50
1:R:24:GLU:OE2	1:R:205:ARG:NH1	2.44	0.50
1:F:24:GLU:OE2	1:F:205:ARG:NH1	2.44	0.50
1:L:24:GLU:OE2	1:L:205:ARG:NH1	2.44	0.50
1:M:107:GLU:OE1	1:M:108:ASP:N	2.44	0.50
1:Q:107:GLU:OE1	1:Q:108:ASP:N	2.44	0.50
1:R:67:GLU:HG2	1:T:105:GLN:CG	2.41	0.50
1:J:120:PHE:CZ	1:L:125:LYS:HA	2.46	0.50
1:P:107:GLU:HB2	1:P:173:HIS:CE1	2.47	0.50
1:T:183:THR:HG23	1:T:185:THR:H	1.77	0.50
1:I:120:PHE:HZ	1:S:125:LYS:HA	1.75	0.50
1:J:24:GLU:HG2	1:J:86:LEU:HD21	1.94	0.50
1:U:127:ILE:HA	1:X:36:LEU:HD13	1.93	0.50
1:A:120:PHE:CZ	1:B:120:PHE:HE1	2.30	0.50
1:J:124:PHE:CZ	1:L:128:TYR:CD1	2.99	0.50
1:L:183:THR:HG23	1:L:185:THR:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:THR:HG23	1:A:185:THR:H	1.76	0.50
1:D:133:ASP:O	1:D:137:VAL:HG13	2.12	0.50
1:N:107:GLU:OE1	1:N:108:ASP:N	2.45	0.50
1:P:120:PHE:CZ	1:R:120:PHE:HE1	2.30	0.50
1:F:183:THR:HG23	1:F:185:THR:H	1.76	0.50
1:G:38:ASP:HA	1:Q:182:GLY:HA3	1.94	0.50
1:J:24:GLU:OE2	1:J:205:ARG:NH1	2.44	0.50
1:C:120:PHE:CE2	1:T:120:PHE:HE2	2.26	0.50
1:W:24:GLU:OE2	1:W:205:ARG:NH1	2.44	0.50
1:D:118:LEU:HD13	1:D:140:GLU:CB	2.42	0.50
1:D:24:GLU:OE2	1:D:205:ARG:NH1	2.45	0.50
1:H:38:ASP:OD1	1:H:38:ASP:N	2.44	0.50
1:M:105:GLN:HG3	1:P:67:GLU:HG2	1.92	0.50
1:M:24:GLU:HG2	1:M:86:LEU:HD21	1.94	0.50
1:T:107:GLU:OE1	1:T:108:ASP:N	2.44	0.50
1:A:13:ILE:HD12	1:B:128:TYR:OH	2.12	0.49
1:C:128:TYR:CD1	1:T:124:PHE:CE1	3.00	0.49
1:F:67:GLU:HG2	1:Q:105:GLN:HG3	1.92	0.49
1:X:118:LEU:HD13	1:X:140:GLU:CB	2.42	0.49
1:A:124:PHE:CD2	1:B:128:TYR:HB2	2.47	0.49
1:E:45:PRO:HA	1:K:190:THR:CG2	2.42	0.49
1:L:24:GLU:HG2	1:L:86:LEU:HD21	1.95	0.49
1:F:24:GLU:HG2	1:F:86:LEU:HD21	1.94	0.49
1:G:186:LYS:O	1:G:187:LYS:C	2.51	0.49
1:I:24:GLU:OE2	1:I:205:ARG:NH1	2.44	0.49
1:K:107:GLU:OE1	1:K:108:ASP:N	2.45	0.49
1:X:186:LYS:HD3	3:X:2013:HOH:O	2.12	0.49
1:X:24:GLU:HG2	1:X:86:LEU:HD21	1.94	0.49
1:V:180:LEU:O	1:V:183:THR:HG22	2.13	0.49
1:C:67:GLU:HG2	1:K:105:GLN:HB3	1.95	0.49
1:G:105:GLN:HG3	1:H:67:GLU:HG2	1.93	0.49
1:W:24:GLU:HG2	1:W:86:LEU:HD21	1.95	0.49
1:E:24:GLU:HG2	1:E:86:LEU:HD21	1.95	0.49
1:Q:118:LEU:HD13	1:Q:140:GLU:CB	2.43	0.49
1:K:24:GLU:HG2	1:K:86:LEU:HD21	1.95	0.49
1:U:183:THR:O	1:U:186:LYS:HG2	2.13	0.49
1:E:36:LEU:HD13	1:W:127:ILE:HA	1.94	0.49
1:G:118:LEU:HD13	1:G:140:GLU:CB	2.43	0.49
1:O:118:LEU:HD13	1:O:140:GLU:CB	2.43	0.49
1:V:24:GLU:HG2	1:V:86:LEU:HD21	1.94	0.49
1:A:24:GLU:HG2	1:A:86:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:THR:HG23	1:B:185:THR:H	1.78	0.49
1:C:24:GLU:HG2	1:C:86:LEU:HD21	1.95	0.49
1:D:122:GLN:OE1	1:D:183:THR:CG2	2.52	0.49
1:D:134:GLU:HA	1:D:137:VAL:HG13	1.94	0.49
1:L:118:LEU:HD13	1:L:140:GLU:CB	2.43	0.49
1:M:118:LEU:HD13	1:M:140:GLU:CB	2.43	0.49
1:T:24:GLU:HG2	1:T:86:LEU:HD21	1.95	0.49
1:I:24:GLU:HG2	1:I:86:LEU:HD21	1.95	0.48
1:J:118:LEU:HD13	1:J:140:GLU:CB	2.43	0.48
1:J:120:PHE:CE1	1:L:120:PHE:CE2	3.00	0.48
1:P:118:LEU:HD13	1:P:140:GLU:CB	2.43	0.48
1:I:107:GLU:OE1	1:I:108:ASP:N	2.46	0.48
1:K:183:THR:O	1:K:186:LYS:HG2	2.14	0.48
1:R:118:LEU:HD13	1:R:140:GLU:CB	2.43	0.48
1:V:183:THR:HG23	1:V:185:THR:H	1.77	0.48
1:H:24:GLU:HG2	1:H:86:LEU:HD21	1.94	0.48
1:I:128:TYR:OH	1:S:13:ILE:HD12	2.12	0.48
1:L:183:THR:O	1:L:186:LYS:HG2	2.14	0.48
1:R:44:GLU:HG3	1:R:45:PRO:HA	1.95	0.48
1:U:180:LEU:O	1:U:183:THR:HG22	2.13	0.48
1:U:128:TYR:CD1	1:X:124:PHE:CZ	3.01	0.48
1:E:128:TYR:CD1	1:W:124:PHE:CE1	3.02	0.48
1:M:183:THR:O	1:M:186:LYS:HG2	2.14	0.48
1:F:54:GLN:HE21	1:Q:110:GLN:NE2	2.11	0.48
1:R:24:GLU:HG2	1:R:86:LEU:HD21	1.95	0.48
1:B:24:GLU:HG2	1:B:86:LEU:HD21	1.95	0.48
1:F:118:LEU:HD13	1:F:140:GLU:CB	2.44	0.48
1:M:180:LEU:O	1:M:183:THR:HG22	2.13	0.48
1:O:120:PHE:CE1	1:V:130:LEU:CD2	2.96	0.48
1:L:180:LEU:O	1:L:183:THR:HG22	2.14	0.48
1:O:128:TYR:HB2	1:V:124:PHE:CE2	2.49	0.48
1:P:107:GLU:OE1	1:P:108:ASP:N	2.47	0.48
1:Q:24:GLU:HG2	1:Q:86:LEU:HD21	1.96	0.48
1:S:183:THR:O	1:S:186:LYS:HG2	2.14	0.48
1:E:128:TYR:HB3	1:W:124:PHE:CE2	2.48	0.48
1:A:180:LEU:O	1:A:183:THR:HG22	2.13	0.48
1:C:183:THR:O	1:C:186:LYS:HG2	2.13	0.48
1:P:24:GLU:HG2	1:P:86:LEU:HD21	1.95	0.48
1:I:118:LEU:HD13	1:I:140:GLU:CB	2.44	0.47
1:K:118:LEU:HD13	1:K:140:GLU:CB	2.44	0.47
1:J:120:PHE:HZ	1:L:125:LYS:HA	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:GLU:HG2	1:G:86:LEU:HD21	1.95	0.47
1:I:128:TYR:CD2	1:I:130:LEU:HD13	2.49	0.47
1:J:124:PHE:CE2	1:L:128:TYR:HB3	2.49	0.47
1:J:180:LEU:O	1:J:183:THR:HG22	2.14	0.47
1:R:183:THR:O	1:R:186:LYS:HG2	2.14	0.47
1:O:120:PHE:CD1	1:V:130:LEU:HD21	2.49	0.47
1:B:180:LEU:O	1:B:183:THR:HG22	2.14	0.47
1:L:107:GLU:OE1	1:L:108:ASP:N	2.48	0.47
1:P:180:LEU:O	1:P:183:THR:HG22	2.14	0.47
1:S:133:ASP:O	1:S:137:VAL:HG12	2.14	0.47
1:U:65:LEU:HD23	1:V:102:ILE:CD1	2.43	0.47
1:F:180:LEU:O	1:F:183:THR:HG22	2.14	0.47
1:V:41:HIS:CD2	1:V:42:LYS:HG2	2.50	0.47
1:A:3:GLY:N	3:A:2001:HOH:O	2.46	0.47
1:T:120:PHE:CD1	1:T:124:PHE:HD2	2.33	0.47
1:U:107:GLU:OE1	1:U:108:ASP:N	2.48	0.47
