



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:11 AM UTC

PDB ID : 1PQ3 / pdb_00001pq3
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.

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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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

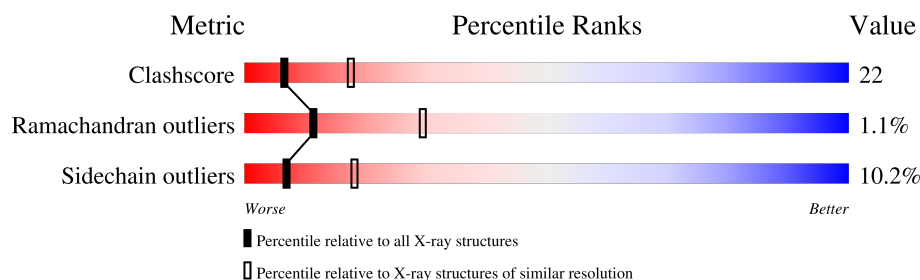
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	306	61% 32% 7%
1	B	306	59% 33% 7% .
1	C	306	63% 27% 9%
1	D	306	60% 33% 7%
1	E	306	58% 34% 7% .
1	F	306	61% 29% 9%

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 crite-

ria:

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

2 Entry composition [i](#)

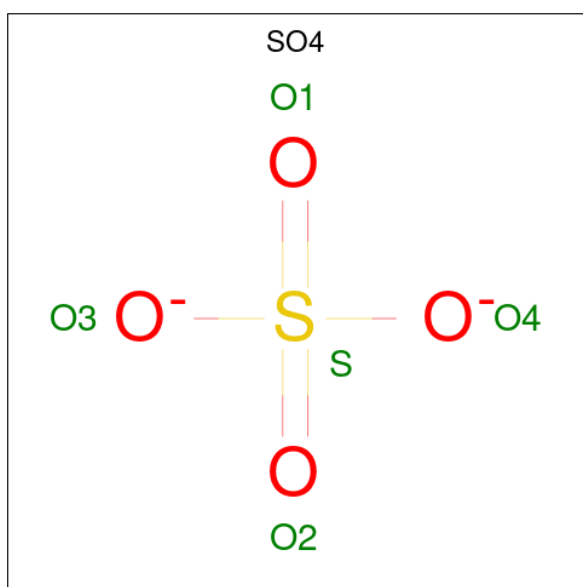
There are 6 unique types of molecules in this entry. The entry contains 14599 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

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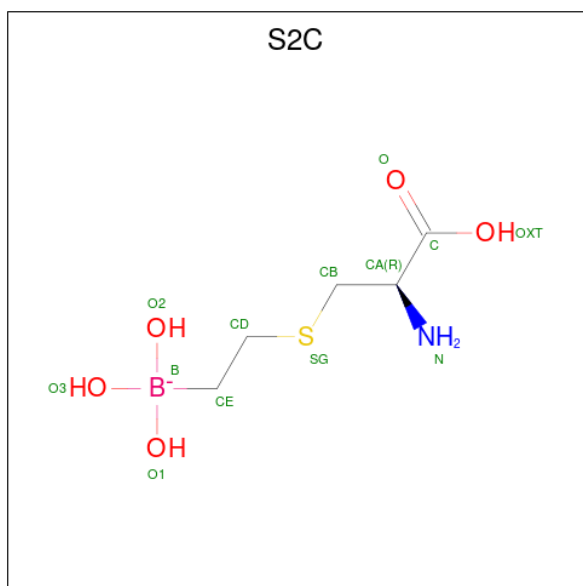
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	2	Total	Mn	0	0
			2	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is S-2-(BORONOETHYL)-L-CYSTEINE (CCD ID: S2C) (formula: C₅H₁₃BNO₅S).



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

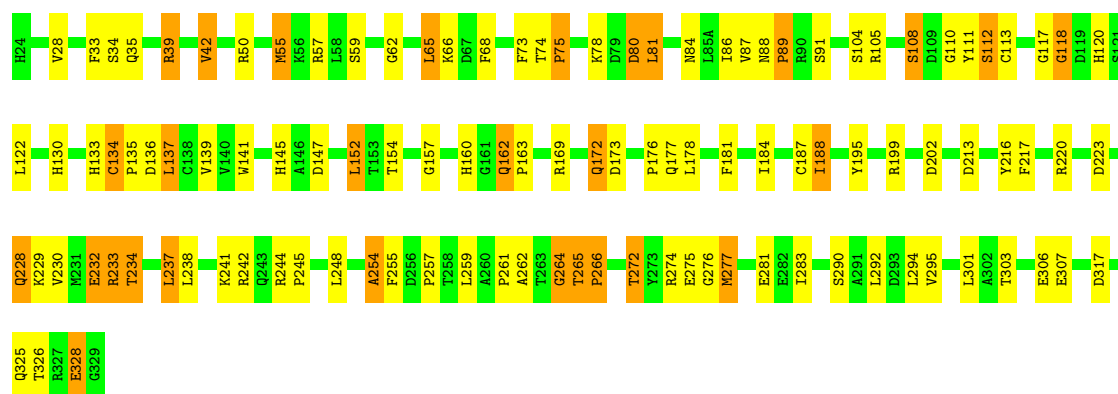
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	D	1	Total 13	B 1	C 5	N 1	O 5	S 1	0	0
5	E	1	Total 13	B 1	C 5	N 1	O 5	S 1	0	0
5	F	1	Total 13	B 1	C 5	N 1	O 5	S 1	0	0

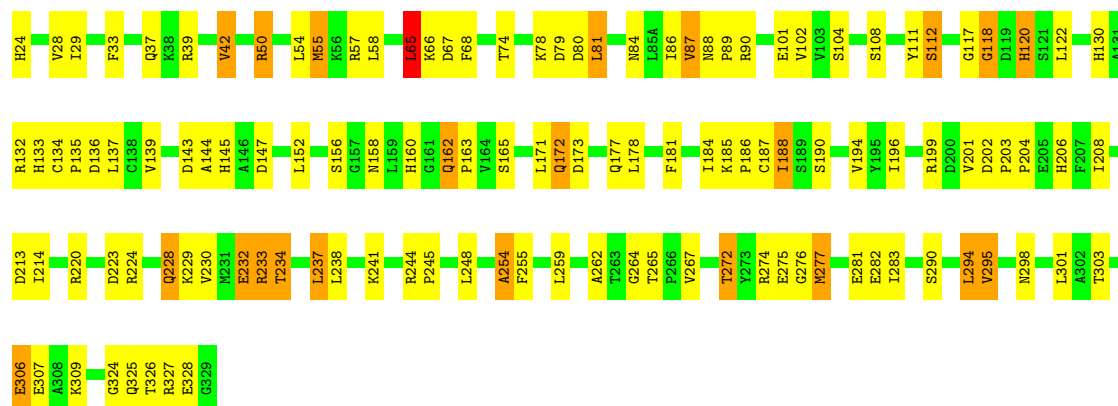
- Molecule 6 is water.

