



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:48 AM UTC

PDB ID : 2VPZ / pdb_00002vpz
Title : Polysulfide reductase native structure
Authors : Jormakka, M.; Yokoyama, K.; Yano, T.; Tamakoshi, M.; Akimoto, S.; Shimamura, T.; Curmi, P.; Iwata, S.
Deposited on : 2008-03-09
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

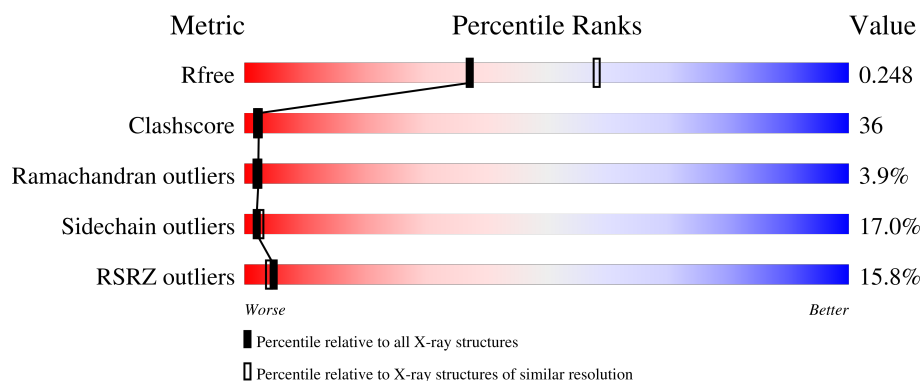
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



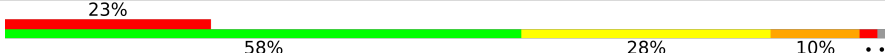
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	765	18% 41% 34% 16% 6% .
1	E	765	15% 41% 35% 14% 6% .
2	B	195	8% 51% 34% 12% ..
2	F	195	6% 52% 34% 11% ..
3	C	253	14% 63% 24% 9% ..

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Mol	Chain	Length	Quality of chain
3	G	253	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	F	1194	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20193 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 THIOSULFATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	0	1
			5896	3802	1032	1043	19			
1	E	735	Total	C	N	O	S	0	0	1
			5896	3802	1032	1043	19			

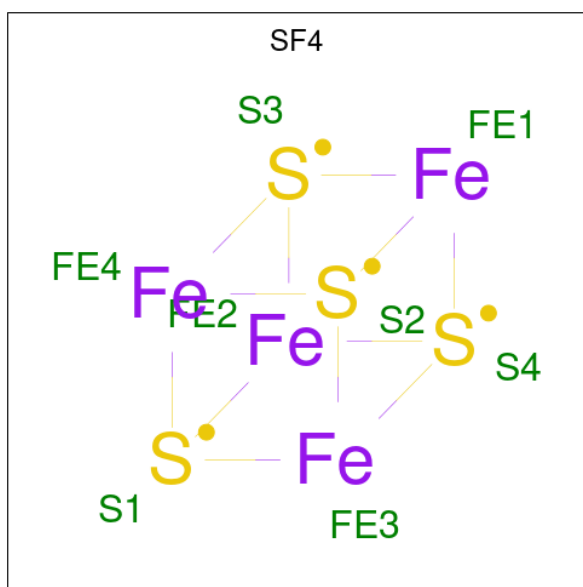
- Molecule 2 is a protein called NRFC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	194	Total	C	N	O	S	0	0	1
			1475	930	256	269	20			
2	F	194	Total	C	N	O	S	0	0	1
			1475	930	256	269	20			

- Molecule 3 is a protein called HYPOTHETICAL MEMBRANE SPANNING PROTEIN.

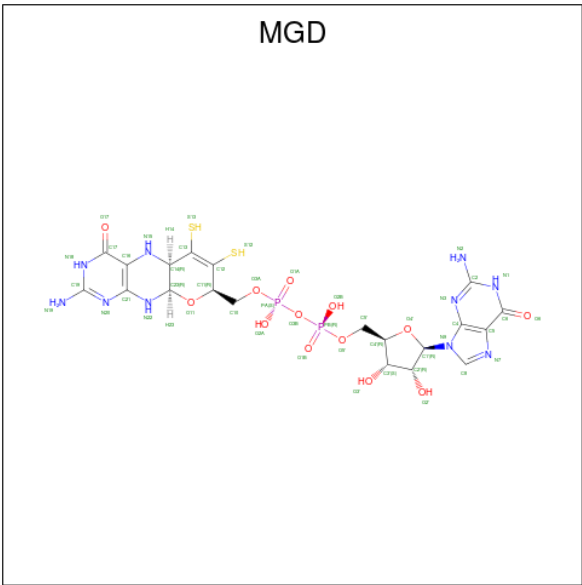
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	251	Total	C	N	O	S	0	0	1
			1948	1323	320	303	2			
3	G	251	Total	C	N	O	S	0	0	1
			1948	1323	320	303	2			

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 6 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mo	0	0
			1	1		
6	E	1	Total	Mo	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	386	Total	O	0	0
			386	386		
7	B	150	Total	O	0	0
			150	150		
7	C	88	Total	O	0	0
			88	88		

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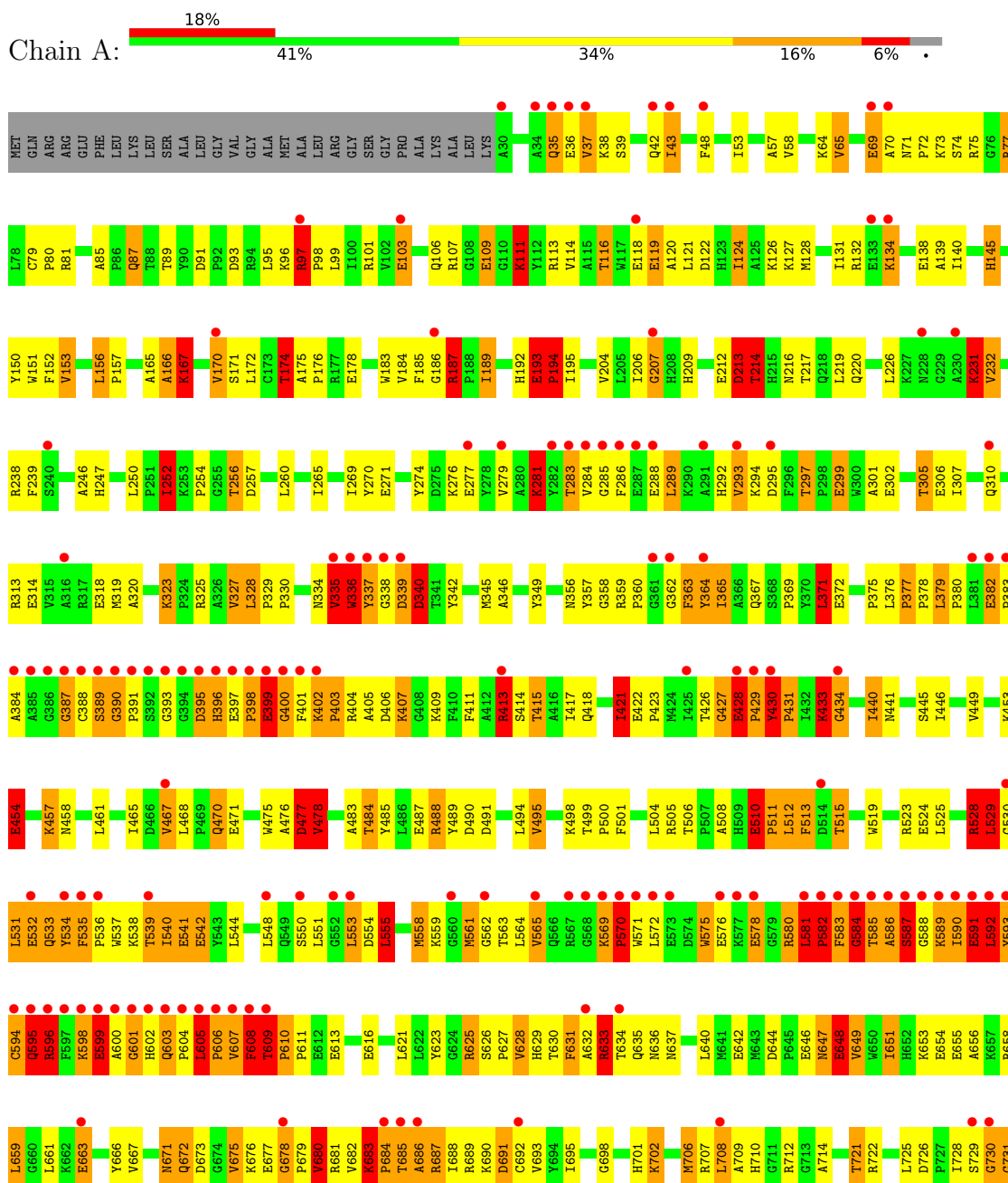
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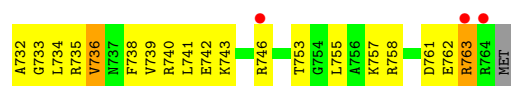
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	452	Total 452	O 452	0	0
7	F	130	Total 130	O 130	0	0
7	G	79	Total 79	O 79	0	0

3 Residue-property plots

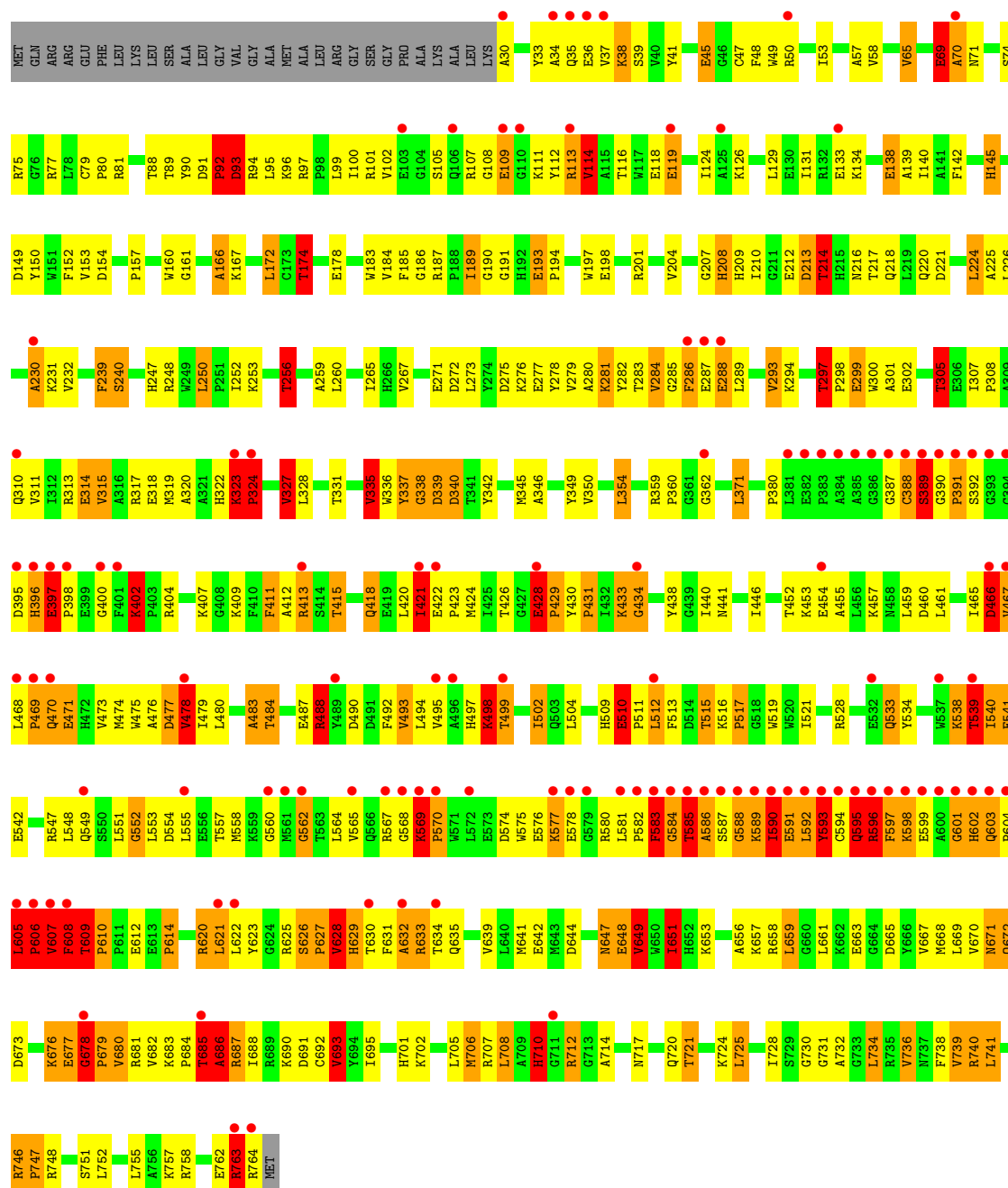
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: THIOSULFATE REDUCTASE



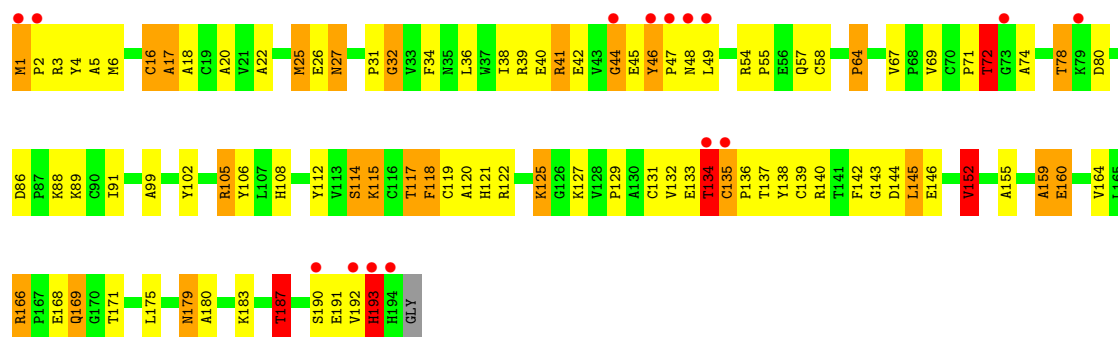


• Molecule 1: THIOSULFATE REDUCTASE

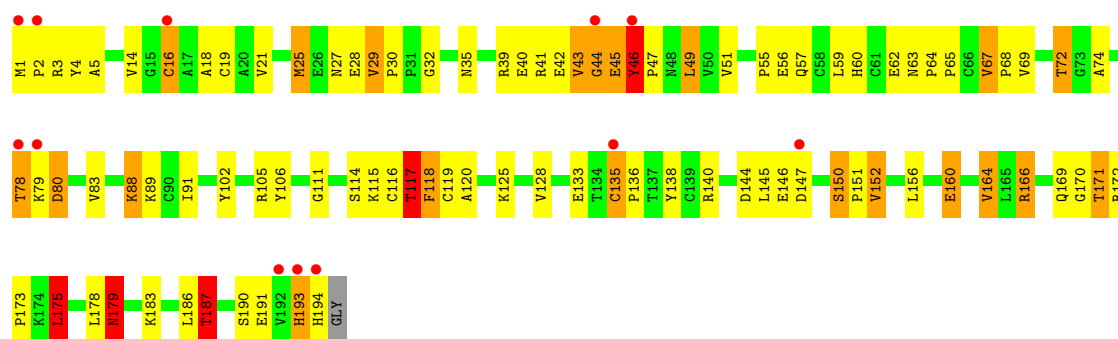


• Molecule 2: NRFC PROTEIN

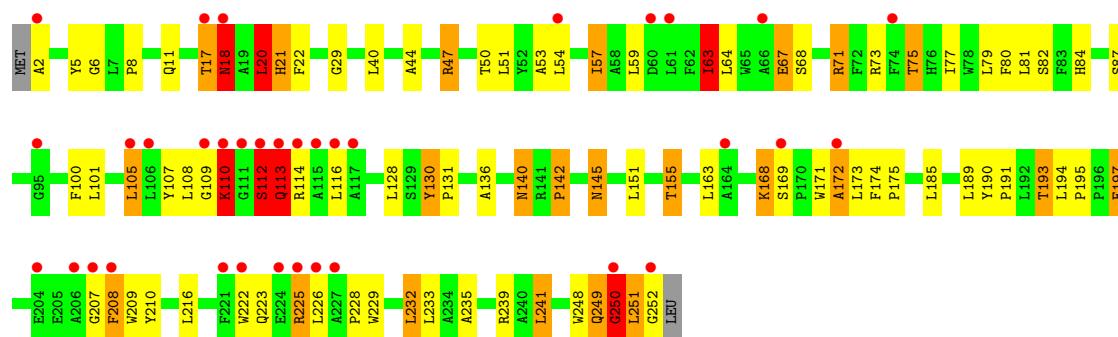




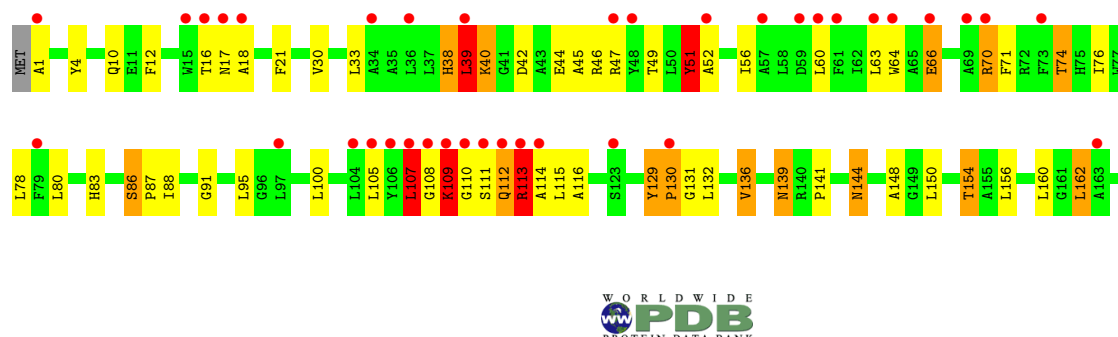
• Molecule 2: NRFC PROTEIN

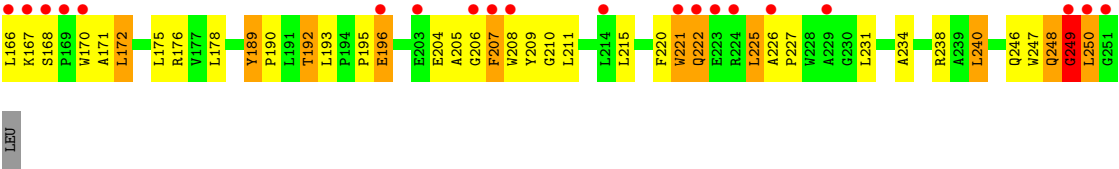


• Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN



• Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.41Å 166.26Å 246.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 2.40 29.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.2 (29.83-2.40) 93.2 (29.83-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.24Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.253 0.241 , 0.248	Depositor DCC
R_{free} test set	4206 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 69.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20193	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MGD, SF4, MO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.40	54/6079 (0.9%)	1.65	149/8267 (1.8%)
1	E	1.52	69/6079 (1.1%)	1.83	200/8267 (2.4%)
2	B	1.25	10/1512 (0.7%)	1.69	33/2058 (1.6%)
2	F	1.27	10/1512 (0.7%)	1.79	41/2058 (2.0%)
3	C	1.35	11/2016 (0.5%)	1.40	26/2764 (0.9%)
3	G	1.18	6/2016 (0.3%)	1.56	31/2764 (1.1%)
All	All	1.39	160/19214 (0.8%)	1.69	480/26178 (1.8%)

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	E	0	3

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	324	PRO	N-CD	17.31	1.72	1.47
1	E	592	LEU	CG-CD1	17.10	2.08	1.52
1	E	323	LYS	C-O	16.69	1.45	1.24
1	E	324	PRO	CA-C	14.88	1.73	1.52
3	C	114	ARG	NE-CZ	14.58	1.49	1.33
1	E	387	GLY	C-N	12.98	1.51	1.33
1	E	240	SER	CA-CB	-12.19	1.35	1.53
3	C	195	PRO	CA-C	11.64	1.58	1.51
1	E	583	PHE	CA-C	10.82	1.67	1.52
1	E	685	THR	CA-C	10.80	1.67	1.52
1	E	324	PRO	N-CA	10.62	1.60	1.47
1	A	581	LEU	CA-C	10.51	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	594	CYS	C-O	-9.67	1.12	1.24
1	E	478	VAL	CA-CB	9.48	1.67	1.54
1	E	586	ALA	CA-C	9.27	1.61	1.53
1	E	114	VAL	CA-CB	9.17	1.64	1.54
1	E	446	ILE	CA-CB	9.12	1.61	1.54
1	E	593	TYR	CA-C	-8.89	1.40	1.52
1	E	594	CYS	CA-C	8.87	1.64	1.52
1	E	231	LYS	CA-CB	-8.82	1.40	1.53
1	E	323	LYS	CA-C	8.82	1.64	1.52
2	F	135	CYS	CB-SG	8.78	2.10	1.81
1	E	324	PRO	CG-CD	8.71	1.80	1.50
1	A	364	TYR	C-O	-8.57	1.13	1.24
1	A	365	ILE	CA-CB	8.49	1.66	1.54
1	E	387	GLY	C-O	-8.43	1.12	1.23
3	G	109	LYS	C-N	8.40	1.45	1.33
1	A	648	GLU	CA-C	8.39	1.62	1.52
1	A	401	PHE	N-CA	8.34	1.56	1.46
1	E	585	THR	CA-C	8.27	1.63	1.52
1	E	230	ALA	C-O	-8.18	1.13	1.23
1	E	388	CYS	CA-CB	-8.13	1.39	1.53
3	C	63	ILE	CA-CB	8.05	1.63	1.54
2	F	91	ILE	CA-CB	8.01	1.65	1.54
3	C	114	ARG	CZ-NH1	7.90	1.43	1.32
1	A	534	TYR	CA-C	7.81	1.62	1.52
1	A	583	PHE	C-O	7.80	1.33	1.24
1	E	421	ILE	CA-CB	-7.78	1.44	1.54
1	E	493	VAL	CA-CB	7.51	1.63	1.54
2	B	67	VAL	CA-CB	7.37	1.63	1.54
1	A	97	ARG	NE-CZ	7.29	1.41	1.33
1	E	594	CYS	N-CA	-7.26	1.37	1.46
2	F	51	VAL	CA-CB	7.22	1.63	1.54
1	A	649	VAL	CA-CB	7.19	1.62	1.54
1	E	595	GLN	CA-CB	-7.04	1.40	1.53
1	A	446	ILE	CA-CB	7.03	1.59	1.54
1	A	402	LYS	CA-C	7.02	1.61	1.52
3	G	112	GLN	CA-C	6.83	1.61	1.52
1	A	583	PHE	N-CA	6.83	1.54	1.46
1	E	585	THR	CA-CB	6.83	1.65	1.53
1	E	586	ALA	CA-CB	-6.78	1.45	1.53
1	E	315	VAL	CA-CB	6.75	1.62	1.54
1	E	35	GLN	CA-C	6.71	1.61	1.52
1	E	131	ILE	CA-CB	6.68	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	67	VAL	CA-C	6.64	1.59	1.52
1	A	377	PRO	CA-C	6.64	1.56	1.52
1	A	582	PRO	CA-C	6.63	1.61	1.52
1	A	581	LEU	N-CA	6.62	1.51	1.45
1	E	210	ILE	CA-CB	6.57	1.61	1.54
2	B	135	CYS	CB-SG	6.55	2.02	1.81
1	A	529	LEU	CA-C	6.50	1.61	1.52
1	A	206	ILE	CA-CB	6.49	1.61	1.53
2	F	152	VAL	CA-CB	6.48	1.61	1.54
1	E	608	PHE	CA-C	6.47	1.61	1.52
1	E	763	ARG	C-N	-6.46	1.24	1.33
1	A	440	ILE	CA-CB	6.42	1.63	1.54
1	A	648	GLU	CB-CG	6.37	1.71	1.52
1	A	337	TYR	CA-C	6.32	1.60	1.52
1	E	388	CYS	CA-C	-6.31	1.44	1.52
2	F	128	VAL	CA-CB	6.31	1.62	1.54
1	E	124	ILE	CA-CB	6.30	1.61	1.54
1	A	97	ARG	C-N	6.30	1.41	1.33
1	A	528	ARG	CA-C	6.28	1.61	1.52
1	A	565	VAL	CA-CB	6.26	1.61	1.54
1	E	331	THR	CA-CB	6.26	1.62	1.53
3	C	110	LYS	CA-C	6.25	1.60	1.52
1	A	265	ILE	CA-CB	6.20	1.61	1.54
3	C	114	ARG	CD-NE	6.18	1.54	1.46
1	E	685	THR	CA-CB	6.18	1.64	1.53
1	E	323	LYS	N-CA	6.17	1.54	1.46
1	E	323	LYS	C-N	6.17	1.48	1.33
1	E	686	ALA	N-CA	5.97	1.53	1.46
1	A	269	ILE	CA-CB	5.95	1.62	1.54
1	A	529	LEU	N-CA	5.95	1.53	1.46
1	E	421	ILE	CA-C	5.95	1.60	1.52
2	F	16	CYS	CB-SG	5.94	2.00	1.81
1	E	595	GLN	CA-C	5.91	1.60	1.52
1	E	594	CYS	C-N	-5.91	1.25	1.33
1	A	608	PHE	CA-C	5.89	1.60	1.52
1	A	601	GLY	CA-C	-5.87	1.43	1.51
1	E	686	ALA	CA-C	5.84	1.60	1.52
3	C	251	LEU	C-N	-5.83	1.25	1.33
1	A	131	ILE	CA-CB	5.80	1.62	1.54
1	A	728	ILE	CA-CB	5.80	1.61	1.55
2	B	91	ILE	CA-CB	5.79	1.62	1.54
1	E	33	TYR	CA-C	5.78	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	112	SER	CA-C	5.78	1.60	1.52
1	E	565	VAL	CA-CB	5.77	1.60	1.54
1	E	350	VAL	CA-CB	5.77	1.61	1.54
1	E	389	SER	CA-C	5.75	1.60	1.52
1	E	648	GLU	CA-C	5.75	1.59	1.52
1	E	583	PHE	CA-CB	-5.75	1.43	1.53
1	A	252	ILE	CA-CB	5.72	1.60	1.54
1	A	430	TYR	CA-C	5.70	1.60	1.52
1	E	140	ILE	CA-CB	5.70	1.61	1.54
1	E	388	CYS	N-CA	-5.68	1.38	1.46
1	A	675	VAL	CA-CB	5.66	1.60	1.54
3	C	18	ASN	CG-OD1	5.64	1.34	1.23
1	E	240	SER	CA-C	5.64	1.61	1.53
1	A	363	PHE	CA-C	5.62	1.59	1.53
3	G	250	LEU	C-N	-5.59	1.25	1.33
1	E	93	ASP	CA-C	5.58	1.60	1.52
1	A	335	VAL	CA-CB	5.57	1.61	1.54
2	B	132	VAL	CA-CB	5.56	1.61	1.54
1	E	214	THR	CA-CB	5.56	1.60	1.53
1	A	114	VAL	CA-CB	5.53	1.59	1.54
1	A	399	GLU	CD-OE2	-5.51	1.14	1.25
1	E	397	GLU	CA-C	5.50	1.59	1.52
2	B	160	GLU	CA-C	5.49	1.60	1.52
2	F	193	HIS	C-N	-5.47	1.25	1.33
2	B	187	THR	CA-C	5.47	1.59	1.52
1	A	417	ILE	CA-CB	5.41	1.61	1.54
1	E	629	HIS	CA-C	5.41	1.59	1.52
2	F	151	PRO	CA-C	5.39	1.60	1.52
1	A	232	VAL	CA-CB	5.39	1.60	1.54
1	A	124	ILE	CA-CB	5.39	1.60	1.54
1	E	584	GLY	CA-C	5.39	1.57	1.52
1	A	609	THR	CA-CB	5.37	1.61	1.53
2	F	21	VAL	CA-CB	5.36	1.61	1.54
2	F	67	VAL	CA-CB	5.35	1.61	1.54
1	A	584	GLY	CA-C	5.35	1.59	1.51
2	B	38	ILE	CA-CB	5.33	1.61	1.54
1	E	539	THR	CA-C	5.33	1.59	1.52
1	A	396	HIS	CA-C	5.32	1.59	1.52
1	A	592	LEU	CA-C	5.32	1.59	1.52
1	A	590	ILE	CA-CB	5.31	1.60	1.54
1	A	37	VAL	CA-CB	5.28	1.63	1.54
1	E	688	ILE	CA-CB	5.28	1.62	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	PHE	CA-C	5.28	1.59	1.52
1	E	517	PRO	CA-C	5.28	1.58	1.52
1	E	521	ILE	CA-CB	5.26	1.61	1.54
1	A	365	ILE	N-CA	5.25	1.52	1.46
1	A	396	HIS	CA-CB	5.25	1.62	1.53
1	A	495	VAL	CA-CB	5.25	1.60	1.54
1	A	763	ARG	C-N	-5.24	1.26	1.33
1	E	324	PRO	CB-CG	-5.24	1.23	1.49
2	B	16	CYS	CB-SG	5.23	1.98	1.81
1	A	401	PHE	CA-CB	-5.21	1.46	1.53
1	E	420	LEU	C-O	-5.21	1.16	1.24
1	E	502	ILE	CA-CB	5.20	1.62	1.54
3	C	113	GLN	N-CA	5.20	1.52	1.46
3	C	63	ILE	CA-C	5.18	1.58	1.52
3	G	189	TYR	CA-C	5.12	1.59	1.52
1	E	628	VAL	CA-CB	5.09	1.61	1.54
2	B	193	HIS	C-N	-5.06	1.26	1.33
3	G	110	GLY	N-CA	5.05	1.52	1.45
1	E	728	ILE	CA-CB	5.04	1.61	1.54
1	A	91	ASP	CA-C	5.03	1.58	1.52
3	G	221	TRP	CA-C	5.03	1.58	1.52
1	A	140	ILE	CA-CB	5.02	1.60	1.54