1:B:128:TYR:CD2	1:B:130:LEU:HD13	2.49	0.47
1:H:36:LEU:CD2	1:H:41:HIS:CB	2.81	0.47
1:M:133:ASP:O	1:M:137:VAL:HG12	2.15	0.47
1:T:36:LEU:HD23	1:T:41:HIS:CD2	2.50	0.47
1:U:24:GLU:HG2	1:U:86:LEU:HD21	1.95	0.47
1:X:180:LEU:O	1:X:183:THR:HG22	2.14	0.47
1:S:24:GLU:HG2	1:S:86:LEU:HD21	1.95	0.47
1:T:180:LEU:O	1:T:183:THR:HG22	2.14	0.47
1:K:133:ASP:O	1:K:137:VAL:HG12	2.15	0.47
1:V:118:LEU:HD13	1:V:140:GLU:CB	2.44	0.47
1:E:45:PRO:HG3	1:K:191:GLU:HA	1.95	0.47
1:N:24:GLU:HG2	1:N:86:LEU:HD21	1.95	0.47
1:S:107:GLU:OE1	1:S:108:ASP:N	2.48	0.47
1:W:180:LEU:O	1:W:183:THR:HG22	2.14	0.47
1:I:133:ASP:O	1:I:137:VAL:HG12	2.15	0.47
1:I:143:LYS:HE2	1:J:133:ASP:OD1	2.14	0.47
1:U:67:GLU:OE2	1:V:109:HIS:ND1	2.47	0.47
1:J:133:ASP:O	1:J:137:VAL:HG12	2.15	0.46
1:U:13:ILE:HD12	1:X:128:TYR:CZ	2.50	0.46
1:O:73:GLN:HA	1:O:168:LEU:HD11	1.97	0.46
1:W:44:GLU:OE1	1:W:47:LEU:HB2	2.15	0.46
1:W:133:ASP:OD2	1:W:136:VAL:HG23	2.14	0.46
1:I:127:ILE:HA	1:S:36:LEU:HD13	1.97	0.46
1:U:116:SER:HA	1:X:128:TYR:OH	2.16	0.46
1:D:183:THR:HG22	1:D:184:PRO:CD	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:GLN:HG3	1:J:67:GLU:HG2	1.96	0.46
1:K:36:LEU:HD13	1:M:127:ILE:HG12	1.98	0.46
1:B:73:GLN:HA	1:B:168:LEU:HD11	1.97	0.46
1:P:128:TYR:OH	1:R:13:ILE:CD1	2.64	0.46
1:P:128:TYR:CD2	1:P:130:LEU:HD13	2.50	0.46
1:F:54:GLN:HE21	1:Q:110:GLN:HE22	1.63	0.46
1:D:118:LEU:HD13	1:D:140:GLU:HB2	1.98	0.46
1:G:73:GLN:HA	1:G:168:LEU:HD11	1.97	0.46
1:I:105:GLN:HG3	1:L:67:GLU:HG2	1.98	0.46
1:O:133:ASP:O	1:O:137:VAL:HG12	2.16	0.46
1:P:124:PHE:CZ	1:R:128:TYR:CD1	3.03	0.46
1:E:133:ASP:O	1:E:137:VAL:HG12	2.15	0.45
1:A:73:GLN:HA	1:A:168:LEU:HD11	1.98	0.45
1:U:36:LEU:HD13	1:X:127:ILE:HA	1.97	0.45
1:G:187:LYS:O	1:G:190:THR:N	2.49	0.45
1:S:44:GLU:OE1	1:S:47:LEU:HB2	2.16	0.45
1:C:73:GLN:HA	1:C:168:LEU:HD11	1.97	0.45
1:I:105:GLN:HB3	1:L:67:GLU:HG2	1.97	0.45
1:C:63:LEU:CD1	1:K:99:ILE:HD11	2.46	0.45
1:N:73:GLN:HA	1:N:168:LEU:HD11	1.98	0.45
1:W:133:ASP:OD2	1:W:135:ALA:HB3	2.16	0.45
1:A:125:LYS:HG2	1:B:120:PHE:CZ	2.51	0.45
1:A:120:PHE:CZ	1:B:120:PHE:CE1	3.04	0.45
1:I:128:TYR:CZ	1:S:13:ILE:CD1	2.98	0.45
1:I:67:GLU:HG2	1:L:105:GLN:HG3	1.99	0.45
1:J:124:PHE:CE1	1:L:128:TYR:CD1	3.05	0.45
1:P:118:LEU:HD13	1:P:140:GLU:HB2	1.99	0.45
1:X:118:LEU:HD13	1:X:140:GLU:HB2	1.99	0.45
1:A:36:LEU:HD13	1:B:127:ILE:HA	1.99	0.45
1:E:196:ASN:O	1:E:199:VAL:HG12	2.17	0.45
1:M:44:GLU:HB3	1:O:157:GLU:O	2.16	0.45
1:P:44:GLU:OE1	1:P:47:LEU:HB2	2.16	0.45
1:U:128:TYR:CD1	1:X:124:PHE:CE1	3.05	0.45
1:X:128:TYR:CD2	1:X:130:LEU:HD13	2.51	0.45
1:E:109:HIS:HE1	1:O:108:ASP:OD1	2.00	0.45
1:G:118:LEU:HD13	1:G:140:GLU:HB2	1.99	0.45
1:K:120:PHE:CE1	1:M:120:PHE:CE2	3.05	0.45
1:V:36:LEU:HD23	1:V:41:HIS:ND1	2.32	0.44
1:Q:44:GLU:OE1	1:Q:47:LEU:HB2	2.16	0.44
1:R:118:LEU:HD13	1:R:140:GLU:HB2	1.99	0.44
1:C:102:ILE:HD11	1:K:65:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:44:GLU:OE1	1:I:47:LEU:HB2	2.16	0.44
1:P:124:PHE:CE1	1:R:128:TYR:CE1	3.05	0.44
1:O:128:TYR:HB2	1:V:124:PHE:CD2	2.52	0.44
1:U:116:SER:HB3	1:X:128:TYR:HE2	1.83	0.44
1:Q:118:LEU:HD13	1:Q:140:GLU:HB2	1.99	0.44
1:Q:81:ASN:OD1	1:Q:81:ASN:N	2.50	0.44
1:V:73:GLN:HA	1:V:168:LEU:HD21	1.98	0.44
1:O:139:GLU:HG3	1:W:135:ALA:CB	2.47	0.44
1:Q:73:GLN:HA	1:Q:168:LEU:HD11	2.00	0.44
1:I:67:GLU:HG2	1:L:105:GLN:HB3	1.99	0.44
1:I:81:ASN:OD1	1:I:81:ASN:N	2.50	0.44
1:L:118:LEU:HD13	1:L:140:GLU:HB2	1.99	0.44
1:U:105:GLN:HG2	1:V:67:GLU:HG2	2.00	0.44
1:A:130:LEU:HD22	1:B:120:PHE:CD2	2.52	0.44
1:I:118:LEU:HD13	1:I:140:GLU:HB2	2.00	0.44
1:M:212:GLN:NE2	3:M:2012:HOH:O	2.50	0.44
1:P:128:TYR:CZ	1:R:13:ILE:CD1	2.99	0.44
1:M:118:LEU:HD13	1:M:140:GLU:HB2	1.98	0.44
1:V:36:LEU:HD23	1:V:41:HIS:CG	2.53	0.43
1:H:36:LEU:O	1:H:39:GLY:N	2.51	0.43
1:M:152:GLU:OE1	1:M:195:VAL:HG23	2.19	0.43
1:D:118:LEU:CD1	1:D:140:GLU:HB2	2.49	0.43
1:F:81:ASN:OD1	1:F:81:ASN:N	2.49	0.43
1:J:124:PHE:CE1	1:L:128:TYR:CE1	3.07	0.43
1:X:81:ASN:OD1	1:X:81:ASN:N	2.50	0.43
1:C:108:ASP:CG	1:K:109:HIS:HE2	2.22	0.43
1:L:118:LEU:CD1	1:L:140:GLU:HB2	2.49	0.43
1:M:118:LEU:CD1	1:M:140:GLU:HB2	2.49	0.43
1:X:183:THR:O	1:X:186:LYS:HG2	2.18	0.43
1:B:152:GLU:OE1	1:B:195:VAL:HG23	2.19	0.43
1:K:36:LEU:HD13	1:M:127:ILE:HA	2.01	0.43
1:O:118:LEU:HD13	1:O:140:GLU:HB2	2.00	0.43
1:U:152:GLU:HG3	1:U:192:ARG:HB3	2.01	0.43
1:A:152:GLU:OE1	1:A:195:VAL:HG23	2.19	0.42
1:A:13:ILE:HD11	1:B:128:TYR:OH	2.18	0.42
1:B:95:SER:OG	1:J:63:LEU:HD22	2.19	0.42
1:I:152:GLU:OE1	1:I:195:VAL:HG23	2.19	0.42
1:J:152:GLU:OE1	1:J:195:VAL:HG23	2.19	0.42
1:C:67:GLU:HG2	1:K:105:GLN:CG	2.49	0.42
1:O:128:TYR:CG	1:V:120:PHE:CD1	3.06	0.42
1:A:118:LEU:HA	1:A:118:LEU:HD23	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:152:GLU:OE1	1:K:195:VAL:HG23	2.19	0.42
1:J:118:LEU:HD13	1:J:140:GLU:HB2	2.00	0.42
1:K:118:LEU:HD13	1:K:140:GLU:HB2	2.00	0.42
1:P:128:TYR:HB2	1:R:124:PHE:CD2	2.54	0.42
1:F:118:LEU:HD13	1:F:140:GLU:HB2	2.00	0.42
1:H:152:GLU:OE1	1:H:195:VAL:HG23	2.19	0.42
