



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:35 PM UTC

PDB ID : 3C8H / pdb_00003c8h
Title : Crystal structure of the enterobactin esterase FES from *Shigella flexneri* in the presence of 2,3-Di-hydroxy-N-benzoyl-serine
Authors : Kim, Y.; Maltseva, N.; Abergel, R.; Holzle, D.; Raymond, K.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2008-02-12
Resolution : 2.48 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

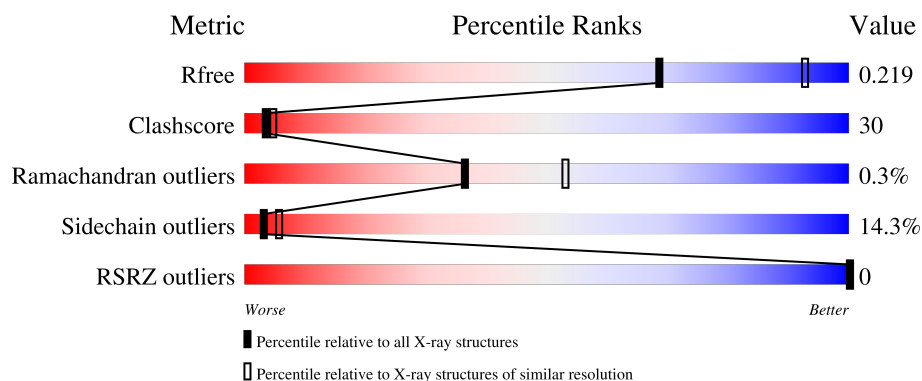
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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

Mol	Chain	Length	Quality of chain
1	A	403	
1	B	403	
1	C	403	
1	D	403	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12711 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 Enterochelin esterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	Se	0	0	0
			3091	1988	543	548	5	7			
1	B	383	Total	C	N	O	S	Se	0	0	0
			3090	1987	542	549	5	7			
1	C	383	Total	C	N	O	S	Se	0	0	0
			3091	1988	543	548	5	7			
1	D	383	Total	C	N	O	S	Se	0	2	0
			3106	1996	544	554	5	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q83SB9
A	-1	ASN	-	expression tag	UNP Q83SB9
A	0	ALA	-	expression tag	UNP Q83SB9
B	-2	SER	-	expression tag	UNP Q83SB9
B	-1	ASN	-	expression tag	UNP Q83SB9
B	0	ALA	-	expression tag	UNP Q83SB9
C	-2	SER	-	expression tag	UNP Q83SB9
C	-1	ASN	-	expression tag	UNP Q83SB9
C	0	ALA	-	expression tag	UNP Q83SB9
D	-2	SER	-	expression tag	UNP Q83SB9
D	-1	ASN	-	expression tag	UNP Q83SB9
D	0	ALA	-	expression tag	UNP Q83SB9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	80	Total	O	0	0
			80	80		
2	B	85	Total	O	0	0
			85	85		