All (480) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	171	THR	N-CA-C	23.93	139.58	111.82
1	E	324	PRO	CA-N-CD	-23.05	79.73	112.00
1	E	467	VAL	N-CA-C	18.56	129.85	110.36
2	F	44	GLY	N-CA-C	18.38	138.18	112.81
1	E	323	LYS	O-C-N	-18.18	100.42	121.32
3	G	114	ALA	N-CA-C	-17.25	92.65	114.56
1	A	401	PHE	N-CA-C	16.16	133.76	113.88
1	E	594	CYS	N-CA-C	16.16	128.60	111.14
1	E	323	LYS	C-N-CD	-15.86	59.98	125.00
1	A	189	ILE	N-CA-C	-15.59	98.40	111.81
2	B	169	GLN	N-CA-C	-15.16	89.43	110.35
1	E	583	PHE	CA-C-N	14.73	132.34	122.18
1	E	583	PHE	C-N-CA	14.73	132.34	122.18
1	E	324	PRO	N-CA-CB	14.36	118.33	103.25
1	E	189	ILE	N-CA-C	-13.95	98.47	111.45
1	E	659	LEU	N-CA-C	-13.83	91.27	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	225	LEU	N-CA-C	-13.73	93.73	112.12
1	E	582	PRO	N-CA-C	13.71	131.77	113.40
1	A	364	TYR	N-CA-C	13.63	127.63	111.82
1	E	324	PRO	N-CA-C	-13.62	84.41	112.47
1	E	323	LYS	CA-C-N	13.40	136.59	119.84
1	E	323	LYS	C-N-CA	13.40	136.59	119.84
1	E	185	PHE	N-CA-C	-12.70	89.83	109.65
3	G	249	GLY	N-CA-C	12.64	143.14	113.18
3	C	114	ARG	N-CA-C	-12.58	96.45	113.18
1	A	583	PHE	CA-C-N	12.44	145.79	121.41
1	A	583	PHE	C-N-CA	12.44	145.79	121.41
2	B	46	TYR	N-CA-C	12.26	136.91	109.81
1	A	659	LEU	N-CA-C	-12.08	95.21	110.19
1	E	387	GLY	CA-C-O	11.92	141.30	120.57
1	A	608	PHE	N-CA-C	-11.84	98.09	112.54
1	A	109	GLU	N-CA-C	-11.31	95.54	110.24
2	F	16	CYS	N-CA-C	-11.22	94.68	110.50
3	G	171	ALA	N-CA-C	11.19	124.57	111.71
2	B	44	GLY	N-CA-C	11.06	124.68	112.29
1	A	592	LEU	N-CA-C	11.05	134.34	110.80
2	F	64	PRO	N-CA-C	11.00	124.11	110.70
1	E	665	ASP	N-CA-C	10.98	125.28	110.35
2	B	72	THR	N-CA-C	-10.71	93.26	109.86
1	E	585	THR	CB-CA-C	10.63	131.58	110.42
1	E	387	GLY	CA-C-N	-10.46	101.55	121.54
1	E	387	GLY	C-N-CA	-10.46	101.55	121.54
1	A	644	ASP	CA-C-N	10.29	131.15	120.04
1	A	644	ASP	C-N-CA	10.29	131.15	120.04
1	E	686	ALA	N-CA-C	10.28	132.70	110.80
1	E	388	CYS	N-CA-C	10.28	132.70	110.80
1	A	731	GLY	N-CA-C	10.19	123.28	111.36
1	A	401	PHE	CA-C-O	-10.14	107.78	119.24
2	F	152	VAL	CB-CA-C	-10.02	99.15	111.97
1	E	680	VAL	CB-CA-C	-9.97	95.77	110.62
1	A	433	LYS	N-CA-C	-9.90	95.81	110.46
1	E	340	ASP	N-CA-C	9.87	123.06	111.71
3	G	193	LEU	CA-C-N	-9.85	110.24	120.38
3	G	193	LEU	C-N-CA	-9.85	110.24	120.38
2	B	1	MET	CA-C-N	-9.82	107.57	119.84
2	B	1	MET	C-N-CA	-9.82	107.57	119.84
1	E	583	PHE	N-CA-C	9.69	131.44	110.80
1	E	323	LYS	CA-C-O	-9.67	106.91	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	594	CYS	O-C-N	-9.66	111.66	122.09
1	A	213	ASP	N-CA-C	-9.60	94.56	109.25
1	E	184	VAL	N-CA-C	9.58	121.44	111.00
1	E	685	THR	CA-C-N	9.54	139.75	121.54
1	E	685	THR	C-N-CA	9.54	139.75	121.54
1	A	683	LYS	CA-C-N	9.42	131.62	119.84
1	A	683	LYS	C-N-CA	9.42	131.62	119.84
3	G	18	ALA	N-CA-C	-9.28	102.09	113.41
1	A	477	ASP	N-CA-C	-9.21	94.32	108.96
3	G	109	LYS	O-C-N	9.20	132.32	122.20
1	E	608	PHE	N-CA-C	-9.11	101.26	111.82
1	E	466	ASP	CA-C-N	9.08	132.32	120.60
1	E	466	ASP	C-N-CA	9.08	132.32	120.60
1	E	174	THR	N-CA-C	9.05	124.45	113.23
3	C	113	GLN	N-CA-C	9.02	130.01	110.80
1	E	590	ILE	CB-CA-C	-9.00	99.75	110.91
1	E	590	ILE	N-CA-CB	8.95	120.48	110.72
1	E	213	ASP	N-CA-C	-8.93	94.84	108.67
3	C	195	PRO	N-CA-C	-8.84	101.98	110.47
2	B	152	VAL	CB-CA-C	-8.81	100.06	112.22
1	A	409	LYS	N-CA-C	8.79	123.31	112.23
1	E	409	LYS	N-CA-C	8.77	123.76	112.89
1	A	174	THR	N-CA-C	8.72	124.10	113.38
1	A	193	GLU	CA-C-N	8.66	130.67	119.84
1	A	193	GLU	C-N-CA	8.66	130.67	119.84
1	E	327	VAL	CB-CA-C	-8.65	96.86	110.69
1	E	603	GLN	N-CA-C	8.65	128.92	109.81
1	E	736	VAL	N-CA-CB	-8.62	100.81	112.28
1	A	327	VAL	CB-CA-C	-8.56	97.32	110.50
1	E	96	LYS	N-CA-C	8.55	124.32	113.55
3	G	83	HIS	CA-C-N	8.51	130.48	119.84
3	G	83	HIS	C-N-CA	8.51	130.48	119.84
1	E	593	TYR	N-CA-CB	8.50	124.85	110.49
1	E	216	ASN	N-CA-C	8.48	121.36	111.02
1	E	240	SER	N-CA-CB	-8.46	96.88	110.51
2	F	29	VAL	CA-C-N	8.34	128.97	120.38
2	F	29	VAL	C-N-CA	8.34	128.97	120.38
1	A	340	ASP	N-CA-C	8.33	128.53	110.80
1	A	736	VAL	N-CA-CB	-8.31	101.54	112.26
1	A	153	VAL	N-CA-C	8.28	120.35	111.58
3	G	207	PHE	CB-CA-C	-8.26	93.99	110.42
2	F	16	CYS	CA-C-N	-8.22	107.98	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	16	CYS	C-N-CA	-8.22	107.98	122.62
1	E	212	GLU	N-CA-C	-8.18	101.80	112.68
1	E	692	CYS	N-CA-C	8.18	121.33	109.14
1	E	428	GLU	N-CA-C	8.16	127.84	109.81
1	A	691	ASP	CB-CA-C	-8.15	93.27	110.31
2	F	43	VAL	N-CA-C	-8.14	95.72	107.77
1	A	591	GLU	N-CA-C	-8.10	102.46	111.28
1	A	582	PRO	N-CA-C	8.08	129.11	112.47
1	E	734	LEU	N-CA-C	8.07	122.40	112.23
1	E	338	GLY	N-CA-C	8.04	126.48	115.30
2	F	152	VAL	N-CA-CB	8.04	119.96	110.55
1	E	34	ALA	CA-C-N	8.04	136.89	121.54
1	E	34	ALA	C-N-CA	8.04	136.89	121.54
1	E	678	GLY	CA-C-N	-8.01	111.18	119.83
1	E	678	GLY	C-N-CA	-8.01	111.18	119.83
1	E	592	LEU	N-CA-C	7.99	122.04	109.81
1	A	467	VAL	CB-CA-C	-7.95	103.12	110.91
1	A	628	VAL	N-CA-CB	-7.88	103.54	112.21
2	F	46	TYR	N-CA-C	7.88	127.22	109.81
1	E	281	LYS	N-CA-C	7.86	123.17	113.50
2	B	46	TYR	CB-CA-C	-7.82	94.77	110.17
2	F	18	ALA	N-CA-C	7.82	119.80	111.28
1	A	364	TYR	CA-C-N	7.82	136.04	121.97
1	A	364	TYR	C-N-CA	7.82	136.04	121.97
1	E	92	PRO	N-CA-C	-7.81	96.38	112.47
1	E	390	GLY	N-CA-C	-7.79	96.44	112.34
1	E	731	GLY	N-CA-C	7.79	131.65	113.18
2	B	46	TYR	CA-C-N	7.75	129.77	120.94
2	B	46	TYR	C-N-CA	7.75	129.77	120.94
1	E	428	GLU	CA-C-N	-7.74	110.17	119.84
1	E	428	GLU	C-N-CA	-7.74	110.17	119.84
3	C	136	ALA	N-CA-C	7.66	122.30	112.34
1	E	593	TYR	CB-CA-C	-7.66	95.18	110.42
1	E	207	GLY	N-CA-C	-7.62	99.88	111.24
1	E	187	ARG	CA-C-N	7.62	127.78	120.31
1	E	187	ARG	C-N-CA	7.62	127.78	120.31
1	A	328	LEU	CA-C-N	-7.60	112.55	120.38
1	A	328	LEU	C-N-CA	-7.60	112.55	120.38
2	B	64	PRO	N-CA-C	7.58	119.95	110.70
1	A	207	GLY	CA-C-O	7.53	127.44	119.00
1	A	232	VAL	N-CA-C	7.51	118.70	107.80
3	G	248	GLN	N-CA-CB	-7.51	100.23	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	154	ASP	N-CA-C	7.50	122.43	113.28
1	A	281	LYS	N-CA-C	7.49	122.42	113.28
1	E	150	TYR	N-CA-C	-7.47	103.21	111.36
3	G	170	TRP	N-CA-C	7.47	120.30	111.71
1	E	323	LYS	CB-CA-C	7.45	124.85	110.17
1	E	278	TYR	N-CA-C	-7.44	103.10	111.14
1	E	712	ARG	N-CA-C	7.44	121.05	109.07
1	E	191	GLY	N-CA-C	7.41	121.09	112.50
1	A	212	GLU	N-CA-C	-7.40	102.84	112.68
1	E	707	ARG	N-CA-C	7.40	120.22	111.71
3	G	166	LEU	N-CA-C	-7.40	105.13	112.97
1	A	648	GLU	N-CA-CB	-7.34	98.47	110.81
1	E	288	GLU	N-CA-C	-7.31	104.22	113.43
1	E	606	PRO	N-CA-C	-7.29	97.45	112.47
1	E	594	CYS	CA-C-N	7.29	135.62	121.18
1	E	594	CYS	C-N-CA	7.29	135.62	121.18
2	B	71	PRO	N-CA-C	7.27	123.14	113.40
1	A	707	ARG	N-CA-C	7.25	120.05	111.71
1	E	594	CYS	N-CA-CB	-7.25	99.56	110.07
3	C	226	LEU	N-CA-C	-7.24	104.58	113.41
1	E	214	THR	N-CA-CB	-7.24	99.30	111.17
2	B	180	ALA	CA-C-N	7.20	127.04	119.05
2	B	180	ALA	C-N-CA	7.20	127.04	119.05
1	A	365	ILE	N-CA-CB	7.19	123.10	111.23
1	E	562	GLY	CA-C-N	7.18	132.32	122.77
1	E	562	GLY	C-N-CA	7.18	132.32	122.77
1	E	593	TYR	N-CA-C	-7.14	95.59	110.80
1	E	276	LYS	N-CA-C	7.12	119.13	111.36
1	E	337	TYR	N-CA-C	7.10	125.93	110.80
3	C	250	GLY	N-CA-C	7.08	129.96	113.18
1	E	431	PRO	N-CA-C	7.08	121.49	110.80
3	G	4	TYR	N-CA-C	-7.06	95.67	108.02
1	E	335	VAL	N-CA-CB	-7.04	99.61	111.23
3	G	130	PRO	N-CA-C	-7.04	97.98	112.47
1	E	595	GLN	N-CA-CB	-7.02	98.10	110.39
1	A	534	TYR	N-CA-C	-6.99	97.85	109.46
1	A	476	ALA	N-CA-C	6.91	121.31	110.32
1	E	690	LYS	CA-C-N	6.88	133.19	121.14
1	E	690	LYS	C-N-CA	6.88	133.19	121.14
1	E	411	PHE	N-CA-C	6.88	118.86	111.36
1	A	570	PRO	O-C-N	-6.86	113.38	122.64
1	A	690	LYS	CA-C-N	6.83	132.13	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	690	LYS	C-N-CA	6.83	132.13	120.72
2	F	16	CYS	O-C-N	-6.79	114.85	122.86
1	E	297	THR	N-CA-CB	-6.76	101.85	110.03
1	A	596	ARG	N-CA-C	-6.76	103.69	112.68
1	E	710	HIS	N-CA-C	6.72	125.12	110.80
1	A	356	ASN	N-CA-C	6.71	121.47	113.28
3	C	6	GLY	N-CA-C	-6.70	100.05	112.37
1	A	595	GLN	N-CA-C	6.64	121.39	113.16
3	C	47	ARG	N-CA-C	6.63	118.59	111.36
1	E	152	PHE	N-CA-C	6.63	121.22	113.20
2	F	111	GLY	N-CA-C	6.62	126.01	114.76
1	A	663	GLU	N-CA-C	6.61	122.21	111.37
1	A	69	GLU	N-CA-C	6.61	119.08	111.02
1	E	285	GLY	N-CA-C	6.60	125.09	115.32
1	A	576	GLU	N-CA-C	6.60	118.13	111.07
1	E	402	LYS	N-CA-C	6.59	118.20	109.83
3	C	169	SER	CA-C-N	6.57	126.34	119.05
3	C	169	SER	C-N-CA	6.57	126.34	119.05
1	E	214	THR	CB-CA-C	6.53	121.64	111.13
3	G	131	GLY	N-CA-C	-6.53	97.71	113.18
1	A	488	ARG	N-CA-C	6.52	119.33	109.23
2	B	171	THR	N-CA-C	6.52	121.06	113.18
1	E	388	CYS	CA-C-O	6.51	129.82	120.51
1	E	585	THR	CA-C-O	-6.51	111.21	120.51
1	A	692	CYS	N-CA-C	6.48	119.26	109.41
1	A	649	VAL	CB-CA-C	-6.48	103.50	111.08
1	E	428	GLU	CA-C-O	-6.47	111.30	120.16
1	E	498	LYS	N-CA-C	-6.47	100.76	111.37
3	G	42	ASP	N-CA-C	6.47	119.75	110.24
1	E	588	GLY	CA-C-N	-6.46	113.58	122.30
1	E	588	GLY	C-N-CA	-6.46	113.58	122.30
1	E	105	SER	CA-C-N	6.45	129.91	120.82
1	E	105	SER	C-N-CA	6.45	129.91	120.82
1	E	492	PHE	N-CA-C	6.45	119.37	110.35
1	E	335	VAL	CB-CA-C	6.43	121.84	111.29
1	E	198	GLU	N-CA-C	6.42	119.09	111.71
2	F	5	ALA	N-CA-C	6.42	118.82	109.07
2	B	4	TYR	N-CA-C	6.39	119.55	109.96
3	C	116	LEU	N-CA-C	-6.38	105.63	113.41
1	E	297	THR	N-CA-C	6.33	119.02	110.29
2	F	43	VAL	CA-C-N	-6.32	116.12	122.69
2	F	43	VAL	C-N-CA	-6.32	116.12	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	PHE	CA-C-N	-6.31	109.03	121.41
1	A	185	PHE	C-N-CA	-6.31	109.03	121.41
1	A	231	LYS	CA-C-N	6.29	131.30	123.12
1	A	231	LYS	C-N-CA	6.29	131.30	123.12
1	A	417	ILE	N-CA-C	6.29	117.79	110.62
2	F	135	CYS	CA-C-N	6.25	125.99	119.05
2	F	135	CYS	C-N-CA	6.25	125.99	119.05
2	F	186	LEU	CA-C-N	6.25	129.58	120.71
2	F	186	LEU	C-N-CA	6.25	129.58	120.71
1	E	354	LEU	N-CA-C	-6.23	105.32	113.17
1	E	174	THR	N-CA-CB	-6.22	100.73	110.44
1	E	661	LEU	N-CA-C	6.22	119.60	109.59
1	E	679	PRO	N-CA-C	6.21	120.60	111.03
1	A	411	PHE	N-CA-C	6.20	117.83	111.14
1	A	219	LEU	N-CA-C	-6.19	104.45	111.14
1	A	570	PRO	N-CA-C	6.18	125.21	112.47
1	A	327	VAL	N-CA-C	6.18	117.67	108.46
1	A	334	ASN	N-CA-C	6.17	120.43	112.41
1	E	433	LYS	N-CA-C	-6.17	99.66	109.59
1	E	478	VAL	CA-C-N	6.15	133.56	122.43
1	E	478	VAL	C-N-CA	6.15	133.56	122.43
3	G	86	SER	N-CA-C	6.14	120.62	108.59
3	C	168	LYS	N-CA-C	6.12	120.33	112.86
1	E	585	THR	CA-CB-CG2	-6.11	100.11	110.50
1	A	513	PHE	CB-CA-C	-6.11	109.55	116.63
1	E	294	LYS	N-CA-C	6.11	118.44	111.11
1	A	633	ARG	N-CA-C	6.09	123.78	110.80
3	G	141	PRO	N-CA-C	6.09	122.64	113.81
1	A	359	ARG	CA-C-N	-6.08	112.75	120.23
1	A	359	ARG	C-N-CA	-6.08	112.75	120.23
1	A	583	PHE	N-CA-C	6.06	123.72	110.80
1	E	172	LEU	CA-CB-CG	-6.06	95.09	116.30
2	B	72	THR	N-CA-CB	-6.06	100.76	110.39
1	E	193	GLU	N-CA-C	6.06	118.20	109.48
3	G	109	LYS	N-CA-C	6.05	118.65	109.63
1	A	270	TYR	N-CA-C	6.05	119.92	112.54
1	E	601	GLY	N-CA-C	6.05	127.51	113.18
3	G	172	LEU	N-CA-C	6.04	117.54	111.07
3	C	225	ARG	N-CA-C	6.03	120.25	113.02
1	E	757	LYS	N-CA-C	6.02	120.36	112.89
1	A	601	GLY	CA-C-N	-6.02	113.35	122.81
1	A	601	GLY	C-N-CA	-6.02	113.35	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	179	ASN	N-CA-C	6.02	123.62	110.80
2	F	105	ARG	N-CA-C	6.01	119.61	109.76
3	C	51	LEU	CA-C-N	6.00	128.25	120.44
3	C	51	LEU	C-N-CA	6.00	128.25	120.44
1	A	254	PRO	N-CA-C	6.00	120.63	111.15
2	B	134	THR	CB-CA-C	-6.00	100.92	111.05
1	A	498	LYS	N-CA-C	-5.98	103.93	111.11
1	E	402	LYS	CA-C-N	-5.98	114.45	120.31
1	E	402	LYS	C-N-CA	-5.98	114.45	120.31
1	E	93	ASP	N-CA-C	5.97	123.52	110.80
1	E	596	ARG	N-CA-C	-5.97	104.75	112.68
1	E	632	ALA	N-CA-C	5.96	120.29	113.19
2	F	187	THR	N-CA-CB	-5.96	100.83	109.83
1	A	569	LYS	N-CA-C	5.96	118.89	108.82
2	B	16	CYS	N-CA-C	-5.94	97.53	107.99
1	A	252	ILE	N-CA-C	5.94	118.18	109.63
3	G	113	ARG	N-CA-C	5.92	123.42	110.80
1	E	584	GLY	CA-C-N	5.92	132.84	121.54
1	E	584	GLY	C-N-CA	5.92	132.84	121.54
3	G	51	TYR	N-CA-C	-5.91	98.20	110.80
1	E	193	GLU	CA-C-N	5.90	127.22	119.84
1	E	193	GLU	C-N-CA	5.90	127.22	119.84
1	E	499	THR	CB-CA-C	-5.90	103.12	109.85
2	F	4	TYR	N-CA-C	5.90	118.80	109.96
1	E	33	TYR	N-CA-C	5.89	120.31	113.18
2	B	27	ASN	N-CA-C	5.89	120.59	113.17
1	A	246	ALA	N-CA-C	5.88	119.67	110.32
1	A	736	VAL	CB-CA-C	5.88	118.49	111.20
1	A	491	ASP	N-CA-C	-5.86	102.38	110.35
1	A	97	ARG	N-CA-C	5.86	119.40	110.50
3	C	87	SER	N-CA-C	5.85	119.22	108.69
2	F	117	THR	N-CA-CB	-5.84	101.57	111.27
1	A	706	MET	N-CA-C	-5.84	97.00	107.98
2	F	102	TYR	N-CA-C	5.83	122.35	113.61
3	C	142	PRO	N-CA-C	5.82	122.25	113.81
1	A	294	LYS	N-CA-C	5.82	118.09	111.11
2	B	102	TYR	N-CA-C	5.81	121.14	112.94
1	A	734	LEU	N-CA-C	5.81	120.51	112.90
3	C	44	ALA	N-CA-C	5.79	118.37	111.71
1	A	427	GLY	N-CA-C	-5.79	107.26	115.30
1	E	239	PHE	CB-CA-C	-5.78	101.28	111.05
3	G	70	ARG	N-CA-C	5.78	118.08	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	542	GLU	CA-C-N	5.78	127.96	120.44
1	A	542	GLU	C-N-CA	5.78	127.96	120.44
1	E	35	GLN	CA-C-N	5.78	128.97	120.82
1	E	35	GLN	C-N-CA	5.78	128.97	120.82
1	E	256	THR	N-CA-CB	-5.78	101.88	110.61
1	E	710	HIS	CA-C-N	-5.78	110.08	121.41
1	E	710	HIS	C-N-CA	-5.78	110.08	121.41
1	E	280	ALA	N-CA-C	5.77	118.31	111.33
1	E	231	LYS	CA-CB-CG	5.77	125.63	114.10
1	A	194	PRO	N-CA-C	5.76	124.33	112.47
1	E	580	ARG	N-CA-C	5.75	117.93	109.24
1	A	661	LEU	N-CA-C	5.75	118.33	109.07
1	E	38	LYS	N-CA-C	-5.74	98.15	108.48
1	A	454	GLU	N-CA-C	-5.73	104.94	111.07
2	F	156	LEU	N-CA-C	-5.73	104.94	111.07
1	E	538	LYS	N-CA-C	5.73	117.61	111.36
3	C	5	TYR	N-CA-C	-5.73	98.00	108.02
1	E	190	GLY	N-CA-C	5.72	122.88	112.58
2	F	175	LEU	N-CA-C	-5.70	98.99	108.34
1	A	626	SER	N-CA-C	-5.70	101.36	109.62
1	E	594	CYS	CA-C-O	5.68	126.55	120.70
1	A	166	ALA	N-CA-C	5.67	117.69	109.07
1	A	555	LEU	N-CA-C	5.67	117.14	111.07
1	E	397	GLU	N-CA-C	5.66	122.32	109.81
1	A	413	ARG	N-CA-C	5.66	120.30	113.17
1	E	610	PRO	N-CA-C	5.65	117.59	110.70
3	G	168	SER	N-CA-C	-5.65	101.43	109.62
1	E	400	GLY	N-CA-C	-5.64	99.80	113.18
1	A	680	VAL	CB-CA-C	-5.63	102.15	110.82
1	A	421	ILE	CB-CA-C	-5.63	103.72	111.65
1	A	407	LYS	N-CA-C	5.63	118.95	111.75
1	A	167	LYS	CA-C-N	5.60	125.27	119.56
1	A	167	LYS	C-N-CA	5.60	125.27	119.56
1	A	648	GLU	CB-CA-C	5.60	119.45	109.65
1	A	590	ILE	N-CA-C	5.59	116.23	110.36
1	A	257	ASP	N-CA-C	5.58	118.13	111.71
2	F	29	VAL	N-CA-C	-5.58	103.48	108.95
2	F	160	GLU	N-CA-C	-5.58	105.20	112.23
1	A	730	GLY	N-CA-C	5.58	126.41	113.18
1	A	510	GLU	N-CA-C	5.57	117.76	110.08
1	A	111	LYS	N-CA-C	5.56	117.36	108.41
1	E	739	VAL	N-CA-CB	-5.56	101.53	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	371	LEU	N-CA-C	-5.55	98.58	108.13
1	A	628	VAL	N-CA-C	5.55	119.48	113.43
2	B	137	THR	N-CA-C	5.55	119.89	113.18
1	E	687	ARG	CB-CG-CD	-5.55	98.55	111.30
2	B	32	GLY	N-CA-C	5.54	126.32	113.18
1	A	606	PRO	N-CA-C	-5.52	106.96	113.86
1	E	477	ASP	CA-C-O	5.51	125.72	119.27
2	F	83	VAL	N-CA-C	-5.51	100.48	108.36
2	B	105	ARG	N-CA-C	5.51	118.53	109.72
1	A	400	GLY	CA-C-N	-5.50	112.90	122.36
1	A	400	GLY	C-N-CA	-5.50	112.90	122.36
1	E	478	VAL	CB-CA-C	5.49	120.29	111.29
3	C	20	LEU	N-CA-C	-5.49	105.21	111.14
1	E	387	GLY	O-C-N	-5.49	115.57	122.70
1	A	403	PRO	N-CA-C	5.48	119.92	111.21
1	E	194	PRO	N-CA-C	5.47	123.74	112.47
1	A	274	TYR	N-CA-C	5.46	117.73	110.53
1	A	383	PRO	N-CA-C	5.46	119.86	111.57
1	E	477	ASP	O-C-N	-5.46	114.99	122.46
1	A	376	LEU	N-CA-C	5.45	114.57	108.25
1	A	265	ILE	N-CA-C	-5.45	105.19	110.42
2	B	143	GLY	N-CA-C	5.43	118.40	110.63
1	A	585	THR	N-CA-C	5.43	119.69	112.30
1	E	597	PHE	CA-C-N	5.43	127.83	120.44
1	E	597	PHE	C-N-CA	5.43	127.83	120.44
3	C	8	PRO	N-CA-C	-5.43	103.32	111.57
1	E	184	VAL	CB-CA-C	-5.43	104.97	112.24
1	E	49	TRP	N-CA-C	-5.42	106.16	112.89
1	E	166	ALA	N-CA-C	5.42	117.50	108.99
1	E	668	MET	N-CA-C	-5.41	100.89	109.59
1	E	629	HIS	CA-C-N	5.40	129.87	122.84
1	E	629	HIS	C-N-CA	5.40	129.87	122.84
1	E	388	CYS	N-CA-CB	-5.40	101.36	110.49
1	E	651	ILE	CB-CA-C	-5.40	101.04	110.71
1	A	214	THR	N-CA-C	5.38	119.46	111.87
1	A	679	PRO	N-CA-C	5.38	119.32	111.03
1	A	489	TYR	N-CA-C	-5.37	101.52	110.17
1	E	226	LEU	N-CA-C	-5.37	105.50	111.36
2	F	19	CYS	N-CA-C	-5.37	105.32	111.07
1	E	339	ASP	N-CA-C	-5.37	104.15	111.56
1	E	483	ALA	CA-C-N	5.37	128.86	120.75
1	E	483	ALA	C-N-CA	5.37	128.86	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	712	ARG	N-CA-C	5.37	117.71	109.07
3	C	29	GLY	N-CA-C	5.37	119.13	112.64
1	E	582	PRO	CA-C-N	5.36	131.79	121.54
1	E	582	PRO	C-N-CA	5.36	131.79	121.54
3	G	225	LEU	N-CA-CB	5.36	121.04	110.63
1	A	226	LEU	CA-C-N	5.35	127.70	120.38
1	A	226	LEU	C-N-CA	5.35	127.70	120.38
1	E	498	LYS	CA-C-N	5.35	130.17	121.83
1	E	498	LYS	C-N-CA	5.35	130.17	121.83
3	G	248	GLN	O-C-N	5.34	128.94	122.48
2	F	64	PRO	CA-C-N	-5.34	114.17	119.56
2	F	64	PRO	C-N-CA	-5.34	114.17	119.56
1	A	458	ASN	N-CA-C	5.32	119.52	113.19
1	A	599	GLU	N-CA-C	5.32	119.92	113.38
1	E	614	PRO	N-CA-C	5.31	117.18	110.70
1	A	35	GLN	N-CA-C	-5.29	103.40	110.55
2	B	108	HIS	N-CA-C	-5.28	102.53	110.24
1	E	706	MET	N-CA-C	-5.28	97.33	107.57
1	A	583	PHE	CB-CA-C	-5.26	99.94	110.42
1	E	629	HIS	N-CA-C	5.26	117.82	109.24
2	F	170	GLY	N-CA-C	5.26	120.46	114.67
1	A	150	TYR	N-CA-C	-5.26	105.44	111.07
2	B	179	ASN	N-CA-C	5.26	118.45	111.30
1	A	686	ALA	N-CA-C	5.25	117.83	109.96
1	E	271	GLU	N-CA-C	-5.25	106.65	113.16
1	A	375	PRO	N-CA-C	5.24	119.44	110.95
1	E	69	GLU	N-CA-C	-5.23	103.12	110.50
1	E	685	THR	N-CA-CB	-5.23	101.65	110.49
1	A	575	TRP	CA-C-N	5.23	127.23	120.44
1	A	575	TRP	C-N-CA	5.23	127.23	120.44
3	G	107	LEU	N-CA-C	-5.23	105.61	112.72
3	C	80	PHE	N-CA-C	5.22	119.74	113.17
3	C	194	LEU	N-CA-C	5.21	117.16	110.39
1	E	569	LYS	CA-C-N	5.20	126.33	119.84
1	E	569	LYS	C-N-CA	5.20	126.33	119.84
2	B	169	GLN	CA-C-N	-5.19	111.23	121.41
2	B	169	GLN	C-N-CA	-5.19	111.23	121.41
1	E	39	SER	N-CA-C	5.19	118.13	107.69
2	F	16	CYS	CA-C-O	-5.19	115.90	121.56
1	E	231	LYS	N-CA-CB	-5.18	101.98	110.43
1	E	187	ARG	N-CA-C	5.17	116.61	108.55
1	A	187	ARG	N-CA-C	5.16	121.22	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	84	HIS	CA-C-N	5.16	124.83	119.56
3	C	84	HIS	C-N-CA	5.16	124.83	119.56
2	F	25	MET	CA-C-N	5.16	127.15	120.44
2	F	25	MET	C-N-CA	5.16	127.15	120.44
1	E	725	LEU	CA-CB-CG	5.16	134.34	116.30
1	E	488	ARG	N-CA-C	5.14	117.23	109.41
1	E	747	PRO	N-CA-C	5.14	119.39	111.57
1	A	428	GLU	CA-C-N	-5.14	113.42	119.84
1	A	428	GLU	C-N-CA	-5.14	113.42	119.84
1	E	161	GLY	N-CA-C	5.14	123.01	114.48
1	A	613	GLU	N-CA-C	5.13	117.12	110.40
1	E	585	THR	N-CA-C	-5.12	99.89	110.80
1	A	336	TRP	N-CA-C	5.12	121.71	110.80
1	E	693	VAL	CB-CA-C	5.12	118.96	110.30
1	A	389	SER	N-CA-C	5.12	121.71	110.80
1	E	510	GLU	N-CA-C	5.12	117.15	110.08
1	A	339	ASP	N-CA-C	5.12	119.24	112.89
1	E	677	GLU	CA-C-N	5.11	129.89	121.87
1	E	677	GLU	C-N-CA	5.11	129.89	121.87
1	E	588	GLY	O-C-N	-5.10	119.00	122.62
1	A	495	VAL	N-CA-C	5.09	115.19	107.75
1	E	45	GLU	N-CA-C	-5.09	106.82	112.57
1	E	583	PHE	N-CA-CB	-5.08	101.90	110.49
1	E	649	VAL	CB-CA-C	-5.08	104.54	111.15
1	E	678	GLY	CA-C-O	-5.08	114.26	121.52
1	A	728	ILE	N-CA-C	5.07	116.49	111.67
1	E	644	ASP	CA-C-N	5.07	125.14	119.87
1	E	644	ASP	C-N-CA	5.07	125.14	119.87
2	B	159	ALA	N-CA-C	5.05	117.76	110.28
1	A	625	ARG	N-CA-C	5.05	118.29	110.17
1	A	508	ALA	N-CA-C	-5.04	106.98	113.23
3	G	162	LEU	N-CA-C	-5.04	105.48	110.97
1	A	325	ARG	N-CA-C	5.04	119.57	112.72
2	B	99	ALA	N-CA-C	5.04	118.58	112.23
1	A	271	GLU	N-CA-C	-5.03	106.83	113.17
3	G	78	LEU	N-CA-C	-5.03	105.92	111.71
1	A	98	PRO	CA-N-CD	-5.02	104.97	112.00
1	A	390	GLY	N-CA-C	5.02	122.57	112.34
2	B	135	CYS	CA-C-N	5.02	125.04	119.32
2	B	135	CYS	C-N-CA	5.02	125.04	119.32
2	F	14	VAL	N-CA-C	-5.01	108.08	112.90
1	E	305	THR	N-CA-CB	-5.00	102.80	110.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ARG	CA-C-N	-5.00	114.57	119.92
1	A	97	ARG	C-N-CA	-5.00	114.57	119.92