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



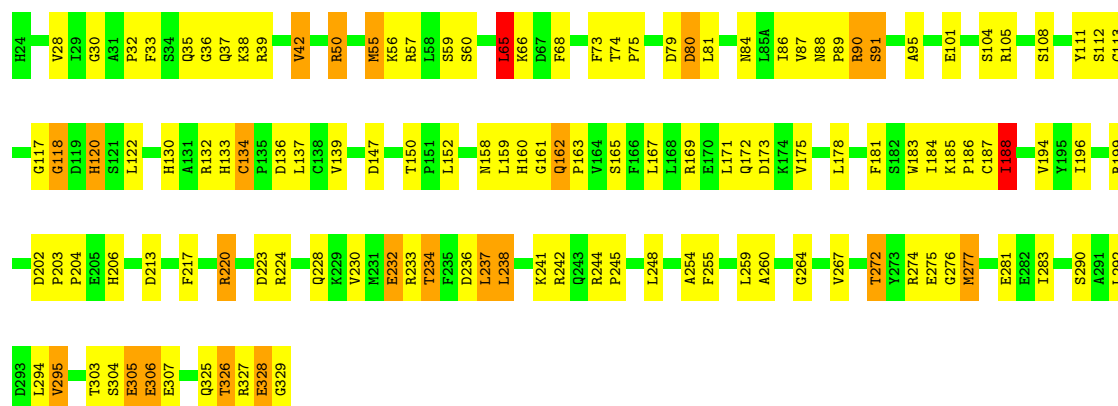
- Molecule 1: Arginase II, mitochondrial precursor

Chain D: 60% 33% 7%



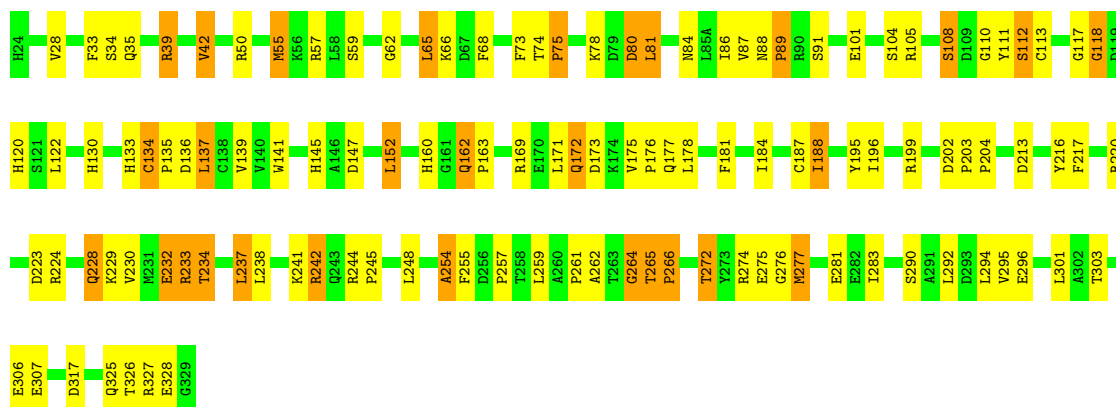
- Molecule 1: Arginase II, mitochondrial precursor

Chain E: 58% 34% 7%



- Molecule 1: Arginase II, mitochondrial precursor

Chain F: 61% 29% 9%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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: SO4, CL, S2C, MN

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	0.51	0/2387	1.06	14/3245 (0.4%)
1	B	0.47	0/2387	1.02	19/3245 (0.6%)
1	C	0.46	0/2387	1.04	15/3245 (0.5%)
1	D	0.53	0/2387	1.07	13/3245 (0.4%)
1	E	0.49	0/2387	1.02	20/3245 (0.6%)
1	F	0.50	0/2387	1.04	16/3245 (0.5%)
All	All	0.49	0/14322	1.04	97/19470 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	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 (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	LEU	N-CA-C	9.16	121.03	111.14
1	D	238	LEU	N-CA-C	9.12	120.99	111.14
1	C	55	MET	N-CA-C	7.55	119.15	111.07
1	F	55	MET	N-CA-C	7.55	119.14	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	265	THR	CA-C-N	7.42	127.40	119.76
1	F	265	THR	C-N-CA	7.42	127.40	119.76
1	A	112	SER	N-CA-C	-7.21	97.49	108.96
1	C	265	THR	CA-C-N	7.10	127.07	119.76
1	C	265	THR	C-N-CA	7.10	127.07	119.76
1	D	295	VAL	N-CA-C	7.07	118.99	108.96
1	D	264	GLY	N-CA-C	7.06	122.48	113.24
1	A	264	GLY	N-CA-C	7.05	122.48	113.24
1	D	112	SER	N-CA-C	-7.03	97.78	108.96
1	A	295	VAL	N-CA-C	6.93	118.80	108.96
1	E	295	VAL	N-CA-C	6.90	118.87	108.80
1	B	264	GLY	N-CA-C	6.66	120.73	112.73
1	B	295	VAL	N-CA-C	6.61	118.44	108.80
1	B	238	LEU	N-CA-C	6.39	119.48	111.24
1	E	260	ALA	CA-C-N	6.39	125.81	118.85
1	E	260	ALA	C-N-CA	6.39	125.81	118.85
1	E	264	GLY	N-CA-C	6.38	120.39	112.73
1	B	260	ALA	CA-C-N	6.38	125.80	118.85
1	B	260	ALA	C-N-CA	6.38	125.80	118.85
1	C	84	ASN	N-CA-C	6.31	120.92	113.23
1	D	55	MET	N-CA-C	6.28	118.68	111.02
1	B	65	LEU	N-CA-C	6.27	120.05	109.76
1	F	87	VAL	N-CA-C	6.27	117.73	109.21
1	E	238	LEU	N-CA-C	6.26	119.31	111.24
1	C	113	CYS	N-CA-C	6.20	118.82	108.96
1	A	55	MET	N-CA-C	6.19	118.57	111.02
1	A	201	VAL	N-CA-C	6.17	116.81	108.17
1	D	201	VAL	N-CA-C	6.17	116.81	108.17
1	E	84	ASN	N-CA-C	6.16	120.75	113.23
1	F	113	CYS	N-CA-C	6.15	118.75	108.96
1	B	84	ASN	N-CA-C	6.12	120.70	113.23
1	C	139	VAL	N-CA-C	6.12	116.67	108.11
1	A	254	ALA	N-CA-C	-6.11	105.31	112.89
1	E	65	LEU	N-CA-C	6.11	120.00	110.17
1	C	87	VAL	N-CA-C	6.09	117.49	109.21
1	F	84	ASN	N-CA-C	6.08	120.65	113.23
1	C	112	SER	N-CA-C	-6.07	99.31	108.96
1	C	238	LEU	N-CA-C	6.07	118.81	111.40
1	D	87	VAL	N-CA-C	6.01	116.95	108.36
1	D	324	GLY	N-CA-C	6.00	120.00	113.58
1	E	36	GLY	N-CA-C	-5.98	105.20	115.61
1	F	112	SER	N-CA-C	-5.98	99.45	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	GLY	N-CA-C	-5.96	105.25	115.61
1	F	238	LEU	N-CA-C	5.92	118.62	111.40
1	A	324	GLY	N-CA-C	5.90	119.89	113.58
1	F	233	ARG	N-CA-C	5.84	117.45	111.14
1	F	139	VAL	N-CA-C	5.82	116.26	108.11
1	A	65	LEU	N-CA-C	5.79	119.25	109.76
1	B	112	SER	N-CA-C	-5.77	99.78	108.96
1	D	65	LEU	N-CA-C	5.77	119.22	109.76
1	D	233	ARG	N-CA-C	5.77	117.64	111.36
1	C	254	ALA	N-CA-C	-5.74	105.16	111.82
1	E	112	SER	N-CA-C	-5.74	99.84	108.96
1	D	254	ALA	N-CA-C	-5.73	105.55	112.54
1	C	233	ARG	N-CA-C	5.69	117.28	111.14
1	D	139	VAL	N-CA-C	5.69	116.07	108.11
1	A	139	VAL	N-CA-C	5.68	116.06	108.11
1	B	113	CYS	N-CA-C	5.68	117.98	108.96
1	F	254	ALA	N-CA-C	-5.66	105.26	111.82
1	A	233	ARG	N-CA-C	5.62	117.48	111.36
1	E	113	CYS	N-CA-C	5.61	117.88	108.96
1	A	84	ASN	N-CA-C	5.57	120.02	113.23
1	B	55	MET	N-CA-C	5.48	117.71	111.02
1	F	264	GLY	N-CA-C	5.47	120.69	113.37
1	E	55	MET	N-CA-C	5.42	117.64	111.02
1	C	264	GLY	N-CA-C	5.41	120.62	113.37
1	A	87	VAL	N-CA-C	5.39	116.75	108.71
1	F	65	LEU	N-CA-C	5.39	118.85	110.17
1	B	232	GLU	N-CA-C	-5.36	105.34	111.07
1	A	144	ALA	N-CA-C	-5.34	106.27	112.89
1	E	139	VAL	N-CA-C	5.33	115.57	108.11
1	E	183	TRP	N-CA-C	5.29	117.79	111.71
1	B	188	ILE	N-CA-C	5.26	116.80	109.80
1	C	65	LEU	N-CA-C	5.23	118.60	110.17
1	D	84	ASN	N-CA-C	5.22	119.60	113.23
1	E	134	CYS	CA-C-N	5.18	125.48	119.47
1	E	134	CYS	C-N-CA	5.18	125.48	119.47
1	E	91	SER	N-CA-C	-5.16	105.35	111.69
1	E	80	ASP	N-CA-C	5.11	117.99	110.59
1	E	232	GLU	N-CA-C	-5.09	105.62	111.07
1	C	134	CYS	CA-C-N	5.08	125.36	119.47
1	C	134	CYS	C-N-CA	5.08	125.36	119.47
1	B	139	VAL	N-CA-C	5.06	115.20	108.11
1	B	159	LEU	N-CA-C	5.06	118.56	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	ASP	N-CA-C	5.06	117.92	110.59
1	B	134	CYS	CA-C-N	5.05	125.33	119.47
1	B	134	CYS	C-N-CA	5.05	125.33	119.47
1	E	159	LEU	N-CA-C	5.04	118.53	112.38
1	F	296	GLU	N-CA-C	5.04	119.38	113.23
1	B	183	TRP	N-CA-C	5.02	117.48	111.71
1	E	188	ILE	N-CA-C	5.00	116.45	109.80
1	F	134	CYS	CA-C-N	5.00	125.27	119.47
1	F	134	CYS	C-N-CA	5.00	125.27	119.47