1:H:209:GLU:HA	1:H:212:GLN:HG2	2.00	0.42
1:Q:100:MET:HE1	1:Q:168:LEU:HG	2.01	0.42
1:I:128:TYR:OH	1:S:13:ILE:CD1	2.68	0.42
1:V:118:LEU:HD13	1:V:140:GLU:HB2	2.00	0.42
1:V:22:LEU:HD13	1:V:75:ILE:HD13	2.02	0.42
1:X:41:HIS:CD2	1:X:42:LYS:HG2	2.54	0.42
1:C:152:GLU:OE1	1:C:195:VAL:HG23	2.19	0.42
1:D:152:GLU:OE1	1:D:195:VAL:HG23	2.19	0.42
1:K:130:LEU:HD11	1:M:116:SER:HB3	2.02	0.42
1:R:111:PHE:CZ	1:R:177:ILE:HD13	2.54	0.42
1:I:120:PHE:CZ	1:S:125:LYS:HA	2.54	0.42
1:T:118:LEU:HD23	1:T:118:LEU:HA	1.89	0.42
1:I:120:PHE:HE1	1:S:120:PHE:CE2	2.37	0.42
1:S:36:LEU:HD23	1:S:41:HIS:CG	2.54	0.42
1:U:144:LEU:HD22	1:U:144:LEU:O	2.20	0.42
1:F:22:LEU:HD13	1:F:75:ILE:HD13	2.01	0.42
1:R:118:LEU:CD1	1:R:140:GLU:HB2	2.49	0.42
1:B:41:HIS:CD2	1:B:42:LYS:HG2	2.55	0.42
1:D:120:PHE:CD1	1:D:124:PHE:HD2	2.37	0.42
1:D:133:ASP:O	1:D:137:VAL:CG1	2.68	0.42
1:D:22:LEU:HD13	1:D:75:ILE:HD13	2.02	0.42
1:F:120:PHE:CD1	1:F:124:PHE:HD2	2.37	0.42
1:H:40:GLU:C	1:H:42:LYS:N	2.73	0.42
1:K:124:PHE:CE2	1:M:128:TYR:CB	3.03	0.42
1:L:152:GLU:OE1	1:L:195:VAL:HG23	2.20	0.42
1:O:118:LEU:CD1	1:O:140:GLU:HB2	2.50	0.42
1:E:118:LEU:HA	1:E:118:LEU:HD23	1.88	0.42
1:E:205:ARG:NH2	3:E:2019:HOH:O	2.52	0.42
1:F:152:GLU:OE1	1:F:195:VAL:HG23	2.20	0.42
1:G:118:LEU:CD1	1:G:140:GLU:HB2	2.50	0.42
1:H:40:GLU:O	1:H:42:LYS:N	2.53	0.42
1:S:152:GLU:OE1	1:S:195:VAL:HG23	2.20	0.42
1:D:73:GLN:HA	1:D:168:LEU:HD21	2.02	0.42
1:H:212:GLN:HE21	1:H:212:GLN:HB3	1.63	0.42
1:I:22:LEU:HD13	1:I:75:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:118:LEU:CD1	1:X:140:GLU:HB2	2.49	0.42
1:A:67:GLU:OE2	1:S:109:HIS:ND1	2.53	0.41
1:C:105:GLN:HG3	1:K:67:GLU:HG2	2.01	0.41
1:E:109:HIS:CD2	1:O:67:GLU:OE2	2.73	0.41
1:E:73:GLN:HA	1:E:168:LEU:HD21	2.02	0.41
1:H:22:LEU:HD13	1:H:75:ILE:HD13	2.02	0.41
1:Q:118:LEU:CD1	1:Q:140:GLU:HB2	2.50	0.41
1:U:13:ILE:HD12	1:X:128:TYR:OH	2.20	0.41
1:W:120:PHE:CD1	1:W:124:PHE:HD2	2.37	0.41
1:W:152:GLU:OE1	1:W:195:VAL:HG23	2.20	0.41
1:E:22:LEU:HD13	1:E:75:ILE:HD13	2.02	0.41
1:F:22:LEU:HD13	1:F:75:ILE:CD1	2.50	0.41
1:J:22:LEU:HD13	1:J:75:ILE:CD1	2.50	0.41
1:E:45:PRO:CA	1:K:190:THR:CG2	2.97	0.41
1:L:43:LYS:HD2	1:N:156:LYS:HE2	2.02	0.41
1:P:120:PHE:CD1	1:P:124:PHE:HD2	2.38	0.41
1:S:36:LEU:HD23	1:S:41:HIS:ND1	2.35	0.41
1:U:128:TYR:CE1	1:X:124:PHE:CE1	3.08	0.41
1:W:22:LEU:HD13	1:W:75:ILE:CD1	2.51	0.41
1:A:128:TYR:CD1	1:B:124:PHE:CZ	3.08	0.41
1:K:118:LEU:CD1	1:K:140:GLU:HB2	2.51	0.41
1:N:120:PHE:CD1	1:N:124:PHE:HD2	2.38	0.41
1:P:118:LEU:CD1	1:P:140:GLU:HB2	2.50	0.41
1:Q:22:LEU:HD13	1:Q:75:ILE:CD1	2.51	0.41
1:X:118:LEU:HD13	1:X:140:GLU:HB3	2.02	0.41
1:U:73:GLN:HA	1:U:168:LEU:HD21	2.03	0.41
1:A:22:LEU:HD13	1:A:75:ILE:CD1	2.51	0.41
1:A:22:LEU:HD13	1:A:75:ILE:HD13	2.02	0.41
1:J:118:LEU:CD1	1:J:140:GLU:HB2	2.51	0.41
1:V:22:LEU:HD13	1:V:75:ILE:CD1	2.51	0.41
1:E:22:LEU:HD13	1:E:75:ILE:CD1	2.51	0.41
1:I:118:LEU:CD1	1:I:140:GLU:HB2	2.51	0.41
1:K:212:GLN:NE2	3:K:2013:HOH:O	2.54	0.41
1:O:37:LYS:HA	1:V:126:SER:CB	2.51	0.41
1:V:118:LEU:CD1	1:V:140:GLU:HB2	2.51	0.41
1:J:22:LEU:HD13	1:J:75:ILE:HD13	2.02	0.41
1:N:181:LEU:HA	1:N:181:LEU:HD12	1.93	0.41
1:O:22:LEU:HD13	1:O:75:ILE:HD13	2.03	0.41
1:W:73:GLN:HA	1:W:168:LEU:HD21	2.03	0.41
1:L:22:LEU:HD13	1:L:75:ILE:HD13	2.03	0.41
1:L:73:GLN:HA	1:L:168:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:22:LEU:HD13	1:N:75:ILE:HD13	2.03	0.41
1:G:118:LEU:HD13	1:G:140:GLU:HB3	2.03	0.41
1:B:67:GLU:HG2	1:J:105:GLN:HB3	2.02	0.41
1:K:187:LYS:O	1:K:191:GLU:HG3	2.21	0.41
1:L:22:LEU:HD13	1:L:75:ILE:CD1	2.51	0.41
1:R:73:GLN:HA	1:R:168:LEU:HD21	2.03	0.41
1:C:22:LEU:HD13	1:C:75:ILE:HD13	2.03	0.41
1:D:22:LEU:HD13	1:D:75:ILE:CD1	2.51	0.41
1:L:36:LEU:HD23	1:L:41:HIS:ND1	2.36	0.41
1:M:22:LEU:HD13	1:M:75:ILE:HD13	2.03	0.41
1:P:22:LEU:HD13	1:P:75:ILE:HD13	2.03	0.41
1:F:118:LEU:CD1	1:F:140:GLU:HB2	2.51	0.41
1:G:105:GLN:HG2	1:H:67:GLU:HG2	2.02	0.41
1:W:22:LEU:HD13	1:W:75:ILE:HD13	2.02	0.41
1:D:120:PHE:CE2	1:F:120:PHE:CE2	3.09	0.40
1:M:22:LEU:HD13	1:M:75:ILE:CD1	2.52	0.40
1:S:22:LEU:HD13	1:S:75:ILE:CD1	2.51	0.40
1:X:22:LEU:HD13	1:X:75:ILE:CD1	2.51	0.40
1:G:22:LEU:HD13	1:G:75:ILE:HD13	2.02	0.40
1:M:187:LYS:O	1:M:191:GLU:HG3	2.21	0.40
1:P:73:GLN:HA	1:P:168:LEU:HD21	2.03	0.40
1:R:41:HIS:CD2	1:R:42:LYS:HG2	2.57	0.40
1:X:22:LEU:HD13	1:X:75:ILE:HD13	2.03	0.40
1:I:120:PHE:CE2	1:S:130:LEU:CD1	3.03	0.40
1:Q:22:LEU:HD13	1:Q:75:ILE:HD13	2.02	0.40
1:R:109:HIS:NE2	1:T:108:ASP:OD2	2.53	0.40
1:V:74:TYR:CZ	1:V:78:ARG:HD2	2.56	0.40
1:I:181:LEU:HD12	1:I:181:LEU:HA	1.92	0.40
1:L:36:LEU:HD23	1:L:41:HIS:CG	2.57	0.40
1:U:22:LEU:HD13	1:U:75:ILE:HD13	2.02	0.40
1:V:152:GLU:HG2	1:V:195:VAL:HG23	2.03	0.40
1:C:22:LEU:HD13	1:C:75:ILE:CD1	2.52	0.40
1:I:22:LEU:HD13	1:I:75:ILE:CD1	2.52	0.40
1:Q:118:LEU:HD13	1:Q:140:GLU:HB3	2.03	0.40
1:R:118:LEU:HD13	1:R:140:GLU:HB3	2.03	0.40
1:U:186:LYS:HE2	3:U:2016:HOH:O	2.21	0.40
1:V:152:GLU:HG3	1:V:192:ARG:HB3	2.04	0.40

