



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:35 PM GMT

PDB ID : 1PQ3
Title : Human Arginase II: Crystal Structure and Physiological Role in Male and Female Sexual Arousal
Authors : Cama, E.; Colletuori, D.M.; Emig, F.A.; Shin, H.; Kim, S.W.; Kim, N.N.; Traish, A.M.; Ash, D.E.; Christianson, D.W.
Deposited on : 2003-06-17
Resolution : 2.70 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

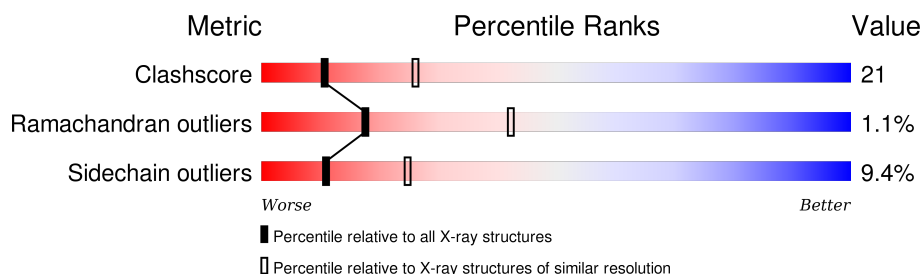
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	306	 64% 31% 6%
1	B	306	 63% 32% 5%
1	C	306	 66% 28% 6%
1	D	306	 62% 32% 6%
1	E	306	 62% 33% 5%
1	F	306	 64% 30% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	F	3074	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14599 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 Arginase II, mitochondrial precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2337	1474	407	447	9			
1	B	306	Total	C	N	O	S	0	0	0
			2337	1474	407	447	9			
1	C	306	Total	C	N	O	S	0	0	0
			2337	1474	407	447	9			
1	D	306	Total	C	N	O	S	0	0	0
			2337	1474	407	447	9			
1	E	306	Total	C	N	O	S	0	0	0
			2337	1474	407	447	9			
1	F	306	Total	C	N	O	S	0	0	0
			2337	1474	407	447	9			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	2	Total Mn 2 2	0	0
3	E	2	Total Mn 2 2	0	0
3	B	2	Total Mn 2 2	0	0
3	C	2	Total Mn 2 2	0	0
3	A	2	Total Mn 2 2	0	0

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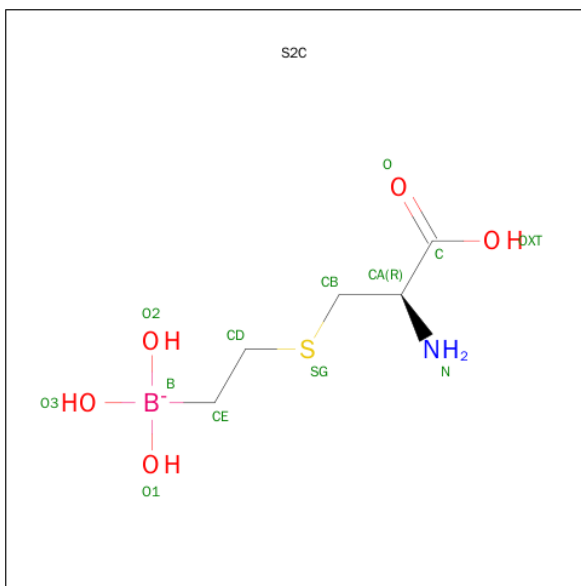
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	2	Total	Mn	0	0
			2	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		

- Molecule 5 is S-2-(BORONOETHYL)-L-CYSTEINE (three-letter code: S2C) (formula: C₅H₁₃BN₂O₅S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	B	C	N	O	S	0	0
			13	1	5	1	5	1		
5	B	1	Total	B	C	N	O	S	0	0
			13	1	5	1	5	1		
5	C	1	Total	B	C	N	O	S	0	0
			13	1	5	1	5	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	D	1	Total 13	B 1	C 5	N 1	O 5	S 1	0	0
5	E	1	Total 13	B 1	C 5	N 1	O 5	S 1	0	0
5	F	1	Total 13	B 1	C 5	N 1	O 5	S 1	0	0

- Molecule 6 is water.

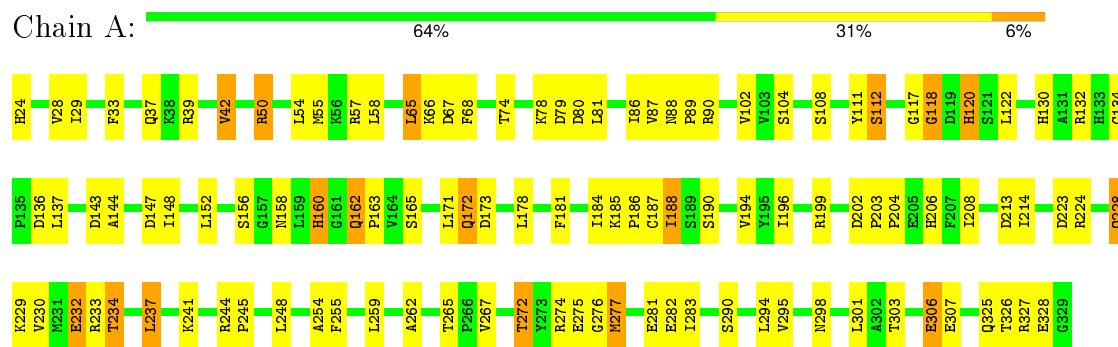
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	69	Total 69	O 69	0	0
6	B	75	Total 75	O 75	0	0
6	C	63	Total 63	O 63	0	0
6	D	74	Total 74	O 74	0	0
6	E	67	Total 67	O 67	0	0
6	F	59	Total 59	O 59	0	0

3 Residue-property plots

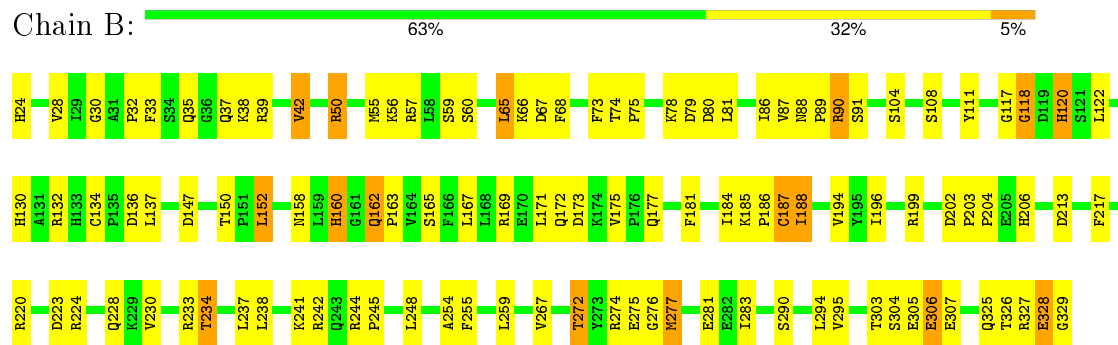
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

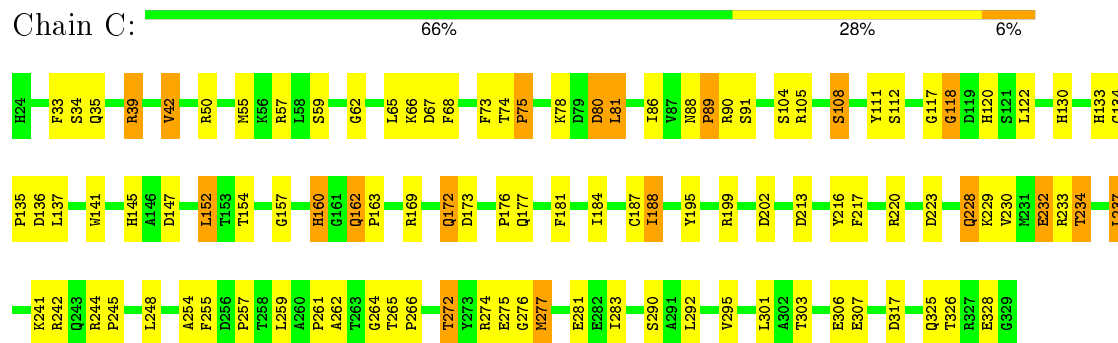
- Molecule 1: Arginase II, mitochondrial precursor



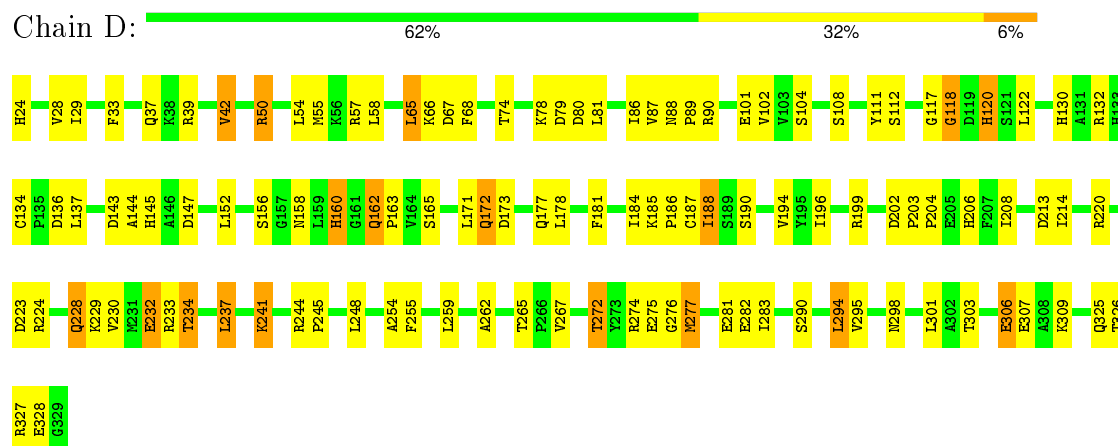
- Molecule 1: Arginase II, mitochondrial precursor