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2337	0	2318	102	0
1	B	2337	0	2318	114	0
1	C	2337	0	2318	110	0
1	D	2337	0	2318	110	0
1	E	2337	0	2318	113	0
1	F	2337	0	2318	122	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	7	0
6	F	59	0	0	8	0
All	All	14599	0	13979	612	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 22.

All (612) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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:HD12	1:F:81:LEU:H	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:C:81:LEU:H	1:C:81:LEU:HD12	1.13	1.06
1:E:326:THR:HG22	1:E:328:GLU:H	1.18	1.06
1:C:80:ASP:OD2	1:E:59:SER:HB2	1.55	1.04
1:D:81:LEU:HD12	1:D:81:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	1:A:50:ARG:HH11	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:HG2	1:D:50:ARG:HH11	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
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:B:326:THR:CG2	1:B:328:GLU:H	1.86	0.89
1:E:326:THR:CG2	1:E:328:GLU:H	1.85	0.89
1:C:73:PHE:O	1:C:75:PRO:HD3	1.73	0.88
1:F:73:PHE:O	1:F:75:PRO:HD3	1.74	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:H	1:C:81:LEU:CD1	1.90	0.83
1:B:50:ARG:HH11	1:B:50:ARG:HG2	1.42	0.83
1:A:326:THR:CG2	1:A:328:GLU:H	1.90	0.83
1:F:81:LEU:H	1:F:81:LEU:CD1	1.91	0.83
1:C:152:LEU:HD22	1:C:176:PRO:HG3	1.62	0.82
1:C:80:ASP:CG	1:E:59:SER:HB2	2.05	0.82
1:D:50:ARG:HH11	1:D:50:ARG:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:THR:HG22	1:A:328:GLU:N	1.95	0.79
1:A:265:THR:HG23	6:A:1197:HOH:O	1.81	0.79
1:D:272:THR:HG21	6:D:903:HOH:O	1.83	0.79
1:C:81:LEU:HD12	1:C:81:LEU:N	1.96	0.79
1:A:162:GLN:N	1:A:163:PRO:HD3	1.97	0.79
1:D:185:LYS:HE3	6:D:889:HOH:O	1.82	0.79
1:E:50:ARG:HH11	1:E:50:ARG:CG	1.96	0.79
1:B:59:SER:HB2	1:F:80:ASP:CG	2.06	0.78
1:F:328:GLU:HG2	1:F:328:GLU:O	1.84	0.78
1:D:57:ARG:HE	1:D:325:GLN:HE22	1.31	0.78
1:C:328:GLU:O	1:C:328:GLU:HG2	1.83	0.78
1:C:78:LYS:HZ3	1:E:55:MET:HE3	1.48	0.78
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
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:HH11	1:B:50:ARG:CG	1.98	0.76
1:E:162:GLN:N	1:E:163:PRO:HD3	2.00	0.76
1:F:81:LEU:HD12	1:F:81:LEU:N	1.97	0.76
1:D:277:MET:HE3	1:D:277:MET:HA	1.69	0.75
1:D:81:LEU:H	1:D:81:LEU:CD1	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:A:277:MET:HE3	1:A:277:MET:HA	1.68	0.74
1:B:55:MET:HE3	1:F:78:LYS:HZ3	1.52	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:A:228:GLN:O	1:A:232:GLU:HG2	1.89	0.72
1:D:162:GLN:H	1:D:163:PRO:HD3	1.54	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:D:228:GLN:O	1:D:232:GLU:HG2	1.89	0.71
1:E:147:ASP:HB3	1:E:163:PRO:HD2	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:171:LEU:HG	1:A:208:ILE:HD11	1.72	0.70
1:A:265:THR:CG2	6:A:1197:HOH:O	2.37	0.70
1:A:79:ASP:OD1	1:A:90:ARG:HG2	1.92	0.70
1:C:57:ARG:HE	1:C:325:GLN:NE2	1.90	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
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: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:E:57:ARG:HE	1:E:325:GLN:NE2	1.89	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:HD12	1:B:81:LEU:N	2.09	0.65
1:B:137:LEU:HD12	1:B:137:LEU:C	2.22	0.65
1:E:162:GLN:H	1:E:163:PRO:HD3	1.60	0.64
1:C:188:ILE:HD13	1:C:188:ILE:H	1.62	0.64
1:A:79:ASP:HA	1:A:90:ARG:HH11	1.62	0.64
1:A:223:ASP:OD1	1:C:274:ARG:HD2	1.97	0.64
1:F:188:ILE:HD13	1:F:188:ILE:H	1.62	0.64
1:B:327:ARG:O	1:C:199:ARG:HA	1.98	0.64
1:F:147:ASP:HB3	1:F:163:PRO:HD2	1.80	0.64
1:E:327:ARG:O	1:F:199:ARG:HA	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:MET:HE3	1:C:277:MET:HA	1.80	0.63
1:E:137:LEU:HD12	1:E:137:LEU:C	2.23	0.63
1:D:223:ASP:OD1	1:F:274:ARG:HD2	1.98	0.63
1:C:162:GLN:H	1:C:163:PRO:HD3	1.63	0.63
1:F:162:GLN:H	1:F:163:PRO:HD3	1.64	0.63
1:A:188:ILE:HD13	1:A:188:ILE:H	1.63	0.63
1:C:147:ASP:HB3	1:C:163:PRO:HD2	1.80	0.63
1:D:104:SER:O	1:D:108:SER:HB2	1.99	0.63
1:A:230:VAL:O	1:A:234:THR:HG23	1.99	0.63
1:B:33:PHE:O	1:B:118:GLY:HA3	1.99	0.63
1:B:81:LEU:H	1:B:81:LEU:CD1	2.05	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:A:137:LEU:C	1:A:137:LEU:HD12	2.25	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
1:B:188:ILE:HD13	1:B:188:ILE:H	1.65	0.62
1:E:199:ARG:NH1	1:E:267:VAL:O	2.31	0.62
1:D:137:LEU:HD12	1:D:137:LEU:C	2.25	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:28:VAL:HB	1:C:55:MET:HE1	1.82	0.61
1:A:277:MET:O	1:A:281:GLU:HG3	2.01	0.61
1:C:241:LYS:H	1:C:241:LYS:HD2	1.65	0.61
1:C:272:THR:HG22	1:C:275:GLU:N	2.09	0.61
1:D:66:LYS:HG3	1:D:111:TYR:OH	2.01	0.61
1:D:79:ASP:HA	1:D:90:ARG:HH11	1.63	0.61
1:F:277:MET:HE3	1:F:277:MET:HA	1.81	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:F:137:LEU:C	1:F:137:LEU:HD12	2.25	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:277:MET:HE3	1:E:277:MET:HA	1.82	0.61
1:A:55:MET:HE3	1:A:67:ASP:OD2	2.01	0.61
1:E:81:LEU:H	1:E:81:LEU:CD1	2.06	0.61
1:B:277:MET:HE3	1:B:277:MET:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:VAL:O	1:D:234:THR:HG23	2.01	0.60