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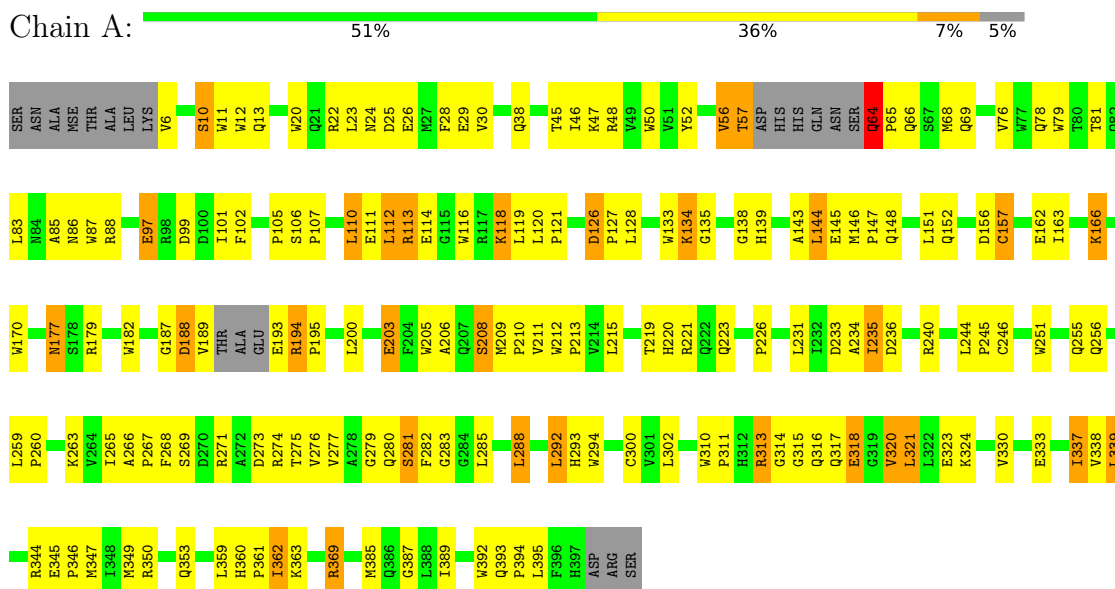
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	90	Total	O	0	0
			90	90		
2	D	78	Total	O	0	0
			78	78		