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	323	LYS	Peptide,Mainchain
1	E	428	GLU	Mainchain

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	5896	0	5814	515	3
1	E	5896	0	5815	459	3
2	B	1475	0	1453	115	0
2	F	1475	0	1454	87	0
3	C	1948	0	2001	92	0
3	G	1948	0	2004	99	0
4	A	8	0	0	0	0
4	B	32	0	0	3	0
4	E	8	0	0	1	0
4	F	32	0	0	3	0
5	A	94	0	44	7	0
5	E	94	0	44	7	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	A	386	0	0	68	0
7	B	150	0	0	35	0
7	C	88	0	0	5	0
7	E	452	0	0	105	0
7	F	130	0	0	20	0
7	G	79	0	0	21	0
All	All	20193	0	18629	1335	3

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 36.

All (1335) 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:E:324:PRO:CD	1:E:324:PRO:CG	1.80	1.60
2:B:135:CYS:SG	2:B:135:CYS:CB	2.02	1.47
1:A:602:HIS:CE1	1:A:606:PRO:HG3	1.52	1.43
1:E:592:LEU:HA	1:E:603:GLN:NE2	1.27	1.41
2:F:135:CYS:CB	2:F:135:CYS:SG	2.10	1.40
1:E:605:LEU:H	1:E:605:LEU:CD2	1.28	1.39
1:A:186:GLY:HA3	1:A:583:PHE:C	1.47	1.36
1:A:591:GLU:OE2	1:A:604:PRO:HG3	1.26	1.34
1:A:184:VAL:CG2	1:A:592:LEU:HD23	1.61	1.30
1:A:582:PRO:HB2	7:A:2277:HOH:O	1.27	1.29
1:E:591:GLU:OE1	1:E:604:PRO:HB3	1.23	1.27
2:B:46:TYR:HB2	7:B:2032:HOH:O	1.33	1.26
1:E:323:LYS:O	7:E:2213:HOH:O	1.53	1.24
1:E:477:ASP:O	1:E:478:VAL:HG23	1.33	1.22
1:E:605:LEU:HD23	1:E:605:LEU:N	1.43	1.21
1:A:601:GLY:HA2	7:A:2285:HOH:O	1.06	1.20
1:A:604:PRO:O	1:A:606:PRO:HD2	1.40	1.20
1:E:388:CYS:HB2	1:E:593:TYR:OH	1.40	1.18
2:B:41:ARG:HH11	2:B:187:THR:CG2	1.56	1.18
1:E:36:GLU:O	1:E:58:VAL:HG22	1.01	1.18
3:G:207:PHE:CE2	3:G:211:LEU:HD13	1.78	1.18
3:C:171:TRP:O	3:C:171:TRP:CE3	1.98	1.17
1:E:602:HIS:CE1	1:E:606:PRO:HG3	1.81	1.15
1:E:562:GLY:O	7:E:2316:HOH:O	1.60	1.15
1:A:584:GLY:HA2	7:A:2278:HOH:O	0.97	1.14
1:A:337:TYR:O	1:A:340:ASP:OD2	1.62	1.14
1:E:477:ASP:O	1:E:478:VAL:CG2	1.96	1.13
1:E:36:GLU:O	1:E:58:VAL:CG2	1.96	1.13
1:E:592:LEU:CA	1:E:603:GLN:HE21	1.59	1.13
1:A:97:ARG:HH21	1:A:763:ARG:NH2	1.47	1.12
1:A:395:ASP:O	1:A:399:GLU:HB2	1.46	1.12
1:A:583:PHE:CE2	1:A:588:GLY:N	2.17	1.12
1:A:69:GLU:O	7:A:2034:HOH:O	1.66	1.12
2:B:134:THR:O	2:B:134:THR:CG2	1.98	1.12
2:B:134:THR:O	2:B:134:THR:HG23	1.48	1.11
1:A:42:GLN:O	1:A:53:ILE:HG13	1.51	1.10
1:E:116:THR:HG22	1:E:119:GLU:HB3	1.25	1.10
1:E:607:VAL:CG1	1:E:607:VAL:O	2.00	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1:ALA:HB1	7:G:2001:HOH:O	1.52	1.09
1:A:601:GLY:CA	7:A:2285:HOH:O	1.69	1.09
2:F:57:GLN:NE2	2:F:140:ARG:HH22	1.49	1.09
1:A:284:VAL:O	1:A:590:ILE:HG22	1.51	1.09
1:A:397:GLU:HB3	1:A:398:PRO:HD3	1.18	1.09
1:E:607:VAL:O	1:E:607:VAL:HG12	1.49	1.08
1:A:395:ASP:HA	1:A:399:GLU:CG	1.83	1.08
1:E:591:GLU:OE1	1:E:604:PRO:CB	2.01	1.08
1:A:184:VAL:HG23	1:A:592:LEU:CD2	1.84	1.07
1:A:428:GLU:HB3	1:A:429:PRO:HD2	1.37	1.07
1:E:591:GLU:CD	1:E:604:PRO:HB3	1.77	1.07
1:A:43:ILE:HG13	1:A:505:ARG:HB3	1.27	1.07
1:E:97:ARG:HG3	7:E:2194:HOH:O	1.53	1.07
1:A:604:PRO:O	1:A:606:PRO:CD	2.04	1.06
1:E:605:LEU:CD2	1:E:605:LEU:N	1.93	1.06
1:A:395:ASP:HA	1:A:399:GLU:HG3	1.06	1.05
1:A:77:ARG:NH1	2:B:138:TYR:HE2	1.54	1.04
1:E:323:LYS:HD3	1:E:354:LEU:CA	1.87	1.03
1:E:602:HIS:HE1	1:E:606:PRO:HG3	0.88	1.03
1:A:467:VAL:HB	7:A:2230:HOH:O	1.58	1.03
1:A:97:ARG:NH2	1:A:763:ARG:HH22	1.55	1.03
2:B:46:TYR:CD1	7:B:2032:HOH:O	2.10	1.03
1:A:186:GLY:HA3	1:A:583:PHE:O	1.59	1.02
1:A:288:GLU:HB3	1:A:591:GLU:HG3	1.41	1.02
1:A:591:GLU:OE2	1:A:604:PRO:CG	2.06	1.02
1:E:602:HIS:CD2	1:E:604:PRO:HD2	1.93	1.02
1:E:602:HIS:NE2	1:E:604:PRO:HD2	1.75	1.02
1:A:632:ALA:O	1:A:635:GLN:HG2	1.61	1.01
1:E:323:LYS:HD3	1:E:354:LEU:HA	1.06	1.01
1:E:592:LEU:CA	1:E:603:GLN:NE2	2.20	1.01
1:E:763:ARG:HG2	7:E:2442:HOH:O	1.59	1.01
2:F:57:GLN:HE22	2:F:140:ARG:NH2	1.57	1.01
1:E:95:LEU:HD12	1:E:466:ASP:O	1.60	1.00
1:E:626:SER:HB2	7:E:2350:HOH:O	1.59	1.00
1:A:602:HIS:CE1	1:A:606:PRO:CG	2.44	1.00
3:G:207:PHE:HE2	3:G:211:LEU:HD13	1.14	1.00
1:A:685:THR:HB	2:B:42:GLU:OE2	1.62	1.00
3:C:17:THR:CG2	3:C:67:GLU:HG3	1.91	1.00
2:B:41:ARG:HD2	2:B:187:THR:HG21	1.40	0.99
1:E:511:PRO:HB3	1:E:515:THR:HG22	1.44	0.99
1:A:279:VAL:HG13	1:A:283:THR:HG21	1.42	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:ASP:HB2	1:E:607:VAL:HG11	1.44	0.99
1:E:429:PRO:HD2	7:E:2259:HOH:O	1.61	0.99
1:A:569:LYS:O	7:A:2271:HOH:O	1.81	0.99
2:B:41:ARG:HD2	2:B:187:THR:CG2	1.91	0.99
1:E:413:ARG:HD3	7:E:2250:HOH:O	1.62	0.98
1:A:165:ALA:O	1:A:415:THR:HG21	1.62	0.98
1:A:592:LEU:O	1:A:593:TYR:HB2	1.60	0.98
3:C:22:PHE:O	3:C:239:ARG:NH1	1.96	0.98
3:G:154:THR:CG2	3:G:238:ARG:HE	1.77	0.97
1:E:230:ALA:O	7:E:2141:HOH:O	1.80	0.97
3:G:38:HIS:HD2	3:G:45:ALA:HB1	1.28	0.97
1:E:598:LYS:HD2	7:E:2331:HOH:O	1.65	0.97
1:A:395:ASP:CA	1:A:399:GLU:HG3	1.93	0.97
1:A:603:GLN:HB3	1:A:604:PRO:HD3	1.43	0.97
1:E:47:CYS:HB2	7:E:2452:HOH:O	1.63	0.97
1:E:116:THR:CG2	1:E:119:GLU:H	1.78	0.97
1:E:608:PHE:O	7:E:2337:HOH:O	1.82	0.97
1:E:592:LEU:HD23	1:E:603:GLN:HE22	1.28	0.96
1:E:602:HIS:HE1	1:E:606:PRO:CG	1.78	0.96
1:A:186:GLY:CA	1:A:583:PHE:C	2.38	0.96
1:A:583:PHE:HE2	1:A:588:GLY:N	1.59	0.96
1:A:172:LEU:HD13	1:A:445:SER:O	1.66	0.96
1:E:224:LEU:HD12	7:E:2135:HOH:O	1.64	0.96
1:A:763:ARG:HG2	7:A:2378:HOH:O	1.65	0.95
2:B:41:ARG:HH11	2:B:187:THR:HG22	1.28	0.95
1:E:653:LYS:HD2	1:E:686:ALA:HB2	1.47	0.94
2:B:46:TYR:CE2	7:B:2029:HOH:O	2.20	0.94
1:E:424:MET:HE2	1:E:455:ALA:HB1	1.50	0.94
3:C:171:TRP:O	3:C:171:TRP:CD2	2.20	0.94
1:A:170:VAL:O	1:A:175:ALA:HB2	1.65	0.94
2:F:57:GLN:NE2	2:F:140:ARG:NH2	2.15	0.94
1:E:342:TYR:CD1	1:E:607:VAL:HB	2.02	0.94
1:A:591:GLU:CD	1:A:604:PRO:HG3	1.93	0.94
1:A:97:ARG:HH21	1:A:763:ARG:HH22	1.00	0.93
3:G:221:TRP:HE3	3:G:225:LEU:HD22	1.31	0.93
1:E:764:ARG:N	7:E:2446:HOH:O	2.01	0.93
2:B:192:VAL:HG21	7:B:2019:HOH:O	1.69	0.93
1:A:632:ALA:O	1:A:635:GLN:CG	2.16	0.93
1:E:590:ILE:HG13	7:E:2181:HOH:O	1.69	0.92
1:A:585:THR:O	1:A:586:ALA:HB3	1.70	0.92
1:E:428:GLU:O	1:E:430:TYR:N	2.02	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:41:ARG:HD2	2:F:187:THR:CG2	2.00	0.92
1:A:651:ILE:HD11	1:A:682:VAL:HG13	1.50	0.92
2:F:41:ARG:HD2	2:F:187:THR:HG23	1.49	0.92
1:A:42:GLN:O	1:A:53:ILE:CG1	2.17	0.91
3:C:155:THR:HG22	3:C:239:ARG:HE	1.35	0.91
3:G:206:GLY:O	3:G:209:TYR:N	2.03	0.91
1:A:531:LEU:O	1:A:534:TYR:O	1.88	0.91
1:A:116:THR:HG22	1:A:119:GLU:H	1.30	0.91
2:B:46:TYR:CB	7:B:2032:HOH:O	2.01	0.91
2:F:46:TYR:HB3	7:F:2036:HOH:O	1.69	0.91
3:G:111:SER:HB3	7:G:2036:HOH:O	1.69	0.91
1:A:360:PRO:HD3	1:A:571:TRP:CE3	2.06	0.90
1:A:599:GLU:O	7:A:2284:HOH:O	1.89	0.90
1:E:551:LEU:O	1:E:553:LEU:N	2.04	0.90
2:B:160:GLU:H	2:B:179:ASN:HD21	1.20	0.90
1:E:324:PRO:CD	1:E:324:PRO:CB	2.23	0.90
1:A:345:MET:HE2	1:A:605:LEU:HD22	1.52	0.89
1:A:608:PHE:O	1:A:608:PHE:CD1	2.25	0.89
1:E:112:TYR:OH	1:E:474:MET:O	1.91	0.89
1:A:184:VAL:HG23	1:A:592:LEU:HD23	0.91	0.89
3:C:207:GLY:O	3:C:210:TYR:N	2.04	0.89
1:E:349:TYR:OH	1:E:591:GLU:HA	1.73	0.89
1:E:397:GLU:HB3	1:E:398:PRO:HD3	1.54	0.89
1:A:434:GLY:HA2	1:A:461:LEU:O	1.72	0.88
1:E:533:GLN:H	1:E:533:GLN:HE21	1.20	0.88
1:E:92:PRO:O	1:E:94:ARG:N	2.06	0.88
1:E:116:THR:HG23	1:E:119:GLU:H	1.39	0.88
1:A:680:VAL:HG11	7:A:2312:HOH:O	1.73	0.88
1:A:763:ARG:HB2	7:A:2380:HOH:O	1.72	0.88
2:B:25:MET:HA	2:B:25:MET:HE2	1.55	0.88
1:A:580:ARG:CB	1:A:580:ARG:HH11	1.87	0.88
1:A:349:TYR:OH	1:A:591:GLU:O	1.92	0.87
1:A:335:VAL:CG1	1:A:732:ALA:O	2.23	0.87
1:A:591:GLU:HB3	1:A:603:GLN:NE2	1.88	0.87
1:A:604:PRO:C	1:A:606:PRO:CD	2.48	0.87
1:E:604:PRO:O	1:E:606:PRO:HD3	1.75	0.87
1:A:729:SER:O	1:A:731:GLY:N	2.08	0.87
1:E:569:LYS:HD2	7:E:2322:HOH:O	1.73	0.87
1:A:77:ARG:HH11	2:B:138:TYR:HE2	1.04	0.86
2:B:146:GLU:HG2	7:B:2110:HOH:O	1.76	0.86
3:C:17:THR:HG21	3:C:67:GLU:HG3	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:THR:CG2	1:A:119:GLU:H	1.87	0.86
2:B:72:THR:HG22	2:B:74:ALA:H	1.38	0.86
1:A:186:GLY:HA3	1:A:584:GLY:N	1.91	0.86
1:A:276:LYS:HA	7:A:2152:HOH:O	1.75	0.86
1:E:297:THR:HG22	1:E:300:TRP:H	1.41	0.86
1:E:605:LEU:N	1:E:605:LEU:HD22	1.90	0.86
3:G:221:TRP:CE3	3:G:225:LEU:HD22	2.11	0.86
1:A:314:GLU:O	1:A:318:GLU:HG3	1.75	0.86
1:E:324:PRO:HD3	7:E:2170:HOH:O	1.74	0.85
1:E:635:GLN:O	1:E:641:MET:CG	2.23	0.85
2:F:41:ARG:HH11	2:F:187:THR:CG2	1.90	0.85
1:A:397:GLU:CB	1:A:398:PRO:HD3	2.06	0.85
1:A:607:VAL:HG12	1:A:607:VAL:O	1.77	0.85
2:B:16:CYS:O	2:B:16:CYS:SG	2.34	0.85
1:E:428:GLU:O	1:E:429:PRO:C	2.15	0.85
1:E:635:GLN:O	1:E:641:MET:HG3	1.77	0.85
1:E:95:LEU:CD1	1:E:466:ASP:O	2.24	0.85
1:E:493:VAL:HG13	7:E:2016:HOH:O	1.76	0.85
3:G:38:HIS:CD2	3:G:45:ALA:HB1	2.11	0.85
1:E:209:HIS:HE1	1:E:625:ARG:H	1.24	0.85
3:C:108:LEU:O	3:C:110:LYS:HG2	1.75	0.85
1:E:606:PRO:O	1:E:608:PHE:N	2.09	0.84
2:F:57:GLN:HE22	2:F:140:ARG:HH22	1.15	0.84
1:E:562:GLY:C	7:E:2316:HOH:O	2.08	0.84
3:C:140:ASN:H	3:C:140:ASN:HD22	1.24	0.84
3:C:128:LEU:HB3	7:C:2061:HOH:O	1.75	0.84
2:F:160:GLU:H	2:F:179:ASN:HD21	1.23	0.84
2:B:159:ALA:O	2:F:183:LYS:HE2	1.78	0.83
1:A:601:GLY:N	7:A:2285:HOH:O	1.94	0.83
2:B:41:ARG:NH1	2:B:187:THR:CG2	2.41	0.83
1:A:604:PRO:C	1:A:606:PRO:HD3	2.03	0.83
3:C:168:LYS:HE2	7:C:2063:HOH:O	1.77	0.83
2:B:46:TYR:HD1	7:B:2032:HOH:O	1.51	0.83
3:G:139:ASN:H	3:G:139:ASN:HD22	1.27	0.83
1:A:42:GLN:NE2	1:A:505:ARG:HD3	1.92	0.83
1:E:590:ILE:CG1	7:E:2181:HOH:O	2.25	0.83
1:A:400:GLY:HA3	7:A:2196:HOH:O	1.79	0.83
1:E:614:PRO:HG2	7:E:2343:HOH:O	1.78	0.83
1:E:608:PHE:CD1	1:E:608:PHE:C	2.57	0.82
1:E:608:PHE:O	1:E:608:PHE:CD1	2.32	0.82
3:G:196:GLU:HG2	7:G:2058:HOH:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:ALA:HA	3:C:175:PRO:HG2	1.60	0.82
1:E:116:THR:CG2	1:E:119:GLU:HB3	2.09	0.82
1:A:335:VAL:O	1:A:733:GLY:HA2	1.79	0.82
1:A:184:VAL:CG2	1:A:592:LEU:CD2	2.52	0.82
1:A:284:VAL:HG23	1:A:587:SER:HB3	1.61	0.82
1:E:498:LYS:HE2	7:E:2297:HOH:O	1.80	0.82
1:A:519:TRP:CE2	1:A:540:ILE:HG12	2.14	0.82
1:A:629:HIS:ND1	1:A:634:THR:HG23	1.93	0.82
3:G:206:GLY:O	3:G:210:GLY:N	2.12	0.82
2:F:47:PRO:HD2	7:F:2036:HOH:O	1.78	0.81
2:F:2:PRO:HD2	2:F:80:ASP:OD2	1.80	0.81
1:A:335:VAL:HG11	1:A:732:ALA:O	1.78	0.81
2:B:46:TYR:HE2	7:B:2029:HOH:O	1.59	0.81
1:E:510:GLU:HG3	7:E:2301:HOH:O	1.78	0.81
2:B:25:MET:HA	2:B:25:MET:CE	2.11	0.81
2:F:65:PRO:HD2	4:F:1196:SF4:S4	2.20	0.81
1:A:97:ARG:NH2	1:A:763:ARG:NH2	2.19	0.81
2:B:117:THR:HG21	7:B:2095:HOH:O	1.81	0.81
1:A:653:LYS:HG3	1:A:684:PRO:O	1.81	0.81
3:G:154:THR:HG22	3:G:238:ARG:HE	1.45	0.80
1:A:607:VAL:HG13	1:A:609:THR:OG1	1.81	0.80
1:E:116:THR:HG22	1:E:119:GLU:CB	2.11	0.80
1:A:42:GLN:NE2	1:A:485:TYR:O	2.15	0.80
2:F:146:GLU:HG2	7:F:2004:HOH:O	1.80	0.80
1:E:283:THR:HG22	7:E:2182:HOH:O	1.80	0.80
1:A:207:GLY:O	5:A:1766:MGD:O5'	2.00	0.79
1:A:397:GLU:HB3	1:A:398:PRO:CD	2.06	0.79
1:E:388:CYS:SG	1:E:413:ARG:NE	2.55	0.79
1:A:186:GLY:CA	1:A:583:PHE:O	2.30	0.79
1:E:301:ALA:O	1:E:305:THR:HB	1.82	0.79
1:E:685:THR:HG22	2:F:42:GLU:CD	2.07	0.79
1:E:342:TYR:HD1	1:E:607:VAL:HB	1.46	0.79
1:E:494:LEU:HD22	1:E:502:ILE:HG12	1.65	0.79
1:A:48:PHE:CE1	1:A:145:HIS:CE1	2.71	0.79
1:A:429:PRO:O	1:A:430:TYR:CD2	2.35	0.79
1:A:686:ALA:HB3	7:A:2331:HOH:O	1.82	0.78
1:E:95:LEU:HD21	7:E:2278:HOH:O	1.82	0.78
1:A:183:TRP:CH2	1:A:596:ARG:HD3	2.17	0.78
1:A:413:ARG:H	1:A:413:ARG:CD	1.97	0.78
1:A:116:THR:HG22	1:A:119:GLU:HB3	1.64	0.78
3:C:53:ALA:O	3:C:57:ILE:HG13	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:PHE:HE2	1:A:588:GLY:H	1.25	0.78
1:A:591:GLU:HB3	1:A:603:GLN:HE22	1.48	0.78
1:A:602:HIS:HE1	1:A:606:PRO:HG3	1.03	0.78
7:B:2145:HOH:O	3:C:251:LEU:HD11	1.82	0.78
1:A:93:ASP:OD1	1:A:758:ARG:NH2	2.16	0.78
1:E:109:GLU:HG3	7:E:2068:HOH:O	1.83	0.78
1:A:605:LEU:HD23	1:A:605:LEU:H	1.48	0.78
1:A:602:HIS:ND1	1:A:606:PRO:HG3	1.98	0.78
2:F:72:THR:HG22	2:F:74:ALA:H	1.49	0.77
1:E:89:THR:OG1	1:E:484:THR:HG21	1.85	0.77
1:E:308:PRO:HB2	7:E:2198:HOH:O	1.84	0.77
1:A:591:GLU:O	1:A:592:LEU:HD12	1.83	0.77
1:A:740:ARG:NH1	7:A:2360:HOH:O	2.15	0.77
1:A:183:TRP:HH2	1:A:596:ARG:HD3	1.50	0.77
1:A:345:MET:HE3	1:A:592:LEU:HD11	1.67	0.77
1:A:256:THR:HG21	1:A:305:THR:HA	1.67	0.77
1:E:648:GLU:HG2	1:E:681:ARG:HH12	1.47	0.77
1:A:585:THR:O	1:A:586:ALA:CB	2.32	0.77
1:E:305:THR:HG22	1:E:307:ILE:H	1.50	0.77
1:E:323:LYS:C	7:E:2213:HOH:O	2.17	0.77
1:A:629:HIS:HA	1:A:634:THR:HG21	1.67	0.76
1:A:647:ASN:C	1:A:648:GLU:HG3	2.11	0.76
2:B:41:ARG:NH1	2:B:187:THR:HG22	2.00	0.76
1:A:70:ALA:O	7:A:2037:HOH:O	2.01	0.76
3:C:140:ASN:H	3:C:140:ASN:ND2	1.84	0.76
3:C:241:LEU:C	3:C:241:LEU:HD12	2.10	0.76
1:A:605:LEU:H	1:A:605:LEU:CD2	1.99	0.76
3:C:155:THR:HG21	3:C:239:ARG:HG2	1.68	0.76
3:G:206:GLY:O	3:G:207:PHE:C	2.29	0.76
1:A:633:ARG:HD2	5:A:1765:MGD:O2B	1.85	0.75
1:E:305:THR:CG2	1:E:307:ILE:H	1.99	0.75
3:C:155:THR:CG2	3:C:239:ARG:HE	1.99	0.75
1:A:75:ARG:HD2	1:A:220:GLN:HE22	1.49	0.75
1:E:629:HIS:ND1	1:E:634:THR:HG23	2.02	0.75
3:C:207:GLY:O	3:C:209:TRP:N	2.19	0.75
1:A:580:ARG:HH11	1:A:580:ARG:HB3	1.49	0.75
1:E:81:ARG:HG2	1:E:628:VAL:O	1.86	0.75
1:E:311:VAL:HB	7:E:2198:HOH:O	1.85	0.75
1:A:390:GLY:H	1:A:595:GLN:HE22	1.34	0.75
1:E:421:ILE:HG23	1:E:421:ILE:O	1.84	0.75
1:A:393:GLY:HA3	1:A:407:LYS:HE3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:GLU:O	1:A:678:GLY:O	2.05	0.75
1:E:488:ARG:HD3	1:E:490:ASP:OD2	1.87	0.74
1:E:95:LEU:HD11	7:E:2278:HOH:O	1.85	0.74
1:E:438:TYR:HD2	7:E:2094:HOH:O	1.69	0.74
1:E:605:LEU:H	1:E:605:LEU:HD23	0.59	0.74
1:E:256:THR:HG21	1:E:305:THR:HA	1.68	0.74
1:A:279:VAL:HG13	1:A:283:THR:CG2	2.14	0.74
1:E:469:PRO:O	1:E:706:MET:HG3	1.87	0.74
1:A:138:GLU:OE2	1:A:402:LYS:HB2	1.87	0.74
1:A:428:GLU:O	1:A:429:PRO:C	2.28	0.74
3:C:173:LEU:HG	3:C:173:LEU:O	1.87	0.74
2:B:41:ARG:HH11	2:B:187:THR:HG23	1.51	0.74
3:G:111:SER:O	3:G:115:LEU:HD12	1.88	0.74
1:E:109:GLU:CG	7:E:2068:HOH:O	2.34	0.74
1:A:388:CYS:HA	1:A:593:TYR:OH	1.86	0.73
1:A:336:TRP:H	1:A:336:TRP:CD1	2.06	0.73
1:A:608:PHE:CD1	1:A:608:PHE:C	2.66	0.73
1:A:457:LYS:HA	7:A:2224:HOH:O	1.88	0.73
1:E:297:THR:HG23	1:E:299:GLU:H	1.52	0.73
1:A:42:GLN:HE22	1:A:505:ARG:HD3	1.52	0.73
1:E:592:LEU:CD2	1:E:603:GLN:HE22	2.02	0.73
2:B:57:GLN:HE22	2:B:140:ARG:HH22	1.34	0.73
2:F:1:MET:HA	7:F:2001:HOH:O	1.89	0.73
1:E:671:ASN:C	1:E:671:ASN:HD22	1.96	0.73
1:A:75:ARG:HH11	1:A:220:GLN:NE2	1.86	0.73
1:E:421:ILE:O	1:E:421:ILE:CG2	2.35	0.73
3:C:235:ALA:O	3:C:239:ARG:HG3	1.89	0.73
1:E:453:LYS:HG2	1:E:475:TRP:CH2	2.24	0.73
1:A:320:ALA:O	1:A:323:LYS:HG2	1.90	0.72
1:A:651:ILE:HD11	1:A:682:VAL:CG1	2.19	0.72
1:E:277:GLU:O	1:E:281:LYS:HG2	1.88	0.72
1:E:539:THR:HG23	1:E:542:GLU:H	1.54	0.72
1:A:393:GLY:HA3	1:A:407:LYS:CE	2.20	0.72
1:E:397:GLU:HB3	1:E:398:PRO:CD	2.19	0.72
1:E:592:LEU:HD23	1:E:603:GLN:NE2	2.04	0.72
1:E:604:PRO:O	1:E:606:PRO:CD	2.37	0.72
3:G:234:ALA:O	3:G:238:ARG:HG3	1.88	0.72
3:C:155:THR:HG21	3:C:239:ARG:CG	2.20	0.72
2:B:16:CYS:O	2:B:18:ALA:N	2.21	0.72
3:C:145:ASN:C	3:C:145:ASN:HD22	1.95	0.72
1:A:153:VAL:HG11	1:A:167:LYS:HE2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ASP:O	1:A:399:GLU:CB	2.32	0.71
1:A:604:PRO:C	1:A:606:PRO:HD2	2.12	0.71
1:E:69:GLU:O	1:E:70:ALA:HB3	1.90	0.71
1:E:75:ARG:HH11	1:E:220:GLN:HE21	1.38	0.71
1:E:431:PRO:HD2	7:E:2262:HOH:O	1.90	0.71
1:E:239:PHE:HB3	1:E:687:ARG:HB3	1.72	0.71
1:A:285:GLY:O	1:A:590:ILE:HG23	1.90	0.71
1:A:170:VAL:O	1:A:175:ALA:CB	2.39	0.71
1:A:519:TRP:NE1	1:A:540:ILE:HG12	2.04	0.71
2:B:160:GLU:H	2:B:179:ASN:ND2	1.86	0.71
1:E:397:GLU:CB	1:E:398:PRO:HD3	2.21	0.71
1:A:428:GLU:HB3	1:A:429:PRO:CD	2.17	0.71
1:A:672:GLN:NE2	1:A:738:PHE:H	1.89	0.71
2:F:67:VAL:HB	2:F:68:PRO:HD3	1.71	0.71
1:E:473:VAL:HG11	7:E:2278:HOH:O	1.90	0.71
1:A:183:TRP:HE1	1:A:413:ARG:HH22	1.39	0.71
1:A:231:LYS:HA	1:A:247:HIS:CD2	2.25	0.70
1:A:342:TYR:CD1	1:A:607:VAL:HB	2.27	0.70
1:A:595:GLN:CG	1:A:595:GLN:O	2.39	0.70
2:F:117:THR:HG23	2:F:120:ALA:H	1.56	0.70
3:G:222:GLN:OE1	3:G:222:GLN:HA	1.91	0.70
1:A:427:GLY:O	1:A:428:GLU:O	2.08	0.70
1:E:38:LYS:HG3	7:E:2024:HOH:O	1.91	0.70
1:E:717:ASN:HD22	5:E:1765:MGD:H192	1.39	0.70
1:A:184:VAL:HG22	1:A:592:LEU:HD23	1.72	0.70
1:E:100:ILE:HG12	1:E:478:VAL:HG22	1.72	0.70
2:F:41:ARG:HH11	2:F:187:THR:HG23	1.55	0.70
3:G:107:LEU:O	3:G:109:LYS:N	2.23	0.70
1:E:113:ARG:NH1	1:E:114:VAL:HG13	2.06	0.70
1:E:478:VAL:HG23	7:E:2283:HOH:O	1.91	0.70
1:E:511:PRO:HB3	1:E:515:THR:CG2	2.21	0.70
1:A:721:THR:HG22	1:A:722:ARG:HG3	1.73	0.70
1:E:75:ARG:HH11	1:E:220:GLN:NE2	1.88	0.70
3:G:206:GLY:HA2	3:G:209:TYR:HB3	1.72	0.70
3:G:21:PHE:O	3:G:238:ARG:NH1	2.25	0.69
2:B:6:MET:HE3	7:B:2045:HOH:O	1.91	0.69
1:E:297:THR:CG2	1:E:299:GLU:H	2.04	0.69
1:A:510:GLU:HG3	7:A:2024:HOH:O	1.92	0.69
1:A:595:GLN:O	1:A:595:GLN:HG3	1.92	0.69
1:A:651:ILE:HD13	1:A:656:ALA:HB2	1.72	0.69
2:B:190:SER:HB3	3:C:252:GLY:N	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:171:TRP:O	3:C:172:ALA:HB2	1.92	0.69
1:E:339:ASP:CB	1:E:607:VAL:HG11	2.22	0.69
1:A:346:ALA:HB2	1:A:605:LEU:CD1	2.22	0.69
1:A:605:LEU:HD23	1:A:605:LEU:N	2.07	0.69
3:C:101:LEU:O	3:C:105:LEU:HD12	1.92	0.69
1:A:209:HIS:HE1	1:A:625:ARG:H	1.41	0.69
1:A:345:MET:HE2	1:A:605:LEU:CD2	2.23	0.69
1:A:625:ARG:HH22	5:A:1765:MGD:H15	1.41	0.69
1:A:377:PRO:HG2	1:A:533:GLN:HG3	1.75	0.69
1:A:395:ASP:C	1:A:399:GLU:HB2	2.18	0.69
1:E:635:GLN:NE2	1:E:635:GLN:H	1.91	0.69
1:A:561:MET:O	1:A:563:THR:N	2.25	0.69
1:A:390:GLY:N	1:A:595:GLN:HE22	1.91	0.68
1:A:467:VAL:HG13	7:A:2050:HOH:O	1.93	0.68
2:B:41:ARG:HD2	2:B:187:THR:HG23	1.75	0.68
3:C:108:LEU:O	3:C:110:LYS:CG	2.42	0.68
1:E:116:THR:HG21	7:E:2074:HOH:O	1.93	0.68
1:A:611:PRO:HB3	7:A:2138:HOH:O	1.91	0.68
1:A:629:HIS:CA	1:A:634:THR:HG21	2.23	0.68
1:A:729:SER:O	1:A:729:SER:OG	2.03	0.68
1:E:183:TRP:HH2	1:E:596:ARG:HD3	1.57	0.68
1:A:367:GLN:HG3	7:A:2272:HOH:O	1.93	0.68
3:C:21:HIS:HE1	3:C:64:LEU:HD11	1.59	0.68
1:E:91:ASP:O	1:E:92:PRO:O	2.12	0.68
1:A:393:GLY:HA3	1:A:407:LYS:NZ	2.07	0.68
3:C:197:GLU:HG2	7:C:2073:HOH:O	1.92	0.68
2:F:40:GLU:HB2	7:F:2022:HOH:O	1.94	0.68
1:E:591:GLU:OE2	1:E:604:PRO:HG3	1.94	0.68
3:G:139:ASN:H	3:G:139:ASN:ND2	1.92	0.68
1:A:232:VAL:H	1:A:247:HIS:HD2	1.40	0.68
1:E:100:ILE:HG23	1:E:478:VAL:HG22	1.74	0.68
1:E:673:ASP:OD2	1:E:721:THR:CG2	2.42	0.68
1:A:166:ALA:HB2	1:A:415:THR:HG23	1.75	0.67
1:E:539:THR:HG22	1:E:542:GLU:CB	2.24	0.67
3:G:76:ILE:O	3:G:80:LEU:HG	1.94	0.67
1:E:388:CYS:HB2	1:E:593:TYR:HH	1.58	0.67
1:E:69:GLU:O	1:E:70:ALA:CB	2.42	0.67
1:A:382:GLU:HA	7:A:2188:HOH:O	1.93	0.67
1:E:577:LYS:HE2	7:E:2323:HOH:O	1.94	0.67
2:F:72:THR:HG23	2:F:89:LYS:HB3	1.77	0.67
2:F:169:GLN:NE2	7:F:2108:HOH:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ARG:NH1	2:B:138:TYR:CE2	2.39	0.67
1:A:422:GLU:HB3	1:A:423:PRO:HD3	1.76	0.67
1:A:79:CYS:HB2	1:A:80:PRO:HD2	1.77	0.67
2:B:47:PRO:O	2:B:48:ASN:OD1	2.13	0.67
1:E:88:THR:HG23	1:E:468:LEU:HD21	1.76	0.67
1:E:648:GLU:HG2	1:E:681:ARG:NH1	2.10	0.67
1:E:734:LEU:HD22	7:E:2420:HOH:O	1.94	0.67
1:A:653:LYS:HD2	1:A:686:ALA:H	1.59	0.66
1:E:118:GLU:HG3	7:E:2307:HOH:O	1.95	0.66
1:A:36:GLU:O	1:A:58:VAL:HG22	1.96	0.66
1:A:209:HIS:O	1:A:213:ASP:HB3	1.94	0.66
1:E:762:GLU:HB2	7:E:2445:HOH:O	1.94	0.66
2:F:3:ARG:HG2	7:F:2003:HOH:O	1.95	0.66
3:G:51:TYR:N	7:G:2015:HOH:O	2.29	0.66
1:E:639:VAL:HG11	2:F:25:MET:HE3	1.78	0.66
2:F:55:PRO:HG2	4:F:1194:SF4:S2	2.34	0.66
3:G:206:GLY:HA2	3:G:209:TYR:CB	2.25	0.66
1:A:673:ASP:OD2	1:A:721:THR:HG21	1.95	0.66
1:E:183:TRP:CH2	1:E:596:ARG:HD3	2.31	0.66
1:E:438:TYR:CD2	7:E:2094:HOH:O	2.47	0.66
1:E:465:ILE:O	1:E:466:ASP:HB3	1.94	0.66
2:F:117:THR:HG21	7:F:2078:HOH:O	1.94	0.66
3:G:115:LEU:HD13	7:G:2032:HOH:O	1.95	0.66
1:E:259:ALA:HB3	7:E:2196:HOH:O	1.96	0.66
1:E:297:THR:CG2	1:E:299:GLU:HG2	2.26	0.66
3:G:12:PHE:CZ	3:G:246:GLN:HG2	2.30	0.66
1:A:301:ALA:O	1:A:305:THR:HB	1.96	0.66
1:A:413:ARG:H	1:A:413:ARG:HD2	1.59	0.66