All (1) 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:L:210:LYS:NZ	1:R:81:ASN:OD1[1_556]	1.99	0.21

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	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	B	209/212 (99%)	205 (98%)	4 (2%)	0	100	100
1	C	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	D	205/212 (97%)	201 (98%)	4 (2%)	0	100	100
1	E	208/212 (98%)	203 (98%)	5 (2%)	0	100	100
1	F	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	G	209/212 (99%)	204 (98%)	5 (2%)	0	100	100
1	H	208/212 (98%)	200 (96%)	7 (3%)	1 (0%)	29	58
1	I	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	J	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	K	208/212 (98%)	203 (98%)	5 (2%)	0	100	100
1	L	208/212 (98%)	203 (98%)	5 (2%)	0	100	100
1	M	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	N	200/212 (94%)	196 (98%)	4 (2%)	0	100	100
1	O	197/212 (93%)	193 (98%)	4 (2%)	0	100	100
1	P	208/212 (98%)	203 (98%)	5 (2%)	0	100	100
1	Q	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	R	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	S	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	T	198/212 (93%)	194 (98%)	4 (2%)	0	100	100
1	U	208/212 (98%)	204 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	W	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	X	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
All	All	4962/5088 (98%)	4857 (98%)	104 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	41	HIS

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	156/182 (86%)	145 (93%)	11 (7%)	14	36
1	B	169/182 (93%)	158 (94%)	11 (6%)	17	41
1	C	159/182 (87%)	152 (96%)	7 (4%)	28	58
1	D	154/182 (85%)	140 (91%)	14 (9%)	9	25
1	E	143/182 (79%)	132 (92%)	11 (8%)	13	32
1	F	160/182 (88%)	147 (92%)	13 (8%)	11	30
1	G	139/182 (76%)	129 (93%)	10 (7%)	14	36
1	H	136/182 (75%)	124 (91%)	12 (9%)	10	27
1	I	168/182 (92%)	152 (90%)	16 (10%)	8	23
1	J	168/182 (92%)	150 (89%)	18 (11%)	6	18
1	K	165/182 (91%)	149 (90%)	16 (10%)	8	22
1	L	169/182 (93%)	152 (90%)	17 (10%)	7	20
1	M	167/182 (92%)	153 (92%)	14 (8%)	11	29
1	N	138/182 (76%)	133 (96%)	5 (4%)	35	66
1	O	128/182 (70%)	120 (94%)	8 (6%)	18	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	162/182 (89%)	148 (91%)	14 (9%)	10	28
1	Q	162/182 (89%)	152 (94%)	10 (6%)	18	44
1	R	164/182 (90%)	152 (93%)	12 (7%)	14	35
1	S	171/182 (94%)	157 (92%)	14 (8%)	11	30
1	T	129/182 (71%)	120 (93%)	9 (7%)	15	37
1	U	168/182 (92%)	154 (92%)	14 (8%)	11	29
1	V	165/182 (91%)	149 (90%)	16 (10%)	8	22
1	W	168/182 (92%)	154 (92%)	14 (8%)	11	29
1	X	168/182 (92%)	152 (90%)	16 (10%)	8	23
All	All	3776/4368 (86%)	3474 (92%)	302 (8%)	12	31

All (302) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	19	LEU
1	A	22	LEU
1	A	25	LYS
1	A	65	LEU
1	A	105	GLN
1	A	107	GLU
1	A	121	GLU
1	A	131	THR
1	A	139	GLU
1	A	183	THR
1	B	19	LEU
1	B	22	LEU
1	B	44	GLU
1	B	65	LEU
1	B	75	ILE
1	B	105	GLN
1	B	107	GLU
1	B	121	GLU
1	B	131	THR
1	B	183	THR
1	B	209	GLU
1	C	22	LEU
1	C	35	GLU
1	C	65	LEU

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Mol	Chain	Res	Type
1	C	105	GLN
1	C	107	GLU
1	C	121	GLU
1	C	131	THR
1	D	19	LEU
1	D	22	LEU
1	D	25	LYS
1	D	44	GLU
1	D	47	LEU
1	D	65	LEU
1	D	105	GLN
1	D	107	GLU
1	D	117	LYS
1	D	118	LEU
1	D	132	THR
1	D	168	LEU
1	D	181	LEU
1	D	194	ARG
1	E	19	LEU
1	E	22	LEU
1	E	25	LYS
1	E	65	LEU
1	E	67	GLU
1	E	105	GLN
1	E	107	GLU
1	E	131	THR
1	E	137	VAL
1	E	168	LEU
1	E	181	LEU
1	F	19	LEU
1	F	22	LEU
1	F	25	LYS
1	F	43	LYS
1	F	65	LEU
1	F	105	GLN
1	F	107	GLU
1	F	118	LEU
1	F	131	THR
1	F	132	THR
1	F	168	LEU
1	F	183	THR
1	F	186	LYS

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Mol	Chain	Res	Type
1	G	5	LYS
1	G	22	LEU
1	G	25	LYS
1	G	44	GLU
1	G	65	LEU
1	G	105	GLN
1	G	107	GLU
1	G	118	LEU
1	G	132	THR
1	G	181	LEU
1	H	19	LEU
1	H	22	LEU
1	H	35	GLU
1	H	38	ASP
1	H	44	GLU
1	H	65	LEU
1	H	105	GLN
1	H	107	GLU
1	H	131	THR
1	H	168	LEU
1	H	181	LEU
1	H	183	THR
1	I	5	LYS
1	I	19	LEU
1	I	22	LEU
1	I	25	LYS
1	I	43	LYS
1	I	44	GLU
1	I	65	LEU
1	I	105	GLN
1	I	107	GLU
1	I	118	LEU
1	I	120	PHE
1	I	131	THR
1	I	137	VAL
1	I	168	LEU
1	I	181	LEU
1	I	212	GLN
1	J	5	LYS
1	J	19	LEU
1	J	22	LEU
1	J	25	LYS

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Mol	Chain	Res	Type
1	J	43	LYS
1	J	44	GLU
1	J	65	LEU
1	J	105	GLN
1	J	107	GLU
1	J	118	LEU
1	J	120	PHE
1	J	121	GLU
1	J	130	LEU
1	J	131	THR
1	J	137	VAL
1	J	168	LEU
1	J	181	LEU
1	J	183	THR
1	K	5	LYS
1	K	19	LEU
1	K	22	LEU
1	K	25	LYS
1	K	43	LYS
1	K	44	GLU
1	K	82	GLN
1	K	105	GLN
1	K	107	GLU
1	K	118	LEU
1	K	120	PHE
1	K	121	GLU
1	K	131	THR
1	K	137	VAL
1	K	168	LEU
1	K	181	LEU
1	L	5	LYS
1	L	19	LEU
1	L	22	LEU
1	L	25	LYS
1	L	43	LYS
1	L	44	GLU
1	L	65	LEU
1	L	82	GLN
1	L	105	GLN
1	L	107	GLU
1	L	118	LEU
1	L	121	GLU

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Mol	Chain	Res	Type
1	L	130	LEU
1	L	131	THR
1	L	168	LEU
1	L	181	LEU
1	L	183	THR
1	M	19	LEU
1	M	22	LEU
1	M	43	LYS
1	M	44	GLU
1	M	65	LEU
1	M	105	GLN
1	M	107	GLU
1	M	118	LEU
1	M	121	GLU
1	M	131	THR
1	M	137	VAL
1	M	168	LEU
1	M	181	LEU
1	M	183	THR
1	N	22	LEU
1	N	65	LEU
1	N	105	GLN
1	N	107	GLU
1	N	181	LEU
1	O	19	LEU
1	O	22	LEU
1	O	65	LEU
1	O	105	GLN
1	O	107	GLU
1	O	118	LEU
1	O	137	VAL
1	O	181	LEU
1	P	19	LEU
1	P	22	LEU
1	P	25	LYS
1	P	43	LYS
1	P	44	GLU
1	P	65	LEU
1	P	81	ASN
1	P	105	GLN
1	P	107	GLU
1	P	118	LEU

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Mol	Chain	Res	Type
1	P	131	THR
1	P	168	LEU
1	P	181	LEU
1	P	183	THR
1	Q	22	LEU
1	Q	25	LYS
1	Q	44	GLU
1	Q	65	LEU
1	Q	89	THR
1	Q	105	GLN
1	Q	107	GLU
1	Q	118	LEU
1	Q	120	PHE
1	Q	131	THR
1	R	5	LYS
1	R	19	LEU
1	R	25	LYS
1	R	43	LYS
1	R	44	GLU
1	R	105	GLN
1	R	107	GLU
1	R	118	LEU
1	R	120	PHE
1	R	130	LEU
1	R	131	THR
1	R	168	LEU
1	S	5	LYS
1	S	19	LEU
1	S	22	LEU
1	S	25	LYS
1	S	37	LYS
1	S	44	GLU
1	S	65	LEU
1	S	105	GLN
1	S	107	GLU
1	S	121	GLU
1	S	130	LEU
1	S	131	THR
1	S	137	VAL
1	S	168	LEU
1	T	19	LEU
1	T	65	LEU