1:A:130:HIS:CE1	1:A:290:SER:HB2	2.36	0.60
1:D:194:VAL:HG11	1:D:234:THR:HB	1.82	0.60
1:E:272:THR:HG23	1:E:274:ARG:H	1.66	0.60
1:C:162:GLN:N	1:C:163:PRO:CD	2.64	0.60
1:C:137:LEU:C	1:C:137:LEU:HD12	2.25	0.60
1:F:241:LYS:H	1:F:241:LYS:HD2	1.66	0.60
1:F:272:THR:HG22	1:F:275:GLU:N	2.10	0.60
1:A:104:SER:O	1:A:108:SER:HB2	2.00	0.60
1:A:28:VAL:HB	1:A:55:MET:HE1	1.84	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:D:130:HIS:CE1	1:D:290:SER:HB2	2.37	0.59
1:E:66:LYS:HG3	1:E:111:TYR:OH	2.02	0.59
1:F:230:VAL:O	1:F:234:THR:HG23	2.02	0.59
1:C:133:HIS:C	1:C:135:PRO:HD3	2.27	0.59
1:D:277:MET:O	1:D:281:GLU:HG3	2.02	0.59
1:F:28:VAL:HB	1:F:55:MET:HE1	1.83	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:HD12	1:E:81:LEU:N	2.09	0.59
1:D:55:MET:HE3	1:D:67:ASP:OD2	2.02	0.58
1:F:104:SER:O	1:F:108:SER:HB2	2.02	0.58
1:D:28:VAL:HB	1:D:55:MET:HE1	1.83	0.58
1:A:274:ARG:HD2	1:B:223:ASP:OD1	2.03	0.58
1:D:274:ARG:HD2	1:E:223:ASP:OD1	2.02	0.58
1:F:133:HIS:C	1:F:135:PRO:HD3	2.28	0.58
1:F:81:LEU:HA	1:F:86:ILE:O	2.04	0.58
1:B:241:LYS:H	1:B:241:LYS:HD2	1.69	0.58
1:B:272:THR:HG21	6:C:1151:HOH:O	2.04	0.58
1:C:78:LYS:NZ	1:E:55:MET:HE3	2.17	0.58
1:C:81:LEU:HA	1:C:86:ILE:O	2.04	0.58
1:F:39:ARG:HD2	6:F:1183:HOH:O	2.04	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:B:274:ARG:HH22	1:C:275:GLU:CD	2.12	0.57
1:E:105:ARG:HG2	6:E:941:HOH:O	2.04	0.57
1:F:57:ARG:NE	1:F:325:GLN:HE22	1.95	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:LYS:HZ3	1:E:55:MET:CE	2.17	0.57
1:E:66:LYS:HD2	1:E:68:PHE:CE1	2.40	0.57
1:B:55:MET:HE3	1:F:78:LYS:NZ	2.17	0.57
1:A:50:ARG:HG2	1:A:50:ARG:NH1	2.07	0.57
1:B:66:LYS:HB2	1:B:111:TYR:CE2	2.40	0.57
1:C:33:PHE:O	1:C:118:GLY:HA3	2.04	0.57
1:A:229:LYS:HA	1:A:232:GLU:HG3	1.86	0.57
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:F:228:GLN:O	1:F:232:GLU:HG2	2.05	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:E:241:LYS:H	1:E:241:LYS:HD2	1.70	0.56
1:A:87:VAL:HG12	1:A:88:ASN:ND2	2.20	0.56
1:D:50:ARG:CG	1:D:50:ARG:NH1	2.61	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:87:VAL:HG12	1:D:88:ASN:ND2	2.21	0.55
1:D:172:GLN:HG2	1:D:186:PRO:HG2	1.88	0.55
1:F:34:SER:HB2	1:F:42:VAL:HG23	1.88	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:112:SER:HA	1:D:290:SER:O	2.07	0.55
1:A:248:LEU:HD13	1:A:283:ILE:CD1	2.37	0.55
1:D:81:LEU:HA	1:D:86:ILE:O	2.07	0.55
1:A:224:ARG:NH2	2:A:3073:SO4:O1	2.40	0.55
1:B:37:GLN:NE2	1:B:42:VAL:CG2	2.70	0.55
1:D:50:ARG:HG2	1:D:50:ARG:NH1	2.08	0.55
1:E:274:ARG:HH22	1:F:275:GLU:CD	2.14	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:A:172:GLN:HG2	1:A:186:PRO:HG2	1.88	0.55
1:F:326:THR:HG23	6:F:1114:HOH:O	2.07	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:B:248:LEU:HD13	1:B:283:ILE:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:305:GLU:H	1:E:305:GLU:CD	2.15	0.55
1:A:303:THR:HB	1:A:307:GLU:OE1	2.07	0.54
1:B:79:ASP:OD2	1:B:91:SER:HB2	2.07	0.54
1:C:136:ASP:O	1:C:244:ARG:HD3	2.07	0.54
1:E:248:LEU:HD13	1:E:283:ILE:CD1	2.36	0.54
1:F:66:LYS:HG3	1:F:111:TYR:OH	2.08	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:B:57:ARG:NE	1:B:325:GLN:HE22	1.92	0.54
1:B:305:GLU:CD	1:B:305:GLU:H	2.15	0.54
1:E:236:ASP:HA	6:E:895:HOH:O	2.07	0.54
1:B:55:MET:CE	1:F:78:LYS:HZ3	2.19	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:A:88:ASN:N	1:A:89:PRO:HD3	2.22	0.53
1:C:66:LYS:HG3	1:C:111:TYR:OH	2.07	0.53
1:C:181:PHE:CD2	1:C:184:ILE:HD12	2.42	0.53
1:D:248:LEU:HD13	1:D:283:ILE:CD1	2.37	0.53
1:D:303:THR:HB	1:D:307:GLU:OE1	2.08	0.53
1:A:57:ARG:HE	1:A:325:GLN:NE2	2.02	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
1:C:134:CYS:HB3	1:C:245:PRO:HG2	1.91	0.53
1:E:37:GLN:NE2	1:E:42:VAL:CG2	2.70	0.53
1:E:79:ASP:OD2	1:E:91:SER:HB2	2.08	0.53
1:F:66:LYS:HD2	1:F:68:PHE:CE1	2.44	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: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:326:THR:HG22	1:E:329:GLY:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:272:THR:CG2	1:F:275:GLU:H	2.12	0.52
1:B:187:CYS:HA	6:B:1141:HOH:O	2.08	0.52
1:E:281:GLU:HB3	1:F:220:ARG:NH1	2.24	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:D:274:ARG:HH22	1:E:275:GLU:CD	2.18	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:A:255:PHE:CE1	1:A:276:GLY:HA3	2.46	0.51
1:C:66:LYS:HB2	1:C:111:TYR:CE2	2.45	0.51
1:D:66:LYS:HB2	1:D:111:TYR:CE2	2.45	0.51
1:E:87:VAL:C	1:E:89:PRO:HD3	2.36	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:B:136:ASP:O	1:B:244:ARG:HD2	2.11	0.50
1:C:39:ARG:HH11	1:C:39:ARG:CG	2.24	0.50
1:C:188:ILE:HD13	1:C:188:ILE:N	2.26	0.50
1:D:177:GLN:HA	6:D:1024:HOH:O	2.10	0.50
1:D:206:HIS:CD2	1:F:328:GLU:O	2.64	0.50
1:A:206:HIS:CD2	1:C:328:GLU:O	2.64	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:B:28:VAL:HB	1:B:55:MET:HE1	1.92	0.50
1:C:145:HIS:HB3	6:C:800:HOH:O	2.11	0.50
1:A:274:ARG:HH22	1:B:275:GLU:CD	2.19	0.50
1:B:38:LYS:HE3	1:B:158:ASN:OD1	2.12	0.50
1:E:88:ASN:N	1:E:89:PRO:HD3	2.27	0.50
1:A:33:PHE:O	1:A:118:GLY:HA3	2.11	0.50
1:D:181:PHE:CD2	1:D:184:ILE:HD12	2.46	0.50