2:B:46:TYR:CE2	7:B:2033:HOH:O	2.49	0.66
1:E:746:ARG:HG3	1:E:746:ARG:HH11	1.61	0.66
1:A:89:THR:OG1	1:A:484:THR:HG21	1.97	0.65
1:A:342:TYR:HD1	1:A:607:VAL:HB	1.60	0.65
1:A:429:PRO:O	1:A:430:TYR:CG	2.49	0.65
2:F:43:VAL:HG23	7:F:2122:HOH:O	1.96	0.65
2:F:72:THR:HG21	2:F:89:LYS:O	1.95	0.65
2:B:47:PRO:HD3	7:B:2034:HOH:O	1.96	0.65
2:B:72:THR:HG21	2:B:89:LYS:O	1.96	0.65
1:E:591:GLU:O	1:E:591:GLU:HG3	1.96	0.65
1:A:286:PHE:HA	1:A:590:ILE:HG21	1.78	0.65
2:F:57:GLN:HE21	2:F:140:ARG:HH22	1.44	0.65
1:A:186:GLY:H	1:A:583:PHE:HA	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:HIS:CE1	3:C:64:LEU:HD21	2.32	0.65
1:E:477:ASP:C	1:E:478:VAL:HG23	2.15	0.65
1:A:293:VAL:HG13	1:A:293:VAL:O	1.95	0.65
1:A:632:ALA:O	1:A:635:GLN:HG3	1.95	0.65
3:C:21:HIS:ND1	3:C:64:LEU:HG	2.11	0.65
1:E:673:ASP:OD2	1:E:721:THR:HG21	1.96	0.65
1:A:95:LEU:HD12	1:A:467:VAL:C	2.22	0.65
1:A:330:PRO:HD2	7:A:2168:HOH:O	1.96	0.65
1:A:396:HIS:HB3	1:A:403:PRO:HB3	1.78	0.65
1:A:305:THR:O	1:A:306:GLU:HB2	1.96	0.65
3:G:129:TYR:CD2	3:G:130:PRO:HD3	2.31	0.65
7:A:2015:HOH:O	2:B:25:MET:HE1	1.96	0.65
1:E:589:LYS:HB3	1:E:592:LEU:HB2	1.78	0.64
1:A:174:THR:HG23	1:A:178:GLU:HG2	1.80	0.64
1:A:400:GLY:CA	7:A:2196:HOH:O	2.39	0.64
1:A:606:PRO:O	1:A:608:PHE:N	2.29	0.64
1:E:97:ARG:NH2	1:E:763:ARG:HD2	2.11	0.64
1:E:139:ALA:O	1:E:433:LYS:O	2.15	0.64
1:E:602:HIS:CD2	1:E:604:PRO:CD	2.75	0.64
2:F:47:PRO:CD	7:F:2036:HOH:O	2.40	0.64
1:A:134:LYS:HE2	7:A:2079:HOH:O	1.96	0.64
2:B:2:PRO:HB3	2:B:144:ASP:CG	2.22	0.64
1:E:232:VAL:H	1:E:247:HIS:CD2	2.16	0.64
1:E:305:THR:HG23	1:E:307:ILE:HG12	1.79	0.64
1:E:589:LYS:NZ	7:E:2326:HOH:O	2.29	0.64
3:C:241:LEU:C	3:C:241:LEU:CD1	2.69	0.64
1:E:315:VAL:HG12	1:E:319:MET:HE3	1.79	0.64
2:F:3:ARG:HD2	2:F:62:GLU:OE2	1.96	0.64
3:G:150:LEU:O	3:G:154:THR:HB	1.98	0.64
1:E:232:VAL:H	1:E:247:HIS:HD2	1.46	0.64
1:E:311:VAL:CB	7:E:2198:HOH:O	2.45	0.64
1:E:323:LYS:CD	1:E:354:LEU:HA	2.02	0.64
1:E:424:MET:HE2	1:E:455:ALA:CB	2.27	0.64
1:E:589:LYS:HG2	1:E:592:LEU:HD12	1.80	0.64
1:A:642:GLU:HG2	2:B:34:PHE:HZ	1.63	0.64
1:E:71:ASN:HD22	1:E:74:SER:H	1.45	0.64
1:E:116:THR:HG22	1:E:119:GLU:H	1.59	0.64
1:E:346:ALA:N	1:E:605:LEU:HD12	2.13	0.64
1:E:153:VAL:HG11	1:E:167:LYS:HE2	1.80	0.64
3:G:154:THR:HG21	3:G:238:ARG:HG2	1.80	0.64
1:A:483:ALA:HA	1:A:515:THR:CG2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:TRP:CE2	1:A:540:ILE:CG1	2.80	0.64
1:E:575:TRP:O	1:E:578:GLU:HB2	1.97	0.64
3:G:225:LEU:HB3	7:G:2070:HOH:O	1.97	0.64
1:E:686:ALA:HB1	7:E:2386:HOH:O	1.97	0.63
1:E:708:LEU:HA	7:E:2408:HOH:O	1.98	0.63
3:G:154:THR:CG2	3:G:238:ARG:NE	2.58	0.63
1:E:434:GLY:HA2	1:E:461:LEU:O	1.97	0.63
1:A:349:TYR:CE2	1:A:590:ILE:O	2.52	0.63
1:E:100:ILE:HG23	1:E:478:VAL:CG2	2.28	0.63
1:E:465:ILE:O	1:E:466:ASP:CB	2.47	0.63
1:A:152:PHE:O	1:A:157:PRO:HD3	1.98	0.63
1:A:336:TRP:H	1:A:336:TRP:HD1	1.46	0.63
1:A:73:LYS:NZ	1:A:192:HIS:HD2	1.95	0.63
1:A:238:ARG:HG3	1:A:688:ILE:HD12	1.80	0.63
1:A:488:ARG:NH2	5:A:1765:MGD:O6	2.31	0.63
1:A:685:THR:HB	2:B:42:GLU:CD	2.23	0.63
1:A:349:TYR:HE1	1:A:605:LEU:HD21	1.64	0.63
1:A:602:HIS:ND1	1:A:606:PRO:CG	2.58	0.63
2:B:17:ALA:HB1	2:B:20:ALA:HB3	1.81	0.63
1:E:97:ARG:HH21	1:E:763:ARG:NH1	1.95	0.63
1:E:608:PHE:C	7:E:2337:HOH:O	2.33	0.63
1:E:651:ILE:HD11	1:E:682:VAL:CG1	2.29	0.63
1:A:495:VAL:HG13	7:A:2020:HOH:O	1.98	0.63
1:A:335:VAL:HG13	1:A:732:ALA:C	2.23	0.63
1:A:511:PRO:HB3	1:A:515:THR:HG22	1.80	0.63
2:B:134:THR:O	2:B:134:THR:HG22	1.93	0.62
3:C:222:TRP:CG	3:C:223:GLN:N	2.62	0.62
1:E:470:GLN:HG2	1:E:706:MET:SD	2.38	0.62
2:F:160:GLU:H	2:F:179:ASN:ND2	1.96	0.62
1:A:37:VAL:HG12	1:A:38:LYS:N	2.13	0.62
1:A:484:THR:HG22	1:A:487:GLU:HG3	1.81	0.62
1:E:424:MET:HG2	1:E:459:LEU:HD21	1.81	0.62
3:G:206:GLY:O	3:G:209:TYR:CA	2.46	0.62
1:A:166:ALA:HB2	1:A:415:THR:CG2	2.28	0.62
1:A:583:PHE:CE2	1:A:587:SER:C	2.77	0.62
1:A:642:GLU:OE2	2:B:31:PRO:O	2.17	0.62
1:E:30:ALA:HB3	7:E:2002:HOH:O	1.98	0.62
1:E:632:ALA:O	1:E:635:GLN:NE2	2.32	0.62
1:A:127:LYS:HE2	7:A:2227:HOH:O	2.00	0.62
1:E:209:HIS:HE1	1:E:625:ARG:N	1.94	0.62
1:E:622:LEU:HD22	5:E:1766:MGD:H8	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:LYS:O	1:E:256:THR:HB	1.99	0.62
1:E:588:GLY:HA3	7:E:2178:HOH:O	1.99	0.62
1:A:95:LEU:HD11	1:A:468:LEU:O	1.99	0.62
1:E:75:ARG:HD2	1:E:220:GLN:HE22	1.65	0.62
2:F:45:GLU:HB2	7:F:2029:HOH:O	1.99	0.62
1:E:720:GLN:HB3	7:E:2420:HOH:O	2.00	0.61
1:A:75:ARG:HH11	1:A:220:GLN:HE21	1.47	0.61
1:A:195:ILE:HA	1:A:362:GLY:O	2.00	0.61
2:B:78:THR:HG21	7:B:2067:HOH:O	2.00	0.61
3:C:222:TRP:CG	3:C:223:GLN:H	2.17	0.61
1:E:591:GLU:CD	1:E:604:PRO:CB	2.63	0.61
1:A:647:ASN:H	1:A:647:ASN:HD22	1.46	0.61
2:B:121:HIS:O	2:B:125:LYS:HE2	2.00	0.61
1:E:391:PRO:O	1:E:413:ARG:HG2	2.00	0.61
1:E:551:LEU:O	1:E:553:LEU:HB2	2.00	0.61
2:B:46:TYR:O	7:B:2030:HOH:O	2.15	0.61
3:C:18:ASN:OD1	3:C:67:GLU:OE2	2.17	0.61
2:F:78:THR:HG21	7:F:2060:HOH:O	2.00	0.61
7:E:2386:HOH:O	2:F:49:LEU:HD11	2.01	0.61
3:G:196:GLU:CD	3:G:196:GLU:H	2.07	0.61
1:A:183:TRP:CB	1:A:592:LEU:HD22	2.30	0.61
1:A:339:ASP:HB3	1:A:607:VAL:HG11	1.82	0.61
3:C:207:GLY:O	3:C:208:PHE:C	2.41	0.61
1:A:578:GLU:HB3	1:A:580:ARG:HD3	1.82	0.61
1:A:603:GLN:HB3	1:A:604:PRO:CD	2.27	0.61
2:B:44:GLY:O	2:B:49:LEU:HD13	2.01	0.61
1:E:589:LYS:HG2	1:E:592:LEU:CD1	2.31	0.61
1:A:387:GLY:O	1:A:593:TYR:CE1	2.54	0.61
1:A:581:LEU:HD11	7:A:2275:HOH:O	2.00	0.61
1:A:604:PRO:O	1:A:606:PRO:HD3	1.95	0.61
2:B:57:GLN:O	2:B:58:CYS:C	2.43	0.61
2:F:193:HIS:HB2	7:F:2130:HOH:O	2.00	0.61
1:A:581:LEU:CD1	7:A:2275:HOH:O	2.49	0.60
1:E:488:ARG:HB2	1:E:517:PRO:HB3	1.82	0.60
2:F:88:LYS:O	3:G:74:THR:HG22	2.00	0.60
1:A:687:ARG:NH2	2:B:40:GLU:OE2	2.33	0.60
1:A:232:VAL:H	1:A:247:HIS:CD2	2.18	0.60
1:A:293:VAL:O	1:A:293:VAL:CG1	2.48	0.60
1:A:635:GLN:O	1:A:709:ALA:HB2	2.01	0.60
2:F:41:ARG:HD2	2:F:187:THR:HG21	1.80	0.60
1:A:580:ARG:HH11	1:A:580:ARG:HB2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:GLN:HE22	1:A:738:PHE:H	1.46	0.60
1:E:174:THR:HG23	1:E:178:GLU:HG2	1.82	0.60
1:E:633:ARG:HD2	5:E:1765:MGD:O2B	2.01	0.60
1:A:239:PHE:HB3	1:A:687:ARG:HB3	1.84	0.60
1:A:561:MET:HE1	1:A:564:LEU:HD12	1.83	0.60
1:A:314:GLU:HG2	7:A:2165:HOH:O	2.01	0.60
1:A:346:ALA:HB2	1:A:605:LEU:HD13	1.82	0.60
2:B:117:THR:HG22	2:B:119:CYS:N	2.16	0.60
1:A:305:THR:HG22	1:A:307:ILE:H	1.67	0.60
1:E:569:LYS:CD	7:E:2322:HOH:O	2.40	0.60
1:A:71:ASN:HD22	1:A:74:SER:H	1.47	0.60
1:A:338:GLY:O	1:A:726:ASP:HA	2.02	0.60
1:A:349:TYR:CE1	1:A:605:LEU:HD21	2.37	0.60
1:A:428:GLU:O	1:A:430:TYR:N	2.35	0.60
2:B:142:PHE:C	2:B:152:VAL:HG22	2.26	0.60
1:E:297:THR:HG21	7:E:2087:HOH:O	2.01	0.60
1:E:474:MET:HE3	7:E:2070:HOH:O	2.02	0.60
3:C:47:ARG:NH1	3:C:107:TYR:O	2.35	0.60
1:E:267:VAL:HG22	7:E:2200:HOH:O	2.01	0.60
2:F:117:THR:HG22	2:F:119:CYS:H	1.66	0.59
1:A:153:VAL:CG1	1:A:167:LYS:HE2	2.33	0.59
1:E:284:VAL:HG12	1:E:592:LEU:CD1	2.32	0.59
1:A:139:ALA:O	1:A:433:LYS:O	2.20	0.59
1:A:580:ARG:CB	1:A:580:ARG:NH1	2.63	0.59
3:C:171:TRP:O	3:C:171:TRP:HE3	1.81	0.59
1:E:639:VAL:HG21	2:F:25:MET:HE1	1.84	0.59
1:A:231:LYS:HA	1:A:247:HIS:NE2	2.17	0.59
1:A:284:VAL:O	1:A:590:ILE:CG2	2.38	0.59
1:E:604:PRO:C	1:E:606:PRO:HD3	2.28	0.59
1:A:391:PRO:O	1:A:413:ARG:HB3	2.03	0.59
1:A:609:THR:O	1:A:610:PRO:C	2.45	0.59
1:A:183:TRP:HB2	1:A:592:LEU:HD22	1.85	0.59
2:B:44:GLY:O	2:B:49:LEU:CD1	2.50	0.59
2:B:47:PRO:CD	7:B:2034:HOH:O	2.50	0.59
3:C:197:GLU:CD	3:C:197:GLU:H	2.10	0.59
1:E:553:LEU:HD21	1:E:557:THR:HG21	1.85	0.59
1:E:79:CYS:HB2	1:E:80:PRO:HD2	1.85	0.59
1:A:428:GLU:CB	1:A:429:PRO:HD2	2.24	0.59
1:A:642:GLU:HG2	2:B:34:PHE:CZ	2.37	0.59
1:A:658:ARG:C	1:A:659:LEU:O	2.39	0.59
1:E:318:GLU:O	1:E:322:HIS:HD2	1.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:539:THR:CG2	1:E:542:GLU:H	2.16	0.59
1:E:740:ARG:NH1	7:E:2427:HOH:O	2.35	0.59
1:E:585:THR:OG1	1:E:589:LYS:HE3	2.02	0.58
1:A:360:PRO:HD3	1:A:571:TRP:CZ3	2.38	0.58
1:E:607:VAL:O	1:E:607:VAL:HG13	1.98	0.58
1:A:99:LEU:O	1:A:478:VAL:HA	2.04	0.58
1:E:495:VAL:CG2	7:E:2299:HOH:O	2.51	0.58
1:E:597:PHE:HB3	7:E:2327:HOH:O	2.02	0.58
3:G:105:LEU:HG	7:G:2032:HOH:O	2.01	0.58
3:G:207:PHE:HE2	3:G:211:LEU:CD1	2.03	0.58
1:A:152:PHE:O	1:A:157:PRO:CD	2.52	0.58
1:A:539:THR:CG2	1:A:541:GLU:HG2	2.34	0.58
1:E:551:LEU:O	1:E:552:GLY:C	2.47	0.58
2:F:43:VAL:CG2	7:F:2122:HOH:O	2.52	0.58
1:A:335:VAL:HG13	1:A:732:ALA:O	2.00	0.58
1:E:282:TYR:O	1:E:587:SER:HB3	2.03	0.58
1:E:490:ASP:O	7:E:2290:HOH:O	2.17	0.58
2:F:194:HIS:N	7:F:2129:HOH:O	2.35	0.58
3:G:105:LEU:HB3	7:G:2011:HOH:O	2.04	0.58
1:E:310:GLN:NE2	1:E:314:GLU:OE2	2.36	0.58
1:E:708:LEU:O	1:E:712:ARG:HD2	2.04	0.58
1:A:413:ARG:H	1:A:413:ARG:NE	2.00	0.58
1:A:582:PRO:C	7:A:2277:HOH:O	2.46	0.58
2:B:192:VAL:HG12	2:B:193:HIS:N	2.19	0.58
1:A:603:GLN:CB	1:A:604:PRO:HD3	2.27	0.58
1:A:755:LEU:O	1:A:758:ARG:HD3	2.04	0.58
2:B:117:THR:HB	7:B:2010:HOH:O	2.03	0.58
2:F:41:ARG:HH11	2:F:187:THR:HG22	1.68	0.58
1:A:53:ILE:HD12	1:A:65:VAL:HG22	1.86	0.57
3:G:206:GLY:C	3:G:209:TYR:H	2.10	0.57
1:A:653:LYS:CG	1:A:684:PRO:O	2.52	0.57
3:C:171:TRP:O	3:C:172:ALA:CB	2.51	0.57
1:E:670:VAL:HG22	1:E:676:LYS:HG3	1.85	0.57
1:E:672:GLN:NE2	1:E:738:PHE:H	2.02	0.57
1:A:116:THR:HG22	1:A:119:GLU:N	2.10	0.57
1:A:388:CYS:HA	1:A:593:TYR:CE1	2.39	0.57
1:A:631:PHE:O	1:A:698:GLY:HA3	2.04	0.57
1:E:606:PRO:CD	1:E:607:VAL:H	2.15	0.57
1:A:121:LEU:HD13	1:A:524:GLU:HB3	1.86	0.57
1:E:108:GLY:HA3	7:E:2066:HOH:O	2.03	0.57
3:G:221:TRP:HZ3	3:G:225:LEU:HD13	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:78:THR:HG22	2:F:80:ASP:H	1.69	0.57
1:A:120:ALA:HB3	7:A:2068:HOH:O	2.04	0.57
1:A:109:GLU:OE2	1:A:111:LYS:HE2	2.03	0.57
1:E:649:VAL:HG13	1:E:695:ILE:CG2	2.35	0.57
3:C:145:ASN:C	3:C:145:ASN:ND2	2.62	0.57
1:E:297:THR:HG23	1:E:299:GLU:HG2	1.87	0.57
3:C:130:TYR:CD2	3:C:131:PRO:HD3	2.39	0.57
1:E:209:HIS:CE1	1:E:625:ARG:H	2.15	0.57
3:G:38:HIS:CE1	7:G:2011:HOH:O	2.57	0.57
1:A:186:GLY:C	1:A:583:PHE:O	2.48	0.57
1:A:427:GLY:O	1:A:430:TYR:O	2.23	0.57
1:E:539:THR:HG22	1:E:542:GLU:HB2	1.87	0.57
1:A:292:HIS:NE2	1:A:604:PRO:HB2	2.20	0.56
3:C:128:LEU:HD22	7:C:2061:HOH:O	2.05	0.56
1:E:669:LEU:CD2	1:E:741:LEU:HD22	2.35	0.56
1:A:594:CYS:O	1:A:598:LYS:HG3	2.05	0.56
1:A:630:THR:H	1:A:634:THR:HG21	1.70	0.56
3:C:171:TRP:O	3:C:171:TRP:CG	2.58	0.56
1:A:607:VAL:O	1:A:607:VAL:CG1	2.48	0.56
2:B:117:THR:CG2	2:B:120:ALA:H	2.18	0.56
1:E:418:GLN:H	1:E:418:GLN:NE2	2.03	0.56
1:E:479:ILE:O	1:E:480:LEU:HD23	2.06	0.56
1:E:642:GLU:HG3	7:E:2436:HOH:O	2.05	0.56
1:E:658:ARG:C	1:E:659:LEU:O	2.37	0.56
1:A:583:PHE:HE2	1:A:588:GLY:CA	2.17	0.56
1:A:646:GLU:O	1:A:648:GLU:OE2	2.23	0.56
2:B:36:LEU:HD11	7:B:2104:HOH:O	2.05	0.56
7:B:2027:HOH:O	3:C:2:ALA:HB1	2.05	0.56
1:A:382:GLU:HB3	7:A:2189:HOH:O	2.05	0.56
1:A:534:TYR:O	1:A:535:PHE:HB2	2.05	0.56
1:E:591:GLU:O	1:E:603:GLN:NE2	2.39	0.56
1:E:647:ASN:HD21	1:E:714:ALA:H	1.52	0.56
1:A:252:ILE:CD1	1:A:256:THR:HG22	2.35	0.56
1:A:428:GLU:O	1:A:430:TYR:O	2.24	0.56
2:B:88:LYS:O	3:C:75:THR:HG22	2.05	0.56
3:C:59:LEU:O	3:C:63:ILE:HG23	2.06	0.56
1:E:511:PRO:CB	1:E:515:THR:HG22	2.28	0.56
1:E:539:THR:HG22	1:E:542:GLU:HB3	1.87	0.56
1:E:311:VAL:CG2	7:E:2198:HOH:O	2.54	0.56
1:A:37:VAL:HG13	1:A:57:ALA:O	2.07	0.56
1:A:379:LEU:O	1:A:380:PRO:C	2.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ARG:CD	5:A:1765:MGD:O2B	2.54	0.56
3:C:155:THR:CG2	3:C:239:ARG:NE	2.69	0.56
1:A:335:VAL:HG13	1:A:733:GLY:HA2	1.88	0.55
1:A:345:MET:HG2	1:A:592:LEU:HD21	1.88	0.55
1:A:558:MET:HE2	1:A:558:MET:HA	1.87	0.55
2:B:27:ASN:HD21	2:B:121:HIS:CE1	2.24	0.55
2:B:72:THR:HG23	2:B:89:LYS:HB3	1.88	0.55
1:E:647:ASN:H	1:E:647:ASN:HD22	1.52	0.55
2:B:3:ARG:HG2	7:B:2001:HOH:O	2.06	0.55
2:B:57:GLN:NE2	7:B:2045:HOH:O	2.39	0.55
3:C:239:ARG:NH2	7:C:2082:HOH:O	2.37	0.55
1:A:319:MET:HE1	1:A:328:LEU:HD11	1.87	0.55
3:C:17:THR:CG2	3:C:67:GLU:CG	2.77	0.55
1:E:77:ARG:NE	7:E:2048:HOH:O	2.39	0.55
2:F:164:VAL:HG22	2:F:173:PRO:HB2	1.88	0.55
1:A:39:SER:HB2	7:A:2005:HOH:O	2.06	0.55
1:A:345:MET:HE3	1:A:592:LEU:CD1	2.36	0.55
2:B:166:ARG:NH2	3:C:249:GLN:NE2	2.54	0.55
3:C:140:ASN:HD22	3:C:140:ASN:N	2.02	0.55
3:C:207:GLY:C	3:C:209:TRP:N	2.64	0.55
2:F:2:PRO:HB3	2:F:144:ASP:CG	2.31	0.55
1:A:319:MET:CE	1:A:328:LEU:HD11	2.36	0.55
1:E:590:ILE:HB	7:E:2181:HOH:O	2.06	0.55
1:E:687:ARG:NH2	2:F:40:GLU:OE2	2.40	0.55
3:G:220:PHE:HD1	7:G:2066:HOH:O	1.90	0.55
1:A:42:GLN:CD	1:A:505:ARG:HB2	2.31	0.55
1:A:635:GLN:HG3	1:A:701:HIS:NE2	2.22	0.55
1:E:671:ASN:ND2	1:E:673:ASP:H	2.05	0.55
1:E:679:PRO:HG2	1:E:747:PRO:HB3	1.89	0.55
2:B:166:ARG:HH22	3:C:249:GLN:NE2	2.04	0.55
1:E:686:ALA:CB	7:E:2386:HOH:O	2.54	0.55
3:G:30:VAL:HG12	3:G:52:ALA:HB2	1.89	0.55
1:A:42:GLN:O	1:A:53:ILE:HG12	2.06	0.55
3:G:208:TRP:HA	3:G:208:TRP:CE3	2.42	0.55
1:E:90:TYR:OH	1:E:509:HIS:HE1	1.90	0.54
1:E:549:GLN:HG3	7:E:2313:HOH:O	2.08	0.54
1:A:519:TRP:CZ2	1:A:540:ILE:HG13	2.43	0.54
1:A:364:TYR:HB2	1:A:570:PRO:HB3	1.89	0.54
1:A:426:THR:HG23	7:A:2052:HOH:O	2.07	0.54
2:B:114:SER:O	2:B:115:LYS:HB3	2.07	0.54
1:E:204:VAL:HB	1:E:328:LEU:HG	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:345:MET:HB2	1:E:605:LEU:HD13	1.89	0.54
1:E:418:GLN:H	1:E:418:GLN:HE21	1.54	0.54
1:E:684:PRO:O	1:E:685:THR:C	2.49	0.54
1:E:724:LYS:HG2	7:E:2424:HOH:O	2.07	0.54
1:A:427:GLY:C	1:A:428:GLU:O	2.51	0.54
1:E:116:THR:CG2	1:E:119:GLU:N	2.60	0.54
1:E:391:PRO:HG3	1:E:411:PHE:CZ	2.43	0.54
3:G:207:PHE:C	3:G:207:PHE:CD2	2.84	0.54
2:F:44:GLY:O	2:F:45:GLU:HB2	2.08	0.54
1:A:367:GLN:O	1:A:500:PRO:HG3	2.07	0.54
1:A:708:LEU:HD22	1:A:755:LEU:HB3	1.89	0.54
3:G:49:THR:HG21	7:G:2011:HOH:O	2.06	0.54
1:A:75:ARG:NH1	1:A:220:GLN:NE2	2.54	0.54
1:A:204:VAL:HB	1:A:328:LEU:HG	1.90	0.54
1:A:384:ALA:N	7:A:2190:HOH:O	2.32	0.54
1:A:558:MET:CE	1:A:561:MET:SD	2.96	0.54
2:B:57:GLN:HE22	2:B:140:ARG:NH2	2.03	0.54
3:C:112:SER:O	3:C:113:GLN:HG2	2.08	0.54
1:E:204:VAL:HG21	1:E:319:MET:HE2	1.89	0.54
1:E:483:ALA:N	1:E:516:LYS:O	2.30	0.54
1:A:80:PRO:HD3	2:B:18:ALA:HB2	1.90	0.53
1:A:107:ARG:HG2	1:A:475:TRP:O	2.07	0.53
1:A:256:THR:CG2	1:A:305:THR:HA	2.36	0.53
1:A:483:ALA:HA	1:A:515:THR:HG21	1.90	0.53
3:G:156:LEU:HD12	3:G:178:LEU:HD13	1.91	0.53
3:G:240:LEU:C	3:G:240:LEU:HD12	2.33	0.53
1:E:470:GLN:NE2	7:E:2279:HOH:O	2.41	0.53
1:A:471:GLU:O	1:A:471:GLU:HG2	2.09	0.53
1:A:540:ILE:O	1:A:544:LEU:HG	2.08	0.53
1:A:467:VAL:CG2	7:A:2230:HOH:O	2.56	0.53
1:E:129:LEU:O	1:E:133:GLU:HG2	2.07	0.53
1:E:320:ALA:O	1:E:323:LYS:HB2	2.08	0.53
2:F:41:ARG:CD	2:F:187:THR:HG23	2.33	0.53
3:G:115:LEU:HB3	7:G:2032:HOH:O	2.08	0.53
1:A:81:ARG:HE	1:A:214:THR:HG22	1.73	0.53
1:A:592:LEU:O	1:A:593:TYR:CB	2.40	0.53
1:E:109:GLU:HG2	7:E:2068:HOH:O	2.04	0.53
1:E:342:TYR:HD1	1:E:607:VAL:CB	2.18	0.53
1:E:671:ASN:C	1:E:671:ASN:ND2	2.66	0.53
2:F:39:ARG:HD2	2:F:56:GLU:OE2	2.08	0.53
3:G:189:TYR:O	3:G:192:THR:HB	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:PRO:HD3	1:A:534:TYR:OH	2.08	0.53
1:E:186:GLY:HA3	1:E:584:GLY:N	2.24	0.53
1:E:339:ASP:HB2	1:E:607:VAL:CG1	2.27	0.53
1:E:346:ALA:H	1:E:605:LEU:HD12	1.73	0.53
1:E:591:GLU:OE1	1:E:604:PRO:CA	2.56	0.53
2:F:166:ARG:HH22	3:G:248:GLN:HE21	1.57	0.53
1:A:357:TYR:HA	1:A:363:PHE:HB2	1.90	0.53
1:E:497:HIS:O	1:E:498:LYS:C	2.51	0.53
1:E:590:ILE:O	1:E:592:LEU:HG	2.09	0.53
1:E:632:ALA:C	1:E:635:GLN:NE2	2.66	0.53
1:A:122:ASP:OD1	1:A:528:ARG:NH1	2.41	0.53
1:A:193:GLU:HG2	7:A:2120:HOH:O	2.09	0.53
1:A:346:ALA:HB2	1:A:605:LEU:HD12	1.91	0.53
1:A:519:TRP:CD1	1:A:540:ILE:HG21	2.44	0.53
1:A:602:HIS:CD2	1:A:604:PRO:HD2	2.44	0.53
3:C:207:GLY:HA2	3:C:210:TYR:HB3	1.91	0.53
1:A:277:GLU:HB3	1:A:281:LYS:HZ2	1.74	0.52
1:E:91:ASP:C	1:E:92:PRO:O	2.52	0.52
1:E:651:ILE:HD13	1:E:656:ALA:HB2	1.89	0.52
1:A:231:LYS:HB2	1:A:247:HIS:CD2	2.45	0.52
1:A:428:GLU:OE2	1:A:428:GLU:HA	2.03	0.52
2:B:57:GLN:NE2	2:B:140:ARG:HH22	2.05	0.52
1:E:286:PHE:C	1:E:288:GLU:H	2.16	0.52
1:E:607:VAL:HG23	7:E:2149:HOH:O	2.09	0.52
1:A:388:CYS:HA	1:A:593:TYR:CZ	2.44	0.52
1:A:607:VAL:HG13	1:A:609:THR:CB	2.38	0.52
3:G:226:ALA:HB3	3:G:227:PRO:HD3	1.90	0.52
1:A:285:GLY:C	1:A:590:ILE:HG23	2.34	0.52
1:A:558:MET:HE2	1:A:561:MET:SD	2.50	0.52
1:A:583:PHE:CZ	1:A:587:SER:HA	2.45	0.52
2:B:117:THR:HG22	2:B:119:CYS:H	1.75	0.52
1:E:286:PHE:CB	7:E:2181:HOH:O	2.57	0.52
1:E:519:TRP:CE2	1:E:540:ILE:CG1	2.92	0.52
1:A:53:ILE:HD12	1:A:65:VAL:CG2	2.40	0.52
1:A:295:ASP:HB2	7:A:2160:HOH:O	2.09	0.52
1:A:413:ARG:HD2	1:A:413:ARG:N	2.24	0.52
3:G:70:ARG:HG2	3:G:71:PHE:H	1.74	0.52
3:G:39:LEU:HD13	3:G:116:ALA:HB3	1.92	0.52
1:E:279:VAL:O	1:E:283:THR:HB	2.09	0.52
1:E:586:ALA:HB3	7:E:2326:HOH:O	2.09	0.52
1:E:622:LEU:HD22	7:E:2426:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:GLU:HB2	7:A:2205:HOH:O	2.09	0.52
1:A:636:ASN:HB2	1:A:706:MET:HE2	1.92	0.52
1:E:81:ARG:HE	1:E:214:THR:HG22	1.75	0.51
3:G:222:GLN:C	7:G:2070:HOH:O	2.53	0.51
1:A:678:GLY:HA3	7:A:2329:HOH:O	2.10	0.51
1:E:539:THR:HG23	1:E:541:GLU:HG2	1.93	0.51
1:A:708:LEU:HD23	1:A:708:LEU:N	2.25	0.51
2:B:140:ARG:NH2	7:B:2045:HOH:O	2.43	0.51
1:E:209:HIS:CG	5:E:1766:MGD:H5'1	2.46	0.51
1:A:187:ARG:NH2	1:A:367:GLN:NE2	2.58	0.51
1:A:286:PHE:CA	1:A:590:ILE:HG21	2.40	0.51
1:E:273:LEU:O	1:E:323:LYS:NZ	2.35	0.51
2:B:192:VAL:HG12	2:B:193:HIS:H	1.75	0.51
1:E:93:ASP:OD1	1:E:758:ARG:NH2	2.44	0.51
1:E:281:LYS:HG3	1:E:282:TYR:CE1	2.46	0.51
1:E:474:MET:HE2	1:E:705:LEU:CD1	2.40	0.51
1:A:118:GLU:H	1:A:118:GLU:CD	2.17	0.51
1:A:630:THR:N	1:A:634:THR:HG21	2.26	0.51
1:E:345:MET:CB	1:E:605:LEU:HD13	2.41	0.51
1:A:93:ASP:CG	1:A:758:ARG:HH22	2.18	0.51
1:A:134:LYS:CE	7:A:2079:HOH:O	2.56	0.51
1:A:358:GLY:O	1:A:571:TRP:HA	2.11	0.51
2:B:183:LYS:HE3	7:B:2143:HOH:O	2.11	0.51
1:E:45:GLU:HG3	7:E:2012:HOH:O	2.10	0.51
1:E:359:ARG:HD3	7:E:2101:HOH:O	2.10	0.51
1:E:635:GLN:O	1:E:641:MET:HG2	2.05	0.51
1:E:635:GLN:NE2	1:E:635:GLN:N	2.56	0.51
1:E:642:GLU:OE2	2:F:32:GLY:N	2.28	0.51
3:G:207:PHE:O	3:G:211:LEU:N	2.44	0.51
1:A:113:ARG:NH2	7:A:2066:HOH:O	2.43	0.51
1:A:421:ILE:HG22	1:A:421:ILE:O	2.10	0.51
1:A:429:PRO:C	1:A:430:TYR:CD2	2.88	0.51
1:A:457:LYS:HD3	7:A:2225:HOH:O	2.11	0.51
1:A:635:GLN:C	1:A:709:ALA:HB2	2.36	0.51
3:C:67:GLU:O	3:C:67:GLU:HG2	2.11	0.51
3:C:140:ASN:O	3:C:142:PRO:HD3	2.11	0.51
1:E:519:TRP:CE2	1:E:540:ILE:HG13	2.46	0.51
1:A:519:TRP:CG	1:A:540:ILE:HG21	2.46	0.51
2:B:2:PRO:HB3	2:B:144:ASP:HB2	1.93	0.51
2:F:67:VAL:CB	2:F:68:PRO:HD3	2.41	0.51
1:A:535:PHE:N	1:A:536:PRO:CD	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:TRP:O	1:A:156:LEU:HB2	2.11	0.50
1:A:336:TRP:O	1:A:735:ARG:HB2	2.10	0.50
1:A:580:ARG:HB2	1:A:580:ARG:NH1	2.25	0.50
1:E:396:HIS:CE1	1:E:404:ARG:H	2.29	0.50
1:E:553:LEU:CD2	1:E:557:THR:HG21	2.40	0.50
3:G:66:GLU:O	3:G:66:GLU:HG2	2.12	0.50
2:B:2:PRO:HD2	2:B:80:ASP:OD2	2.10	0.50
2:B:121:HIS:O	2:B:125:LYS:CE	2.58	0.50
1:E:99:LEU:O	1:E:478:VAL:HA	2.12	0.50
1:E:422:GLU:H	1:E:423:PRO:HD2	1.76	0.50
1:E:396:HIS:HB3	1:E:407:LYS:HE3	1.94	0.50
1:E:568:GLY:O	1:E:570:PRO:HD3	2.12	0.50
1:A:483:ALA:CA	1:A:515:THR:HG23	2.42	0.50
1:A:605:LEU:N	1:A:606:PRO:CD	2.73	0.50
2:B:72:THR:CG2	2:B:74:ALA:H	2.18	0.50
1:E:397:GLU:CG	1:E:398:PRO:HD3	2.42	0.50
3:G:46:ARG:HG3	7:G:2014:HOH:O	2.10	0.50
1:A:152:PHE:O	1:A:157:PRO:CG	2.60	0.50
1:E:336:TRP:O	1:E:340:ASP:OD1	2.30	0.50
3:G:189:TYR:HB3	3:G:190:PRO:HD3	1.94	0.50
1:E:37:VAL:HA	1:E:57:ALA:O	2.12	0.49
1:E:284:VAL:HG12	1:E:592:LEU:HD12	1.93	0.49
2:F:46:TYR:CD1	2:F:46:TYR:C	2.88	0.49
3:G:76:ILE:HG12	3:G:80:LEU:HD11	1.94	0.49
2:B:32:GLY:N	7:B:2011:HOH:O	2.43	0.49
2:B:117:THR:O	2:B:117:THR:HG23	2.12	0.49
1:E:88:THR:HG21	1:E:467:VAL:HG11	1.92	0.49
3:G:144:ASN:C	3:G:144:ASN:HD22	2.19	0.49
1:A:285:GLY:C	1:A:590:ILE:CG2	2.86	0.49