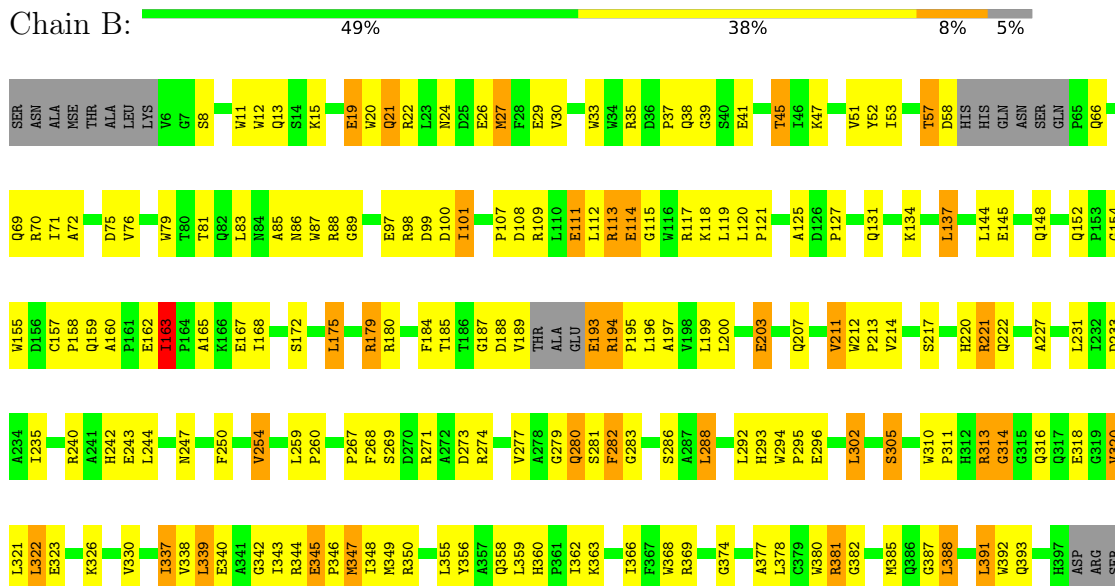
3 Residue-property plots

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

• Molecule 1: Enterochelin esterase

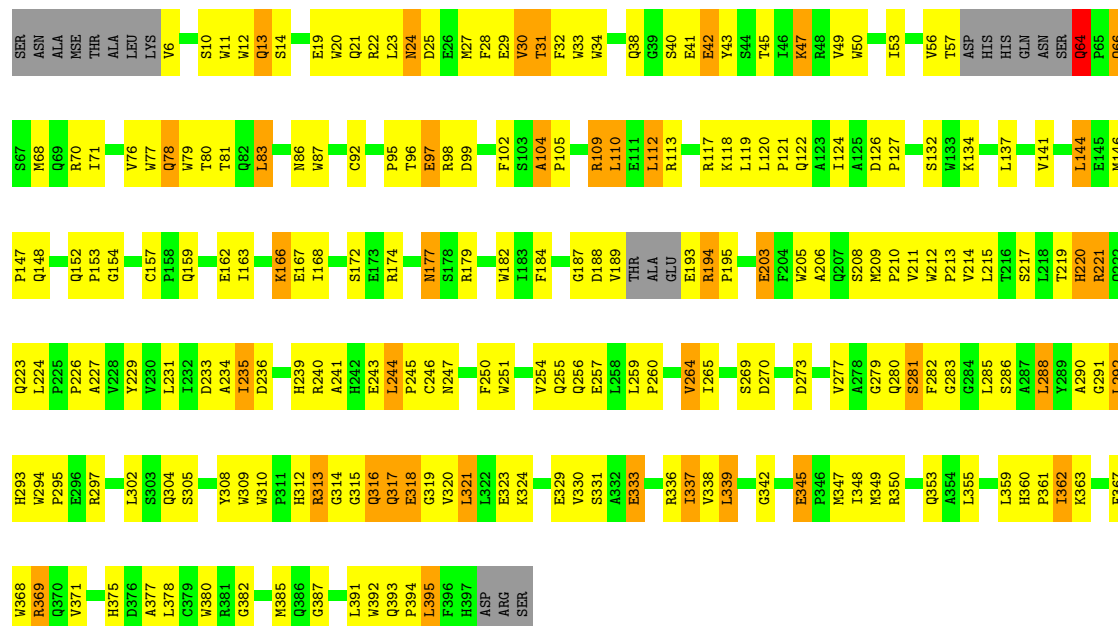


• Molecule 1: Enterochelin esterase



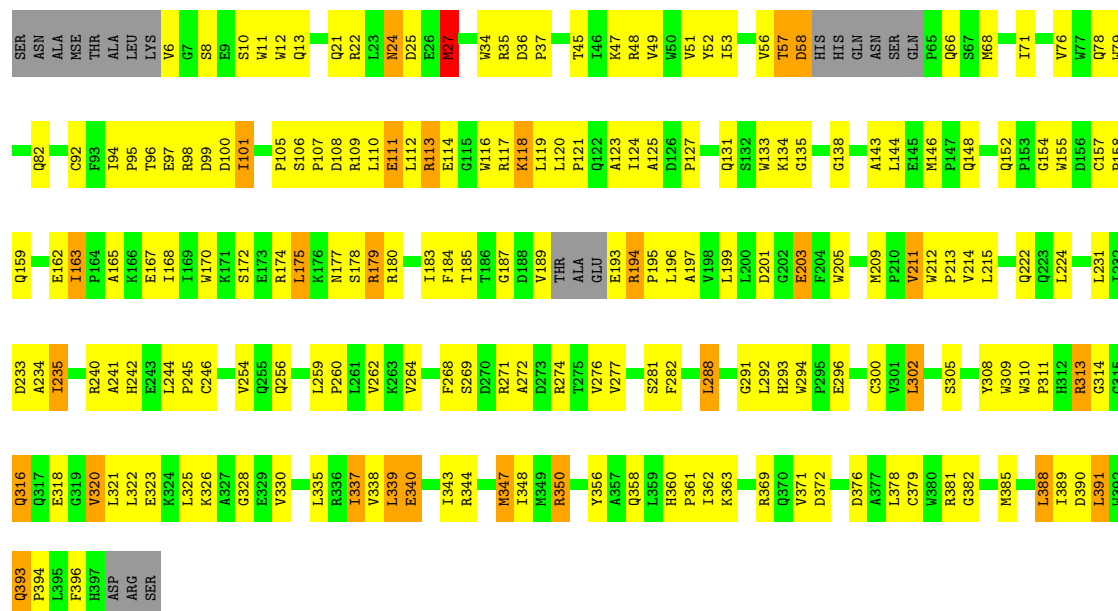
• Molecule 1: Enterochelin esterase

Chain C: 