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Mol	Chain	Res	Type
1	T	105	GLN
1	T	107	GLU
1	T	130	LEU
1	T	131	THR
1	T	168	LEU
1	T	181	LEU
1	T	183	THR
1	U	19	LEU
1	U	22	LEU
1	U	25	LYS
1	U	67	GLU
1	U	105	GLN
1	U	107	GLU
1	U	121	GLU
1	U	130	LEU
1	U	144	LEU
1	U	152	GLU
1	U	168	LEU
1	U	181	LEU
1	U	183	THR
1	U	212	GLN
1	V	19	LEU
1	V	22	LEU
1	V	25	LYS
1	V	44	GLU
1	V	65	LEU
1	V	78	ARG
1	V	105	GLN
1	V	107	GLU
1	V	118	LEU
1	V	130	LEU
1	V	131	THR
1	V	152	GLU
1	V	157	GLU
1	V	168	LEU
1	V	181	LEU
1	V	183	THR
1	W	19	LEU
1	W	22	LEU
1	W	25	LYS
1	W	44	GLU
1	W	65	LEU

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Mol	Chain	Res	Type
1	W	81	ASN
1	W	105	GLN
1	W	107	GLU
1	W	121	GLU
1	W	131	THR
1	W	132	THR
1	W	168	LEU
1	W	181	LEU
1	W	183	THR
1	X	22	LEU
1	X	25	LYS
1	X	43	LYS
1	X	44	GLU
1	X	65	LEU
1	X	67	GLU
1	X	105	GLN
1	X	107	GLU
1	X	118	LEU
1	X	120	PHE
1	X	122	GLN
1	X	131	THR
1	X	168	LEU
1	X	181	LEU
1	X	183	THR
1	X	186	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	B	105	GLN
1	C	122	GLN
1	D	105	GLN
1	E	109	HIS
1	F	122	GLN
1	G	26	ASN
1	H	212	GLN
1	J	122	GLN
1	K	82	GLN
1	K	196	ASN
1	K	212	GLN
1	M	212	GLN

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Mol	Chain	Res	Type
1	N	109	HIS
1	N	122	GLN
1	O	41	HIS
1	O	105	GLN
1	P	122	GLN
1	Q	105	GLN
1	Q	110	GLN
1	Q	122	GLN
1	S	122	GLN
1	S	212	GLN
1	T	105	GLN
1	U	122	GLN
1	V	122	GLN
1	W	81	ASN
1	X	26	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

24 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	7WB	A	1213	-	15,16,16	3.36	7 (46%)	14,22,22	2.58	5 (35%)
2	7WB	L	1213	-	15,16,16	3.55	8 (53%)	14,22,22	2.45	5 (35%)
2	7WB	I	1213	-	15,16,16	3.35	8 (53%)	14,22,22	2.74	5 (35%)
2	7WB	T	1212	-	15,16,16	2.76	7 (46%)	14,22,22	2.54	5 (35%)
2	7WB	R	1213	-	15,16,16	3.59	8 (53%)	14,22,22	2.27	5 (35%)
2	7WB	X	1213	-	15,16,16	3.16	8 (53%)	14,22,22	2.53	5 (35%)
2	7WB	U	1213	-	15,16,16	3.44	8 (53%)	14,22,22	2.44	5 (35%)
2	7WB	Q	1213	-	15,16,16	3.50	8 (53%)	14,22,22	2.19	5 (35%)
2	7WB	N	1213	-	15,16,16	3.05	8 (53%)	14,22,22	2.09	5 (35%)
2	7WB	J	1213	-	15,16,16	2.80	8 (53%)	14,22,22	2.49	5 (35%)
2	7WB	V	1213	-	15,16,16	2.82	7 (46%)	14,22,22	2.24	5 (35%)
2	7WB	G	1213	-	15,16,16	3.51	8 (53%)	14,22,22	2.22	5 (35%)
2	7WB	K	1213	-	15,16,16	3.37	8 (53%)	14,22,22	2.38	5 (35%)
2	7WB	F	1213	-	15,16,16	4.22	8 (53%)	14,22,22	2.38	5 (35%)
2	7WB	S	1213	-	15,16,16	3.74	7 (46%)	14,22,22	2.52	5 (35%)
2	7WB	D	1213	-	15,16,16	2.72	8 (53%)	14,22,22	2.67	5 (35%)
2	7WB	P	1213	-	15,16,16	3.55	8 (53%)	14,22,22	2.35	5 (35%)
2	7WB	C	1213	-	15,16,16	3.09	8 (53%)	14,22,22	2.37	5 (35%)
2	7WB	M	1213	-	15,16,16	3.09	8 (53%)	14,22,22	2.51	5 (35%)
2	7WB	O	1213	-	15,16,16	2.84	8 (53%)	14,22,22	2.39	5 (35%)
2	7WB	W	1213	-	15,16,16	3.85	8 (53%)	14,22,22	2.62	6 (42%)
2	7WB	B	1213	-	15,16,16	3.25	8 (53%)	14,22,22	2.60	5 (35%)
2	7WB	H	1213	-	15,16,16	2.91	7 (46%)	14,22,22	2.06	5 (35%)
2	7WB	E	1213	-	15,16,16	3.54	8 (53%)	14,22,22	2.20	5 (35%)

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	7WB	A	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	L	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	I	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	T	1212	-	-	0/0/13/13	0/3/3/3
2	7WB	R	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	X	1213	-	-	0/0/13/13	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	7WB	U	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	Q	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	N	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	J	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	V	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	G	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	K	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	F	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	S	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	D	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	P	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	C	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	M	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	O	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	W	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	B	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	H	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	E	1213	-	-	0/0/13/13	0/3/3/3