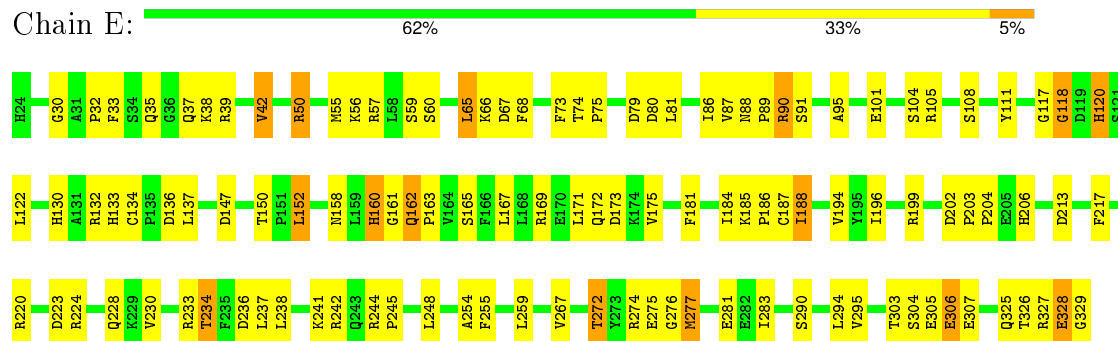
- Molecule 1: Arginase II, mitochondrial precursor



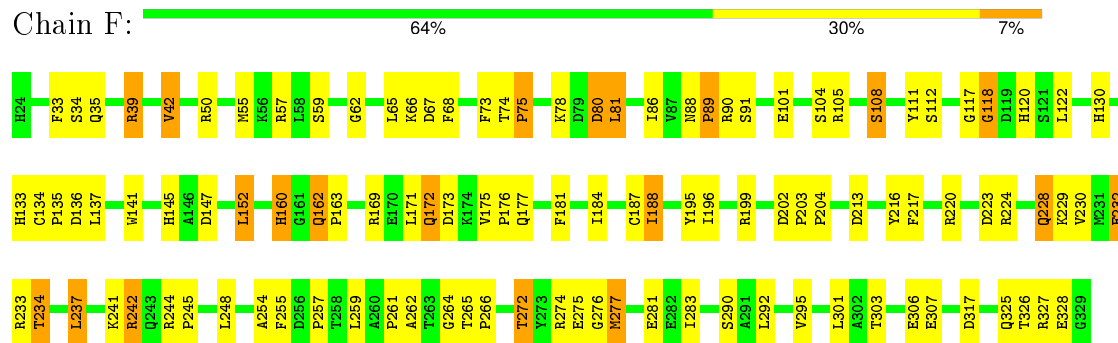
- Molecule 1: Arginase II, mitochondrial precursor