1:A:415:THR:HG22	7:A:2204:HOH:O	2.13	0.49
1:A:689:ARG:NH2	1:A:691:ASP:OD2	2.41	0.49
1:E:209:HIS:CD2	5:E:1766:MGD:H5'1	2.48	0.49
1:E:632:ALA:C	1:E:635:GLN:HE22	2.20	0.49
1:A:79:CYS:CB	1:A:80:PRO:HD2	2.42	0.49
1:A:337:TYR:O	1:A:340:ASP:CG	2.47	0.49
1:A:536:PRO:HG2	1:A:537:TRP:H	1.77	0.49
1:A:647:ASN:HD21	1:A:714:ALA:H	1.61	0.49
2:B:2:PRO:HB3	2:B:144:ASP:CB	2.42	0.49
1:E:208:HIS:HE1	1:E:218:GLN:NE2	2.10	0.49
1:E:635:GLN:H	1:E:635:GLN:HE21	1.60	0.49
2:F:72:THR:HG22	2:F:74:ALA:N	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:CYS:O	1:A:391:PRO:HD3	2.12	0.49
1:A:525:LEU:O	1:A:529:LEU:HG	2.12	0.49
1:E:311:VAL:HG23	7:E:2198:HOH:O	2.10	0.49
1:A:320:ALA:O	1:A:323:LYS:CG	2.60	0.49
3:C:20:LEU:HD13	3:C:63:ILE:HD13	1.94	0.49
1:A:395:ASP:CA	1:A:399:GLU:CG	2.72	0.49
1:A:583:PHE:CE2	1:A:588:GLY:CA	2.93	0.49
1:E:324:PRO:HD2	7:E:2213:HOH:O	2.10	0.49
1:A:36:GLU:O	1:A:36:GLU:HG2	2.13	0.49
7:E:2167:HOH:O	2:F:46:TYR:HB2	2.12	0.49
1:A:48:PHE:HE1	1:A:145:HIS:CE1	2.30	0.49
2:B:22:ALA:HB2	2:B:134:THR:HG21	1.95	0.49
2:B:57:GLN:CD	7:B:2045:HOH:O	2.56	0.49
1:E:69:GLU:HA	7:E:2042:HOH:O	2.11	0.49
1:E:598:LYS:HB3	1:E:599:GLU:OE1	2.13	0.49
3:G:144:ASN:OD1	3:G:192:THR:CG2	2.61	0.49
1:A:554:ASP:OD2	1:A:554:ASP:N	2.46	0.49
1:A:69:GLU:C	7:A:2034:HOH:O	2.37	0.48
1:E:621:LEU:HD22	1:E:622:LEU:O	2.12	0.48
1:A:468:LEU:HD13	1:A:706:MET:HE3	1.94	0.48
1:A:710:HIS:O	7:A:2345:HOH:O	2.20	0.48
1:E:186:GLY:H	1:E:583:PHE:HA	1.78	0.48
1:E:81:ARG:HD2	1:E:630:THR:OG1	2.13	0.48
1:E:454:GLU:HG2	7:E:2274:HOH:O	2.13	0.48
1:E:467:VAL:HG12	1:E:468:LEU:HG	1.94	0.48
1:E:519:TRP:NE1	1:E:540:ILE:HG12	2.28	0.48
3:G:38:HIS:CE1	3:G:105:LEU:HD22	2.48	0.48
1:A:345:MET:CE	1:A:592:LEU:HD11	2.41	0.48
1:A:572:LEU:HD22	7:A:2275:HOH:O	2.13	0.48
1:A:647:ASN:C	1:A:648:GLU:CG	2.85	0.48
1:E:685:THR:HG22	2:F:42:GLU:OE2	2.13	0.48
1:A:81:ARG:HE	1:A:214:THR:CG2	2.27	0.48
1:A:96:LYS:HB3	1:A:513:PHE:HB3	1.96	0.48
3:C:21:HIS:CD2	3:C:21:HIS:C	2.92	0.48
3:G:221:TRP:HD1	7:G:2035:HOH:O	1.96	0.48
3:G:225:LEU:CB	7:G:2070:HOH:O	2.59	0.48
1:A:81:ARG:HH21	1:A:214:THR:HG22	1.77	0.48
1:A:284:VAL:CG2	1:A:587:SER:HB3	2.38	0.48
1:E:225:ALA:O	1:E:230:ALA:HB3	2.14	0.48
1:E:342:TYR:CE1	1:E:607:VAL:HB	2.46	0.48
1:E:371:LEU:HD13	1:E:547:ARG:CZ	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:512:LEU:O	1:E:515:THR:HB	2.14	0.48
3:G:206:GLY:CA	3:G:209:TYR:CB	2.90	0.48
1:E:100:ILE:HG12	1:E:478:VAL:CG2	2.42	0.48
1:E:345:MET:HB3	1:E:605:LEU:CD1	2.44	0.48
3:G:40:LYS:HG3	3:G:40:LYS:O	2.14	0.48
1:A:183:TRP:HB3	1:A:592:LEU:HD22	1.95	0.48
1:A:519:TRP:CZ2	1:A:540:ILE:CG1	2.97	0.48
1:A:585:THR:O	1:A:585:THR:HG22	2.12	0.48
2:B:122:ARG:HB3	2:B:127:LYS:HB2	1.95	0.48
3:C:174:PHE:H	3:C:175:PRO:HD2	1.79	0.48
1:E:41:TYR:HE1	1:E:560:GLY:O	1.97	0.48
1:E:391:PRO:HG2	1:E:392:SER:H	1.77	0.48
1:E:701:HIS:O	1:E:710:HIS:O	2.30	0.48
1:A:71:ASN:HD21	1:A:73:LYS:HB2	1.78	0.48
1:A:454:GLU:HG2	7:A:2101:HOH:O	2.14	0.48
1:A:673:ASP:OD2	1:A:721:THR:CG2	2.61	0.48
2:B:155:ALA:HB1	7:B:2113:HOH:O	2.14	0.48
3:C:140:ASN:ND2	3:C:140:ASN:N	2.59	0.48
3:G:172:LEU:O	3:G:176:ARG:HG3	2.14	0.48
1:A:591:GLU:CB	1:A:603:GLN:HE22	2.23	0.48
1:A:592:LEU:C	1:A:592:LEU:HD13	2.38	0.48
1:A:599:GLU:HB2	7:A:2281:HOH:O	2.14	0.48
2:F:115:LYS:HG3	2:F:116:CYS:O	2.14	0.47
1:A:393:GLY:HA3	1:A:407:LYS:HZ1	1.80	0.47
2:B:36:LEU:CD1	7:B:2104:HOH:O	2.62	0.47
1:A:305:THR:HG23	1:A:307:ILE:HD12	1.96	0.47
1:A:390:GLY:H	1:A:595:GLN:NE2	2.09	0.47
1:A:422:GLU:HB3	1:A:423:PRO:CD	2.43	0.47
2:B:27:ASN:HD21	2:B:121:HIS:HE1	1.61	0.47
1:E:474:MET:HE2	1:E:705:LEU:HD11	1.96	0.47
1:A:276:LYS:CA	7:A:2152:HOH:O	2.49	0.47
1:A:428:GLU:CB	1:A:429:PRO:CD	2.89	0.47
1:A:73:LYS:NZ	1:A:192:HIS:CD2	2.79	0.47
2:B:117:THR:CG2	2:B:117:THR:O	2.60	0.47
1:E:606:PRO:CG	1:E:607:VAL:N	2.77	0.47
1:A:239:PHE:O	1:A:687:ARG:HD2	2.15	0.47
1:A:364:TYR:HB2	1:A:570:PRO:CB	2.45	0.47
1:A:671:ASN:HD21	1:A:675:VAL:H	1.63	0.47
7:B:2075:HOH:O	3:C:82:SER:HB3	2.14	0.47
1:E:160:TRP:O	1:E:160:TRP:CG	2.67	0.47
1:A:654:GLU:HG3	7:A:2317:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:GLU:HB3	7:E:2005:HOH:O	2.14	0.47
1:E:81:ARG:HE	1:E:214:THR:CG2	2.27	0.47
1:E:81:ARG:NE	1:E:214:THR:HG22	2.29	0.47
1:E:100:ILE:HG12	1:E:478:VAL:HG13	1.96	0.47
1:E:201:ARG:HD3	7:E:2124:HOH:O	2.14	0.47
2:F:190:SER:O	2:F:194:HIS:N	2.47	0.47
1:A:195:ILE:HG12	1:A:329:PRO:HB3	1.97	0.47
1:A:548:LEU:C	1:A:553:LEU:O	2.58	0.47
1:A:683:LYS:HA	1:A:684:PRO:HD2	1.67	0.47
2:F:16:CYS:SG	2:F:16:CYS:O	2.73	0.47
3:G:70:ARG:HG2	3:G:71:PHE:N	2.29	0.47
1:A:396:HIS:CB	1:A:403:PRO:HB3	2.44	0.47
1:E:677:GLU:O	1:E:678:GLY:O	2.33	0.47
1:A:214:THR:HG23	1:A:214:THR:O	2.15	0.47
1:A:336:TRP:CD1	1:A:336:TRP:N	2.73	0.47
7:A:2041:HOH:O	2:B:133:GLU:HG3	2.15	0.47
1:E:119:GLU:HG2	7:E:2076:HOH:O	2.15	0.47
1:E:519:TRP:CE2	1:E:540:ILE:HG12	2.49	0.47
1:A:103:GLU:OE1	1:A:103:GLU:HA	2.15	0.46
1:A:519:TRP:CG	1:A:540:ILE:CG2	2.97	0.46
1:A:655:GLU:CD	1:A:658:ARG:HH22	2.23	0.46
2:B:47:PRO:CG	7:B:2034:HOH:O	2.63	0.46
2:F:78:THR:CG2	2:F:79:LYS:N	2.79	0.46
1:A:289:LEU:HD12	1:A:590:ILE:HD11	1.97	0.46
1:A:470:GLN:HE21	1:A:470:GLN:HB3	1.39	0.46
2:B:86:ASP:OD1	2:B:88:LYS:HB2	2.15	0.46
1:E:606:PRO:HG2	1:E:607:VAL:N	2.31	0.46
2:F:172:ARG:N	2:F:173:PRO:HD3	2.30	0.46
1:A:530:GLY:HA2	1:A:532:GLU:OE2	2.15	0.46
1:A:592:LEU:O	1:A:592:LEU:HD13	2.15	0.46
2:B:46:TYR:CD2	7:B:2033:HOH:O	2.68	0.46
1:A:187:ARG:HH22	1:A:367:GLN:NE2	2.13	0.46
1:A:231:LYS:CA	1:A:247:HIS:CD2	2.98	0.46
3:C:17:THR:HG22	3:C:18:ASN:N	2.31	0.46
3:C:68:SER:O	3:C:71:ARG:HB3	2.16	0.46
3:C:151:LEU:O	3:C:155:THR:HB	2.16	0.46
1:E:142:PHE:CG	1:E:157:PRO:HG3	2.50	0.46
1:E:755:LEU:O	1:E:758:ARG:HD3	2.15	0.46
1:E:651:ILE:HD11	1:E:682:VAL:HG13	1.96	0.46
2:F:29:VAL:HA	2:F:30:PRO:HD3	1.71	0.46
2:F:166:ARG:HH22	3:G:248:GLN:NE2	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LYS:HB2	1:A:247:HIS:CG	2.50	0.46
1:A:558:MET:HE1	1:A:561:MET:SD	2.56	0.46
1:E:576:GLU:C	1:E:578:GLU:H	2.23	0.46
3:G:107:LEU:C	3:G:109:LYS:H	2.22	0.46
1:A:132:ARG:CD	7:A:2077:HOH:O	2.63	0.46
1:E:627:PRO:HB2	2:F:16:CYS:HA	1.97	0.46
1:E:630:THR:HG23	7:E:2452:HOH:O	2.15	0.46
1:A:523:ARG:HG3	1:A:535:PHE:HB3	1.97	0.46
1:A:583:PHE:HB3	1:A:584:GLY:H	1.10	0.46
2:B:139:CYS:SG	4:B:1194:SF4:S3	3.13	0.46
1:E:724:LYS:CG	7:E:2424:HOH:O	2.64	0.46
3:G:70:ARG:CG	3:G:71:PHE:N	2.78	0.46
1:A:75:ARG:HD2	1:A:220:GLN:NE2	2.25	0.46
1:A:195:ILE:N	1:A:195:ILE:HD12	2.30	0.46
1:A:231:LYS:HB3	1:A:231:LYS:HE3	1.68	0.46
1:A:310:GLN:HG3	7:A:2164:HOH:O	2.16	0.46
1:A:519:TRP:CD2	1:A:540:ILE:HG23	2.50	0.46
1:E:252:ILE:HG12	1:E:256:THR:HG22	1.98	0.46
1:E:336:TRP:O	1:E:338:GLY:N	2.49	0.46
1:A:627:PRO:HB2	2:B:16:CYS:HA	1.98	0.45
1:E:153:VAL:CG1	1:E:167:LYS:HE2	2.46	0.45
1:E:495:VAL:HG21	7:E:2299:HOH:O	2.15	0.45
2:F:35:ASN:HD22	2:F:106:TYR:HE2	1.64	0.45
7:B:2081:HOH:O	3:C:251:LEU:HD11	2.15	0.45
3:C:50:THR:O	3:C:54:LEU:HG	2.16	0.45
1:E:97:ARG:HH22	1:E:763:ARG:HD2	1.80	0.45
1:E:305:THR:HG23	1:E:307:ILE:H	1.78	0.45
1:E:345:MET:CB	1:E:605:LEU:CD1	2.94	0.45
1:E:247:HIS:CE1	7:E:2150:HOH:O	2.69	0.45
1:A:183:TRP:HB3	1:A:592:LEU:O	2.16	0.45
1:E:81:ARG:NH1	1:E:630:THR:OG1	2.39	0.45
1:E:166:ALA:HB2	1:E:415:THR:CG2	2.45	0.45
1:E:647:ASN:HD22	1:E:647:ASN:N	2.10	0.45
3:G:86:SER:O	3:G:87:PRO:C	2.57	0.45
1:A:647:ASN:HD22	1:A:647:ASN:N	2.10	0.45
3:C:208:PHE:C	3:C:208:PHE:CD2	2.93	0.45
3:C:222:TRP:CD1	3:C:222:TRP:C	2.94	0.45
1:E:397:GLU:HB3	7:E:2242:HOH:O	2.16	0.45
1:E:591:GLU:OE2	1:E:604:PRO:HB3	2.15	0.45
1:E:592:LEU:HA	1:E:603:GLN:HE21	0.65	0.45
3:G:139:ASN:ND2	7:G:2043:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLU:OE2	1:A:313:ARG:NH2	2.30	0.45
1:A:369:PRO:HG2	1:A:494:LEU:HB3	1.99	0.45
1:A:483:ALA:HA	1:A:515:THR:HG23	1.95	0.45
1:E:93:ASP:O	1:E:469:PRO:HD3	2.16	0.45
1:E:149:ASP:CB	7:E:2094:HOH:O	2.64	0.45
1:E:335:VAL:HG13	1:E:732:ALA:O	2.17	0.45
1:A:37:VAL:CG1	1:A:38:LYS:N	2.78	0.45
1:A:305:THR:CG2	1:A:307:ILE:HB	2.47	0.45
2:B:41:ARG:NH1	2:B:187:THR:HG23	2.21	0.45
1:E:265:ILE:HD11	1:E:349:TYR:HB2	1.98	0.45
2:F:35:ASN:ND2	2:F:106:TYR:HE2	2.15	0.45
1:E:426:THR:C	1:E:428:GLU:N	2.75	0.45
1:E:591:GLU:OE2	1:E:604:PRO:CG	2.64	0.45
2:F:88:LYS:O	3:G:74:THR:CG2	2.63	0.45
2:F:27:ASN:O	2:F:28:GLU:C	2.60	0.45
3:G:100:LEU:HB3	7:G:2031:HOH:O	2.17	0.45
1:A:548:LEU:HD13	1:A:558:MET:HB2	1.99	0.45
2:B:55:PRO:HB2	7:B:2104:HOH:O	2.16	0.45
3:C:77:ILE:HG12	3:C:81:LEU:HD11	1.99	0.45
3:C:108:LEU:HB3	3:C:110:LYS:HG3	1.99	0.45
3:C:190:TYR:HB3	3:C:191:PRO:HD3	1.99	0.45
1:E:553:LEU:HD21	1:E:557:THR:CG2	2.47	0.45
3:G:132:LEU:O	3:G:136:VAL:HB	2.17	0.45
1:A:335:VAL:HG13	1:A:733:GLY:CA	2.46	0.44
1:E:97:ARG:HH21	1:E:763:ARG:CZ	2.31	0.44
1:E:380:PRO:HD3	1:E:534:TYR:OH	2.16	0.44
3:G:206:GLY:HA2	3:G:209:TYR:HB2	1.98	0.44
2:B:191:GLU:HG3	7:B:2144:HOH:O	2.17	0.44
3:C:21:HIS:CE1	3:C:64:LEU:CG	3.00	0.44
1:E:397:GLU:CB	1:E:398:PRO:CD	2.88	0.44
1:E:591:GLU:O	1:E:591:GLU:CG	2.64	0.44
1:A:64:LYS:HE2	2:B:26:GLU:HB2	1.98	0.44
1:A:107:ARG:HB2	7:A:2224:HOH:O	2.16	0.44
1:E:651:ILE:HD11	1:E:682:VAL:HG12	1.99	0.44
3:C:248:TRP:CE2	3:C:250:GLY:HA3	2.53	0.44
1:E:48:PHE:CZ	1:E:145:HIS:CE1	3.05	0.44
1:E:620:ARG:HB3	7:E:2392:HOH:O	2.17	0.44
1:A:449:VAL:O	1:A:453:LYS:HG3	2.17	0.44
1:A:512:LEU:O	1:A:515:THR:HB	2.17	0.44
1:A:686:ALA:CB	7:A:2331:HOH:O	2.52	0.44
1:E:308:PRO:CB	7:E:2198:HOH:O	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LYS:CE	2:B:26:GLU:HB2	2.47	0.44
1:A:349:TYR:HH	1:A:591:GLU:C	2.10	0.44
1:E:186:GLY:HA3	1:E:583:PHE:C	2.43	0.44
1:E:197:TRP:CG	1:E:221:ASP:HB3	2.53	0.44
3:C:172:ALA:CA	3:C:175:PRO:HG2	2.39	0.44
1:E:469:PRO:O	1:E:706:MET:CG	2.63	0.44
3:G:52:ALA:O	3:G:56:ILE:HG13	2.18	0.44
1:A:116:THR:HG23	1:A:118:GLU:N	2.33	0.44
1:A:305:THR:CG2	1:A:307:ILE:H	2.31	0.44
1:A:540:ILE:HG13	1:A:540:ILE:H	1.63	0.44
3:C:108:LEU:O	3:C:109:GLY:C	2.61	0.44
1:E:519:TRP:CZ2	1:E:540:ILE:HG13	2.53	0.44
1:A:75:ARG:NH1	1:A:220:GLN:HE21	2.11	0.44
1:A:81:ARG:HH21	1:A:214:THR:CG2	2.30	0.44
1:A:232:VAL:N	1:A:247:HIS:HD2	2.11	0.44
1:E:75:ARG:NH1	1:E:220:GLN:HE21	2.11	0.44
1:E:239:PHE:CB	1:E:687:ARG:HB3	2.44	0.44
1:E:327:VAL:HG13	1:E:362:GLY:HA2	1.99	0.44
1:E:428:GLU:O	1:E:430:TYR:CA	2.65	0.44
1:A:43:ILE:HB	1:A:505:ARG:HH21	1.83	0.43
1:A:116:THR:HG22	1:A:119:GLU:CB	2.43	0.43
1:A:124:ILE:HD11	1:A:478:VAL:HG11	2.00	0.43
1:A:404:ARG:HG3	1:A:406:ASP:OD2	2.18	0.43
1:A:534:TYR:O	1:A:535:PHE:CB	2.66	0.43
1:A:569:LYS:HA	1:A:570:PRO:HD3	1.76	0.43
1:E:256:THR:CG2	1:E:305:THR:HA	2.42	0.43
1:E:412:ALA:HB1	1:E:413:ARG:NH1	2.33	0.43
1:E:214:THR:HG21	1:E:627:PRO:O	2.17	0.43
1:E:287:GLU:OE1	1:E:287:GLU:N	2.51	0.43
1:E:601:GLY:HA2	7:E:2334:HOH:O	2.18	0.43
1:E:606:PRO:CG	1:E:607:VAL:H	2.31	0.43
1:E:606:PRO:CD	1:E:607:VAL:N	2.81	0.43
1:E:623:TYR:HA	1:E:695:ILE:O	2.18	0.43
1:A:284:VAL:HG12	1:A:285:GLY:N	2.33	0.43
1:A:548:LEU:O	1:A:553:LEU:O	2.36	0.43
3:C:222:TRP:CD1	3:C:223:GLN:N	2.86	0.43
2:F:63:ASN:HB2	7:F:2111:HOH:O	2.18	0.43
3:G:240:LEU:C	3:G:240:LEU:CD1	2.91	0.43
1:A:256:THR:HG23	1:A:256:THR:O	2.17	0.43
1:A:483:ALA:CA	1:A:515:THR:CG2	2.95	0.43
1:E:299:GLU:OE2	1:E:313:ARG:NH2	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:609:THR:HG23	7:E:2338:HOH:O	2.18	0.43
1:E:672:GLN:NE2	1:E:672:GLN:H	2.17	0.43
3:G:227:PRO:O	3:G:231:LEU:HB2	2.18	0.43
1:A:430:TYR:HB2	1:A:431:PRO:HD3	2.01	0.43
3:C:21:HIS:CE1	3:C:64:LEU:HD11	2.45	0.43
1:E:81:ARG:HB2	4:E:1764:SF4:S3	2.58	0.43
1:E:107:ARG:O	1:E:108:GLY:C	2.58	0.43
1:E:112:TYR:CZ	1:E:474:MET:O	2.71	0.43
3:G:46:ARG:CG	7:G:2014:HOH:O	2.67	0.43
1:A:583:PHE:CZ	1:A:587:SER:CA	3.01	0.43
1:A:591:GLU:O	1:A:592:LEU:CD1	2.62	0.43
1:A:596:ARG:NH1	1:A:600:ALA:CB	2.81	0.43
1:E:95:LEU:CD1	7:E:2278:HOH:O	2.58	0.43
1:E:116:THR:HG23	1:E:119:GLU:N	2.19	0.43
1:E:149:ASP:HA	7:E:2094:HOH:O	2.17	0.43
1:E:313:ARG:HD3	1:E:317:ARG:NH2	2.34	0.43
1:E:647:ASN:H	1:E:647:ASN:ND2	2.17	0.43
2:F:117:THR:HG23	2:F:117:THR:O	2.17	0.43
3:G:207:PHE:HB3	3:G:208:TRP:H	1.43	0.43
1:A:605:LEU:CD2	1:A:605:LEU:N	2.70	0.43
1:A:761:ASP:C	1:A:763:ARG:H	2.26	0.43
1:E:470:GLN:O	1:E:471:GLU:C	2.60	0.43
1:E:622:LEU:HB2	1:E:693:VAL:O	2.19	0.43
2:F:147:ASP:O	2:F:150:SER:HB2	2.17	0.43
1:A:193:GLU:CG	7:A:2120:HOH:O	2.65	0.43
1:A:286:PHE:HA	1:A:590:ILE:CG2	2.47	0.43
1:E:346:ALA:N	1:E:605:LEU:CD1	2.79	0.43
1:E:453:LYS:HG2	1:E:475:TRP:CZ2	2.53	0.43
1:E:620:ARG:O	1:E:620:ARG:CG	2.66	0.43
1:E:708:LEU:HD22	7:E:2408:HOH:O	2.18	0.43
1:E:717:ASN:ND2	5:E:1765:MGD:H192	2.11	0.43
1:A:342:TYR:CD2	1:A:605:LEU:HA	2.54	0.43
1:E:466:ASP:HA	5:E:1765:MGD:N2	2.34	0.43
1:E:669:LEU:HD23	1:E:741:LEU:HD22	1.99	0.43
2:F:55:PRO:CG	4:F:1194:SF4:S2	3.05	0.43
1:A:488:ARG:HD3	1:A:490:ASP:OD2	2.19	0.43
1:A:677:GLU:C	1:A:678:GLY:O	2.62	0.43
1:E:574:ASP:HA	1:E:577:LYS:HD3	2.00	0.43
1:E:683:LYS:HE2	1:E:685:THR:HB	1.99	0.43
1:A:122:ASP:HB2	7:A:2071:HOH:O	2.18	0.42
1:A:138:GLU:CD	1:A:402:LYS:HB2	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ALA:HB2	1:A:515:THR:CG2	2.49	0.42
1:A:555:LEU:O	1:A:559:LYS:HG3	2.18	0.42
3:C:57:ILE:HG21	3:C:100:PHE:HB2	2.01	0.42
1:E:397:GLU:CB	7:E:2242:HOH:O	2.67	0.42
1:E:468:LEU:HB3	1:E:469:PRO:HD2	2.00	0.42
1:A:85:ALA:HA	7:A:2044:HOH:O	2.18	0.42
1:A:124:ILE:O	1:A:128:MET:HG3	2.19	0.42
1:A:184:VAL:HG22	1:A:592:LEU:CG	2.49	0.42
1:A:533:GLN:HG2	1:A:534:TYR:N	2.33	0.42
1:A:623:TYR:HA	1:A:695:ILE:O	2.19	0.42
1:A:702:LYS:HG3	7:A:2232:HOH:O	2.18	0.42
3:C:155:THR:CG2	3:C:239:ARG:CG	2.93	0.42
3:G:148:ALA:HA	7:G:2049:HOH:O	2.19	0.42
3:G:205:ALA:HB1	3:G:240:LEU:CD2	2.49	0.42
1:E:138:GLU:CD	1:E:402:LYS:HB2	2.44	0.42
1:E:302:GLU:O	1:E:302:GLU:HG2	2.19	0.42
2:F:57:GLN:HE22	2:F:140:ARG:HH21	1.58	0.42
3:G:160:LEU:HB3	3:G:175:LEU:HB2	2.00	0.42
1:A:595:GLN:HA	1:A:598:LYS:HD2	2.02	0.42
1:A:647:ASN:H	1:A:647:ASN:ND2	2.14	0.42
1:E:100:ILE:CG2	1:E:478:VAL:HG22	2.48	0.42
1:E:275:ASP:C	1:E:275:ASP:OD1	2.63	0.42
1:E:433:LYS:HB3	1:E:460:ASP:HB2	2.01	0.42
1:E:553:LEU:HD23	1:E:553:LEU:HA	1.86	0.42
2:F:135:CYS:HA	2:F:136:PRO:HD3	1.76	0.42
1:A:209:HIS:CE1	1:A:625:ARG:H	2.29	0.42
1:A:586:ALA:O	1:A:587:SER:CB	2.66	0.42
2:F:125:LYS:HE2	7:F:2079:HOH:O	2.20	0.42
3:G:91:GLY:O	3:G:95:LEU:HD12	2.19	0.42
3:G:206:GLY:CA	3:G:209:TYR:HB2	2.49	0.42
1:A:391:PRO:O	1:A:413:ARG:CB	2.67	0.42
2:B:106:TYR:CE1	2:B:114:SER:HB3	2.54	0.42
1:E:79:CYS:CB	1:E:80:PRO:HD2	2.49	0.42
1:E:275:ASP:N	1:E:323:LYS:HE3	2.34	0.42
1:E:604:PRO:C	1:E:605:LEU:CD2	2.82	0.42
2:F:118:PHE:HD1	2:F:118:PHE:HA	1.63	0.42
7:F:2030:HOH:O	3:G:250:LEU:HD12	2.18	0.42
3:G:206:GLY:O	3:G:209:TYR:CB	2.68	0.42
1:A:77:ARG:NH2	7:A:2041:HOH:O	2.42	0.42
1:A:87:GLN:HG3	1:A:637:ASN:CG	2.45	0.42
1:A:671:ASN:ND2	1:A:675:VAL:H	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:PHE:CE1	1:E:145:HIS:CE1	3.08	0.42
7:E:2135:HOH:O	2:F:138:TYR:CE1	2.73	0.42
1:A:682:VAL:HG12	1:A:684:PRO:HD3	2.02	0.42
3:G:247:TRP:CE2	3:G:249:GLY:HA3	2.55	0.42
1:A:72:PRO:HG2	1:A:501:PHE:CD2	2.54	0.42
1:A:422:GLU:N	1:A:423:PRO:HD2	2.34	0.42
1:A:628:VAL:HG13	1:A:640:LEU:HD22	2.02	0.42
1:E:166:ALA:HB2	1:E:415:THR:HG21	2.02	0.42
2:F:72:THR:HG21	2:F:89:LYS:C	2.44	0.42
2:B:5:ALA:HB3	2:B:145:LEU:HD13	2.02	0.41
2:B:64:PRO:HB3	4:B:1196:SF4:S3	2.60	0.41
2:B:88:LYS:O	3:C:75:THR:CG2	2.67	0.41
1:E:297:THR:HG21	1:E:299:GLU:HG2	2.00	0.41
1:E:730:GLY:HA3	7:E:2253:HOH:O	2.19	0.41
1:E:734:LEU:CD2	7:E:2420:HOH:O	2.62	0.41
1:A:101:ARG:HB2	1:A:477:ASP:HA	2.02	0.41
1:A:156:LEU:HB3	1:A:157:PRO:HD3	2.02	0.41
1:E:250:LEU:HD13	1:E:307:ILE:HG21	2.02	0.41
1:E:388:CYS:O	1:E:389:SER:C	2.63	0.41
1:E:391:PRO:HD3	1:E:595:GLN:CD	2.45	0.41
2:B:78:THR:HG22	2:B:80:ASP:H	1.86	0.41
3:C:21:HIS:CE1	3:C:64:LEU:CD2	3.00	0.41
1:E:256:THR:HG23	7:E:2196:HOH:O	2.19	0.41
1:E:569:LYS:HA	1:E:570:PRO:HD3	1.85	0.41
2:F:166:ARG:HD2	7:F:2106:HOH:O	2.20	0.41
1:A:113:ARG:NE	7:A:2066:HOH:O	2.54	0.41
1:A:194:PRO:O	1:A:363:PHE:HA	2.20	0.41
1:A:676:LYS:NZ	1:A:742:GLU:OE1	2.53	0.41
1:E:112:TYR:OH	1:E:476:ALA:O	2.38	0.41
1:E:247:HIS:CD2	1:E:247:HIS:N	2.87	0.41
1:E:651:ILE:HD12	1:E:684:PRO:HA	2.02	0.41
3:G:208:TRP:HA	3:G:208:TRP:HE3	1.85	0.41
2:B:129:PRO:HB3	4:B:1195:SF4:S3	2.61	0.41
3:C:229:TRP:O	3:C:233:LEU:HG	2.19	0.41
1:E:116:THR:HG22	1:E:119:GLU:N	2.30	0.41
1:E:293:VAL:O	1:E:293:VAL:HG13	2.19	0.41
1:E:412:ALA:HB1	1:E:413:ARG:HH12	1.85	0.41
1:E:484:THR:HB	1:E:487:GLU:OE1	2.20	0.41
2:F:117:THR:HB	7:F:2012:HOH:O	2.19	0.41
1:A:575:TRP:O	1:A:580:ARG:HG2	2.21	0.41
1:E:248:ARG:NH1	1:E:318:GLU:OE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:533:GLN:HE21	1:E:533:GLN:N	2.02	0.41
1:A:39:SER:C	7:A:2005:HOH:O	2.64	0.41
1:A:252:ILE:HG13	1:A:307:ILE:HD11	2.02	0.41
2:B:168:GLU:C	2:B:169:GLN:O	2.52	0.41
3:C:173:LEU:O	3:C:173:LEU:CG	2.65	0.41
1:E:100:ILE:CG1	1:E:478:VAL:HG22	2.48	0.41
1:E:113:ARG:HB3	7:E:2046:HOH:O	2.21	0.41
1:E:142:PHE:CD1	1:E:157:PRO:HB3	2.56	0.41
1:E:591:GLU:O	1:E:603:GLN:CD	2.63	0.41
1:A:295:ASP:O	1:A:297:THR:HG22	2.21	0.41
2:B:46:TYR:HE2	7:B:2033:HOH:O	1.96	0.41
1:E:421:ILE:HD11	1:E:452:THR:HG23	2.03	0.41
1:A:42:GLN:OE1	1:A:506:THR:N	2.53	0.41
1:A:175:ALA:HB3	1:A:176:PRO:HD3	2.02	0.41
1:A:284:VAL:HB	1:A:589:LYS:HA	2.03	0.41
1:A:499:THR:HB	1:A:565:VAL:CG1	2.51	0.41
1:A:510:GLU:HG3	1:A:510:GLU:H	1.77	0.41
2:B:118:PHE:HD1	2:B:118:PHE:HA	1.72	0.41
2:B:135:CYS:HA	2:B:136:PRO:HD3	1.89	0.41
2:B:190:SER:CB	3:C:252:GLY:N	2.81	0.41
3:C:185:LEU:O	3:C:189:LEU:HG	2.20	0.41
1:E:88:THR:CG2	1:E:467:VAL:HG11	2.51	0.41
1:E:97:ARG:NH2	1:E:763:ARG:NH1	2.64	0.41
1:E:288:GLU:HG3	7:E:2186:HOH:O	2.21	0.41
1:E:622:LEU:O	1:E:623:TYR:HB3	2.21	0.41
1:A:116:THR:HG23	1:A:118:GLU:H	1.85	0.41
1:A:279:VAL:HA	1:A:283:THR:HB	2.03	0.41
1:E:50:ARG:HD2	7:E:2016:HOH:O	2.20	0.41
2:F:59:LEU:O	2:F:60:HIS:C	2.64	0.41
3:G:16:THR:HG21	3:G:66:GLU:HB2	2.03	0.41
3:G:195:PRO:HD2	3:G:196:GLU:OE2	2.20	0.41
1:E:93:ASP:CG	1:E:758:ARG:HH22	2.28	0.40
1:E:239:PHE:O	1:E:687:ARG:HD2	2.21	0.40
1:E:591:GLU:O	1:E:603:GLN:HG2	2.20	0.40
1:A:587:SER:O	1:A:589:LYS:HE2	2.21	0.40
1:A:666:TYR:CZ	1:A:681:ARG:HG3	2.56	0.40
1:A:753:THR:CG2	1:A:757:LYS:HE2	2.51	0.40
2:B:112:TYR:HB3	3:C:73:ARG:NH2	2.35	0.40
3:C:145:ASN:OD1	3:C:193:THR:CG2	2.68	0.40
3:C:207:GLY:HA2	3:C:210:TYR:CB	2.52	0.40
1:E:53:ILE:HD12	1:E:65:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:VAL:HG21	1:E:319:MET:CE	2.50	0.40
2:F:35:ASN:ND2	2:F:106:TYR:CE2	2.88	0.40
3:G:112:GLN:N	7:G:2036:HOH:O	2.53	0.40
3:G:205:ALA:HB1	3:G:240:LEU:HD22	2.02	0.40
1:A:43:ILE:HB	1:A:505:ARG:NH2	2.36	0.40
1:A:371:LEU:HD23	1:A:551:LEU:CD1	2.52	0.40
1:A:405:ALA:HB2	1:A:430:TYR:CZ	2.57	0.40
2:B:25:MET:CE	2:B:25:MET:CA	2.92	0.40
2:B:166:ARG:HG2	7:B:2145:HOH:O	2.22	0.40
3:C:174:PHE:N	3:C:175:PRO:HD2	2.37	0.40
3:C:228:PRO:O	3:C:232:LEU:HD12	2.22	0.40
1:E:553:LEU:CD2	1:E:557:THR:CG2	2.99	0.40
2:F:175:LEU:HD12	2:F:175:LEU:C	2.46	0.40
1:A:207:GLY:O	5:A:1766:MGD:PB	2.79	0.40
1:E:95:LEU:CD2	7:E:2278:HOH:O	2.53	0.40
1:E:548:LEU:HD23	1:E:548:LEU:HA	1.89	0.40
3:G:44:GLU:OE1	3:G:47:ARG:NH1	2.54	0.40
1:A:113:ARG:CZ	7:A:2066:HOH:O	2.70	0.40
1:A:170:VAL:HG12	1:A:171:SER:N	2.36	0.40
1:A:209:HIS:HD2	5:A:1766:MGD:O2A	2.04	0.40
1:A:506:THR:CG2	7:A:2248:HOH:O	2.69	0.40
1:A:671:ASN:C	1:A:671:ASN:HD22	2.29	0.40
1:E:746:ARG:HH11	1:E:746:ARG:CG	2.32	0.40
2:F:117:THR:HG22	2:F:119:CYS:N	2.34	0.40
3:G:33:LEU:HD23	3:G:33:LEU:HA	1.75	0.40
3:G:60:LEU:HD23	3:G:63:LEU:HD12	2.02	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLU:OE2	1:E:134:LYS:N[2_674]	1.60	0.60
1:A:399:GLU:OE2	1:E:133:GLU:C[2_674]	1.61	0.59
1:A:399:GLU:OE2	1:E:133:GLU:O[2_674]	2.10	0.10