1:E:28:VAL:HB	1:E:55:MET:HE1	1.94	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:B:66:LYS:HG3	1:B:111:TYR:CZ	2.46	0.50
1:B:217:PHE:CE1	1:B:234:THR:HG22	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:277:MET:HA	1:A:277:MET:CE	2.41	0.49
1:B:87:VAL:C	1:B:89:PRO:HD3	2.37	0.49
1:C:292:LEU:C	1:C:292:LEU:HD23	2.37	0.49
1:C:169:ARG:O	1:C:172:GLN:HG2	2.12	0.49
1:D:326:THR:CG2	1:D:327:ARG:N	2.74	0.49
1:F:248:LEU:HD22	1:F:283:ILE:HD12	1.93	0.49
1:B:88:ASN:N	1:B:89:PRO:HD3	2.27	0.49
1:C:33:PHE:CZ	1:C:35:GLN:HB2	2.47	0.49
1:C:326:THR:CG2	1:C:328:GLU:HB3	2.41	0.49
1:F:188:ILE:HD13	1:F:188:ILE:N	2.26	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: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: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:D:160:HIS:CE1	5:D:554:S2C:HE2	2.48	0.49
1:B:120:HIS:CG	1:B:295:VAL:HG21	2.48	0.49
1:C:277:MET:HA	1:C:277:MET:CE	2.42	0.49
1:D:275:GLU:OE1	1:F:274:ARG:NH2	2.46	0.49
1:E:150:THR:C	1:E:152:LEU:N	2.71	0.49
1:F:224:ARG:NH2	2:F:3074:SO4:S	2.85	0.49
1:F:274:ARG:HG3	6:F:993:HOH:O	2.12	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:39:ARG:NH1	1:F:39:ARG:HG3	2.27	0.49
1:D:190:SER:HB2	1:D:214:ILE:HG12	1.94	0.48
1:F:33:PHE:CB	1:F:122:LEU:HD21	2.41	0.48
1:B:33:PHE:HB3	1:B:122:LEU:HD21	1.94	0.48
1:B:304:SER:OG	1:B:306:GLU:HG3	2.14	0.48
1:E:120:HIS:CG	1:E:295:VAL:HG21	2.48	0.48
1:E:136:ASP:O	1:E:244:ARG:HD2	2.12	0.48
1:F:224:ARG:NH2	2:F:3074:SO4:O3	2.46	0.48
1:F:277:MET:HA	1:F:277:MET:CE	2.42	0.48
1:B:272:THR:HG23	1:B:274:ARG:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:65:LEU:HD23	1:F:78:LYS:CD	2.43	0.48
1:C:39:ARG:NH1	1:C:39:ARG:HG3	2.28	0.48
1:E:272:THR:HG23	1:E:274:ARG:N	2.27	0.48
1:D:171:LEU:O	1:D:172:GLN:C	2.57	0.48
1:D:277:MET:HA	1:D:277:MET:CE	2.42	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:199:ARG:NH1	1:A:267:VAL:O	2.46	0.48
1:A:328:GLU:O	1:B:206:HIS:CD2	2.67	0.48
1:D:327:ARG:O	1:E:199:ARG:HA	2.13	0.48
1:D:328:GLU:O	1:E:206:HIS:CD2	2.67	0.48
1:F:101:GLU:HG3	6:F:1164:HOH:O	2.14	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:B:50:ARG:HH12	1:B:55:MET:HE2	1.77	0.47
1:D:282:GLU:OE2	1:E:220:ARG:NH2	2.47	0.47
1:F:292:LEU:C	1:F:292:LEU:HD23	2.39	0.47
1:A:171:LEU:O	1:A:172:GLN:C	2.57	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:C:154:THR:HG21	1:C:157:GLY:HA2	1.95	0.47
1:D:274:ARG:NH2	1:E:275:GLU:OE1	2.48	0.47
1:E:50:ARG:HH12	1:E:55:MET:HE2	1.79	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:B:150:THR:C	1:B:152:LEU:N	2.70	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:275:GLU:CD	1:F:274:ARG:HH22	2.23	0.47
1:D:233:ARG:O	1:D:237:LEU:HD22	2.14	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
1:A:188:ILE:H	1:A:188:ILE:CD1	2.27	0.47
1:B:150:THR:C	1:B:152:LEU:H	2.22	0.47
1:C:188:ILE:H	1:C:188:ILE:CD1	2.26	0.47
1:C:217:PHE:CE1	1:C:234:THR:HG22	2.49	0.47
1:D:203:PRO:HB2	1:D:204:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:199:ARG:HH22	1:C:254:ALA:C	2.23	0.47
1:D:265:THR:O	1:D:265:THR:HG22	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:E:150:THR:C	1:E:152:LEU:H	2.22	0.47
1:F:199:ARG:HH22	1:F:254:ALA:C	2.23	0.47
1:A:233:ARG:O	1:A:237:LEU:HD22	2.15	0.47
1:C:160:HIS:CE1	5:C:553:S2C:HE2	2.50	0.47
1:A:282:GLU:OE2	1:B:220:ARG:NH2	2.48	0.46
1:D:188:ILE:HD13	1:D:188:ILE:N	2.28	0.46
1:F:272:THR:HG23	1:F:274:ARG:H	1.79	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: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:A:306:GLU:HG3	1:A:307:GLU:N	2.31	0.46
1:D:136:ASP:O	1:D:244:ARG:HD3	2.15	0.46
1:D:328:GLU:O	1:E:206:HIS:HD2	1.98	0.46
1:D:188:ILE:H	1:D:188:ILE:CD1	2.28	0.46
1:D:306:GLU:HG3	1:D:307:GLU:N	2.31	0.46
1:A:275:GLU:CD	1:C:274:ARG:HH22	2.24	0.46
1:B:233:ARG:O	1:B:237:LEU:HD22	2.16	0.46
1:A:203:PRO:HB2	1:A:204:PRO:HD3	1.98	0.46
1:F:112:SER:HA	1:F:290:SER:O	2.16	0.46
1:A:136:ASP:O	1:A:244:ARG:HD3	2.16	0.45
1:D:202:ASP:HB3	1:D:204:PRO:HD2	1.98	0.45
1:B:130:HIS:CE1	1:B:290:SER:HB2	2.51	0.45
1:C:112:SER:HA	1:C:290:SER:O	2.16	0.45
1:D:29:ILE:HD13	1:D:102:VAL:HG12	1.97	0.45
1:A:143:ASP:OD1	1:A:144:ALA:N	2.49	0.45
1:C:50:ARG:HG2	1:C:50:ARG:HH11	1.82	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:E:274:ARG:NH2	1:F:275:GLU:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:277:MET:HA	1:B:277:MET:CE	2.46	0.45
1:F:39:ARG:CG	1:F:39:ARG:NH1	2.79	0.45
1:A:199:ARG:NH2	1:A:254:ALA:O	2.50	0.45
1:A:206:HIS:HD2	1:C:328:GLU:O	2.00	0.45
1:B:79:ASP:OD1	1:B:90:ARG:HG2	2.17	0.45
1:C:257:PRO:O	1:C:261:PRO:HG3	2.17	0.45
1:D:37:GLN:NE2	1:D:42:VAL:HG21	2.32	0.45
1:F:137:LEU:HD12	1:F:137:LEU:O	2.15	0.45
1:F:199:ARG:NH2	1:F:254:ALA:O	2.49	0.45
1:A:120:HIS:CG	1:A:295:VAL:HG21	2.52	0.45
1:B:202:ASP:OD2	5:B:552:S2C:N	2.50	0.45
1:C:199:ARG:NH2	1:C:254:ALA:O	2.49	0.45
1:F:50:ARG:HG2	1:F:50:ARG:HH11	1.82	0.45
1:C:28:VAL:CB	1:C:55:MET:HE1	2.47	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: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:C:272:THR:CG2	1:C:275:GLU:H	2.12	0.44
1:F:257:PRO:O	1:F:261:PRO:HG3	2.17	0.44