- Molecule 1: Arginase II, mitochondrial precursor



- Molecule 1: Arginase II, mitochondrial precursor



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	142.99Å 142.99Å 127.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.227 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14599	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: S2C, MN, SO4, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/2387	0.70	1/3245 (0.0%)
1	B	0.38	0/2387	0.68	1/3245 (0.0%)
1	C	0.37	0/2387	0.67	0/3245
1	D	0.42	0/2387	0.71	0/3245
1	E	0.39	0/2387	0.68	1/3245 (0.0%)
1	F	0.40	0/2387	0.67	0/3245
All	All	0.39	0/14322	0.69	3/19470 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	152	LEU	CA-CB-CG	5.57	128.11	115.30
1	B	152	LEU	CA-CB-CG	5.49	127.93	115.30
1	A	112	SER	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	GLY	Peptide
1	B	117	GLY	Peptide
1	C	117	GLY	Peptide
1	D	117	GLY	Peptide
1	E	117	GLY	Peptide
1	F	117	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2337	0	2318	100	0
1	B	2337	0	2318	111	0
1	C	2337	0	2318	107	0
1	D	2337	0	2318	108	0
1	E	2337	0	2318	110	0
1	F	2337	0	2318	118	0
2	A	20	0	0	1	0
2	B	5	0	0	0	0
2	C	10	0	0	0	0
2	D	20	0	0	1	0
2	F	20	0	0	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	13	0	12	1	0
5	B	13	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	13	0	11	2	0
5	D	13	0	12	1	0
5	E	13	0	12	2	0
5	F	13	0	12	2	0
6	A	69	0	0	7	0
6	B	75	0	0	4	0
6	C	63	0	0	3	0
6	D	74	0	0	10	0
6	E	67	0	0	6	0
6	F	59	0	0	8	0
All	All	14599	0	13979	596	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (596) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:THR:HG22	1:C:328:GLU:H	1.07	1.13
1:F:326:THR:HG22	1:F:328:GLU:H	1.07	1.11
1:F:81:LEU:H	1:F:81:LEU:HD12	1.13	1.08
1:A:326:THR:HG22	1:A:328:GLU:H	1.17	1.08
1:D:326:THR:HG22	1:D:328:GLU:H	1.16	1.07
1:E:326:THR:HG22	1:E:328:GLU:H	1.18	1.06
1:C:81:LEU:HD12	1:C:81:LEU:H	1.13	1.06
1:C:80:ASP:OD2	1:E:59:SER:HB2	1.55	1.04
1:D:81:LEU:H	1:D:81:LEU:HD12	1.23	1.04
1:B:59:SER:HB2	1:F:80:ASP:OD2	1.56	1.03
1:B:326:THR:HG22	1:B:328:GLU:H	1.18	1.03
1:A:81:LEU:HD12	1:A:81:LEU:H	1.22	1.01
1:F:272:THR:HG22	1:F:275:GLU:H	1.28	0.99
1:C:272:THR:HG22	1:C:275:GLU:H	1.28	0.98
1:E:272:THR:HG22	1:E:275:GLU:H	1.28	0.97
1:B:272:THR:HG22	1:B:275:GLU:H	1.28	0.96
1:A:50:ARG:HH11	1:A:50:ARG:HG2	1.27	0.96
1:B:81:LEU:HD12	1:B:81:LEU:H	1.28	0.96
1:E:81:LEU:H	1:E:81:LEU:HD12	1.29	0.96
1:D:50:ARG:HH11	1:D:50:ARG:HG2	1.29	0.95
1:C:57:ARG:HE	1:C:325:GLN:HE22	1.14	0.95
1:F:57:ARG:HE	1:F:325:GLN:HE22	1.15	0.95
1:D:272:THR:HG22	1:D:275:GLU:H	1.29	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:THR:HG22	1:A:275:GLU:H	1.30	0.94
1:B:57:ARG:HE	1:B:325:GLN:HE22	1.10	0.92
1:C:326:THR:HG22	1:C:328:GLU:N	1.86	0.90
1:E:57:ARG:HE	1:E:325:GLN:HE22	1.10	0.90
1:F:326:THR:HG22	1:F:328:GLU:N	1.86	0.90
1:A:185:LYS:HE3	6:A:814:HOH:O	1.72	0.89
1:E:326:THR:CG2	1:E:328:GLU:H	1.85	0.89
1:B:326:THR:CG2	1:B:328:GLU:H	1.86	0.89
1:F:73:PHE:O	1:F:75:PRO:HD3	1.74	0.88
1:C:73:PHE:O	1:C:75:PRO:HD3	1.73	0.88
1:D:101:GLU:HG2	6:D:1169:HOH:O	1.72	0.86
1:F:326:THR:CG2	1:F:328:GLU:H	1.88	0.86
1:E:50:ARG:HH11	1:E:50:ARG:HG2	1.40	0.86
1:D:326:THR:CG2	1:D:328:GLU:H	1.89	0.85
1:C:326:THR:CG2	1:C:328:GLU:H	1.89	0.84
1:A:50:ARG:HH11	1:A:50:ARG:CG	1.90	0.84
6:D:1079:HOH:O	1:F:328:GLU:HB2	1.78	0.83
1:C:81:LEU:CD1	1:C:81:LEU:H	1.90	0.83
1:B:50:ARG:HG2	1:B:50:ARG:HH11	1.42	0.83
1:A:326:THR:CG2	1:A:328:GLU:H	1.90	0.83
1:F:81:LEU:CD1	1:F:81:LEU:H	1.91	0.83
1:C:152:LEU:HD22	1:C:176:PRO:HG3	1.62	0.82
1:D:50:ARG:CG	1:D:50:ARG:HH11	1.92	0.82
1:B:326:THR:HG22	1:B:328:GLU:N	1.95	0.81
1:D:326:THR:HG22	1:D:328:GLU:N	1.94	0.81
1:E:326:THR:HG22	1:E:328:GLU:N	1.95	0.81
1:F:152:LEU:HD22	1:F:176:PRO:HG3	1.63	0.81
1:A:39:ARG:HD3	6:A:1042:HOH:O	1.81	0.80
1:A:326:THR:HG22	1:A:328:GLU:N	1.95	0.79
1:D:272:THR:HG21	6:D:903:HOH:O	1.83	0.79
1:A:265:THR:HG23	6:A:1197:HOH:O	1.81	0.79
1:C:81:LEU:HD12	1:C:81:LEU:N	1.96	0.79
1:E:50:ARG:HH11	1:E:50:ARG:CG	1.96	0.79
1:D:185:LYS:HE3	6:D:889:HOH:O	1.82	0.79
1:A:162:GLN:N	1:A:163:PRO:HD3	1.97	0.79
1:F:328:GLU:O	1:F:328:GLU:HG2	1.84	0.78
1:D:57:ARG:HE	1:D:325:GLN:HE22	1.31	0.78
1:C:328:GLU:HG2	1:C:328:GLU:O	1.83	0.78
1:C:80:ASP:CG	1:E:59:SER:HB2	2.05	0.77
1:A:57:ARG:HE	1:A:325:GLN:HE22	1.31	0.77
1:D:162:GLN:N	1:D:163:PRO:HD3	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:LEU:HD22	1:C:176:PRO:CG	2.15	0.77
1:F:152:LEU:HD22	1:F:176:PRO:CG	2.16	0.76
1:B:162:GLN:N	1:B:163:PRO:HD3	2.00	0.76
1:B:50:ARG:CG	1:B:50:ARG:HH11	1.98	0.76
1:F:81:LEU:N	1:F:81:LEU:HD12	1.97	0.76
1:E:162:GLN:N	1:E:163:PRO:HD3	2.00	0.76
1:D:81:LEU:CD1	1:D:81:LEU:H	2.00	0.75
1:B:230:VAL:O	1:B:234:THR:HG23	1.86	0.75
1:E:230:VAL:O	1:E:234:THR:HG23	1.87	0.75
1:B:59:SER:HB2	1:F:80:ASP:CG	2.06	0.73
1:A:228:GLN:OE1	1:B:224:ARG:HD2	1.88	0.73
1:D:228:GLN:OE1	1:E:224:ARG:HD2	1.87	0.73
1:D:81:LEU:HD12	1:D:81:LEU:N	2.02	0.73
1:D:162:GLN:H	1:D:163:PRO:HD3	1.54	0.72
1:A:228:GLN:O	1:A:232:GLU:HG2	1.89	0.72
1:B:274:ARG:HD2	1:C:223:ASP:OD1	1.90	0.72
1:B:37:GLN:NE2	1:B:42:VAL:HG21	2.05	0.72
1:D:147:ASP:HB3	1:D:163:PRO:HD2	1.72	0.72
1:B:57:ARG:HE	1:B:325:GLN:NE2	1.88	0.71
1:E:147:ASP:HB3	1:E:163:PRO:HD2	1.72	0.71
1:D:228:GLN:O	1:D:232:GLU:HG2	1.89	0.71
1:F:33:PHE:HB3	1:F:122:LEU:HD21	1.72	0.71
1:E:274:ARG:HD2	1:F:223:ASP:OD1	1.90	0.71
1:A:81:LEU:HD12	1:A:81:LEU:N	2.02	0.71
1:D:171:LEU:HG	1:D:208:ILE:HD11	1.73	0.71
1:A:162:GLN:H	1:A:163:PRO:HD3	1.54	0.71
1:B:147:ASP:HB3	1:B:163:PRO:HD2	1.71	0.71
1:E:37:GLN:NE2	1:E:42:VAL:HG21	2.05	0.71
1:A:147:ASP:HB3	1:A:163:PRO:HD2	1.73	0.70
1:B:24:HIS:HB3	6:B:856:HOH:O	1.92	0.70
1:C:33:PHE:HB3	1:C:122:LEU:HD21	1.71	0.70
1:A:265:THR:CG2	6:A:1197:HOH:O	2.37	0.70
1:A:171:LEU:HG	1:A:208:ILE:HD11	1.72	0.70
1:C:57:ARG:HE	1:C:325:GLN:NE2	1.90	0.70
1:A:79:ASP:OD1	1:A:90:ARG:HG2	1.92	0.70
1:F:162:GLN:N	1:F:163:PRO:HD3	2.07	0.69
1:C:162:GLN:N	1:C:163:PRO:HD3	2.07	0.69
1:D:79:ASP:OD1	1:D:90:ARG:HG2	1.93	0.69
1:E:133:HIS:HB3	6:E:855:HOH:O	1.93	0.69
1:A:272:THR:HG21	6:A:881:HOH:O	1.94	0.68
1:F:57:ARG:HE	1:F:325:GLN:NE2	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:H	1:A:81:LEU:CD1	2.00	0.67
1:F:242:ARG:NH2	2:F:3084:SO4:O4	2.28	0.67
1:E:162:GLN:N	1:E:163:PRO:CD	2.58	0.67
1:E:326:THR:HG22	1:E:329:GLY:H	1.59	0.67
1:F:277:MET:O	1:F:281:GLU:HG3	1.95	0.67
1:F:224:ARG:HD3	6:F:973:HOH:O	1.94	0.66
1:C:277:MET:O	1:C:281:GLU:HG3	1.96	0.66
1:B:326:THR:HG22	1:B:329:GLY:H	1.59	0.66
1:C:229:LYS:HA	1:C:232:GLU:HG3	1.77	0.66
1:E:57:ARG:HE	1:E:325:GLN:NE2	1.89	0.66
1:A:162:GLN:N	1:A:163:PRO:CD	2.58	0.66
1:B:162:GLN:N	1:B:163:PRO:CD	2.58	0.66
1:B:162:GLN:H	1:B:163:PRO:HD3	1.61	0.66
1:D:162:GLN:N	1:D:163:PRO:CD	2.59	0.65
1:F:229:LYS:HA	1:F:232:GLU:HG3	1.77	0.65
1:B:81:LEU:N	1:B:81:LEU:HD12	2.09	0.65
1:E:162:GLN:H	1:E:163:PRO:HD3	1.60	0.64
1:C:188:ILE:H	1:C:188:ILE:HD13	1.62	0.64