All (187) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1213	7WB	CAK-SAJ	-12.37	1.54	1.74
2	S	1213	7WB	CAK-SAJ	-10.06	1.57	1.74
2	E	1213	7WB	CAK-SAJ	-9.39	1.59	1.74
2	W	1213	7WB	CAK-SAJ	-8.73	1.60	1.74
2	A	1213	7WB	CAK-SAJ	-8.49	1.60	1.74
2	P	1213	7WB	CAK-SAJ	-8.29	1.60	1.74
2	G	1213	7WB	CAK-SAJ	-8.07	1.61	1.74
2	R	1213	7WB	CAK-SAJ	-8.01	1.61	1.74
2	Q	1213	7WB	CAK-SAJ	-7.80	1.61	1.74
2	U	1213	7WB	CAK-SAJ	-6.97	1.63	1.74
2	L	1213	7WB	CAK-SAJ	-6.50	1.63	1.74
2	C	1213	7WB	CAK-SAJ	-6.48	1.63	1.74
2	I	1213	7WB	CAK-SAJ	-6.35	1.64	1.74
2	K	1213	7WB	CAK-SAJ	-6.16	1.64	1.74
2	L	1213	7WB	CAE-CAL	-5.91	1.33	1.40
2	W	1213	7WB	CAE-CAL	-5.88	1.33	1.40
2	L	1213	7WB	CAN-CAL	-5.85	1.34	1.47
2	G	1213	7WB	CAN-CAL	-5.84	1.34	1.47
2	M	1213	7WB	CAN-CAL	-5.80	1.34	1.47
2	W	1213	7WB	CAN-CAL	-5.77	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1213	7WB	CAN-CAL	-5.77	1.34	1.47
2	I	1213	7WB	CAE-CAL	-5.75	1.33	1.40
2	F	1213	7WB	CAN-CAL	-5.74	1.34	1.47
2	I	1213	7WB	CAN-CAL	-5.71	1.34	1.47
2	R	1213	7WB	CAN-CAL	-5.70	1.34	1.47
2	N	1213	7WB	CAN-CAL	-5.70	1.34	1.47
2	P	1213	7WB	CAN-CAL	-5.69	1.34	1.47
2	X	1213	7WB	CAK-SAJ	-5.68	1.65	1.74
2	B	1213	7WB	CAE-CAL	-5.67	1.33	1.40
2	U	1213	7WB	CAN-CAL	-5.66	1.34	1.47
2	H	1213	7WB	CAE-CAL	-5.65	1.33	1.40
2	G	1213	7WB	CAE-CAL	-5.64	1.33	1.40
2	B	1213	7WB	CAN-CAL	-5.63	1.34	1.47
2	H	1213	7WB	CAN-CAL	-5.61	1.34	1.47
2	U	1213	7WB	CAE-CAL	-5.61	1.33	1.40
2	C	1213	7WB	CAN-CAL	-5.59	1.34	1.47
2	D	1213	7WB	CAE-CAL	-5.55	1.33	1.40
2	K	1213	7WB	CAE-CAL	-5.55	1.33	1.40
2	V	1213	7WB	CAE-CAL	-5.52	1.33	1.40
2	W	1213	7WB	CAN-CAM	-5.51	1.33	1.41
2	Q	1213	7WB	CAN-CAL	-5.51	1.34	1.47
2	T	1212	7WB	CAE-CAL	-5.48	1.33	1.40
2	L	1213	7WB	CAN-CAM	-5.47	1.33	1.41
2	E	1213	7WB	CAN-CAL	-5.45	1.35	1.47
2	B	1213	7WB	CAK-SAJ	-5.44	1.65	1.74
2	N	1213	7WB	CAK-SAJ	-5.38	1.65	1.74
2	T	1212	7WB	CAN-CAL	-5.37	1.35	1.47
2	P	1213	7WB	CAE-CAL	-5.34	1.33	1.40
2	O	1213	7WB	CAE-CAL	-5.34	1.33	1.40
2	V	1213	7WB	CAN-CAL	-5.32	1.35	1.47
2	M	1213	7WB	CAE-CAL	-5.31	1.33	1.40
2	S	1213	7WB	CAN-CAL	-5.30	1.35	1.47
2	X	1213	7WB	CAE-CAL	-5.30	1.34	1.40
2	R	1213	7WB	CAE-CAL	-5.27	1.34	1.40
2	U	1213	7WB	CAN-CAM	-5.26	1.34	1.41
2	O	1213	7WB	CAN-CAL	-5.19	1.35	1.47
2	S	1213	7WB	CAN-CAM	-5.18	1.34	1.41
2	J	1213	7WB	CAN-CAL	-5.18	1.35	1.47
2	Q	1213	7WB	CAE-CAL	-5.16	1.34	1.40
2	X	1213	7WB	CAN-CAL	-5.13	1.35	1.47
2	D	1213	7WB	CAN-CAL	-5.11	1.35	1.47
2	F	1213	7WB	CAE-CAL	-5.10	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1213	7WB	CAN-CAM	-5.09	1.34	1.41
2	M	1213	7WB	CAN-CAM	-5.09	1.34	1.41
2	K	1213	7WB	CAN-CAM	-5.05	1.34	1.41
2	A	1213	7WB	CAN-CAL	-5.04	1.35	1.47
2	V	1213	7WB	CAN-CAM	-5.04	1.34	1.41
2	R	1213	7WB	CAN-CAM	-5.02	1.34	1.41
2	N	1213	7WB	CAE-CAL	-4.97	1.34	1.40
2	I	1213	7WB	CAN-CAM	-4.91	1.34	1.41
2	H	1213	7WB	CAN-CAM	-4.89	1.34	1.41
2	T	1212	7WB	CAN-CAM	-4.82	1.34	1.41
2	F	1213	7WB	CAN-CAM	-4.82	1.34	1.41
2	S	1213	7WB	CAE-CAL	-4.79	1.34	1.40
2	J	1213	7WB	CAE-CAL	-4.78	1.34	1.40
2	Q	1213	7WB	CAN-CAM	-4.70	1.34	1.41
2	A	1213	7WB	CAN-CAM	-4.67	1.34	1.41
2	E	1213	7WB	CAE-CAL	-4.65	1.34	1.40
2	X	1213	7WB	CAN-CAM	-4.59	1.35	1.41
2	P	1213	7WB	CAN-CAM	-4.57	1.35	1.41
2	O	1213	7WB	CAN-CAM	-4.56	1.35	1.41
2	A	1213	7WB	CAE-CAL	-4.54	1.34	1.40
2	N	1213	7WB	CAN-CAM	-4.48	1.35	1.41
2	C	1213	7WB	CAE-CAL	-4.34	1.35	1.40
2	G	1213	7WB	CAN-CAM	-4.24	1.35	1.41
2	Q	1213	7WB	CAF-CAM	-4.24	1.33	1.39
2	J	1213	7WB	CAN-CAM	-4.17	1.35	1.41
2	D	1213	7WB	CAN-CAM	-4.11	1.35	1.41
2	W	1213	7WB	CAG-CAN	-4.07	1.33	1.39
2	C	1213	7WB	CAN-CAM	-4.03	1.35	1.41
2	E	1213	7WB	CAN-CAM	-4.00	1.35	1.41
2	J	1213	7WB	CAK-SAJ	-4.00	1.67	1.74
2	X	1213	7WB	CAF-CAM	-3.94	1.33	1.39
2	L	1213	7WB	CAF-CAM	-3.77	1.33	1.39
2	R	1213	7WB	CAF-CAM	-3.73	1.33	1.39
2	I	1213	7WB	CAK-CAL	-3.65	1.32	1.39
2	K	1213	7WB	CAF-CAM	-3.62	1.34	1.39
2	M	1213	7WB	CAG-CAN	-3.50	1.34	1.39
2	H	1213	7WB	CAF-CAM	-3.49	1.34	1.39
2	V	1213	7WB	CAF-CAM	-3.47	1.34	1.39
2	U	1213	7WB	CAF-CAM	-3.47	1.34	1.39
2	M	1213	7WB	CAK-SAJ	-3.46	1.68	1.74
2	O	1213	7WB	CAK-SAJ	-3.44	1.68	1.74
2	L	1213	7WB	CAG-CAN	-3.43	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	1213	7WB	CAG-CAN	-3.40	1.34	1.39
2	R	1213	7WB	CAG-CAN	-3.39	1.34	1.39
2	E	1213	7WB	CAF-CAM	-3.37	1.34	1.39
2	C	1213	7WB	CAG-CAN	-3.37	1.34	1.39
2	W	1213	7WB	CAF-CAM	-3.36	1.34	1.39
2	B	1213	7WB	CAG-CAN	-3.36	1.34	1.39
2	P	1213	7WB	CAF-CAM	-3.36	1.34	1.39
2	K	1213	7WB	CAG-CAN	-3.32	1.34	1.39
2	J	1213	7WB	CAG-CAN	-3.31	1.34	1.39
2	M	1213	7WB	CAF-CAM	-3.29	1.34	1.39
2	J	1213	7WB	CAF-CAM	-3.28	1.34	1.39
2	H	1213	7WB	CAM-NAI	-3.26	1.33	1.39
2	L	1213	7WB	CAK-CAL	-3.23	1.32	1.39
2	M	1213	7WB	CAK-CAL	-3.20	1.32	1.39
2	Q	1213	7WB	CAM-NAI	-3.18	1.34	1.39
2	L	1213	7WB	CAM-NAI	-3.17	1.34	1.39
2	R	1213	7WB	CAK-CAL	-3.17	1.33	1.39
2	N	1213	7WB	CAF-CAM	-3.16	1.34	1.39
2	F	1213	7WB	CAG-CAN	-3.16	1.34	1.39
2	O	1213	7WB	CAF-CAM	-3.15	1.34	1.39
2	S	1213	7WB	CAF-CAM	-3.14	1.34	1.39
2	G	1213	7WB	CAM-NAI	-3.14	1.34	1.39
2	C	1213	7WB	CAF-CAM	-3.11	1.34	1.39
2	K	1213	7WB	CAM-NAI	-3.09	1.34	1.39
2	G	1213	7WB	CAF-CAM	-3.07	1.35	1.39
2	U	1213	7WB	CAM-NAI	-3.06	1.34	1.39
2	W	1213	7WB	CAM-NAI	-3.06	1.34	1.39
2	U	1213	7WB	CAG-CAN	-3.05	1.35	1.39
2	B	1213	7WB	CAM-NAI	-3.04	1.34	1.39
2	B	1213	7WB	CAF-CAM	-3.01	1.35	1.39
2	O	1213	7WB	CAM-NAI	-3.01	1.34	1.39
2	Q	1213	7WB	CAG-CAN	-3.01	1.35	1.39
2	N	1213	7WB	CAM-NAI	-3.00	1.34	1.39
2	P	1213	7WB	CAK-CAL	-3.00	1.33	1.39
2	X	1213	7WB	CAG-CAN	-2.99	1.35	1.39
2	A	1213	7WB	CAF-CAM	-2.98	1.35	1.39
2	W	1213	7WB	CAK-CAL	-2.97	1.33	1.39
2	I	1213	7WB	CAG-CAN	-2.95	1.35	1.39
2	S	1213	7WB	CAG-CAN	-2.95	1.35	1.39
2	V	1213	7WB	CAM-NAI	-2.95	1.34	1.39
2	D	1213	7WB	CAM-NAI	-2.93	1.34	1.39
2	O	1213	7WB	CAG-CAN	-2.92	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1213	7WB	CAK-CAL	-2.90	1.33	1.39
2	M	1213	7WB	CAM-NAI	-2.89	1.34	1.39
2	G	1213	7WB	CAG-CAN	-2.87	1.35	1.39
2	R	1213	7WB	CAM-NAI	-2.86	1.34	1.39
2	E	1213	7WB	CAK-CAL	-2.85	1.33	1.39
2	X	1213	7WB	CAM-NAI	-2.85	1.34	1.39
2	I	1213	7WB	CAF-CAM	-2.80	1.35	1.39
2	H	1213	7WB	CAG-CAN	-2.79	1.35	1.39
2	T	1212	7WB	CAK-CAL	-2.78	1.33	1.39
2	D	1213	7WB	CAF-CAM	-2.74	1.35	1.39
2	C	1213	7WB	CAK-CAL	-2.71	1.33	1.39
2	V	1213	7WB	CAG-CAN	-2.71	1.35	1.39
2	S	1213	7WB	CAK-CAL	-2.68	1.34	1.39
2	X	1213	7WB	CAK-CAL	-2.67	1.34	1.39
2	T	1212	7WB	CAM-NAI	-2.64	1.34	1.39
2	F	1213	7WB	CAF-CAM	-2.63	1.35	1.39
2	B	1213	7WB	CAK-CAL	-2.61	1.34	1.39
2	K	1213	7WB	CAK-CAL	-2.60	1.34	1.39
2	G	1213	7WB	CAK-CAL	-2.53	1.34	1.39
2	F	1213	7WB	CAK-CAL	-2.52	1.34	1.39
2	D	1213	7WB	CAG-CAN	-2.51	1.35	1.39
2	I	1213	7WB	CAM-NAI	-2.51	1.35	1.39
2	E	1213	7WB	CAM-NAI	-2.51	1.35	1.39
2	F	1213	7WB	CAM-NAI	-2.48	1.35	1.39
2	A	1213	7WB	CAG-CAN	-2.48	1.35	1.39
2	H	1213	7WB	CAK-CAL	-2.47	1.34	1.39
2	N	1213	7WB	CAG-CAN	-2.44	1.36	1.39
2	E	1213	7WB	CAG-CAN	-2.43	1.36	1.39
2	D	1213	7WB	CAK-CAL	-2.40	1.34	1.39
2	Q	1213	7WB	CAK-CAL	-2.38	1.34	1.39
2	T	1212	7WB	CAF-CAM	-2.36	1.36	1.39
2	P	1213	7WB	CAM-NAI	-2.35	1.35	1.39
2	V	1213	7WB	CAK-CAL	-2.35	1.34	1.39
2	J	1213	7WB	CAM-NAI	-2.34	1.35	1.39
2	J	1213	7WB	CAK-CAL	-2.30	1.34	1.39
2	T	1212	7WB	CAG-CAN	-2.26	1.36	1.39
2	O	1213	7WB	CAK-CAL	-2.23	1.34	1.39
2	U	1213	7WB	CAK-CAL	-2.21	1.35	1.39
2	D	1213	7WB	CAK-SAJ	-2.11	1.71	1.74
2	C	1213	7WB	CAM-NAI	-2.08	1.35	1.39
2	N	1213	7WB	CAK-CAL	-2.03	1.35	1.39