• Molecule 1: Enterochelin esterase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.51Å 48.78Å 156.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.23 – 2.48 47.23 – 2.48	Depositor EDS
% Data completeness (in resolution range)	94.2 (47.23-2.48) 94.2 (47.23-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.183 , 0.225 0.184 , 0.219	Depositor DCC
R_{free} test set	2889 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.429 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12711	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7823e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.61	2/3184 (0.1%)	0.93	12/4334 (0.3%)
1	B	0.59	0/3183	0.90	7/4332 (0.2%)
1	C	0.61	0/3184	0.94	8/4334 (0.2%)
1	D	0.61	0/3198	0.93	5/4351 (0.1%)
All	All	0.61	2/12749 (0.0%)	0.93	32/17351 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	THR	C-O	6.61	1.36	1.23
1	A	56	VAL	C-O	-5.04	1.18	1.24

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	GLU	CA-C-N	8.08	129.94	119.84
1	A	345	GLU	C-N-CA	8.08	129.94	119.84
1	B	160	ALA	CA-C-N	7.94	127.96	119.78
1	B	160	ALA	C-N-CA	7.94	127.96	119.78
1	A	266	ALA	CA-C-N	7.58	127.56	119.76
1	A	266	ALA	C-N-CA	7.58	127.56	119.76
1	C	104	ALA	CA-C-N	7.36	126.89	119.24
1	C	104	ALA	C-N-CA	7.36	126.89	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	294	TRP	CA-C-N	6.56	126.18	119.56
1	B	294	TRP	C-N-CA	6.56	126.18	119.56
1	C	163	ILE	CA-C-N	6.45	126.41	120.21
1	C	163	ILE	C-N-CA	6.45	126.41	120.21
1	D	27	MSE	N-CA-C	6.36	120.00	110.14
1	A	163	ILE	CA-C-N	6.24	126.20	120.03
1	A	163	ILE	C-N-CA	6.24	126.20	120.03
1	A	126	ASP	CA-C-N	6.11	127.48	119.84
1	A	126	ASP	C-N-CA	6.11	127.48	119.84
1	A	188	ASP	N-CA-C	6.09	120.74	112.88
1	B	345	GLU	CA-C-N	6.08	125.47	118.85
1	B	345	GLU	C-N-CA	6.08	125.47	118.85
1	A	113	ARG	N-CA-C	-5.84	104.10	111.11
1	D	146	MSE	CA-C-N	5.73	126.11	119.47
1	D	146	MSE	C-N-CA	5.73	126.11	119.47
1	B	163	ILE	CB-CA-C	-5.68	104.31	110.85
1	A	64	GLN	N-CA-C	-5.68	95.10	111.00
1	D	294	TRP	CA-C-N	5.62	125.29	119.56
1	D	294	TRP	C-N-CA	5.62	125.29	119.56
1	C	310	TRP	N-CA-C	5.51	115.93	109.60
1	C	64	GLN	CA-C-N	-5.37	113.75	120.51
1	C	64	GLN	C-N-CA	-5.37	113.75	120.51
1	C	64	GLN	N-CA-C	-5.17	96.53	111.00
1	A	46	ILE	N-CA-C	5.04	115.60	107.73