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	733/765 (96%)	651 (89%)	46 (6%)	36 (5%)	1	1
1	E	733/765 (96%)	634 (86%)	63 (9%)	36 (5%)	1	1
2	B	192/195 (98%)	176 (92%)	13 (7%)	3 (2%)	7	11
2	F	192/195 (98%)	179 (93%)	9 (5%)	4 (2%)	5	7
3	C	249/253 (98%)	231 (93%)	13 (5%)	5 (2%)	6	7
3	G	249/253 (98%)	220 (88%)	22 (9%)	7 (3%)	4	3
All	All	2348/2426 (97%)	2091 (89%)	166 (7%)	91 (4%)	2	2

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	TRP
1	A	340	ASP
1	A	428	GLU
1	A	429	PRO
1	A	431	PRO
1	A	535	PHE
1	A	562	GLY
1	A	570	PRO
1	A	586	ALA
1	A	587	SER
1	A	593	TYR
1	A	605	LEU
1	A	678	GLY
1	A	687	ARG
1	A	730	GLY
2	B	17	ALA
3	C	208	PHE
3	C	250	GLY
1	E	92	PRO
1	E	93	ASP

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Mol	Chain	Res	Type
1	E	109	GLU
1	E	324	PRO
1	E	396	HIS
1	E	397	GLU
1	E	428	GLU
1	E	552	GLY
1	E	567	ARG
1	E	583	PHE
1	E	593	TYR
1	E	607	VAL
1	E	631	PHE
1	E	678	GLY
1	E	686	ALA
2	F	46	TYR
3	G	108	GLY
3	G	113	ARG
3	G	222	GLN
1	A	365	ILE
1	A	399	GLU
1	A	430	TYR
1	A	434	GLY
1	A	582	PRO
1	A	592	LEU
1	A	607	VAL
1	A	631	PHE
1	A	633	ARG
2	B	193	HIS
3	C	112	SER
3	C	172	ALA
1	E	337	TYR
1	E	391	PRO
1	E	606	PRO
1	E	685	THR
2	F	178	LEU
2	F	179	ASN
3	G	39	LEU
3	G	51	TYR
3	G	249	GLY
1	A	216	ASN
1	A	389	SER
1	A	398	PRO
1	E	389	SER

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Mol	Chain	Res	Type
1	E	429	PRO
1	E	466	ASP
1	E	469	PRO
1	E	471	GLU
1	E	513	PHE
1	E	570	PRO
2	F	45	GLU
1	A	478	VAL
2	B	115	LYS
1	E	478	VAL
1	E	627	PRO
1	E	710	HIS
1	E	763	ARG
3	G	38	HIS
1	A	387	GLY
3	C	113	GLN
1	E	70	ALA
1	A	598	LYS
1	A	609	THR
1	A	610	PRO
1	A	684	PRO
1	E	138	GLU
1	E	610	PRO
1	A	584	GLY
1	E	605	LEU
1	A	194	PRO
1	E	434	GLY
1	A	511	PRO
1	E	609	THR