1:A:79:ASP:HA	1:A:90:ARG:HH11	1.62	0.64
1:D:55:MET:HE3	1:D:67:ASP:OD2	1.97	0.64
1:A:223:ASP:OD1	1:C:274:ARG:HD2	1.97	0.64
1:F:188:ILE:H	1:F:188:ILE:HD13	1.62	0.64
1:F:147:ASP:HB3	1:F:163:PRO:HD2	1.80	0.64
1:B:327:ARG:O	1:C:199:ARG:HA	1.98	0.64
1:E:327:ARG:O	1:F:199:ARG:HA	1.99	0.63
1:A:55:MET:HE3	1:A:67:ASP:OD2	1.98	0.63
1:D:223:ASP:OD1	1:F:274:ARG:HD2	1.98	0.63
1:F:162:GLN:H	1:F:163:PRO:HD3	1.64	0.63
1:C:162:GLN:H	1:C:163:PRO:HD3	1.63	0.63
1:C:147:ASP:HB3	1:C:163:PRO:HD2	1.80	0.63
1:A:188:ILE:H	1:A:188:ILE:HD13	1.63	0.63
1:D:104:SER:O	1:D:108:SER:HB2	1.99	0.63
1:B:81:LEU:CD1	1:B:81:LEU:H	2.05	0.63
1:B:33:PHE:O	1:B:118:GLY:HA3	1.99	0.63
1:A:230:VAL:O	1:A:234:THR:HG23	1.99	0.63
1:E:150:THR:OG1	1:E:152:LEU:HB3	1.99	0.62
1:B:199:ARG:NH1	1:B:267:VAL:O	2.32	0.62
1:D:39:ARG:HD3	6:D:1116:HOH:O	2.00	0.62
1:C:133:HIS:O	1:C:135:PRO:HD3	1.99	0.62
1:B:150:THR:OG1	1:B:152:LEU:HB3	1.99	0.62
1:E:188:ILE:HD13	1:E:188:ILE:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:ARG:NH1	1:E:267:VAL:O	2.31	0.62
1:B:188:ILE:HD13	1:B:188:ILE:H	1.65	0.62
1:A:194:VAL:HG11	1:A:234:THR:HB	1.81	0.61
1:E:33:PHE:O	1:E:118:GLY:HA3	2.00	0.61
1:C:272:THR:HG22	1:C:275:GLU:N	2.09	0.61
1:D:79:ASP:HA	1:D:90:ARG:HH11	1.63	0.61
1:A:277:MET:O	1:A:281:GLU:HG3	2.01	0.61
1:C:241:LYS:HD2	1:C:241:LYS:H	1.65	0.61
1:D:66:LYS:HG3	1:D:111:TYR:OH	2.01	0.61
1:C:57:ARG:NE	1:C:325:GLN:HE22	1.94	0.61
1:F:162:GLN:N	1:F:163:PRO:CD	2.64	0.61
1:F:133:HIS:O	1:F:135:PRO:HD3	2.00	0.61
1:A:66:LYS:HG3	1:A:111:TYR:OH	2.01	0.61
1:B:272:THR:HG23	1:B:274:ARG:H	1.66	0.61
1:D:188:ILE:HD13	1:D:188:ILE:H	1.65	0.61
1:E:81:LEU:H	1:E:81:LEU:CD1	2.06	0.61
1:D:230:VAL:O	1:D:234:THR:HG23	2.01	0.60
1:E:272:THR:HG23	1:E:274:ARG:H	1.66	0.60
1:D:194:VAL:HG11	1:D:234:THR:HB	1.82	0.60
1:A:130:HIS:CE1	1:A:290:SER:HB2	2.36	0.60
1:C:162:GLN:N	1:C:163:PRO:CD	2.64	0.60
1:F:272:THR:HG22	1:F:275:GLU:N	2.10	0.60
1:F:241:LYS:H	1:F:241:LYS:HD2	1.66	0.60
1:A:104:SER:O	1:A:108:SER:HB2	2.00	0.60
1:C:230:VAL:O	1:C:234:THR:HG23	2.02	0.60
1:E:272:THR:HG21	6:F:1150:HOH:O	2.01	0.60
1:F:272:THR:HG21	6:F:887:HOH:O	2.00	0.60
1:B:137:LEU:HD12	1:B:137:LEU:C	2.22	0.59
1:E:66:LYS:HG3	1:E:111:TYR:OH	2.02	0.59
1:D:130:HIS:CE1	1:D:290:SER:HB2	2.37	0.59
1:F:230:VAL:O	1:F:234:THR:HG23	2.02	0.59
1:D:277:MET:O	1:D:281:GLU:HG3	2.02	0.59
1:B:66:LYS:HG3	1:B:111:TYR:OH	2.01	0.59
1:C:104:SER:O	1:C:108:SER:HB2	2.02	0.59
1:C:233:ARG:O	1:C:237:LEU:HD22	2.02	0.59
1:E:81:LEU:N	1:E:81:LEU:HD12	2.09	0.59
1:F:104:SER:O	1:F:108:SER:HB2	2.02	0.58
1:E:137:LEU:C	1:E:137:LEU:HD12	2.23	0.58
1:D:274:ARG:HD2	1:E:223:ASP:OD1	2.02	0.58
1:A:274:ARG:HD2	1:B:223:ASP:OD1	2.03	0.58
1:F:81:LEU:HA	1:F:86:ILE:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:LEU:HA	1:C:86:ILE:O	2.04	0.58
1:B:272:THR:HG21	6:C:1151:HOH:O	2.04	0.58
1:F:39:ARG:HD2	6:F:1183:HOH:O	2.04	0.58
1:B:241:LYS:HD2	1:B:241:LYS:H	1.69	0.58
1:C:81:LEU:O	1:E:60:SER:HA	2.04	0.58
1:B:272:THR:CG2	1:B:275:GLU:H	2.09	0.58
1:F:233:ARG:O	1:F:237:LEU:HD22	2.03	0.57
1:A:137:LEU:HD12	1:A:137:LEU:C	2.25	0.57
1:F:57:ARG:NE	1:F:325:GLN:HE22	1.95	0.57
1:E:105:ARG:HG2	6:E:941:HOH:O	2.04	0.57
1:E:66:LYS:HD2	1:E:68:PHE:CE1	2.40	0.57
1:D:137:LEU:HD12	1:D:137:LEU:C	2.25	0.57
1:A:50:ARG:HG2	1:A:50:ARG:NH1	2.07	0.57
1:C:33:PHE:O	1:C:118:GLY:HA3	2.04	0.57
1:B:66:LYS:HB2	1:B:111:TYR:CE2	2.40	0.57
1:A:229:LYS:HA	1:A:232:GLU:HG3	1.86	0.57
1:F:228:GLN:O	1:F:232:GLU:HG2	2.05	0.56
1:B:66:LYS:HD2	1:B:68:PHE:CE1	2.40	0.56
1:B:281:GLU:OE1	1:C:220:ARG:HD2	2.05	0.56
1:C:137:LEU:C	1:C:137:LEU:HD12	2.25	0.56
1:F:137:LEU:C	1:F:137:LEU:HD12	2.25	0.56
1:F:33:PHE:O	1:F:118:GLY:HA3	2.04	0.56
1:C:228:GLN:O	1:C:232:GLU:HG2	2.06	0.56
1:B:55:MET:CE	1:F:78:LYS:HZ3	2.19	0.56
1:E:241:LYS:HD2	1:E:241:LYS:H	1.70	0.56
1:D:50:ARG:CG	1:D:50:ARG:NH1	2.61	0.56
1:A:87:VAL:HG12	1:A:88:ASN:ND2	2.20	0.56
1:D:229:LYS:HA	1:D:232:GLU:HG3	1.87	0.56
1:C:130:HIS:CE1	1:C:290:SER:HB2	2.41	0.56
1:B:60:SER:HA	1:F:81:LEU:O	2.04	0.56
1:D:224:ARG:NH2	2:D:3083:SO4:O3	2.39	0.56
1:E:57:ARG:NE	1:E:325:GLN:HE22	1.93	0.56
1:D:172:GLN:HG2	1:D:186:PRO:HG2	1.88	0.55
1:D:87:VAL:HG12	1:D:88:ASN:ND2	2.21	0.55
1:F:34:SER:HB2	1:F:42:VAL:HG23	1.88	0.55
1:D:112:SER:HA	1:D:290:SER:O	2.07	0.55
1:B:104:SER:O	1:B:108:SER:HB2	2.06	0.55
1:C:78:LYS:HG3	6:C:1188:HOH:O	2.06	0.55
1:D:81:LEU:HA	1:D:86:ILE:O	2.07	0.55
1:A:248:LEU:HD13	1:A:283:ILE:CD1	2.37	0.55
1:D:50:ARG:HG2	1:D:50:ARG:NH1	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLN:NE2	1:B:42:VAL:CG2	2.70	0.55
1:A:224:ARG:NH2	2:A:3073:SO4:O1	2.40	0.55
1:E:104:SER:O	1:E:108:SER:HB2	2.06	0.55
1:E:281:GLU:OE1	1:F:220:ARG:HD2	2.07	0.55
1:E:272:THR:CG2	1:E:275:GLU:H	2.09	0.55
1:F:130:HIS:CE1	1:F:290:SER:HB2	2.42	0.55
1:F:326:THR:HG23	6:F:1114:HOH:O	2.07	0.55
1:A:172:GLN:HG2	1:A:186:PRO:HG2	1.88	0.55
1:A:277:MET:HE3	1:A:277:MET:HA	1.88	0.55
1:D:57:ARG:HE	1:D:325:GLN:NE2	2.02	0.55
1:F:181:PHE:CD2	1:F:184:ILE:HD12	2.42	0.55
1:C:133:HIS:C	1:C:135:PRO:HD3	2.27	0.55
1:B:248:LEU:HD13	1:B:283:ILE:CD1	2.37	0.55
1:B:255:PHE:CE1	1:B:276:GLY:HA3	2.42	0.55
1:C:34:SER:HB2	1:C:42:VAL:HG23	1.88	0.55
1:E:255:PHE:CE1	1:E:276:GLY:HA3	2.42	0.55
1:C:136:ASP:O	1:C:244:ARG:HD3	2.07	0.54
1:B:79:ASP:OD2	1:B:91:SER:HB2	2.07	0.54
1:A:303:THR:HB	1:A:307:GLU:OE1	2.07	0.54
1:F:66:LYS:HG3	1:F:111:TYR:OH	2.08	0.54
1:E:248:LEU:HD13	1:E:283:ILE:CD1	2.36	0.54
1:A:112:SER:HA	1:A:290:SER:O	2.07	0.54
1:B:169:ARG:O	1:B:172:GLN:HG2	2.08	0.54
1:E:66:LYS:HB2	1:E:111:TYR:CE2	2.41	0.54
1:D:277:MET:HE3	1:D:277:MET:HA	1.89	0.54
1:C:78:LYS:HZ3	1:E:55:MET:CE	2.19	0.54
1:B:57:ARG:NE	1:B:325:GLN:HE22	1.92	0.54
1:E:236:ASP:HA	6:E:895:HOH:O	2.07	0.54
1:B:56:LYS:HA	1:F:80:ASP:OD2	2.07	0.54
1:C:80:ASP:OD2	1:E:56:LYS:HA	2.08	0.54
1:F:133:HIS:C	1:F:135:PRO:HD3	2.28	0.54
1:A:88:ASN:N	1:A:89:PRO:HD3	2.22	0.53
1:C:181:PHE:CD2	1:C:184:ILE:HD12	2.42	0.53
1:C:66:LYS:HG3	1:C:111:TYR:OH	2.07	0.53
1:D:303:THR:HB	1:D:307:GLU:OE1	2.08	0.53
1:D:248:LEU:HD13	1:D:283:ILE:CD1	2.37	0.53
1:A:57:ARG:HE	1:A:325:GLN:NE2	2.02	0.53
1:B:55:MET:HE3	1:F:78:LYS:HZ3	1.74	0.53
1:D:88:ASN:N	1:D:89:PRO:HD3	2.23	0.53
1:F:136:ASP:O	1:F:244:ARG:HD3	2.08	0.53
1:E:167:LEU:HB3	1:E:188:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:GLN:NE2	1:E:42:VAL:CG2	2.70	0.53
1:C:134:CYS:HB3	1:C:245:PRO:HG2	1.91	0.53
1:F:66:LYS:HD2	1:F:68:PHE:CE1	2.44	0.53
1:E:79:ASP:OD2	1:E:91:SER:HB2	2.08	0.53
1:B:274:ARG:HH22	1:C:275:GLU:CD	2.12	0.53
1:C:78:LYS:HZ3	1:E:55:MET:HE3	1.74	0.53
1:B:160:HIS:CE1	5:B:552:S2C:HE2	2.44	0.53
1:A:81:LEU:HA	1:A:86:ILE:O	2.08	0.53
1:B:81:LEU:HA	1:B:86:ILE:O	2.09	0.53
1:B:326:THR:HG22	1:B:329:GLY:N	2.23	0.52
1:F:134:CYS:HB3	1:F:245:PRO:HG2	1.91	0.52
1:B:167:LEU:HB3	1:B:188:ILE:HD11	1.91	0.52
1:E:326:THR:HG22	1:E:329:GLY:N	2.23	0.52
1:F:272:THR:CG2	1:F:275:GLU:H	2.12	0.52
1:A:66:LYS:HB2	1:A:111:TYR:CE2	2.45	0.52