1:A:265:THR:O	1:A:265:THR:HG22	2.16	0.44
1:B:134:CYS:HB3	1:B:245:PRO:HG2	1.99	0.44
1:E:203:PRO:HB2	1:E:204:PRO:HD3	1.99	0.44
1:B:137:LEU:HD12	1:B:137:LEU:O	2.17	0.44
1:C:88:ASN:N	1:C:89:PRO:HD3	2.32	0.44
1:D:199:ARG:NH2	1:D:254:ALA:O	2.50	0.44
1:E:33:PHE:CB	1:E:122:LEU:HD21	2.48	0.44
1:E:137:LEU:HD12	1:E:137:LEU:O	2.17	0.44
1:E:277:MET:HA	1:E:277:MET:CE	2.46	0.44
1:A:37:GLN:NE2	1:A:42:VAL:HG21	2.33	0.44
1:B:169:ARG:HD3	6:B:997:HOH:O	2.17	0.44
1:B:177:GLN:HA	6:B:1144:HOH:O	2.17	0.44
1:C:264:GLY:HA2	1:C:301:LEU:CD1	2.48	0.44
1:F:255:PHE:CE1	1:F:276:GLY:HA3	2.52	0.44
1:A:54:LEU:O	1:A:57:ARG:HB3	2.18	0.44
1:A:202:ASP:HB3	1:A:204:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:GLY:O	1:E:32:PRO:HD3	2.18	0.44
1:E:79:ASP:OD1	1:E:90:ARG:HG2	2.17	0.44
1:F:120:HIS:CE1	1:F:141:TRP:CZ2	3.06	0.44
1:A:262:ALA:HB1	1:A:298:ASN:O	2.18	0.44
1:B:120:HIS:CD2	1:B:295:VAL:HG21	2.52	0.44
1:D:79:ASP:HA	1:D:90:ARG:NH1	2.32	0.44
1:D:120:HIS:CG	1:D:295:VAL:HG21	2.52	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:B:277:MET:O	1:B:281:GLU:HG3	2.18	0.44
1:C:303:THR:HB	1:C:307:GLU:OE1	2.18	0.44
1:D:54:LEU:O	1:D:57:ARG:HB3	2.18	0.44
1:F:28:VAL:CB	1:F:55:MET:HE1	2.48	0.44
1:F:303:THR:HB	1:F: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:D:134:CYS:HB3	1:D:245:PRO:HG2	1.99	0.43
1:D:145:HIS:HB3	6:D:809:HOH:O	2.18	0.43
1:E:194:VAL:HG23	1:E:238:LEU:HD21	1.99	0.43
1:E:303:THR:HB	1:E:307:GLU:OE1	2.19	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:F:152:LEU:HD12	1:F:152:LEU:HA	1.73	0.43
1:C:177:GLN:H	1:C:177:GLN:HG2	1.70	0.43
1:D:199:ARG:HH22	1:D:254:ALA:C	2.26	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:OE2	1:A:282:GLU:HA	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
1:F:177:GLN:H	1:F:177:GLN:HG2	1.70	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:B:33:PHE:CB	1:B:122:LEU:HD21	2.48	0.43
1:F:224:ARG:NH2	2:F:3074:SO4:O4	2.51	0.43
1:A:196:ILE:HD11	1:A:234:THR:HG21	2.00	0.43
1:C:105:ARG:HG2	1:C:105:ARG:NH1	2.34	0.43
1:D:33:PHE:HB3	1:D:122:LEU:HD21	2.00	0.43
1:D:66:LYS:HG3	1:D:111:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:ILE:HD11	1:E:234:THR:HG21	2.00	0.43
1:A:66:LYS:HG3	1:A:111:TYR:CZ	2.54	0.43
1:A:162:GLN:O	1:A:165:SER:HB2	2.19	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:B:292:LEU:HD23	1:B:292:LEU:C	2.44	0.42
1:C:277:MET:HE3	1:C:277:MET:CA	2.49	0.42
1:D:241:LYS:H	1:D:241:LYS:HD2	1.84	0.42
1:D:309:LYS:HE3	1:D:309:LYS:HB2	1.84	0.42
1:B:50:ARG:CG	1:B:50:ARG:NH1	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:C:78:LYS:HD3	1:E:55:MET:HB3	2.01	0.42
1:B:303:THR:HB	1:B:307:GLU:OE1	2.19	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:A:37:GLN:HB3	1:A:160:HIS:CE1	2.53	0.42
1:A:78:LYS:HB2	1:A:78:LYS:HE3	1.86	0.42
1:C:265:THR:N	1:C:266:PRO:HD3	2.34	0.42
1:F:120:HIS:CG	1:F:295:VAL:HG21	2.53	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: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:F:105:ARG:HG2	1:F:105:ARG:NH1	2.35	0.42
1:C:202:ASP:OD2	5:C:553:S2C:N	2.52	0.42
1:A:199:ARG:HH22	1:A:254:ALA:C	2.27	0.42
1:B:171:LEU:O	1:B:175:VAL:HG23	2.20	0.42
1:A:133:HIS:C	1:A:135:PRO:HD3	2.45	0.42
1:A:134:CYS:HB3	1:A:245:PRO:HG2	2.01	0.42
1:A:136:ASP:O	1:A:244:ARG:CD	2.68	0.42
1:B:55:MET:HB3	1:F:78:LYS:HD3	2.02	0.42
1:B:196:ILE:HD11	1:B:234:THR:HG21	2.02	0.42
1:E:199:ARG:NH2	1:E:254:ALA:O	2.53	0.42
1:F:202:ASP:OD2	5:F:556:S2C:N	2.53	0.42
1:C:108:SER:C	1:C:110:GLY:H	2.28	0.41
1:D:294:LEU:HD22	1:D:294:LEU:HA	1.95	0.41
1:F:196:ILE:HD11	1:F:234:THR:HG21	2.02	0.41
1:C:78:LYS:HE3	1:C:78:LYS:HB2	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:136:ASP:O	1:B:244:ARG:CD	2.69	0.41
1:E:292:LEU:HD23	1:E:292:LEU:C	2.46	0.41
1:F:88:ASN:HB3	1:F:91:SER:HB3	2.03	0.41
1:B:167:LEU:O	1:B:188:ILE:HD13	2.20	0.41
1:D:162:GLN:HG3	6:D:926:HOH:O	2.19	0.41
1:F:171:LEU:O	1:F:175:VAL:HG23	2.21	0.41
1:D:50:ARG:HH12	1:D:55:MET:HE2	1.85	0.41
1:A:148:ILE:HG12	1:A:148:ILE:O	2.21	0.41
1:B:50:ARG:HG2	1:B:50:ARG:NH1	2.20	0.41
1:B:78:LYS:HE3	1:B:78:LYS:HB2	1.81	0.41
1:A:66:LYS:HD2	1:A:68:PHE:CE1	2.56	0.41
1:E:167:LEU:O	1:E:188:ILE:HD13	2.20	0.41
1:F:108:SER:C	1:F:110:GLY:H	2.29	0.41
1:A:58:LEU:HB2	1:A:65:LEU:HD21	2.03	0.40
1:D:133:HIS:C	1:D:135:PRO:HD3	2.46	0.40
1:F:203:PRO:HB2	1:F:204:PRO:HD3	2.04	0.40
1:C:88:ASN:HB3	1:C:91:SER:HB3	2.03	0.40
1:D:66:LYS:HD2	1:D:68:PHE:CE1	2.56	0.40
1:E:101:GLU:CD	6:E:834:HOH:O	2.64	0.40
1:A:156:SER:HB2	1:A:158:ASN:ND2	2.35	0.40
1:B:50:ARG:HH22	1:B:67:ASP:CG	2.30	0.40
1:D:78:LYS:HE3	1:D:78:LYS:HB2	1.86	0.40
1:F:241:LYS:HD2	1:F:241:LYS:N	2.35	0.40
1:D:162:GLN:O	1:D:165:SER:HB2	2.21	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%)	12	32
1	B	304/306 (99%)	285 (94%)	17 (6%)	2 (1%)	18	41
1	C	304/306 (99%)	287 (94%)	12 (4%)	5 (2%)	7	20
1	D	304/306 (99%)	284 (93%)	17 (6%)	3 (1%)	12	32
1	E	304/306 (99%)	285 (94%)	17 (6%)	2 (1%)	18	41
1	F	304/306 (99%)	285 (94%)	14 (5%)	5 (2%)	7	20
All	All	1824/1836 (99%)	1711 (94%)	93 (5%)	20 (1%)	11	29