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1213	7WB	CAM-NAI-CAE	6.25	110.45	106.16
2	B	1213	7WB	CAM-NAI-CAE	5.82	110.16	106.16
2	D	1213	7WB	CAN-CAM-NAI	-5.81	107.20	112.85
2	W	1213	7WB	CAN-CAM-NAI	-5.48	107.52	112.85
2	I	1213	7WB	CAN-CAM-NAI	-5.41	107.58	112.85
2	A	1213	7WB	CAM-NAI-CAE	5.40	109.87	106.16
2	I	1213	7WB	CAM-NAI-CAE	5.38	109.85	106.16
2	B	1213	7WB	CAN-CAM-NAI	-5.36	107.64	112.85
2	W	1213	7WB	CAM-NAI-CAE	5.36	109.84	106.16
2	X	1213	7WB	CAN-CAM-NAI	-5.34	107.66	112.85
2	X	1213	7WB	CAM-NAI-CAE	5.33	109.82	106.16
2	J	1213	7WB	CAN-CAM-NAI	-5.29	107.70	112.85
2	M	1213	7WB	CAN-CAM-NAI	-5.17	107.82	112.85
2	T	1212	7WB	CAM-NAI-CAE	5.09	109.66	106.16
2	M	1213	7WB	CAM-NAI-CAE	5.09	109.66	106.16
2	L	1213	7WB	CAN-CAM-NAI	-5.09	107.90	112.85
2	J	1213	7WB	CAM-NAI-CAE	5.08	109.65	106.16
2	K	1213	7WB	CAN-CAM-NAI	-5.00	107.98	112.85
2	O	1213	7WB	CAN-CAM-NAI	-5.00	107.99	112.85
2	T	1212	7WB	CAN-CAM-NAI	-5.00	107.99	112.85
2	U	1213	7WB	CAN-CAM-NAI	-4.97	108.01	112.85
2	S	1213	7WB	CAM-NAI-CAE	4.92	109.54	106.16
2	F	1213	7WB	CAN-CAM-NAI	-4.89	108.09	112.85
2	A	1213	7WB	CAN-CAM-NAI	-4.85	108.14	112.85
2	L	1213	7WB	CAM-NAI-CAE	4.83	109.48	106.16
2	U	1213	7WB	CAM-NAI-CAE	4.82	109.47	106.16
2	C	1213	7WB	CAN-CAM-NAI	-4.81	108.17	112.85
2	S	1213	7WB	CAN-CAM-NAI	-4.79	108.19	112.85
2	G	1213	7WB	CAN-CAM-NAI	-4.78	108.19	112.85
2	P	1213	7WB	CAN-CAM-NAI	-4.78	108.20	112.85
2	C	1213	7WB	CAM-NAI-CAE	4.73	109.41	106.16
2	K	1213	7WB	CAM-NAI-CAE	4.56	109.29	106.16
2	V	1213	7WB	CAN-CAM-NAI	-4.54	108.44	112.85
2	Q	1213	7WB	CAN-CAM-NAI	-4.44	108.53	112.85
2	V	1213	7WB	CAM-NAI-CAE	4.44	109.21	106.16
2	R	1213	7WB	CAN-CAM-NAI	-4.39	108.58	112.85
2	N	1213	7WB	CAN-CAM-NAI	-4.38	108.59	112.85
2	O	1213	7WB	CAM-NAI-CAE	4.32	109.13	106.16
2	H	1213	7WB	CAN-CAM-NAI	-4.23	108.73	112.85
2	E	1213	7WB	CAN-CAM-NAI	-4.23	108.73	112.85
2	F	1213	7WB	CAC-NAH-CAK	4.08	114.90	104.42
2	R	1213	7WB	CAC-NAH-CAK	4.07	114.87	104.42
2	P	1213	7WB	CAC-NAH-CAK	4.04	114.79	104.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1213	7WB	CAM-NAI-CAE	4.03	108.93	106.16
2	Q	1213	7WB	CAM-NAI-CAE	4.03	108.93	106.16
2	O	1213	7WB	CAC-NAH-CAK	4.02	114.75	104.42
2	P	1213	7WB	CAM-NAI-CAE	4.02	108.92	106.16
2	R	1213	7WB	CAM-NAI-CAE	3.99	108.90	106.16
2	E	1213	7WB	CAC-NAH-CAK	3.92	114.47	104.42
2	S	1213	7WB	CAC-NAH-CAK	3.91	114.47	104.42
2	E	1213	7WB	CAM-NAI-CAE	3.83	108.79	106.16
2	G	1213	7WB	CAM-NAI-CAE	3.79	108.76	106.16
2	Q	1213	7WB	CAC-NAH-CAK	3.77	114.09	104.42
2	G	1213	7WB	CAC-NAH-CAK	3.74	114.01	104.42
2	K	1213	7WB	CAC-NAH-CAK	3.72	113.97	104.42
2	N	1213	7WB	CAC-NAH-CAK	3.65	113.80	104.42
2	A	1213	7WB	CAC-NAH-CAK	3.63	113.75	104.42
2	J	1213	7WB	CAC-NAH-CAK	3.61	113.69	104.42
2	I	1213	7WB	CAC-NAH-CAK	3.61	113.69	104.42
2	W	1213	7WB	CAC-NAH-CAK	3.61	113.69	104.42
2	U	1213	7WB	CAC-NAH-CAK	3.59	113.64	104.42
2	H	1213	7WB	CAM-NAI-CAE	3.55	108.60	106.16
2	C	1213	7WB	CAC-NAH-CAK	3.47	113.32	104.42
2	A	1213	7WB	CAN-CAL-CAE	3.40	111.58	105.82
2	H	1213	7WB	CAC-NAH-CAK	3.38	113.08	104.42
2	N	1213	7WB	CAM-NAI-CAE	3.37	108.48	106.16
2	X	1213	7WB	CAC-NAH-CAK	3.36	113.04	104.42
2	A	1213	7WB	CAL-CAE-NAI	-3.31	105.11	111.79
2	L	1213	7WB	CAC-NAH-CAK	3.31	112.92	104.42
2	M	1213	7WB	CAC-NAH-CAK	3.31	112.91	104.42
2	V	1213	7WB	CAC-NAH-CAK	3.28	112.85	104.42
2	T	1212	7WB	CAC-NAH-CAK	3.24	112.72	104.42
2	B	1213	7WB	CAC-NAH-CAK	3.20	112.63	104.42
2	I	1213	7WB	CAN-CAL-CAE	3.17	111.19	105.82
2	C	1213	7WB	CAN-CAL-CAE	3.15	111.16	105.82
2	S	1213	7WB	CAN-CAL-CAE	3.13	111.12	105.82
2	S	1213	7WB	CAL-CAE-NAI	-3.12	105.49	111.79
2	I	1213	7WB	CAL-CAE-NAI	-3.07	105.60	111.79
2	B	1213	7WB	CAL-CAE-NAI	-3.06	105.63	111.79
2	P	1213	7WB	CAN-CAL-CAE	2.99	110.89	105.82
2	C	1213	7WB	CAL-CAE-NAI	-2.99	105.76	111.79
2	M	1213	7WB	CAL-CAE-NAI	-2.98	105.78	111.79
2	W	1213	7WB	CAL-CAE-NAI	-2.93	105.88	111.79
2	L	1213	7WB	CAL-CAE-NAI	-2.92	105.90	111.79
2	T	1212	7WB	CAN-CAL-CAE	2.91	110.75	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	1212	7WB	CAL-CAE-NAI	-2.90	105.95	111.79
2	B	1213	7WB	CAN-CAL-CAE	2.90	110.73	105.82
2	E	1213	7WB	CAN-CAL-CAE	2.89	110.71	105.82
2	D	1213	7WB	CAC-NAH-CAK	2.86	111.75	104.42
2	U	1213	7WB	CAL-CAE-NAI	-2.83	106.08	111.79
2	D	1213	7WB	CAL-CAE-NAI	-2.82	106.10	111.79
2	X	1213	7WB	CAL-CAE-NAI	-2.82	106.10	111.79
2	J	1213	7WB	CAL-CAE-NAI	-2.81	106.13	111.79
2	M	1213	7WB	CAN-CAL-CAE	2.80	110.56	105.82
2	P	1213	7WB	CAL-CAE-NAI	-2.79	106.16	111.79
2	R	1213	7WB	CAN-CAL-CAE	2.77	110.51	105.82
2	L	1213	7WB	CAN-CAL-CAE	2.74	110.47	105.82
2	R	1213	7WB	CAL-CAE-NAI	-2.74	106.27	111.79
2	K	1213	7WB	CAL-CAE-NAI	-2.72	106.30	111.79
2	E	1213	7WB	CAL-CAE-NAI	-2.70	106.34	111.79
2	V	1213	7WB	CAL-CAE-NAI	-2.69	106.36	111.79
2	W	1213	7WB	CAN-CAL-CAE	2.65	110.31	105.82
2	U	1213	7WB	CAN-CAL-CAE	2.65	110.31	105.82
2	J	1213	7WB	CAN-CAL-CAE	2.64	110.29	105.82
2	V	1213	7WB	CAN-CAL-CAE	2.63	110.28	105.82
2	D	1213	7WB	CAN-CAL-CAE	2.59	110.21	105.82
2	K	1213	7WB	CAN-CAL-CAE	2.54	110.13	105.82
2	F	1213	7WB	CAL-CAE-NAI	-2.54	106.67	111.79
2	F	1213	7WB	CAN-CAL-CAE	2.54	110.12	105.82
2	Q	1213	7WB	CAL-CAE-NAI	-2.50	106.75	111.79
2	X	1213	7WB	CAN-CAL-CAE	2.49	110.03	105.82
2	G	1213	7WB	CAN-CAL-CAE	2.45	109.97	105.82
2	G	1213	7WB	CAL-CAE-NAI	-2.36	107.03	111.79
2	H	1213	7WB	CAN-CAL-CAE	2.35	109.81	105.82
2	Q	1213	7WB	CAN-CAL-CAE	2.35	109.80	105.82
2	H	1213	7WB	CAL-CAE-NAI	-2.31	107.13	111.79
2	O	1213	7WB	CAL-CAE-NAI	-2.25	107.25	111.79
2	N	1213	7WB	CAL-CAE-NAI	-2.22	107.31	111.79
2	N	1213	7WB	CAN-CAL-CAE	2.17	109.50	105.82
2	O	1213	7WB	CAM-CAN-CAL	2.11	106.48	105.05
2	W	1213	7WB	CAM-CAN-CAL	2.01	106.41	105.05