1:C:66:LYS:HD2	1:C:68:PHE:CE1	2.45	0.52
1:D:265:THR:CG2	6:D:1022:HOH:O	2.57	0.52
1:E:281:GLU:HB3	1:F:220:ARG:NH1	2.24	0.52
1:B:187:CYS:HA	6:B:1141:HOH:O	2.08	0.52
1:E:160:HIS:CE1	5:E:555:S2C:HE2	2.45	0.52
6:A:1170:HOH:O	1:C:272:THR:HG21	2.08	0.52
1:F:326:THR:CG2	1:F:328:GLU:HB3	2.40	0.52
1:B:281:GLU:HB3	1:C:220:ARG:NH1	2.25	0.52
1:E:169:ARG:O	1:E:172:GLN:HG2	2.08	0.52
1:B:33:PHE:CZ	1:B:35:GLN:HB2	2.44	0.51
1:A:181:PHE:CD2	1:A:184:ILE:HD12	2.46	0.51
1:D:39:ARG:HD2	1:D:301:LEU:HD11	1.93	0.51
1:E:33:PHE:CZ	1:E:35:GLN:HB2	2.45	0.51
1:D:33:PHE:O	1:D:118:GLY:HA3	2.11	0.51
1:F:39:ARG:CG	1:F:39:ARG:HH11	2.23	0.51
1:C:66:LYS:HB2	1:C:111:TYR:CE2	2.45	0.51
1:A:255:PHE:CE1	1:A:276:GLY:HA3	2.46	0.51
1:D:66:LYS:HB2	1:D:111:TYR:CE2	2.45	0.51
1:E:81:LEU:HA	1:E:86:ILE:O	2.11	0.51
1:F:66:LYS:HB2	1:F:111:TYR:CE2	2.46	0.51
1:D:206:HIS:CD2	1:F:328:GLU:O	2.64	0.50
1:C:188:ILE:N	1:C:188:ILE:HD13	2.26	0.50
1:C:39:ARG:CG	1:C:39:ARG:HH11	2.24	0.50
1:D:177:GLN:HA	6:D:1024:HOH:O	2.10	0.50
1:B:136:ASP:O	1:B:244:ARG:HD2	2.11	0.50
1:A:206:HIS:CD2	1:C:328:GLU:O	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:ARG:HH22	1:F:275:GLU:CD	2.14	0.50
1:A:277:MET:HA	1:A:277:MET:CE	2.41	0.50
1:E:150:THR:HG22	1:E:165:SER:OG	2.11	0.50
1:A:39:ARG:HD2	1:A:301:LEU:HD11	1.93	0.50
1:C:145:HIS:HB3	6:C:800:HOH:O	2.11	0.50
1:E:88:ASN:N	1:E:89:PRO:HD3	2.27	0.50
1:B:38:LYS:HE3	1:B:158:ASN:OD1	2.12	0.50
1:E:217:PHE:CE1	1:E:234:THR:HG22	2.47	0.50
1:F:195:TYR:HB2	1:F:216:TYR:CB	2.42	0.50
1:D:181:PHE:CD2	1:D:184:ILE:HD12	2.46	0.50
1:A:33:PHE:O	1:A:118:GLY:HA3	2.11	0.50
1:B:66:LYS:HG3	1:B:111:TYR:CZ	2.46	0.50
1:E:305:GLU:CD	1:E:305:GLU:H	2.15	0.50
1:B:217:PHE:CE1	1:B:234:THR:HG22	2.47	0.50
1:C:78:LYS:CD	1:E:65:LEU:HD23	2.42	0.49
1:C:195:TYR:HB2	1:C:216:TYR:CB	2.42	0.49
1:C:277:MET:HE3	1:C:277:MET:HA	1.94	0.49
1:D:326:THR:CG2	1:D:327:ARG:N	2.74	0.49
1:D:277:MET:HA	1:D:277:MET:CE	2.42	0.49
1:C:169:ARG:O	1:C:172:GLN:HG2	2.12	0.49
1:F:248:LEU:HD22	1:F:283:ILE:HD12	1.93	0.49
1:C:326:THR:CG2	1:C:328:GLU:HB3	2.41	0.49
1:C:33:PHE:CZ	1:C:35:GLN:HB2	2.47	0.49
1:F:188:ILE:HD13	1:F:188:ILE:N	2.26	0.49
1:B:305:GLU:CD	1:B:305:GLU:H	2.15	0.49
1:B:88:ASN:N	1:B:89:PRO:HD3	2.27	0.49
1:C:277:MET:CE	1:C:277:MET:HA	2.42	0.49
1:E:33:PHE:HB3	1:E:122:LEU:HD21	1.94	0.49
1:E:66:LYS:HG3	1:E:111:TYR:CZ	2.48	0.49
1:B:136:ASP:OD1	1:B:242:ARG:NH1	2.46	0.49
1:C:105:ARG:HG2	1:C:105:ARG:HH11	1.77	0.49
1:A:188:ILE:HD13	1:A:188:ILE:N	2.27	0.49
1:B:150:THR:HG22	1:B:165:SER:OG	2.11	0.49
1:C:248:LEU:HD22	1:C:283:ILE:HD12	1.93	0.49
1:D:255:PHE:CE1	1:D:276:GLY:HA3	2.47	0.49
1:E:136:ASP:OD1	1:E:242:ARG:NH1	2.46	0.49
1:F:169:ARG:O	1:F:172:GLN:HG2	2.12	0.49
1:F:277:MET:CE	1:F:277:MET:HA	2.42	0.49
1:D:160:HIS:CE1	5:D:554:S2C:HE2	2.48	0.49
1:D:275:GLU:OE1	1:F:274:ARG:NH2	2.46	0.49
1:F:274:ARG:HG3	6:F:993:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:ARG:NH2	2:F:3074:SO4:S	2.85	0.49
1:B:120:HIS:CG	1:B:295:VAL:HG21	2.48	0.49
1:F:39:ARG:NH1	1:F:39:ARG:HG3	2.27	0.49
1:A:190:SER:HB2	1:A:214:ILE:HG12	1.94	0.49
1:B:181:PHE:CD2	1:B:184:ILE:HD12	2.48	0.49
1:F:33:PHE:CB	1:F:122:LEU:HD21	2.41	0.48
1:D:190:SER:HB2	1:D:214:ILE:HG12	1.94	0.48
1:F:224:ARG:NH2	2:F:3074:SO4:O3	2.46	0.48
1:B:33:PHE:HB3	1:B:122:LEU:HD21	1.94	0.48
1:E:136:ASP:O	1:E:244:ARG:HD2	2.12	0.48
1:E:120:HIS:CG	1:E:295:VAL:HG21	2.48	0.48
1:B:304:SER:OG	1:B:306:GLU:HG3	2.14	0.48
1:B:272:THR:HG23	1:B:274:ARG:N	2.28	0.48
1:B:274:ARG:NH2	1:C:275:GLU:OE1	2.46	0.48
1:C:57:ARG:NH2	1:C:317:ASP:OD1	2.41	0.48
1:F:57:ARG:NH2	1:F:317:ASP:OD1	2.41	0.48
1:E:272:THR:HG23	1:E:274:ARG:N	2.27	0.48
1:B:65:LEU:HD23	1:F:78:LYS:CD	2.43	0.48
1:C:39:ARG:HG3	1:C:39:ARG:NH1	2.28	0.48
1:F:33:PHE:CZ	1:F:35:GLN:HB2	2.48	0.48
1:E:50:ARG:HG2	1:E:50:ARG:NH1	2.19	0.48
1:A:328:GLU:O	1:B:206:HIS:CD2	2.67	0.48
1:D:328:GLU:O	1:E:206:HIS:CD2	2.67	0.48
1:D:327:ARG:O	1:E:199:ARG:HA	2.13	0.48
1:F:101:GLU:HG3	6:F:1164:HOH:O	2.14	0.48
1:A:199:ARG:NH1	1:A:267:VAL:O	2.46	0.48
1:A:326:THR:CG2	1:A:327:ARG:N	2.75	0.48
1:C:59:SER:O	1:C:62:GLY:N	2.46	0.48
1:C:272:THR:HG23	1:C:274:ARG:H	1.78	0.48
1:D:282:GLU:OE2	1:E:220:ARG:NH2	2.47	0.47
1:A:327:ARG:O	1:B:199:ARG:HA	2.13	0.47
1:E:233:ARG:O	1:E:237:LEU:HD22	2.13	0.47
1:D:274:ARG:NH2	1:E:275:GLU:OE1	2.48	0.47
1:C:154:THR:HG21	1:C:157:GLY:HA2	1.95	0.47
1:E:304:SER:OG	1:E:306:GLU:HG3	2.14	0.47
1:A:160:HIS:CE1	5:A:551:S2C:HE2	2.49	0.47
1:F:105:ARG:HG2	1:F:105:ARG:HH11	1.78	0.47
1:C:33:PHE:CB	1:C:122:LEU:HD21	2.41	0.47
1:D:274:ARG:HH22	1:E:275:GLU:CD	2.18	0.47
1:F:188:ILE:H	1:F:188:ILE:CD1	2.27	0.47
1:F:217:PHE:CE1	1:F:234:THR:HG22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ARG:O	1:D:237:LEU:HD22	2.14	0.47
1:C:188:ILE:H	1:C:188:ILE:CD1	2.26	0.47
1:A:188:ILE:H	1:A:188:ILE:CD1	2.27	0.47
1:C:217:PHE:CE1	1:C:234:THR:HG22	2.49	0.47
1:D:220:ARG:NH1	6:D:1171:HOH:O	2.48	0.47
1:E:181:PHE:CD2	1:E:184:ILE:HD12	2.49	0.47
1:F:160:HIS:CE1	5:F:556:S2C:HE2	2.50	0.47
1:D:203:PRO:HB2	1:D:204:PRO:HD3	1.97	0.47
1:D:265:THR:HG22	1:D:265:THR:O	2.14	0.47
1:A:274:ARG:NH2	1:B:275:GLU:OE1	2.48	0.47
1:C:137:LEU:HD12	1:C:137:LEU:O	2.15	0.47
1:C:160:HIS:CE1	5:C:553:S2C:HE2	2.50	0.47
1:A:233:ARG:O	1:A:237:LEU:HD22	2.15	0.47
1:F:272:THR:HG23	1:F:274:ARG:H	1.79	0.46
1:D:188:ILE:N	1:D:188:ILE:HD13	2.28	0.46
1:A:282:GLU:OE2	1:B:220:ARG:NH2	2.48	0.46
1:A:328:GLU:O	1:B:206:HIS:HD2	1.99	0.46
1:E:38:LYS:HE3	1:E:158:ASN:OD1	2.14	0.46
1:E:95:ALA:HB2	6:E:869:HOH:O	2.16	0.46
1:A:29:ILE:HD13	1:A:102:VAL:HG12	1.97	0.46
1:D:199:ARG:NH1	1:D:267:VAL:O	2.48	0.46
1:D:206:HIS:HD2	1:F:328:GLU:O	1.99	0.46
1:E:55:MET:HE3	1:E:67:ASP:OD2	2.16	0.46
1:E:101:GLU:HG3	6:E:1182:HOH:O	2.14	0.46
1:F:59:SER:O	1:F:62:GLY:N	2.48	0.46
1:D:328:GLU:O	1:E:206:HIS:HD2	1.98	0.46
1:A:306:GLU:HG3	1:A:307:GLU:N	2.31	0.46
1:E:87:VAL:C	1:E:89:PRO:HD3	2.36	0.46
1:D:136:ASP:O	1:D:244:ARG:HD3	2.15	0.46
1:D:188:ILE:CD1	1:D:188:ILE:H	2.28	0.46
1:D:306:GLU:HG3	1:D:307:GLU:N	2.31	0.46
1:B:233:ARG:O	1:B:237:LEU:HD22	2.16	0.46
1:F:112:SER:HA	1:F:290:SER:O	2.16	0.46
1:A:203:PRO:HB2	1:A:204:PRO:HD3	1.98	0.46
1:B:277:MET:HA	1:B:277:MET:HE3	1.98	0.45
1:D:202:ASP:HB3	1:D:204:PRO:HD2	1.98	0.45
1:A:136:ASP:O	1:A:244:ARG:HD3	2.16	0.45
1:A:274:ARG:HH22	1:B:275:GLU:CD	2.19	0.45
1:C:112:SER:HA	1:C:290:SER:O	2.16	0.45
1:B:130:HIS:CE1	1:B:290:SER:HB2	2.51	0.45
1:D:29:ILE:HD13	1:D:102:VAL:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:ARG:NH2	1:F:275:GLU:OE1	2.49	0.45
1:C:152:LEU:HD12	1:C:152:LEU:HA	1.72	0.45
1:C:255:PHE:CE1	1:C:276:GLY:HA3	2.51	0.45
1:C:50:ARG:HG2	1:C:50:ARG:HH11	1.82	0.45
1:A:143:ASP:OD1	1:A:144:ALA:N	2.49	0.45
1:C:120:HIS:CE1	1:C:141:TRP:CZ2	3.05	0.45
1:E:130:HIS:CE1	1:E:290:SER:HB2	2.52	0.45
1:A:275:GLU:OE1	1:C:274:ARG:NH2	2.48	0.45
1:B:203:PRO:HB2	1:B:204:PRO:HD3	1.99	0.45
1:F:39:ARG:CG	1:F:39:ARG:NH1	2.79	0.45
1:B:277:MET:CE	1:B:277:MET:HA	2.46	0.45