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%)	234 (91%)	23 (9%)	9	23
1	B	257/257 (100%)	229 (89%)	28 (11%)	6	16
1	C	257/257 (100%)	230 (90%)	27 (10%)	6	17
1	D	257/257 (100%)	233 (91%)	24 (9%)	8	21
1	E	257/257 (100%)	228 (89%)	29 (11%)	5	14
1	F	257/257 (100%)	231 (90%)	26 (10%)	7	18
All	All	1542/1542 (100%)	1385 (90%)	157 (10%)	7	18

All (157) 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	81	LEU
1	A	132	ARG
1	A	152	LEU
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
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

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Mol	Chain	Res	Type
1	B	120	HIS
1	B	132	ARG
1	B	173	ASP
1	B	178	LEU
1	B	185	LYS
1	B	186	PRO
1	B	187	CYS
1	B	188	ILE
1	B	213	ASP
1	B	220	ARG
1	B	228	GLN
1	B	232	GLU
1	B	234	THR
1	B	259	LEU
1	B	272	THR
1	B	277	MET
1	B	294	LEU
1	B	305	GLU
1	B	306	GLU
1	B	326	THR
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	108	SER
1	C	137	LEU
1	C	152	LEU
1	C	173	ASP
1	C	178	LEU
1	C	187	CYS
1	C	188	ILE
1	C	213	ASP
1	C	228	GLN
1	C	232	GLU
1	C	234	THR
1	C	237	LEU
1	C	242	ARG
1	C	259	LEU