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	210/212 (99%)	-0.11	0 100 100	26, 43, 58, 71	0
1	B	210/212 (99%)	-0.13	1 (0%) 91 90	25, 42, 61, 75	0
1	C	210/212 (99%)	-0.12	1 (0%) 91 90	30, 48, 68, 87	0
1	D	209/212 (98%)	0.12	4 (1%) 66 63	33, 49, 72, 102	0
1	E	210/212 (99%)	0.39	11 (5%) 27 22	42, 60, 76, 84	0
1	F	210/212 (99%)	-0.17	0 100 100	24, 43, 69, 84	0
1	G	210/212 (99%)	0.32	8 (3%) 40 35	37, 62, 84, 96	0
1	H	210/212 (99%)	0.59	20 (9%) 8 5	43, 67, 103, 141	0
1	I	210/212 (99%)	-0.17	0 100 100	20, 41, 59, 77	0
1	J	210/212 (99%)	-0.14	1 (0%) 91 90	23, 38, 51, 68	0
1	K	210/212 (99%)	-0.15	0 100 100	27, 41, 60, 71	0
1	L	210/212 (99%)	-0.19	0 100 100	21, 37, 55, 69	0
1	M	210/212 (99%)	-0.22	0 100 100	21, 36, 53, 68	0
1	N	204/212 (96%)	0.37	11 (5%) 25 20	39, 62, 83, 91	0
1	O	203/212 (95%)	0.48	13 (6%) 19 14	43, 68, 90, 110	0
1	P	210/212 (99%)	-0.01	0 100 100	27, 48, 71, 92	0
1	Q	210/212 (99%)	-0.02	0 100 100	26, 48, 68, 85	0
1	R	210/212 (99%)	-0.09	2 (0%) 82 80	27, 48, 70, 81	0
1	S	210/212 (99%)	-0.26	1 (0%) 91 90	20, 37, 53, 67	0
1	T	206/212 (97%)	0.42	13 (6%) 20 15	36, 70, 90, 103	0
1	U	210/212 (99%)	-0.09	2 (0%) 82 80	24, 42, 61, 71	0
1	V	210/212 (99%)	0.16	8 (3%) 40 35	26, 49, 74, 87	0
1	W	210/212 (99%)	-0.14	0 100 100	23, 39, 61, 85	0
1	X	210/212 (99%)	-0.19	1 (0%) 91 90	21, 38, 55, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	5022/5088 (98%)	0.03	97 (1%) 66 63	20, 47, 77, 141	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	57	ALA	5.1
1	O	41	HIS	4.5
1	G	19	LEU	4.3
1	R	189	PHE	4.3
1	H	48	SER	4.0
1	H	3	GLY	3.9
1	E	3	GLY	3.9
1	V	39	GLY	3.9
1	N	189	PHE	3.8
1	H	39	GLY	3.7
1	H	115	ALA	3.7
1	O	128	TYR	3.7
1	H	202	ILE	3.6
1	H	189	PHE	3.5
1	E	189	PHE	3.5
1	H	6	VAL	3.3
1	T	18	VAL	3.3
1	N	119	ALA	3.3
1	E	166	PHE	3.2
1	T	11	ALA	3.2
1	T	19	LEU	3.2
1	D	45	PRO	3.1
1	H	45	PRO	3.1
1	N	118	LEU	3.0
1	E	198	TRP	3.0
1	H	8	GLY	3.0
1	H	178	GLN	2.9
1	O	118	LEU	2.9
1	H	41	HIS	2.9
1	O	127	ILE	2.9
1	V	179	TYR	2.9
1	G	31	LEU	2.8
1	O	3	GLY	2.8
1	G	23	HIS	2.8
1	H	36	LEU	2.8
1	T	8	GLY	2.8
1	R	212	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	N	120	PHE	2.7
1	T	207	ALA	2.7
1	T	33	HIS	2.6
1	O	181	LEU	2.6
1	O	120	PHE	2.6
1	E	208	SER	2.6
1	V	130	LEU	2.6
1	V	35	GLU	2.6
1	E	100	MET	2.6
1	H	31	LEU	2.5
1	N	181	LEU	2.5
1	G	167	THR	2.5
1	C	128	TYR	2.5
1	O	84	THR	2.5
1	E	75	ILE	2.5
1	N	82	GLN	2.4
1	U	120	PHE	2.4
1	G	166	PHE	2.3
1	T	193	PRO	2.3
1	T	180	LEU	2.3
1	N	18	VAL	2.3
1	H	181	LEU	2.3
1	H	58	PHE	2.3
1	V	40	GLU	2.2
1	G	131	THR	2.2
1	B	128	TYR	2.2
1	N	188	LEU	2.2
1	V	41	HIS	2.2
1	E	128	TYR	2.2
1	O	29	PHE	2.2
1	G	189	PHE	2.2
1	T	23	HIS	2.2
1	O	75	ILE	2.2
1	H	35	GLU	2.2
1	J	95	SER	2.2
1	S	81	ASN	2.2
1	E	148	LEU	2.2
1	V	115	ALA	2.2
1	O	63	LEU	2.1
1	O	39	GLY	2.1
1	T	198	TRP	2.1
1	H	179	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	64	LYS	2.1
1	T	82	GLN	2.1
1	D	128	TYR	2.1
1	H	126	SER	2.1
1	H	102	ILE	2.1
1	D	10	PRO	2.1
1	H	44	GLU	2.1
1	V	6	VAL	2.1
1	N	137	VAL	2.0
1	N	171	LEU	2.0
1	G	75	ILE	2.0
1	X	128	TYR	2.0
1	T	9	HIS	2.0
1	N	206	PRO	2.0
1	D	95	SER	2.0
1	U	124	PHE	2.0
1	O	40	GLU	2.0
1	E	206	PRO	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. 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(\AA^2)	Q<0.9
2	7WB	N	1213	14/14	0.83	0.28	80,87,93,94	0
2	7WB	O	1213	14/14	0.86	0.30	62,71,88,94	0
2	7WB	E	1213	14/14	0.87	0.20	50,59,68,72	0
2	7WB	T	1212	14/14	0.90	0.29	49,54,71,71	0
2	7WB	C	1213	14/14	0.91	0.17	38,46,57,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	7WB	R	1213	14/14	0.91	0.26	62,72,84,85	0
2	7WB	G	1213	14/14	0.91	0.21	54,57,64,69	0
2	7WB	I	1213	14/14	0.92	0.19	35,41,60,62	0
2	7WB	S	1213	14/14	0.92	0.18	42,48,58,69	0
2	7WB	D	1213	14/14	0.92	0.24	46,50,51,57	0
2	7WB	K	1213	14/14	0.93	0.21	48,55,61,66	0
2	7WB	H	1213	14/14	0.93	0.22	63,67,74,78	0
2	7WB	Q	1213	14/14	0.93	0.19	49,54,58,61	0
2	7WB	P	1213	14/14	0.94	0.19	35,42,56,61	0
2	7WB	X	1213	14/14	0.94	0.18	39,44,51,56	0
2	7WB	L	1213	14/14	0.94	0.18	38,40,43,46	0
2	7WB	B	1213	14/14	0.94	0.18	38,42,49,58	0
2	7WB	A	1213	14/14	0.94	0.18	34,37,45,48	0
2	7WB	V	1213	14/14	0.94	0.16	46,48,61,66	0
2	7WB	M	1213	14/14	0.95	0.17	35,38,41,42	0
2	7WB	J	1213	14/14	0.95	0.14	33,40,46,50	0
2	7WB	W	1213	14/14	0.95	0.17	31,35,43,52	0
2	7WB	U	1213	14/14	0.96	0.14	33,37,52,60	0
2	7WB	F	1213	14/14	0.96	0.18	38,42,50,55	0

6.5 Other polymers

There are no such residues in this entry.