1:A:206:HIS:HD2	1:C:328:GLU:O	2.00	0.45
1:F:199:ARG:NH2	1:F:254:ALA:O	2.49	0.45
1:F:137:LEU:O	1:F:137:LEU:HD12	2.15	0.45
1:B:79:ASP:OD1	1:B:90:ARG:HG2	2.17	0.45
1:D:37:GLN:NE2	1:D:42:VAL:HG21	2.32	0.45
1:A:199:ARG:NH2	1:A:254:ALA:O	2.50	0.45
1:C:257:PRO:O	1:C:261:PRO:HG3	2.17	0.45
1:C:199:ARG:NH2	1:C:254:ALA:O	2.49	0.45
1:E:277:MET:CE	1:E:277:MET:HA	2.46	0.45
1:B:202:ASP:OD2	5:B:552:S2C:N	2.50	0.45
1:B:87:VAL:C	1:B:89:PRO:HD3	2.37	0.45
1:A:120:HIS:CG	1:A:295:VAL:HG21	2.52	0.45
1:C:292:LEU:C	1:C:292:LEU:HD23	2.37	0.45
1:F:50:ARG:HG2	1:F:50:ARG:HH11	1.82	0.45
1:B:55:MET:HE3	1:B:67:ASP:OD2	2.15	0.45
1:D:143:ASP:OD1	1:D:144:ALA:N	2.50	0.45
1:E:134:CYS:HB3	1:E:245:PRO:HG2	1.99	0.45
1:E:202:ASP:OD2	5:E:555:S2C:N	2.49	0.45
1:C:272:THR:CG2	1:C:275:GLU:H	2.12	0.44
1:A:57:ARG:NE	1:A:325:GLN:HE22	2.06	0.44
1:B:30:GLY:O	1:B:32:PRO:HD3	2.17	0.44
1:F:257:PRO:O	1:F:261:PRO:HG3	2.17	0.44
1:A:265:THR:HG22	1:A:265:THR:O	2.16	0.44
1:E:203:PRO:HB2	1:E:204:PRO:HD3	1.99	0.44
1:B:134:CYS:HB3	1:B:245:PRO:HG2	1.99	0.44
1:E:33:PHE:CB	1:E:122:LEU:HD21	2.48	0.44
1:B:137:LEU:HD12	1:B:137:LEU:O	2.17	0.44
1:E:137:LEU:O	1:E:137:LEU:HD12	2.17	0.44
1:D:199:ARG:NH2	1:D:254:ALA:O	2.50	0.44
1:C:88:ASN:N	1:C:89:PRO:HD3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ARG:HD3	6:B:997:HOH:O	2.17	0.44
1:A:37:GLN:NE2	1:A:42:VAL:HG21	2.33	0.44
1:B:177:GLN:HA	6:B:1144:HOH:O	2.17	0.44
1:F:255:PHE:CE1	1:F:276:GLY:HA3	2.52	0.44
1:C:264:GLY:HA2	1:C:301:LEU:CD1	2.48	0.44
1:A:54:LEU:O	1:A:57:ARG:HB3	2.18	0.44
1:E:150:THR:C	1:E:152:LEU:N	2.71	0.44
1:E:79:ASP:OD1	1:E:90:ARG:HG2	2.17	0.44
1:A:202:ASP:HB3	1:A:204:PRO:HD2	1.99	0.44
1:F:120:HIS:CE1	1:F:141:TRP:CZ2	3.06	0.44
1:E:30:GLY:O	1:E:32:PRO:HD3	2.18	0.44
1:D:79:ASP:HA	1:D:90:ARG:NH1	2.32	0.44
1:B:120:HIS:CD2	1:B:295:VAL:HG21	2.52	0.44
1:D:120:HIS:CG	1:D:295:VAL:HG21	2.52	0.44
1:A:262:ALA:HB1	1:A:298:ASN:O	2.18	0.44
1:F:78:LYS:HE3	1:F:78:LYS:HB2	1.66	0.44
1:F:145:HIS:HB3	6:F:1126:HOH:O	2.18	0.44
1:F:264:GLY:HA2	1:F:301:LEU:CD1	2.48	0.44
1:D:54:LEU:O	1:D:57:ARG:HB3	2.18	0.44
1:B:277:MET:O	1:B:281:GLU:HG3	2.18	0.44
1:F:303:THR:HB	1:F:307:GLU:OE1	2.18	0.44
1:C:303:THR:HB	1:C:307:GLU:OE1	2.18	0.44
1:C:78:LYS:HG2	1:E:65:LEU:HD23	2.00	0.44
1:E:277:MET:O	1:E:281:GLU:HG3	2.17	0.44
1:D:57:ARG:NE	1:D:325:GLN:HE22	2.07	0.43
1:A:28:VAL:HG11	1:A:55:MET:HE2	1.99	0.43
1:E:303:THR:HB	1:E:307:GLU:OE1	2.19	0.43
1:D:145:HIS:HB3	6:D:809:HOH:O	2.18	0.43
1:D:134:CYS:HB3	1:D:245:PRO:HG2	1.99	0.43
1:E:194:VAL:HG23	1:E:238:LEU:HD21	1.99	0.43
1:F:152:LEU:HD12	1:F:152:LEU:HA	1.73	0.43
1:D:171:LEU:O	1:D:172:GLN:C	2.57	0.43
1:C:120:HIS:CG	1:C:295:VAL:HG21	2.53	0.43
1:D:156:SER:HB2	1:D:158:ASN:ND2	2.34	0.43
1:E:277:MET:HA	1:E:277:MET:HE3	2.00	0.43
1:C:177:GLN:HG2	1:C:177:GLN:H	1.70	0.43
1:D:262:ALA:HB1	1:D:298:ASN:O	2.18	0.43
1:D:196:ILE:HD11	1:D:234:THR:HG21	2.01	0.43
1:A:282:GLU:HA	1:A:282:GLU:OE2	2.17	0.43
1:A:224:ARG:NH1	6:A:1185:HOH:O	2.51	0.43
1:B:194:VAL:HG23	1:B:238:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:GLN:H	1:F:177:GLN:HG2	1.70	0.43
1:F:224:ARG:NH2	2:F:3074:SO4:O4	2.51	0.43
1:B:33:PHE:CB	1:B:122:LEU:HD21	2.48	0.43
1:A:33:PHE:HB3	1:A:122:LEU:HD21	1.99	0.43
1:A:241:LYS:H	1:A:241:LYS:HD2	1.84	0.43
1:F:292:LEU:C	1:F:292:LEU:HD23	2.39	0.43
1:E:196:ILE:HD11	1:E:234:THR:HG21	2.00	0.43
1:A:171:LEU:O	1:A:172:GLN:C	2.57	0.43
1:A:196:ILE:HD11	1:A:234:THR:HG21	2.00	0.43
1:B:150:THR:C	1:B:152:LEU:N	2.70	0.43
1:D:66:LYS:HG3	1:D:111:TYR:CZ	2.53	0.43
1:D:33:PHE:HB3	1:D:122:LEU:HD21	2.00	0.43
1:C:105:ARG:HG2	1:C:105:ARG:NH1	2.34	0.43
1:A:162:GLN:O	1:A:165:SER:HB2	2.19	0.43
1:A:66:LYS:HG3	1:A:111:TYR:CZ	2.54	0.43
1:C:39:ARG:CG	1:C:39:ARG:NH1	2.80	0.43
1:D:37:GLN:HB3	1:D:160:HIS:CE1	2.54	0.43
1:E:120:HIS:CD2	1:E:295:VAL:HG21	2.52	0.43
1:D:309:LYS:HE3	1:D:309:LYS:HB2	1.84	0.42
1:D:241:LYS:HD2	1:D:241:LYS:H	1.84	0.42
1:B:50:ARG:NH1	1:B:50:ARG:CG	2.69	0.42
1:B:65:LEU:HD23	1:F:78:LYS:HG2	2.01	0.42
1:B:199:ARG:NH2	1:B:254:ALA:O	2.52	0.42
1:D:275:GLU:CD	1:F:274:ARG:HH22	2.23	0.42
1:B:150:THR:C	1:B:152:LEU:H	2.22	0.42
1:C:78:LYS:HD3	1:E:55:MET:HB3	2.01	0.42
1:D:282:GLU:OE2	1:D:282:GLU:HA	2.19	0.42
1:E:161:GLY:HA3	6:E:931:HOH:O	2.18	0.42
1:E:171:LEU:O	1:E:175:VAL:HG23	2.20	0.42
1:B:303:THR:HB	1:B:307:GLU:OE1	2.19	0.42
1:A:37:GLN:HB3	1:A:160:HIS:CE1	2.53	0.42
1:F:120:HIS:CG	1:F:295:VAL:HG21	2.53	0.42
1:C:265:THR:N	1:C:266:PRO:HD3	2.34	0.42
1:A:78:LYS:HB2	1:A:78:LYS:HE3	1.86	0.42
1:C:199:ARG:HH22	1:C:254:ALA:C	2.23	0.42
1:F:105:ARG:HG2	1:F:105:ARG:NH1	2.35	0.42
1:D:136:ASP:O	1:D:244:ARG:CD	2.67	0.42
1:F:88:ASN:N	1:F:89:PRO:HD3	2.33	0.42
1:B:73:PHE:O	1:B:75:PRO:HD3	2.20	0.42
1:D:58:LEU:HB2	1:D:65:LEU:HD21	2.02	0.42
1:F:199:ARG:HH22	1:F:254:ALA:C	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:THR:C	1:E:152:LEU:H	2.22	0.42
1:C:202:ASP:OD2	5:C:553:S2C:N	2.52	0.42
1:B:171:LEU:O	1:B:175:VAL:HG23	2.20	0.42
1:E:199:ARG:NH2	1:E:254:ALA:O	2.53	0.42
1:B:196:ILE:HD11	1:B:234:THR:HG21	2.02	0.42
1:D:28:VAL:HG11	1:D:55:MET:HE2	2.00	0.42
1:B:55:MET:HB3	1:F:78:LYS:HD3	2.02	0.42
1:F:202:ASP:OD2	5:F:556:S2C:N	2.53	0.42
1:A:136:ASP:O	1:A:244:ARG:CD	2.68	0.42
1:A:134:CYS:HB3	1:A:245:PRO:HG2	2.01	0.42
1:F:196:ILE:HD11	1:F:234:THR:HG21	2.02	0.41
1:D:294:LEU:HD22	1:D:294:LEU:HA	1.95	0.41
1:C:78:LYS:HE3	1:C:78:LYS:HB2	1.65	0.41
1:F:265:THR:N	1:F:266:PRO:HD3	2.35	0.41
1:D:223:ASP:OD2	1:F:327:ARG:NH1	2.52	0.41
1:E:73:PHE:O	1:E:75:PRO:HD3	2.20	0.41
1:C:55:MET:HE3	1:C:67:ASP:OD2	2.21	0.41
1:B:136:ASP:O	1:B:244:ARG:CD	2.69	0.41
1:F:88:ASN:HB3	1:F:91:SER:HB3	2.03	0.41
1:A:275:GLU:CD	1:C:274:ARG:HH22	2.24	0.41
1:D:162:GLN:HG3	6:D:926:HOH:O	2.19	0.41
1:B:167:LEU:O	1:B:188:ILE:HD13	2.20	0.41
1:F:171:LEU:O	1:F:175:VAL:HG23	2.21	0.41
1:B:50:ARG:NH1	1:B:50:ARG:HG2	2.20	0.41
1:A:148:ILE:O	1:A:148:ILE:HG12	2.21	0.41
1:B:78:LYS:HE3	1:B:78:LYS:HB2	1.81	0.41
1:E:167:LEU:O	1:E:188:ILE:HD13	2.20	0.41
1:A:66:LYS:HD2	1:A:68:PHE:CE1	2.56	0.41
1:B:28:VAL:HG11	1:B:55:MET:HE2	2.03	0.41
1:C:78:LYS:NZ	1:E:55:MET:HE3	2.36	0.40
1:A:58:LEU:HB2	1:A:65:LEU:HD21	2.03	0.40
1:F:203:PRO:HB2	1:F:204:PRO:HD3	2.04	0.40
1:D:66:LYS:HD2	1:D:68:PHE:CE1	2.56	0.40
1:C:88:ASN:HB3	1:C:91:SER:HB3	2.03	0.40
1:F:241:LYS:N	1:F:241:LYS:HD2	2.35	0.40
1:D:78:LYS:HE3	1:D:78:LYS:HB2	1.86	0.40
1:A:156:SER:HB2	1:A:158:ASN:ND2	2.35	0.40
1:D:162:GLN:O	1:D:165:SER:HB2	2.21	0.40
1:D:28:VAL:HB	1:D:55:MET:HE1	2.04	0.40
1:F:55:MET:HE3	1:F:67:ASP:OD2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/306 (99%)	285 (94%)	16 (5%)	3 (1%)	19	45
1	B	304/306 (99%)	285 (94%)	17 (6%)	2 (1%)	26	55
1	C	304/306 (99%)	287 (94%)	12 (4%)	5 (2%)	12	30
1	D	304/306 (99%)	284 (93%)	17 (6%)	3 (1%)	19	45
1	E	304/306 (99%)	285 (94%)	17 (6%)	2 (1%)	26	55
1	F	304/306 (99%)	285 (94%)	14 (5%)	5 (2%)	12	30
All	All	1824/1836 (99%)	1711 (94%)	93 (5%)	20 (1%)	17	42