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Mol	Chain	Res	Type
1	C	266	PRO
1	C	272	THR
1	C	277	MET
1	C	294	LEU
1	C	306	GLU
1	C	328	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	81	LEU
1	D	120	HIS
1	D	132	ARG
1	D	152	LEU
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	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
1	E	173	ASP
1	E	178	LEU
1	E	185	LYS

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Mol	Chain	Res	Type
1	E	186	PRO
1	E	187	CYS
1	E	188	ILE
1	E	213	ASP
1	E	220	ARG
1	E	228	GLN
1	E	232	GLU
1	E	234	THR
1	E	237	LEU
1	E	259	LEU
1	E	272	THR
1	E	277	MET
1	E	294	LEU
1	E	305	GLU
1	E	306	GLU
1	E	326	THR
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	108	SER
1	F	137	LEU
1	F	152	LEU
1	F	173	ASP
1	F	178	LEU
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	266	PRO
1	F	272	THR
1	F	277	MET
1	F	294	LEU

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Mol	Chain	Res	Type
1	F	306	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	162	GLN
1	A	206	HIS
1	A	211	ASN
1	A	284	HIS
1	A	325	GLN
1	B	88	ASN
1	B	162	GLN
1	B	172	GLN
1	B	206	HIS
1	B	211	ASN
1	B	325	GLN
1	C	97	GLN
1	C	162	GLN
1	C	172	GLN
1	C	211	ASN
1	C	284	HIS
1	C	325	GLN
1	D	88	ASN
1	D	158	ASN
1	D	162	GLN
1	D	206	HIS
1	D	211	ASN
1	D	284	HIS
1	D	325	GLN
1	E	88	ASN
1	E	162	GLN
1	E	172	GLN
1	E	206	HIS
1	E	211	ASN
1	E	325	GLN
1	F	88	ASN
1	F	97	GLN
1	F	162	GLN
1	F	172	GLN
1	F	211	ASN
1	F	243	GLN

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Mol	Chain	Res	Type
1	F	284	HIS
1	F	325	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 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	3073	-	4,4,4	0.18	0	6,6,6	1.15	0
5	S2C	D	554	3	11,12,12	1.14	0	9,16,16	0.98	1 (11%)
2	SO4	F	3074	-	4,4,4	0.29	0	6,6,6	1.15	0
2	SO4	F	3084	-	4,4,4	0.42	0	6,6,6	1.20	0
2	SO4	C	3075	-	4,4,4	0.35	0	6,6,6	1.22	0
2	SO4	A	3082	-	4,4,4	0.40	0	6,6,6	1.16	0
2	SO4	C	3078	-	4,4,4	0.40	0	6,6,6	1.12	0
2	SO4	D	3079	-	4,4,4	0.39	0	6,6,6	1.17	0
5	S2C	A	551	3	11,12,12	1.15	0	9,16,16	0.97	1 (11%)
2	SO4	D	3072	-	4,4,4	0.18	0	6,6,6	1.20	0
2	SO4	A	3070	-	4,4,4	0.22	0	6,6,6	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	S2C	B	552	3	11,12,12	1.14	0	9,16,16	0.97	1 (11%)
2	SO4	D	3083	-	4,4,4	0.26	0	6,6,6	1.21	0
5	S2C	E	555	3	11,12,12	1.16	0	9,16,16	0.97	1 (11%)
2	SO4	A	3081	-	4,4,4	0.35	0	6,6,6	1.16	0
5	S2C	C	553	3	11,12,12	1.15	0	9,16,16	0.97	1 (11%)
2	SO4	D	3080	-	4,4,4	0.35	0	6,6,6	1.18	0
2	SO4	F	3071	-	4,4,4	0.24	0	6,6,6	1.15	0
2	SO4	B	3085	-	4,4,4	0.37	0	6,6,6	1.17	0
2	SO4	F	3077	-	4,4,4	0.39	0	6,6,6	1.11	0
5	S2C	F	556	3	11,12,12	1.16	0	9,16,16	0.97	1 (11%)

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
5	S2C	D	554	3	-	4/8/12/12	-
5	S2C	C	553	3	-	4/8/12/12	-
5	S2C	B	552	3	-	4/8/12/12	-
5	S2C	F	556	3	-	4/8/12/12	-
5	S2C	A	551	3	-	4/8/12/12	-
5	S2C	E	555	3	-	4/8/12/12	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	554	S2C	CB-SG-CD	-2.46	94.96	102.26
5	C	553	S2C	CB-SG-CD	-2.45	94.99	102.26
5	A	551	S2C	CB-SG-CD	-2.45	95.00	102.26
5	E	555	S2C	CB-SG-CD	-2.45	95.00	102.26
5	B	552	S2C	CB-SG-CD	-2.44	95.01	102.26
5	F	556	S2C	CB-SG-CD	-2.44	95.02	102.26

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	551	S2C	N-CA-CB-SG
5	B	552	S2C	N-CA-CB-SG
5	C	553	S2C	N-CA-CB-SG
5	D	554	S2C	N-CA-CB-SG
5	E	555	S2C	N-CA-CB-SG
5	F	556	S2C	N-CA-CB-SG
5	A	551	S2C	OXT-C-CA-N
5	B	552	S2C	OXT-C-CA-N
5	C	553	S2C	OXT-C-CA-N
5	D	554	S2C	OXT-C-CA-N
5	E	555	S2C	OXT-C-CA-N
5	F	556	S2C	OXT-C-CA-N
5	A	551	S2C	C-CA-CB-SG
5	B	552	S2C	C-CA-CB-SG
5	C	553	S2C	C-CA-CB-SG
5	D	554	S2C	C-CA-CB-SG
5	E	555	S2C	C-CA-CB-SG
5	F	556	S2C	C-CA-CB-SG
5	A	551	S2C	O-C-CA-N
5	B	552	S2C	O-C-CA-N
5	C	553	S2C	O-C-CA-N
5	D	554	S2C	O-C-CA-N
5	E	555	S2C	O-C-CA-N
5	F	556	S2C	O-C-CA-N

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	D	554	S2C	1	0
2	F	3074	SO4	3	0
2	F	3084	SO4	1	0
5	A	551	S2C	1	0
5	B	552	S2C	2	0
2	D	3083	SO4	1	0
5	E	555	S2C	2	0
5	C	553	S2C	2	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.