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	610/632 (96%)	490 (80%)	120 (20%)	1 2
1	E	610/632 (96%)	495 (81%)	115 (19%)	1 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	162/163 (99%)	140 (86%)	22 (14%)	3	5
2	F	162/163 (99%)	143 (88%)	19 (12%)	5	7
3	C	185/187 (99%)	159 (86%)	26 (14%)	3	4
3	G	185/187 (99%)	162 (88%)	23 (12%)	4	6
All	All	1914/1964 (98%)	1589 (83%)	325 (17%)	2	2

All (325) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	43	ILE
1	A	65	VAL
1	A	77	ARG
1	A	87	GLN
1	A	97	ARG
1	A	103	GLU
1	A	106	GLN
1	A	111	LYS
1	A	116	THR
1	A	119	GLU
1	A	126	LYS
1	A	134	LYS
1	A	145	HIS
1	A	156	LEU
1	A	167	LYS
1	A	170	VAL
1	A	174	THR
1	A	187	ARG
1	A	189	ILE
1	A	193	GLU
1	A	213	ASP
1	A	214	THR
1	A	217	THR
1	A	231	LYS
1	A	250	LEU
1	A	252	ILE
1	A	256	THR
1	A	260	LEU
1	A	281	LYS
1	A	283	THR
1	A	289	LEU

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Mol	Chain	Res	Type
1	A	293	VAL
1	A	297	THR
1	A	299	GLU
1	A	302	GLU
1	A	305	THR
1	A	323	LYS
1	A	327	VAL
1	A	335	VAL
1	A	371	LEU
1	A	372	GLU
1	A	378	PRO
1	A	379	LEU
1	A	382	GLU
1	A	395	ASP
1	A	413	ARG
1	A	414	SER
1	A	415	THR
1	A	418	GLN
1	A	421	ILE
1	A	428	GLU
1	A	433	LYS
1	A	440	ILE
1	A	441	ASN
1	A	454	GLU
1	A	457	LYS
1	A	465	ILE
1	A	470	GLN
1	A	477	ASP
1	A	478	VAL
1	A	484	THR
1	A	504	LEU
1	A	510	GLU
1	A	512	LEU
1	A	515	THR
1	A	528	ARG
1	A	529	LEU
1	A	531	LEU
1	A	532	GLU
1	A	533	GLN
1	A	538	LYS
1	A	539	THR
1	A	540	ILE

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Mol	Chain	Res	Type
1	A	541	GLU
1	A	542	GLU
1	A	550	SER
1	A	553	LEU
1	A	555	LEU
1	A	558	MET
1	A	561	MET
1	A	578	GLU
1	A	580	ARG
1	A	581	LEU
1	A	587	SER
1	A	589	LYS
1	A	591	GLU
1	A	592	LEU
1	A	594	CYS
1	A	595	GLN
1	A	596	ARG
1	A	599	GLU
1	A	603	GLN
1	A	605	LEU
1	A	608	PHE
1	A	616	GLU
1	A	621	LEU
1	A	633	ARG
1	A	647	ASN
1	A	648	GLU
1	A	649	VAL
1	A	651	ILE
1	A	663	GLU
1	A	667	VAL
1	A	671	ASN
1	A	672	GLN
1	A	680	VAL
1	A	683	LYS
1	A	685	THR
1	A	693	VAL
1	A	702	LYS
1	A	708	LEU
1	A	721	THR
1	A	725	LEU
1	A	736	VAL
1	A	739	VAL

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Mol	Chain	Res	Type
1	A	741	LEU
1	A	743	LYS
1	A	746	ARG
1	A	762	GLU
2	B	1	MET
2	B	25	MET
2	B	39	ARG
2	B	41	ARG
2	B	45	GLU
2	B	54	ARG
2	B	69	VAL
2	B	72	THR
2	B	78	THR
2	B	105	ARG
2	B	114	SER
2	B	117	THR
2	B	118	PHE
2	B	125	LYS
2	B	131	CYS
2	B	134	THR
2	B	145	LEU
2	B	152	VAL
2	B	164	VAL
2	B	166	ARG
2	B	175	LEU
2	B	187	THR
3	C	11	GLN
3	C	17	THR
3	C	18	ASN
3	C	20	LEU
3	C	21	HIS
3	C	40	LEU
3	C	57	ILE
3	C	63	ILE
3	C	67	GLU
3	C	71	ARG
3	C	75	THR
3	C	79	LEU
3	C	105	LEU
3	C	110	LYS
3	C	130	TYR
3	C	140	ASN

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Mol	Chain	Res	Type
3	C	145	ASN
3	C	155	THR
3	C	163	LEU
3	C	193	THR
3	C	197	GLU
3	C	216	LEU
3	C	225	ARG
3	C	232	LEU
3	C	241	LEU
3	C	249	GLN
1	E	65	VAL
1	E	69	GLU
1	E	101	ARG
1	E	102	VAL
1	E	111	LYS
1	E	113	ARG
1	E	114	VAL
1	E	119	GLU
1	E	126	LYS
1	E	145	HIS
1	E	172	LEU
1	E	174	THR
1	E	189	ILE
1	E	193	GLU
1	E	208	HIS
1	E	213	ASP
1	E	214	THR
1	E	217	THR
1	E	224	LEU
1	E	240	SER
1	E	250	LEU
1	E	256	THR
1	E	260	LEU
1	E	272	ASP
1	E	284	VAL
1	E	286	PHE
1	E	289	LEU
1	E	293	VAL
1	E	297	THR
1	E	298	PRO
1	E	299	GLU
1	E	305	THR

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Mol	Chain	Res	Type
1	E	314	GLU
1	E	323	LYS
1	E	327	VAL
1	E	335	VAL
1	E	360	PRO
1	E	371	LEU
1	E	389	SER
1	E	395	ASP
1	E	402	LYS
1	E	413	ARG
1	E	415	THR
1	E	418	GLN
1	E	421	ILE
1	E	428	GLU
1	E	440	ILE
1	E	441	ASN
1	E	457	LYS
1	E	466	ASP
1	E	470	GLN
1	E	484	THR
1	E	488	ARG
1	E	498	LYS
1	E	499	THR
1	E	504	LEU
1	E	510	GLU
1	E	512	LEU
1	E	515	THR
1	E	528	ARG
1	E	533	GLN
1	E	538	LYS
1	E	539	THR
1	E	540	ILE
1	E	541	GLU
1	E	554	ASP
1	E	555	LEU
1	E	558	MET
1	E	564	LEU
1	E	569	LYS
1	E	577	LYS
1	E	581	LEU
1	E	585	THR
1	E	589	LYS

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Mol	Chain	Res	Type
1	E	590	ILE
1	E	591	GLU
1	E	595	GLN
1	E	596	ARG
1	E	598	LYS
1	E	602	HIS
1	E	605	LEU
1	E	607	VAL
1	E	608	PHE
1	E	609	THR
1	E	612	GLU
1	E	620	ARG
1	E	621	LEU
1	E	626	SER
1	E	628	VAL
1	E	633	ARG
1	E	647	ASN
1	E	649	VAL
1	E	651	ILE
1	E	657	LYS
1	E	663	GLU
1	E	667	VAL
1	E	671	ASN
1	E	672	GLN
1	E	676	LYS
1	E	680	VAL
1	E	685	THR
1	E	691	ASP
1	E	693	VAL
1	E	702	LYS
1	E	708	LEU
1	E	721	THR
1	E	725	LEU
1	E	736	VAL
1	E	739	VAL
1	E	740	ARG
1	E	741	LEU
1	E	746	ARG
1	E	748	ARG
1	E	751	SER
1	E	752	LEU
2	F	49	LEU

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Mol	Chain	Res	Type
2	F	69	VAL
2	F	72	THR
2	F	78	THR
2	F	80	ASP
2	F	88	LYS
2	F	114	SER
2	F	117	THR
2	F	118	PHE
2	F	133	GLU
2	F	145	LEU
2	F	150	SER
2	F	152	VAL
2	F	164	VAL
2	F	166	ARG
2	F	171	THR
2	F	175	LEU
2	F	187	THR
2	F	191	GLU
3	G	10	GLN
3	G	17	ASN
3	G	39	LEU
3	G	40	LYS
3	G	64	TRP
3	G	66	GLU
3	G	74	THR
3	G	88	ILE
3	G	107	LEU
3	G	109	LYS
3	G	113	ARG
3	G	129	TYR
3	G	136	VAL
3	G	139	ASN
3	G	144	ASN
3	G	154	THR
3	G	162	LEU
3	G	167	LYS
3	G	192	THR
3	G	196	GLU
3	G	204	GLU
3	G	215	LEU
3	G	240	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	71	ASN
1	A	123	HIS
1	A	192	HIS
1	A	209	HIS
1	A	220	GLN
1	A	247	HIS
1	A	322	HIS
1	A	367	GLN
1	A	441	ASN
1	A	470	GLN
1	A	472	HIS
1	A	509	HIS
1	A	533	GLN
1	A	549	GLN
1	A	595	GLN
1	A	602	HIS
1	A	603	GLN
1	A	647	ASN
1	A	671	ASN
1	A	672	GLN
1	A	717	ASN
2	B	27	ASN
2	B	35	ASN
2	B	48	ASN
2	B	57	GLN
2	B	77	GLN
2	B	179	ASN
3	C	11	GLN
3	C	21	HIS
3	C	84	HIS
3	C	140	ASN
3	C	201	HIS
3	C	249	GLN
1	E	35	GLN
1	E	71	ASN
1	E	83	GLN
1	E	209	HIS
1	E	218	GLN
1	E	220	GLN
1	E	247	HIS
1	E	292	HIS

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Mol	Chain	Res	Type
1	E	310	GLN
1	E	322	HIS
1	E	396	HIS
1	E	418	GLN
1	E	444	HIS
1	E	470	GLN
1	E	472	HIS
1	E	509	HIS
1	E	533	GLN
1	E	602	HIS
1	E	603	GLN
1	E	635	GLN
1	E	647	ASN
1	E	671	ASN
1	E	672	GLN
1	E	717	ASN
2	F	27	ASN
2	F	35	ASN
2	F	57	GLN
2	F	77	GLN
2	F	169	GLN
2	F	179	ASN
3	G	10	GLN
3	G	38	HIS
3	G	83	HIS
3	G	137	ASN
3	G	139	ASN
3	G	248	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SF4	B	1197	2	0,12,12	-	-	-		
4	SF4	B	1195	2	0,12,12	-	-	-		
5	MGD	E	1766	6	47,52,52	2.03	12 (25%)	58,81,81	2.67	19 (32%)
4	SF4	F	1194	2	0,12,12	-	-	-		
4	SF4	F	1196	2	0,12,12	-	-	-		
4	SF4	E	1764	1	0,12,12	-	-	-		
5	MGD	E	1765	6	47,52,52	2.04	9 (19%)	58,81,81	3.14	22 (37%)
4	SF4	F	1195	2	0,12,12	-	-	-		
5	MGD	A	1765	6	47,52,52	1.78	9 (19%)	58,81,81	3.03	19 (32%)
4	SF4	B	1194	2	0,12,12	-	-	-		
4	SF4	B	1196	2	0,12,12	-	-	-		
4	SF4	F	1197	2	0,12,12	-	-	-		
5	MGD	A	1766	6	47,52,52	1.79	10 (21%)	58,81,81	3.02	20 (34%)
4	SF4	A	1764	1	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	B	1197	2	-	-	0/6/5/5
4	SF4	B	1195	2	-	-	0/6/5/5
5	MGD	E	1766	6	-	1/22/66/66	0/6/6/6
4	SF4	F	1194	2	-	-	0/6/5/5
4	SF4	F	1196	2	-	-	0/6/5/5
4	SF4	E	1764	1	-	-	0/6/5/5
5	MGD	E	1765	6	-	2/22/66/66	0/6/6/6
4	SF4	F	1195	2	-	-	0/6/5/5
5	MGD	A	1765	6	-	5/22/66/66	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	B	1194	2	-	-	0/6/5/5
4	SF4	B	1196	2	-	-	0/6/5/5
4	SF4	F	1197	2	-	-	0/6/5/5
5	MGD	A	1766	6	-	1/22/66/66	0/6/6/6
4	SF4	A	1764	1	-	-	0/6/5/5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1765	MGD	C16-C21	6.61	1.49	1.38
5	E	1766	MGD	C21-N22	-6.12	1.29	1.35
5	E	1765	MGD	PB-O3B	5.80	1.65	1.59
5	E	1765	MGD	PA-O3B	5.51	1.65	1.59
5	E	1766	MGD	C16-C21	5.49	1.48	1.38
5	A	1765	MGD	C16-C21	5.45	1.47	1.38
5	A	1766	MGD	C16-C21	5.05	1.47	1.38
5	E	1766	MGD	C5-C4	4.47	1.51	1.38
5	A	1766	MGD	O11-C23	4.47	1.50	1.43
5	A	1765	MGD	C23-C14	-4.26	1.50	1.53
5	A	1766	MGD	C14-N15	-3.94	1.42	1.46
5	E	1766	MGD	O3'-C3'	3.93	1.52	1.43
5	A	1765	MGD	C5-C4	3.75	1.49	1.38
5	A	1766	MGD	C5-C4	3.67	1.48	1.38
5	E	1765	MGD	C5-C4	3.64	1.48	1.38
5	E	1766	MGD	PA-O3B	3.48	1.63	1.59
5	E	1765	MGD	C5-N7	-3.47	1.32	1.39
5	A	1766	MGD	C16-C17	3.08	1.51	1.41
5	E	1765	MGD	C10-C11	-2.87	1.47	1.51
5	E	1765	MGD	C8-N9	-2.87	1.31	1.37
5	A	1765	MGD	PA-O3B	2.82	1.62	1.59
5	E	1766	MGD	C19-N20	2.79	1.39	1.33
5	A	1766	MGD	C6-N1	-2.79	1.33	1.38
5	E	1766	MGD	C14-N15	-2.76	1.43	1.46
5	A	1765	MGD	C14-N15	2.72	1.49	1.46
5	A	1766	MGD	C21-N22	-2.70	1.32	1.35
5	A	1765	MGD	C17-N18	-2.67	1.33	1.38
5	A	1765	MGD	O6-C6	2.65	1.28	1.23
5	E	1766	MGD	C5-N7	-2.63	1.33	1.39
5	E	1766	MGD	C19-N18	-2.60	1.31	1.37
5	E	1765	MGD	C16-C17	2.44	1.49	1.41
5	A	1765	MGD	C5-C6	2.43	1.53	1.44
5	E	1766	MGD	C19-N19	-2.42	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1766	MGD	C16-N15	-2.35	1.32	1.37
5	E	1765	MGD	C8-N7	2.30	1.39	1.32
5	A	1766	MGD	PB-O2B	-2.27	1.44	1.55
5	A	1765	MGD	PB-O3B	2.17	1.61	1.59
5	A	1766	MGD	C23-C14	-2.07	1.52	1.53
5	A	1766	MGD	PA-O2A	-2.04	1.45	1.55
5	E	1766	MGD	C6-N1	-2.02	1.35	1.38

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1766	MGD	O11-C23-C14	14.07	118.35	108.96
5	A	1765	MGD	O11-C23-C14	12.57	117.35	108.96
5	E	1765	MGD	O11-C23-N22	-11.15	98.49	108.61
5	E	1766	MGD	O11-C23-C14	10.62	116.05	108.96
5	E	1765	MGD	C23-C14-N15	9.11	116.82	107.87
5	A	1765	MGD	C23-C14-N15	8.00	115.72	107.87
5	A	1765	MGD	C2-N3-C4	7.24	124.77	112.30
5	E	1766	MGD	C5-C4-N3	-7.18	116.97	128.39
5	A	1765	MGD	C5-C4-N3	-7.10	117.09	128.39
5	E	1765	MGD	O11-C23-C14	-7.04	104.27	108.96
5	E	1765	MGD	C5-C4-N3	-6.81	117.55	128.39
5	E	1765	MGD	C2-N3-C4	6.50	123.50	112.30
5	A	1766	MGD	C5-C4-N3	-6.30	118.37	128.39
5	E	1765	MGD	C19-N20-C21	5.94	123.84	113.36
5	E	1766	MGD	O17-C17-C16	-5.58	113.82	127.26
5	A	1765	MGD	C19-N20-C21	5.47	123.01	113.36
5	E	1765	MGD	C6-C5-N7	5.26	139.87	130.29
5	E	1766	MGD	C23-C14-N15	5.25	113.03	107.87
5	A	1766	MGD	C2-N3-C4	5.21	121.28	112.30
5	A	1766	MGD	N9-C4-N3	5.10	136.14	125.95
5	A	1766	MGD	O4'-C1'-N9	4.91	119.48	108.36
5	E	1766	MGD	C2-N3-C4	4.75	120.48	112.30
5	A	1766	MGD	C23-C14-N15	4.74	112.53	107.87
5	A	1766	MGD	O3B-PB-O1B	-4.53	97.07	110.70
5	E	1766	MGD	N9-C4-N3	4.52	135.00	125.95
5	A	1765	MGD	N9-C4-N3	4.46	134.88	125.95
5	A	1766	MGD	O11-C23-N22	4.39	112.59	108.61
5	E	1765	MGD	C4-C5-N7	-4.25	103.93	110.67
5	E	1766	MGD	C19-N20-C21	4.06	120.53	113.36
5	E	1765	MGD	N9-C4-N3	4.02	133.99	125.95
5	A	1765	MGD	C6-C5-N7	3.97	137.51	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1765	MGD	C17-C16-N15	3.93	126.97	116.27
5	A	1766	MGD	C19-N18-C17	-3.72	118.37	125.11
5	A	1765	MGD	C4-C5-N7	-3.63	104.91	110.67
5	E	1766	MGD	C16-C17-N18	3.59	121.98	112.13
5	A	1766	MGD	O6-C6-C5	-3.52	117.25	126.53
5	E	1765	MGD	C17-C16-N15	3.50	125.81	116.27
5	A	1765	MGD	O2B-PB-O3B	3.42	116.53	107.27
5	A	1766	MGD	O2B-PB-O3B	3.33	116.27	107.27
5	E	1766	MGD	O4'-C1'-N9	3.33	115.90	108.36
5	A	1766	MGD	O17-C17-C16	-3.28	119.36	127.26
5	A	1766	MGD	C17-C16-N15	3.26	125.16	116.27
5	A	1765	MGD	N2-C2-N1	3.14	123.39	116.76
5	E	1766	MGD	O11-C23-N22	-3.13	105.77	108.61
5	E	1765	MGD	C16-C17-N18	3.09	120.61	112.13
5	E	1766	MGD	O2A-PA-O1A	3.02	126.50	112.44
5	A	1766	MGD	O5'-C5'-C4'	-2.78	99.54	108.99
5	A	1765	MGD	O17-C17-C16	-2.77	120.57	127.26
5	E	1765	MGD	O2A-PA-O3B	-2.77	99.78	107.27
5	E	1766	MGD	C2-N1-C6	-2.75	120.12	125.11
5	A	1766	MGD	C16-C17-N18	2.75	119.67	112.13
5	E	1765	MGD	O3'-C3'-C4'	-2.73	103.23	111.08
5	A	1765	MGD	O3B-PA-O1A	-2.71	102.54	110.70
5	E	1766	MGD	C19-N18-C17	-2.70	120.21	125.11
5	E	1766	MGD	O3'-C3'-C4'	2.69	118.82	111.08
5	A	1766	MGD	C6-C5-N7	2.67	135.14	130.29
5	A	1765	MGD	O4'-C4'-C5'	-2.65	100.85	109.33
5	E	1765	MGD	C8-N7-C5	2.64	108.96	104.26
5	E	1766	MGD	C4-C5-N7	-2.60	106.55	110.67
5	E	1766	MGD	O6-C6-C5	-2.58	119.72	126.53
5	A	1765	MGD	O4'-C1'-C2'	-2.54	101.17	106.62
5	A	1765	MGD	N19-C19-N18	2.49	122.02	116.76
5	E	1765	MGD	O2B-PB-O1B	2.47	123.95	112.44
5	A	1765	MGD	O3B-PB-O1B	-2.46	103.29	110.70
5	E	1765	MGD	O3B-PB-O1B	-2.43	103.40	110.70
5	E	1765	MGD	O6-C6-C5	-2.42	120.14	126.53
5	A	1766	MGD	C19-N20-C21	2.42	117.63	113.36
5	E	1765	MGD	O17-C17-C16	-2.41	121.45	127.26
5	A	1766	MGD	C5-C6-N1	2.34	119.22	113.25
5	E	1766	MGD	C6-C5-N7	2.34	134.55	130.29
5	A	1766	MGD	O4'-C4'-C5'	-2.31	101.93	109.33
5	E	1765	MGD	C19-N18-C17	-2.28	120.98	125.11
5	E	1765	MGD	O2B-PB-O3B	-2.26	101.16	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1765	MGD	O2A-PA-O1A	2.24	122.84	112.44
5	A	1765	MGD	C16-C17-N18	2.16	118.05	112.13
5	E	1766	MGD	C4'-O4'-C1'	-2.16	104.71	109.47
5	A	1766	MGD	C2'-C1'-N9	2.15	119.23	113.25
5	E	1766	MGD	O17-C17-N18	2.15	124.15	120.11
5	A	1765	MGD	C2'-C1'-N9	2.12	119.15	113.25
5	E	1765	MGD	N2-C2-N1	2.09	121.18	116.76

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1765	MGD	C5'-O5'-PB-O2B
5	A	1765	MGD	C5'-O5'-PB-O3B
5	E	1765	MGD	O4'-C4'-C5'-O5'
5	A	1765	MGD	PA-O3B-PB-O5'
5	E	1765	MGD	PA-O3B-PB-O5'
5	A	1766	MGD	C11-C10-O3A-PA
5	A	1765	MGD	C5'-O5'-PB-O1B
5	E	1766	MGD	C11-C10-O3A-PA
5	A	1765	MGD	PA-O3B-PB-O1B

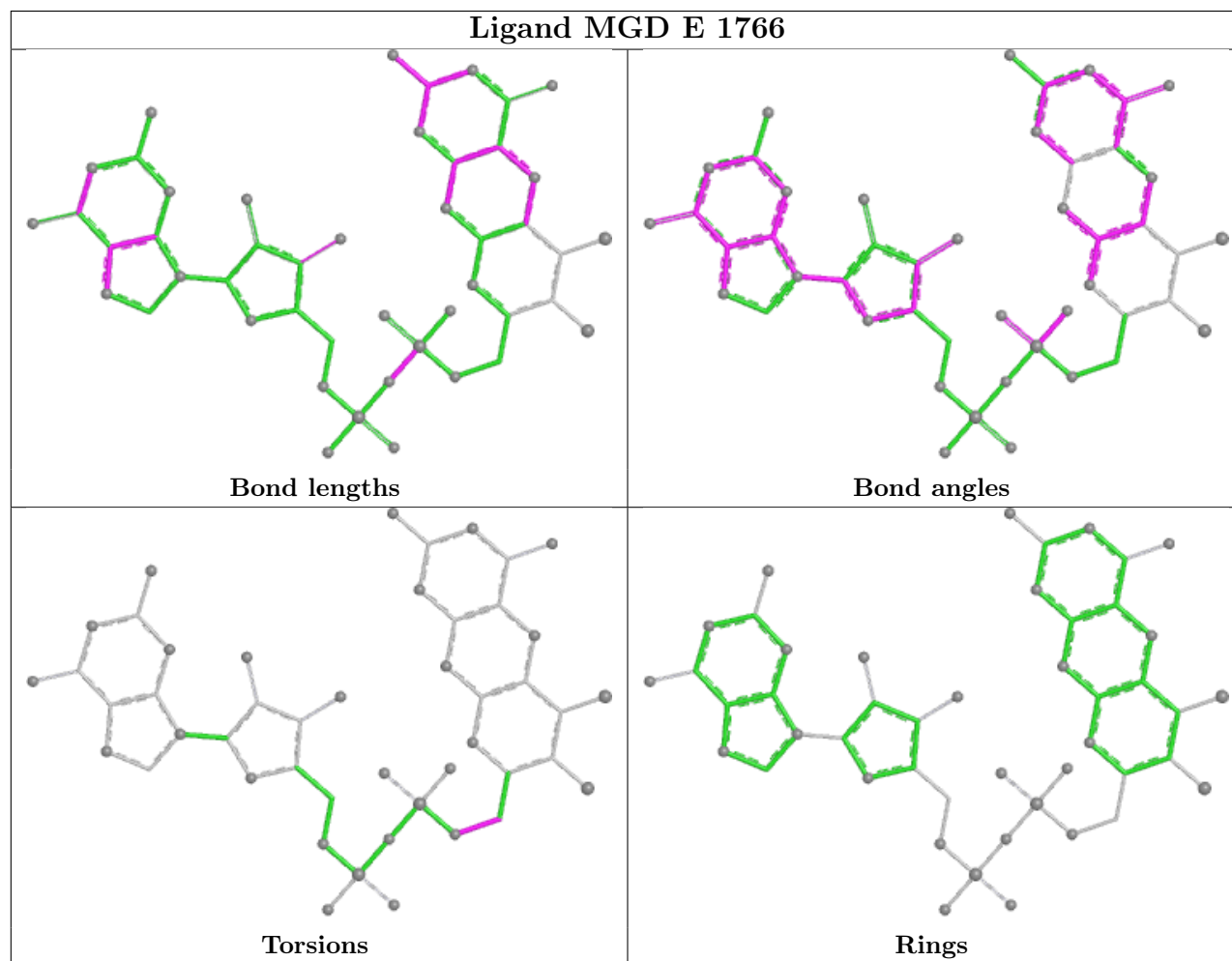
There are no ring outliers.