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	GLY
1	A	172	GLN
1	B	118	GLY
1	C	118	GLY
1	D	118	GLY
1	D	172	GLN
1	E	118	GLY
1	F	118	GLY
1	C	172	GLN
1	F	172	GLN
1	C	262	ALA
1	F	262	ALA
1	A	162	GLN
1	B	162	GLN
1	C	162	GLN
1	D	162	GLN
1	E	162	GLN
1	F	162	GLN
1	C	89	PRO
1	F	89	PRO

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	257/257 (100%)	233 (91%)	24 (9%)	11	25
1	B	257/257 (100%)	233 (91%)	24 (9%)	11	25
1	C	257/257 (100%)	233 (91%)	24 (9%)	11	25
1	D	257/257 (100%)	232 (90%)	25 (10%)	10	23
1	E	257/257 (100%)	233 (91%)	24 (9%)	11	25
1	F	257/257 (100%)	233 (91%)	24 (9%)	11	25
All	All	1542/1542 (100%)	1397 (91%)	145 (9%)	11	25

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	42	VAL
1	A	50	ARG
1	A	65	LEU
1	A	74	THR
1	A	80	ASP
1	A	120	HIS
1	A	132	ARG
1	A	152	LEU
1	A	160	HIS
1	A	173	ASP
1	A	178	LEU
1	A	187	CYS
1	A	188	ILE
1	A	213	ASP
1	A	228	GLN
1	A	232	GLU
1	A	234	THR
1	A	237	LEU
1	A	259	LEU
1	A	272	THR
1	A	277	MET