10 monomers are involved in 21 short contacts:

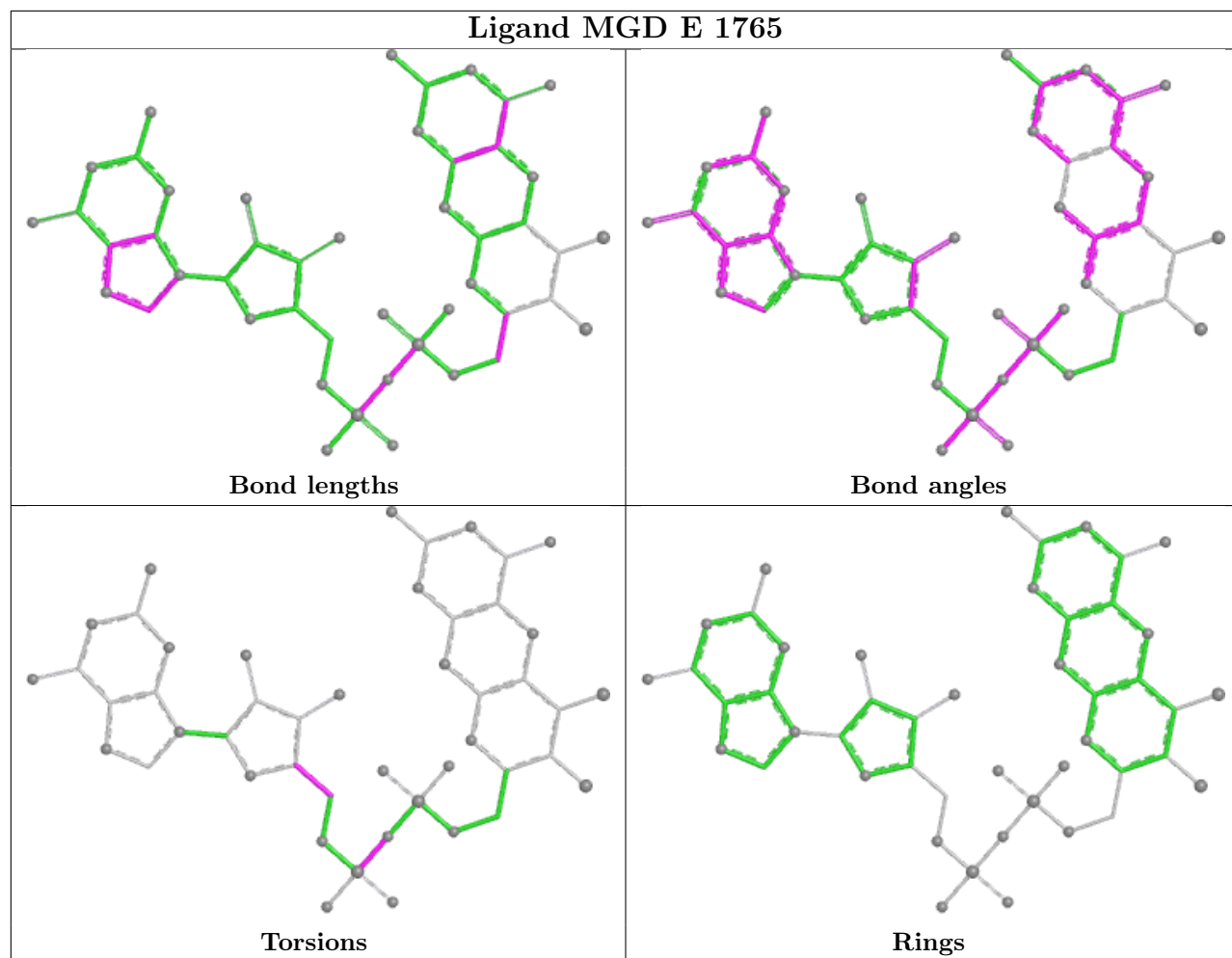
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1195	SF4	1	0
5	E	1766	MGD	3	0
4	F	1194	SF4	2	0
4	F	1196	SF4	1	0
4	E	1764	SF4	1	0
5	E	1765	MGD	4	0
5	A	1765	MGD	4	0
4	B	1194	SF4	1	0
4	B	1196	SF4	1	0
5	A	1766	MGD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

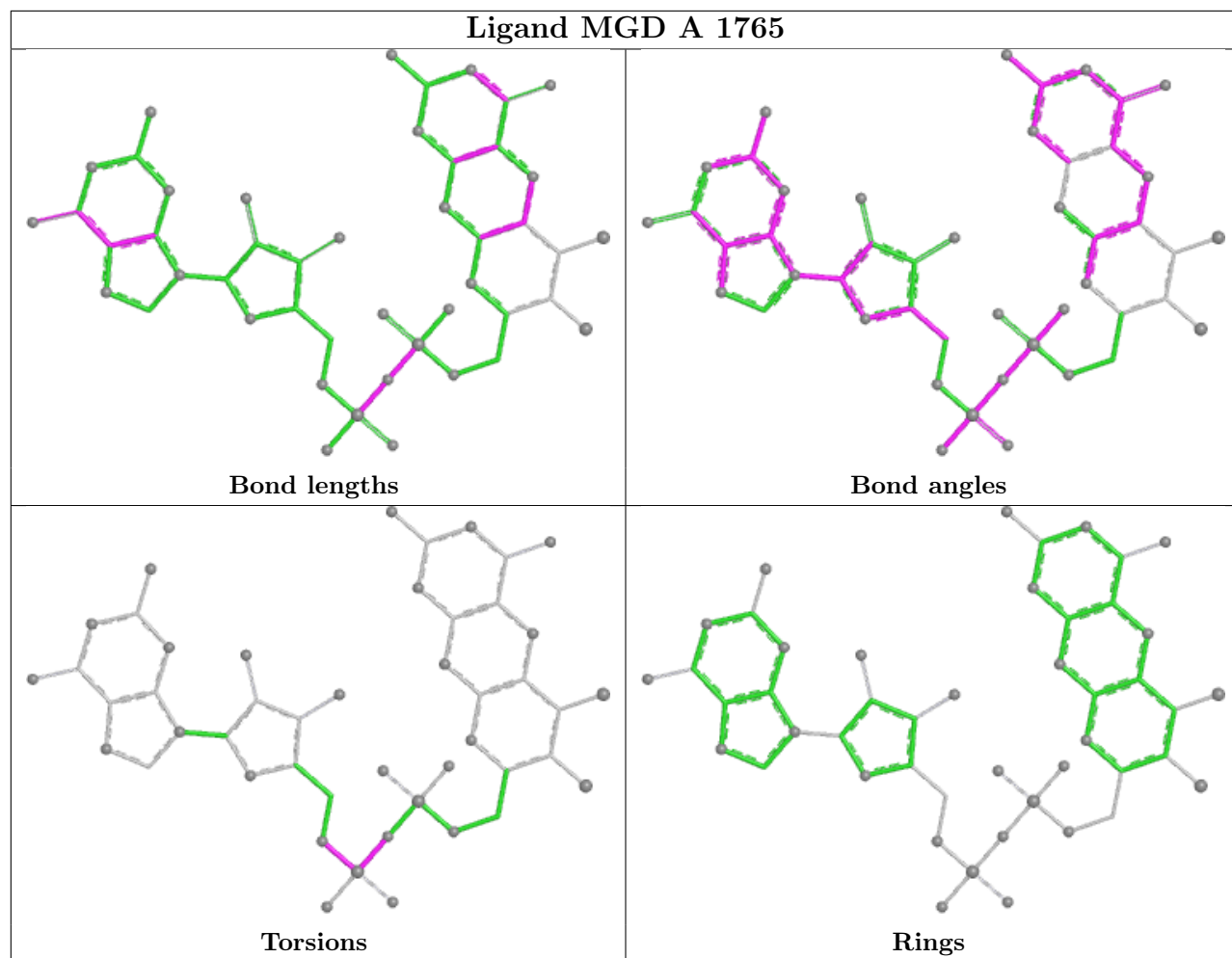
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

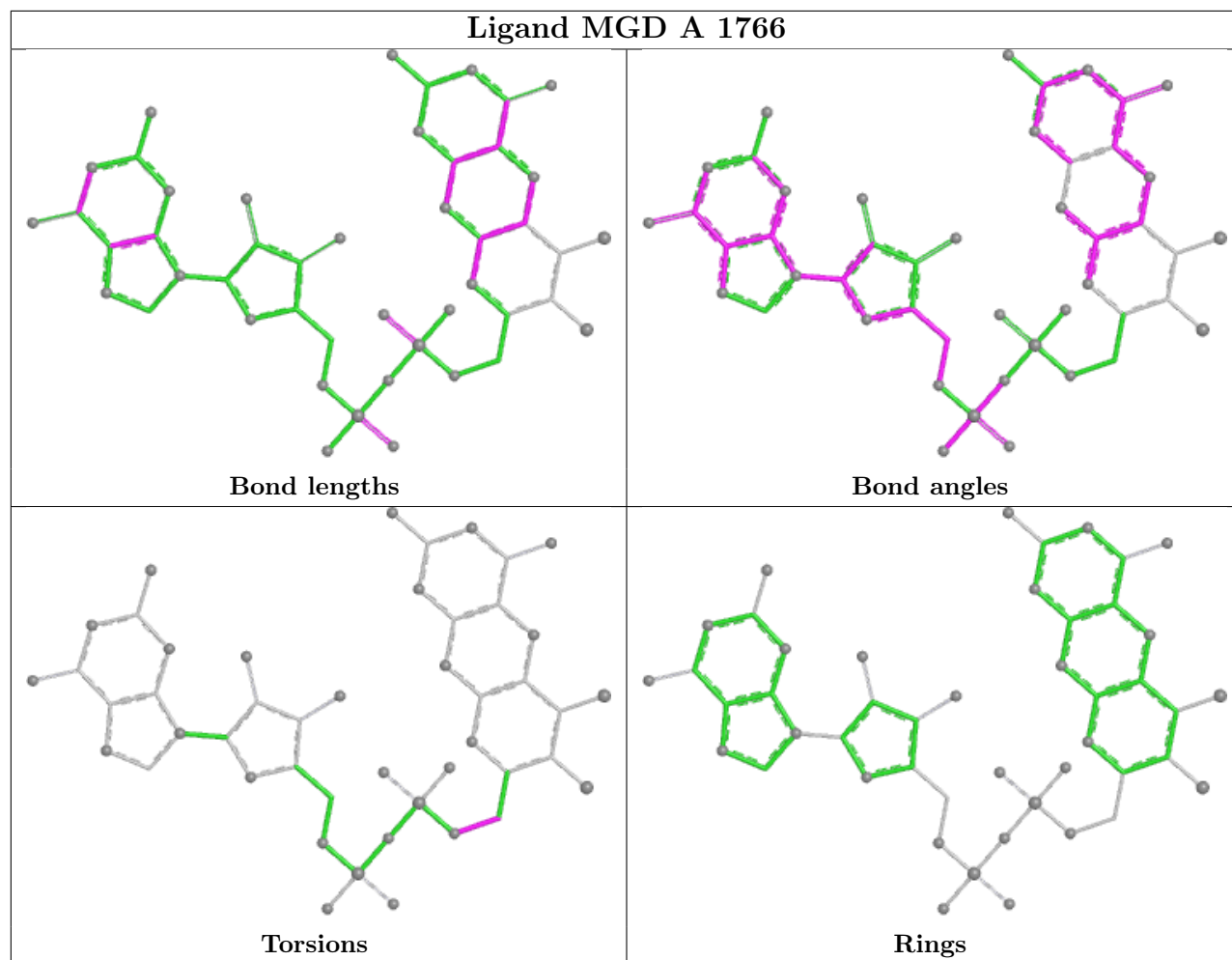


Ligand MGD E 1765



Ligand MGD A 1765





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	735/765 (96%)	1.05	139 (18%) 3 2	25, 48, 80, 134	0
1	E	735/765 (96%)	1.01	115 (15%) 5 4	25, 46, 78, 136	0
2	B	194/195 (99%)	0.57	15 (7%) 19 16	29, 42, 63, 90	0
2	F	194/195 (99%)	0.59	12 (6%) 26 23	31, 46, 67, 90	0
3	C	251/253 (99%)	1.12	35 (13%) 6 5	32, 54, 81, 99	0
3	G	251/253 (99%)	1.34	57 (22%) 2 2	34, 62, 91, 107	0
All	All	2360/2426 (97%)	1.00	373 (15%) 5 4	25, 48, 80, 136	0

All (373) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	251	GLY	17.6
1	A	583	PHE	13.2
1	E	592	LEU	10.7
1	E	607	VAL	10.4
1	A	586	ALA	10.2
1	E	600	ALA	10.0
3	C	252	GLY	9.8
1	A	607	VAL	9.4
1	A	685	THR	8.9
1	E	593	TYR	8.7
1	E	764	ARG	8.3
1	A	764	ARG	8.3
1	E	391	PRO	8.2
1	E	390	GLY	8.0
3	G	206	GLY	7.8
1	A	592	LEU	7.8
1	A	394	GLY	7.7
2	F	1	MET	7.6
1	E	398	PRO	7.5

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Mol	Chain	Res	Type	RSRZ
1	E	323	LYS	7.5
1	A	401	PHE	7.5
3	G	111	SER	7.4
3	G	207	PHE	7.3
1	E	601	GLY	7.2
1	A	590	ILE	7.2
1	A	584	GLY	7.0
1	A	396	HIS	6.9
1	E	591	GLU	6.7
1	E	393	GLY	6.7
1	E	584	GLY	6.7
1	A	585	THR	6.6
1	A	42	GLN	6.5
1	E	599	GLU	6.5
1	E	388	CYS	6.4
1	A	398	PRO	6.4
1	A	606	PRO	6.3
1	E	394	GLY	6.3
1	A	391	PRO	6.1
1	E	590	ILE	6.1
1	A	400	GLY	6.0
1	A	362	GLY	6.0
1	E	37	VAL	6.0
1	E	287	GLU	6.0
1	E	36	GLU	5.9
3	C	111	GLY	5.9
3	G	110	GLY	5.9
1	A	600	ALA	5.8
1	A	588	GLY	5.8
1	A	335	VAL	5.8
1	A	385	ALA	5.8
1	E	585	THR	5.8
1	A	593	TYR	5.7
1	A	686	ALA	5.7
1	E	34	ALA	5.7
1	A	37	VAL	5.6
3	C	95	GLY	5.5
1	A	591	GLU	5.5
1	A	582	PRO	5.5
1	A	399	GLU	5.4
2	B	1	MET	5.4
3	C	109	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	570	PRO	5.4
2	B	46	TYR	5.4
3	C	115	ALA	5.3
1	E	387	GLY	5.3
3	G	223	GLU	5.2
1	E	401	PHE	5.2
1	A	207	GLY	5.2
1	A	589	LYS	5.1
1	E	568	GLY	5.1
1	E	384	ALA	5.1
1	A	285	GLY	5.1
1	E	582	PRO	5.1
3	C	227	ALA	5.1
1	E	400	GLY	5.0
1	A	30	ALA	4.9
1	A	393	GLY	4.9
1	A	361	GLY	4.9
1	E	495	VAL	4.9
1	A	587	SER	4.8
1	E	478	VAL	4.8
1	A	598	LYS	4.7
3	C	110	LYS	4.7
1	E	597	PHE	4.7
1	A	601	GLY	4.7
3	G	169	PRO	4.7
1	A	597	PHE	4.6
3	C	114	ARG	4.6
1	E	632	ALA	4.6
1	A	594	CYS	4.5
1	E	596	ARG	4.5
2	B	47	PRO	4.5
1	A	596	ARG	4.5
1	A	608	PHE	4.5
1	A	397	GLU	4.4
1	E	606	PRO	4.4
2	F	193	HIS	4.4
3	C	74	PHE	4.4
1	A	395	ASP	4.4
1	A	230	ALA	4.4
1	A	632	ALA	4.4
1	E	588	GLY	4.4
3	G	112	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	389	SER	4.4
1	A	384	ALA	4.3
1	E	602	HIS	4.2
1	E	133	GLU	4.2
1	E	386	GLY	4.2
2	B	44	GLY	4.2
1	E	608	PHE	4.1
1	A	595	GLN	4.1
1	E	586	ALA	4.1
3	C	207	GLY	4.0
3	C	208	PHE	4.0
1	A	389	SER	4.0
1	E	383	PRO	4.0
3	C	172	ALA	3.9
1	E	30	ALA	3.9
1	E	685	THR	3.9
1	E	469	PRO	3.9
1	E	595	GLN	3.9
1	A	48	PHE	3.9
3	G	108	GLY	3.9
1	E	392	SER	3.9
1	E	569	LYS	3.8
1	A	364	TYR	3.8
1	E	603	GLN	3.8
1	E	594	CYS	3.8
1	A	602	HIS	3.8
3	C	222	TRP	3.7
1	E	395	ASP	3.7
3	G	17	ASN	3.7
1	E	467	VAL	3.7
2	F	44	GLY	3.7
1	A	134	LYS	3.7
1	A	571	TRP	3.7
3	C	225	ARG	3.7
1	A	133	GLU	3.6
2	F	16	CYS	3.6
3	C	60	ASP	3.6
1	A	429	PRO	3.6
3	G	221	TRP	3.6
1	A	70	ALA	3.6
1	E	549	GLN	3.6
3	G	113	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	135	CYS	3.5
1	E	468	LEU	3.5
1	E	581	LEU	3.5
1	E	583	PHE	3.5
1	A	36	GLU	3.5
1	E	413	ARG	3.5
1	A	387	GLY	3.5
3	G	170	TRP	3.5
1	A	277	GLU	3.5
2	B	134	THR	3.5
1	A	430	TYR	3.5
1	A	386	GLY	3.5
3	G	63	LEU	3.4
3	C	224	GLU	3.4
3	G	222	GLN	3.4
1	A	392	SER	3.4
1	A	729	SER	3.4
1	E	396	HIS	3.4
1	A	283	THR	3.3
1	E	630	THR	3.3
3	G	1	ALA	3.3
1	A	605	LEU	3.3
1	A	284	VAL	3.3
1	A	390	GLY	3.3
1	E	286	PHE	3.3
1	A	186	GLY	3.3
3	C	250	GLY	3.3
1	A	562	GLY	3.3
1	E	466	ASP	3.2
3	G	249	GLY	3.2
1	A	118	GLU	3.2
1	A	663	GLU	3.2
1	A	467	VAL	3.2
1	A	552	GLY	3.2
3	C	112	SER	3.2
2	F	194	HIS	3.2
3	C	226	LEU	3.2
3	G	109	LYS	3.2
1	E	362	GLY	3.2
3	G	34	ALA	3.1
1	A	603	GLN	3.1
1	A	569	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	287	GLU	3.1
1	A	599	GLU	3.1
2	B	193	HIS	3.1
1	E	434	GLY	3.1
3	C	18	ASN	3.1
1	E	499	THR	3.0
1	A	581	LEU	3.0
1	A	240	SER	3.0
3	C	206	ALA	3.0
1	A	97	ARG	3.0
1	E	567	ARG	3.0
1	E	109	GLU	3.0
2	B	49	LEU	3.0
3	G	47	ARG	3.0
1	A	170	VAL	3.0
2	F	2	PRO	3.0
2	B	48	ASN	3.0
1	A	530	GLY	3.0
1	A	428	GLU	2.9
1	E	578	GLU	2.9
3	G	60	LEU	2.9
1	E	103	GLU	2.9
1	E	428	GLU	2.9
1	A	692	CYS	2.9
2	B	192	VAL	2.9
1	A	534	TYR	2.9
1	E	397	GLU	2.9
1	E	562	GLY	2.9
1	E	310	GLN	2.9
2	F	78	THR	2.8
3	C	113	GLN	2.8
3	G	57	ALA	2.8
1	E	470	GLN	2.8
3	G	70	ARG	2.8
3	G	39	LEU	2.8
3	G	114	ALA	2.8
1	A	69	GLU	2.8
2	F	79	LYS	2.8
1	E	604	PRO	2.8
1	E	496	ALA	2.8
3	G	36	LEU	2.8
1	A	730	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
3	G	250	LEU	2.7
1	A	434	GLY	2.7
1	E	381	LEU	2.7
3	G	97	LEU	2.7
3	G	166	LEU	2.7
1	A	291	ALA	2.7
3	C	66	ALA	2.7
3	G	226	ALA	2.7
1	A	560	GLY	2.7
2	B	2	PRO	2.7
1	A	548	LEU	2.7
1	E	605	LEU	2.7
3	C	116	LEU	2.7
1	A	339	ASP	2.7
1	A	388	CYS	2.7
1	A	568	GLY	2.7
1	A	383	PRO	2.7
1	E	421	ILE	2.7
1	A	578	GLU	2.7
3	G	107	LEU	2.6
1	E	70	ALA	2.6
3	G	229	ALA	2.6
3	G	64	TRP	2.6
1	A	604	PRO	2.6
1	E	579	GLY	2.6
1	E	678	GLY	2.6
1	A	565	VAL	2.6
1	A	536	PRO	2.5
1	A	684	PRO	2.5
1	E	560	GLY	2.5
1	A	573	GLU	2.5
1	E	622	LEU	2.5
1	A	577	LYS	2.5
1	A	288	GLU	2.5
1	A	576	GLU	2.5
3	C	221	PHE	2.5
1	E	113	ARG	2.5
3	G	224	ARG	2.5
3	C	204	GLU	2.5
3	G	59	ASP	2.5
3	G	66	GLU	2.5
1	E	577	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	532	GLU	2.5
3	G	48	TYR	2.5
1	A	381	LEU	2.5
1	E	106	GLN	2.5
3	G	18	ALA	2.5
3	G	130	PRO	2.4
1	E	555	LEU	2.4
1	E	385	ALA	2.4
1	A	609	THR	2.4
1	E	539	THR	2.4
1	A	678	GLY	2.4
1	A	310	GLN	2.4
3	G	105	LEU	2.4
1	A	337	TYR	2.4
1	A	103	GLU	2.4
1	A	43	ILE	2.4
1	E	561	MET	2.4
1	A	634	THR	2.3
3	G	16	THR	2.3
2	F	192	VAL	2.3
1	E	570	PRO	2.3
1	A	336	TRP	2.3
1	E	512	LEU	2.3
1	E	565	VAL	2.3
1	A	382	GLU	2.3
1	A	746	ARG	2.3
2	B	190	SER	2.3
3	G	15	TRP	2.3
1	A	425	ILE	2.3
3	C	105	LEU	2.3
2	B	79	LYS	2.3
1	A	535	PHE	2.3
3	G	73	PHE	2.3
3	G	79	PHE	2.3
1	A	282	TYR	2.3
1	E	489	TYR	2.3
1	A	34	ALA	2.3
1	A	567	ARG	2.3
3	C	54	LEU	2.3
3	G	214	LEU	2.3
2	F	147	ASP	2.3
1	E	119	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	164	ALA	2.2
1	A	572	LEU	2.2
3	C	106	LEU	2.2
1	E	537	TRP	2.2
1	E	454	GLU	2.2
3	G	52	ALA	2.2
3	C	17	THR	2.2
3	G	167	LYS	2.2
3	G	168	SER	2.2
1	A	295	ASP	2.2
1	A	293	VAL	2.2
1	E	324	PRO	2.2
1	A	316	ALA	2.2
3	G	163	ALA	2.2
1	A	539	THR	2.2
3	G	106	TYR	2.2
1	A	338	GLY	2.2
1	E	382	GLU	2.2
1	A	413	ARG	2.2
1	A	763	ARG	2.2
2	F	135	CYS	2.2
3	C	61	LEU	2.2
3	G	196	GLU	2.2
3	G	203	GLU	2.2
1	A	402	LYS	2.2
1	E	110	GLY	2.1
1	E	711	GLY	2.1
3	G	104	LEU	2.1
1	E	763	ARG	2.1
3	G	61	PHE	2.1
3	C	117	ALA	2.1
1	E	634	THR	2.1
2	F	46	TYR	2.1
1	A	550	SER	2.1
1	A	286	PHE	2.1
1	A	35	GLN	2.1
1	E	35	GLN	2.1
1	E	125	ALA	2.1
3	C	2	ALA	2.1
1	A	708	LEU	2.1
1	E	587	SER	2.1
1	A	279	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	G	69	ALA	2.1
1	A	228	ASN	2.1
1	E	572	LEU	2.1
1	E	422	GLU	2.1
1	E	532	GLU	2.1
1	E	598	LYS	2.1
3	G	123	SER	2.1
1	E	50	ARG	2.0
1	E	230	ALA	2.0
3	G	208	TRP	2.0
1	A	514	ASP	2.0
1	A	553	LEU	2.0
1	E	288	GLU	2.0
1	E	621	LEU	2.0
1	E	589	LYS	2.0
2	B	73	GLY	2.0
2	B	194	HIS	2.0
3	C	169	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SF4	F	1194	8/8	0.87	0.16	59,63,70,71	0
4	SF4	B	1196	8/8	0.89	0.17	43,45,50,51	0
4	SF4	B	1194	8/8	0.90	0.15	49,52,53,54	0
4	SF4	B	1195	8/8	0.93	0.11	46,48,52,55	0
4	SF4	F	1196	8/8	0.96	0.08	40,42,43,43	0

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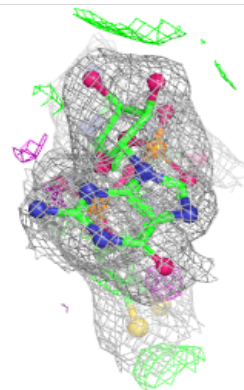
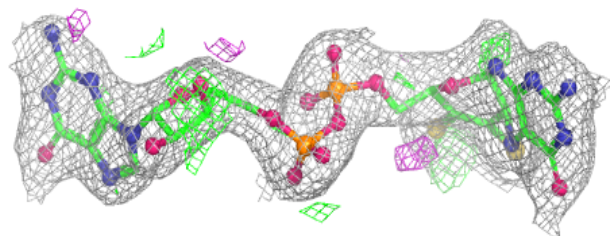
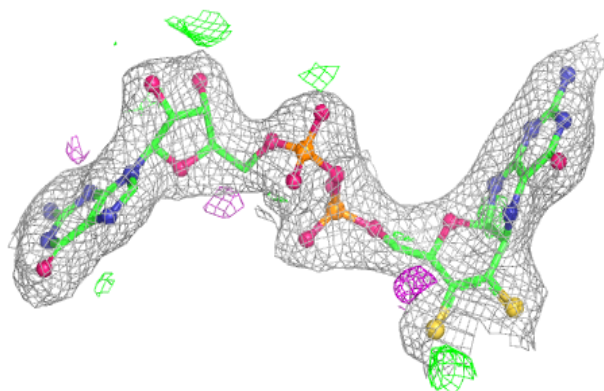
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SF4	B	1197	8/8	0.97	0.07	36,39,43,43	0
4	SF4	F	1195	8/8	0.97	0.07	42,43,43,44	0
4	SF4	E	1764	8/8	0.97	0.08	33,38,40,42	0
5	MGD	E	1765	47/47	0.97	0.07	31,38,40,41	0
5	MGD	E	1766	47/47	0.97	0.08	25,32,36,39	0
5	MGD	A	1765	47/47	0.98	0.07	28,39,42,45	0
5	MGD	A	1766	47/47	0.98	0.07	23,33,40,40	0
4	SF4	A	1764	8/8	0.98	0.07	32,37,40,41	0
4	SF4	F	1197	8/8	0.98	0.06	44,46,48,49	0
6	MO	A	1767	1/1	0.99	0.04	35,35,35,35	0
6	MO	E	1767	1/1	0.99	0.03	31,31,31,31	0

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

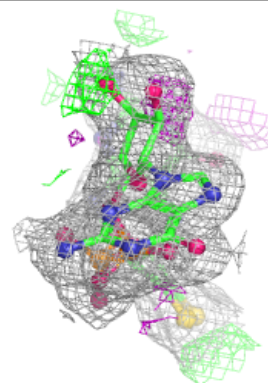
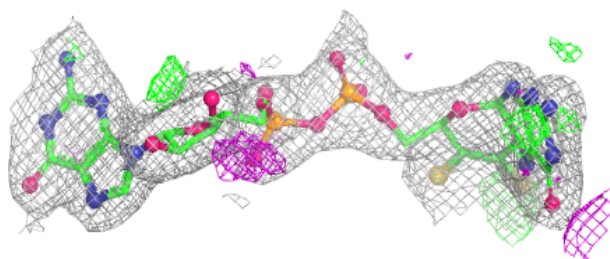
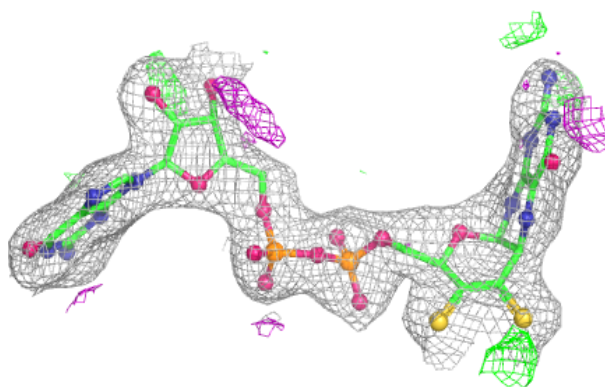
Electron density around MGD E 1765:

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

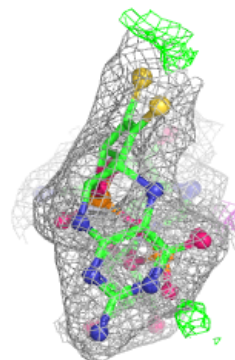
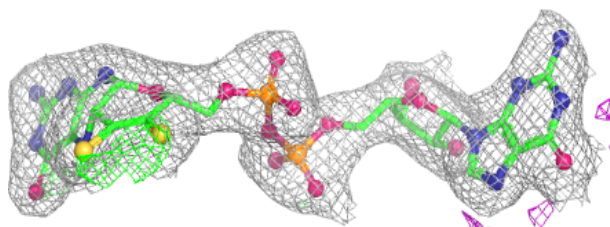
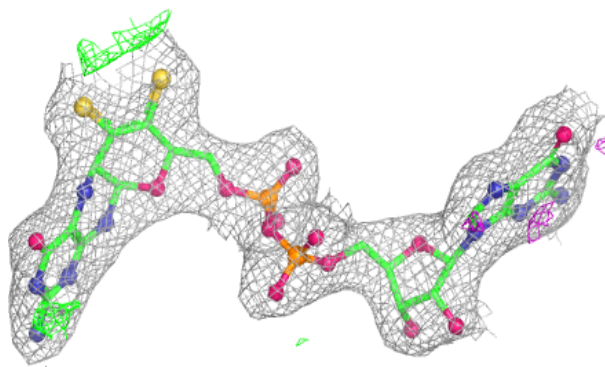


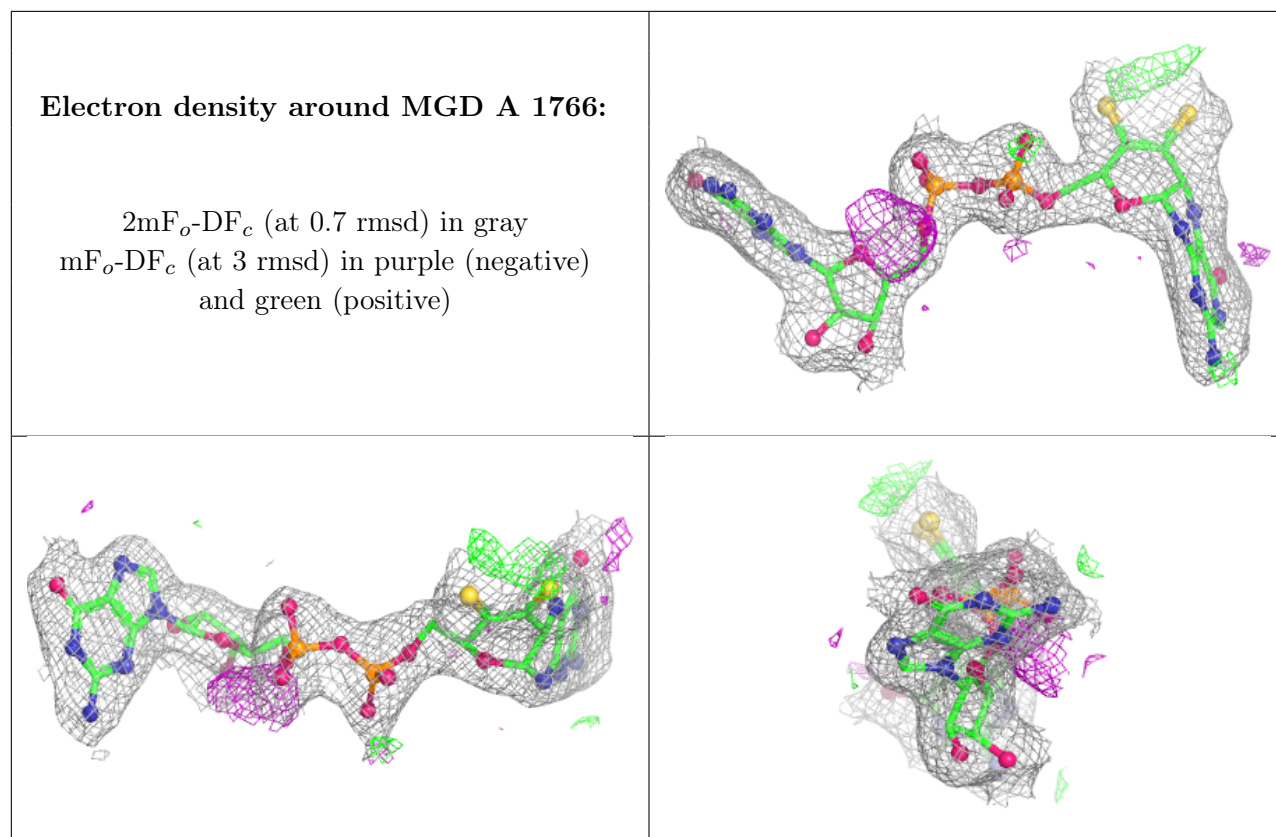
Electron density around MGD E 1766:

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

**Electron density around MGD A 1765:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.