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Mol	Chain	Res	Type
1	A	294	LEU
1	A	306	GLU
1	B	39	ARG
1	B	42	VAL
1	B	50	ARG
1	B	65	LEU
1	B	74	THR
1	B	80	ASP
1	B	90	ARG
1	B	120	HIS
1	B	132	ARG
1	B	160	HIS
1	B	173	ASP
1	B	185	LYS
1	B	186	PRO
1	B	187	CYS
1	B	188	ILE
1	B	213	ASP
1	B	228	GLN
1	B	234	THR
1	B	259	LEU
1	B	272	THR
1	B	277	MET
1	B	294	LEU
1	B	306	GLU
1	B	328	GLU
1	C	39	ARG
1	C	42	VAL
1	C	65	LEU
1	C	74	THR
1	C	75	PRO
1	C	80	ASP
1	C	81	LEU
1	C	90	ARG
1	C	108	SER
1	C	152	LEU
1	C	160	HIS
1	C	173	ASP
1	C	187	CYS
1	C	188	ILE
1	C	213	ASP
1	C	228	GLN

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Mol	Chain	Res	Type
1	C	232	GLU
1	C	234	THR
1	C	237	LEU
1	C	242	ARG
1	C	259	LEU
1	C	272	THR
1	C	277	MET
1	C	306	GLU
1	D	24	HIS
1	D	42	VAL
1	D	50	ARG
1	D	65	LEU
1	D	74	THR
1	D	80	ASP
1	D	120	HIS
1	D	132	ARG
1	D	152	LEU
1	D	160	HIS
1	D	173	ASP
1	D	178	LEU
1	D	187	CYS
1	D	188	ILE
1	D	213	ASP
1	D	228	GLN
1	D	232	GLU
1	D	234	THR
1	D	237	LEU
1	D	241	LYS
1	D	259	LEU
1	D	272	THR
1	D	277	MET
1	D	294	LEU
1	D	306	GLU
1	E	39	ARG
1	E	42	VAL
1	E	50	ARG
1	E	65	LEU
1	E	74	THR
1	E	80	ASP
1	E	90	ARG
1	E	120	HIS
1	E	132	ARG

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Mol	Chain	Res	Type
1	E	160	HIS
1	E	173	ASP
1	E	185	LYS
1	E	186	PRO
1	E	187	CYS
1	E	188	ILE
1	E	213	ASP
1	E	228	GLN
1	E	234	THR
1	E	259	LEU
1	E	272	THR
1	E	277	MET
1	E	294	LEU
1	E	306	GLU
1	E	328	GLU
1	F	39	ARG
1	F	42	VAL
1	F	65	LEU
1	F	74	THR
1	F	75	PRO
1	F	80	ASP
1	F	81	LEU
1	F	90	ARG
1	F	108	SER
1	F	152	LEU
1	F	160	HIS
1	F	173	ASP
1	F	187	CYS
1	F	188	ILE
1	F	213	ASP
1	F	228	GLN
1	F	232	GLU
1	F	234	THR
1	F	237	LEU
1	F	242	ARG
1	F	259	LEU
1	F	272	THR
1	F	277	MET
1	F	306	GLU

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

Mol	Chain	Res	Type
1	A	88	ASN
1	A	206	HIS
1	A	285	ASN
1	B	172	GLN
1	B	206	HIS
1	B	285	ASN
1	B	325	GLN
1	C	88	ASN
1	C	172	GLN
1	C	325	GLN
1	D	88	ASN
1	D	206	HIS
1	D	285	ASN
1	E	172	GLN
1	E	206	HIS
1	E	285	ASN
1	E	325	GLN
1	F	88	ASN
1	F	172	GLN
1	F	325	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 17 are monoatomic - leaving 21 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	3070	-	4,4,4	0.25	0	6,6,6	1.20	1 (16%)
2	SO4	A	3073	-	4,4,4	0.38	0	6,6,6	1.17	1 (16%)
2	SO4	A	3081	-	4,4,4	0.27	0	6,6,6	1.26	1 (16%)
2	SO4	A	3082	-	4,4,4	0.35	0	6,6,6	1.25	1 (16%)
5	S2C	A	551	3	6,12,12	1.30	1 (16%)	4,16,16	1.48	1 (25%)
2	SO4	B	3085	-	4,4,4	0.30	0	6,6,6	1.33	1 (16%)
5	S2C	B	552	3	6,12,12	1.31	1 (16%)	4,16,16	1.48	1 (25%)
2	SO4	C	3075	-	4,4,4	0.32	0	6,6,6	1.31	1 (16%)
2	SO4	C	3078	-	4,4,4	0.26	0	6,6,6	1.25	1 (16%)
5	S2C	C	553	3	6,12,12	1.30	1 (16%)	4,16,16	1.48	1 (25%)
2	SO4	D	3072	-	4,4,4	0.21	0	6,6,6	1.30	1 (16%)
2	SO4	D	3079	-	4,4,4	0.33	0	6,6,6	1.23	1 (16%)
2	SO4	D	3080	-	4,4,4	0.24	0	6,6,6	1.30	1 (16%)
2	SO4	D	3083	-	4,4,4	0.19	0	6,6,6	1.37	1 (16%)
5	S2C	D	554	3	6,12,12	1.29	1 (16%)	4,16,16	1.49	1 (25%)
5	S2C	E	555	3	6,12,12	1.31	1 (16%)	4,16,16	1.48	1 (25%)
2	SO4	F	3071	-	4,4,4	0.22	0	6,6,6	1.26	1 (16%)
2	SO4	F	3074	-	4,4,4	0.33	0	6,6,6	1.20	1 (16%)
2	SO4	F	3077	-	4,4,4	0.25	0	6,6,6	1.21	1 (16%)
2	SO4	F	3084	-	4,4,4	0.26	0	6,6,6	1.23	1 (16%)
5	S2C	F	556	3	6,12,12	1.33	1 (16%)	4,16,16	1.48	1 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	3070	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3073	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3081	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3082	-	-	0/0/0/0	0/0/0/0
5	S2C	A	551	3	-	0/4/12/12	0/0/0/0
2	SO4	B	3085	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	S2C	B	552	3	-	0/4/12/12	0/0/0/0
2	SO4	C	3075	-	-	0/0/0/0	0/0/0/0
2	SO4	C	3078	-	-	0/0/0/0	0/0/0/0
5	S2C	C	553	3	-	0/4/12/12	0/0/0/0
2	SO4	D	3072	-	-	0/0/0/0	0/0/0/0
2	SO4	D	3079	-	-	0/0/0/0	0/0/0/0
2	SO4	D	3080	-	-	0/0/0/0	0/0/0/0
2	SO4	D	3083	-	-	0/0/0/0	0/0/0/0
5	S2C	D	554	3	-	0/4/12/12	0/0/0/0
5	S2C	E	555	3	-	0/4/12/12	0/0/0/0
2	SO4	F	3071	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3074	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3077	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3084	-	-	0/0/0/0	0/0/0/0
5	S2C	F	556	3	-	0/4/12/12	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	556	S2C	CE-CD	-2.23	1.52	1.54
5	E	555	S2C	CE-CD	-2.20	1.52	1.54
5	A	551	S2C	CE-CD	-2.15	1.52	1.54
5	C	553	S2C	CE-CD	-2.14	1.52	1.54
5	B	552	S2C	CE-CD	-2.14	1.52	1.54
5	D	554	S2C	CE-CD	-2.14	1.52	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3083	SO4	O2-S-O1	-3.02	99.94	109.50
2	B	3085	SO4	O2-S-O1	-2.92	100.25	109.50
2	D	3080	SO4	O2-S-O1	-2.84	100.49	109.50
2	C	3075	SO4	O2-S-O1	-2.83	100.53	109.50
2	D	3072	SO4	O2-S-O1	-2.82	100.55	109.50
2	C	3078	SO4	O2-S-O1	-2.74	100.80	109.50
2	F	3071	SO4	O2-S-O1	-2.73	100.83	109.50
2	A	3081	SO4	O2-S-O1	-2.73	100.84	109.50
2	A	3082	SO4	O2-S-O1	-2.70	100.93	109.50
2	D	3079	SO4	O2-S-O1	-2.64	101.13	109.50
2	F	3077	SO4	O2-S-O1	-2.64	101.14	109.50
2	F	3084	SO4	O2-S-O1	-2.61	101.23	109.50
2	A	3070	SO4	O2-S-O1	-2.59	101.28	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3074	SO4	O2-S-O1	-2.58	101.33	109.50
5	D	554	S2C	CB-SG-CD	-2.48	94.96	102.41
5	C	553	S2C	CB-SG-CD	-2.47	94.99	102.41
5	A	551	S2C	CB-SG-CD	-2.47	95.00	102.41
2	A	3073	SO4	O2-S-O1	-2.47	101.68	109.50
5	E	555	S2C	CB-SG-CD	-2.47	95.00	102.41
5	B	552	S2C	CB-SG-CD	-2.46	95.01	102.41
5	F	556	S2C	CB-SG-CD	-2.46	95.02	102.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3073	SO4	1	0
5	A	551	S2C	1	0
5	B	552	S2C	2	0
5	C	553	S2C	2	0
2	D	3083	SO4	1	0
5	D	554	S2C	1	0
5	E	555	S2C	2	0
2	F	3074	SO4	3	0
2	F	3084	SO4	1	0
5	F	556	S2C	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.