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	314	GLY	Peptide
1	C	345	GLU	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	3091	0	2996	176	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3090	0	2993	185	0
1	C	3091	0	2996	213	1
1	D	3106	0	3004	195	0
2	A	80	0	0	14	0
2	B	85	0	0	9	0
2	C	90	0	0	7	0
2	D	78	0	0	8	0
All	All	12711	0	11989	724	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (724) 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:B:221:ARG:O	1:B:222:GLN:HG2	1.46	1.11
1:A:193:GLU:HB3	1:A:269:SER:HB2	1.35	1.08
1:B:152:GLN:OE1	1:B:381:ARG:HD2	1.53	1.06
1:D:337:ILE:HD11	1:D:339:LEU:HG	1.37	1.05
1:B:53:ILE:H	1:B:57:THR:HB	1.24	1.00
1:A:22:ARG:HG2	1:A:24:ASN:O	1.61	0.99
1:B:185:THR:HG21	1:B:194:ARG:HH21	1.24	0.99
1:D:224:LEU:HD21	1:D:389:ILE:HG13	1.46	0.97
1:B:22:ARG:HH12	1:B:148:GLN:HE22	1.02	0.97
1:A:187:GLY:HA3	1:A:226:PRO:HB3	1.47	0.96
1:D:185[A]:THR:HG21	1:D:194:ARG:HH21	1.29	0.96
1:D:316:GLN:HA	1:D:316:GLN:HE21	1.30	0.96
1:B:22:ARG:HH22	1:B:148:GLN:HE21	1.02	0.93
1:D:347:MSE:HA	1:D:350:ARG:HD2	1.52	0.92
1:D:22:ARG:HH12	1:D:148:GLN:NE2	1.67	0.92
1:C:57:THR:HG22	1:C:57:THR:O	1.67	0.92
1:B:107:PRO:HG2	1:B:112:LEU:HD11	1.51	0.91
1:C:38:GLN:NE2	1:C:45:THR:H	1.69	0.90
1:B:212:TRP:HB2	1:B:213:PRO:HD3	1.53	0.90
1:C:313:ARG:HG3	1:D:313:ARG:HB2	1.51	0.89
1:A:313:ARG:NH2	1:A:313:ARG:HB3	1.87	0.89
1:B:337:ILE:HD11	1:B:339:LEU:HG	1.54	0.89
1:B:346:PRO:HD2	2:B:421:HOH:O	1.73	0.88
1:D:152:GLN:OE1	1:D:381:ARG:HD2	1.73	0.88
1:C:359:LEU:HB3	1:C:362:ILE:HD11	1.54	0.88
1:B:152:GLN:OE1	1:B:381:ARG:CD	2.22	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLN:HE22	1:A:106:SER:HA	1.36	0.88
1:B:22:ARG:HH12	1:B:148:GLN:NE2	1.70	0.88
1:D:48:ARG:HB2	1:D:96:THR:HG22	1.56	0.86
1:C:244:LEU:HB2	1:C:245:PRO:HD3	1.54	0.86
1:C:264:VAL:HG12	1:C:265:ILE:HD12	1.56	0.86
1:C:24:ASN:OD1	1:C:27:MSE:HB3	1.77	0.85
1:A:69:GLN:HB3	1:C:264:VAL:HG21	1.57	0.85
1:D:288:LEU:HD13	1:D:292:LEU:HD11	1.59	0.84
1:B:152:GLN:HB3	1:B:382:GLY:HA2	1.59	0.84
1:A:45:THR:HG22	1:A:97:GLU:HB3	1.59	0.84
1:D:48:ARG:HB2	1:D:96:THR:CG2	2.08	0.83
1:A:337:ILE:HD11	1:A:339:LEU:HG	1.60	0.83
1:C:187:GLY:HA3	1:C:226:PRO:HB3	1.60	0.83
1:A:313:ARG:HB3	1:A:313:ARG:HH21	1.45	0.82
1:D:185[A]:THR:CG2	1:D:194:ARG:HH21	1.91	0.82
1:A:38:GLN:NE2	1:A:45:THR:H	1.75	0.82
1:C:38:GLN:HE22	1:C:45:THR:HB	1.44	0.82
1:B:101:ILE:HD13	1:B:119:LEU:HG	1.63	0.81
1:C:12:TRP:CZ2	1:C:76:VAL:HG22	2.16	0.81
1:B:22:ARG:HH22	1:B:148:GLN:NE2	1.79	0.81
1:C:215:LEU:O	1:C:219:THR:HG23	1.81	0.80
1:A:256:GLN:O	1:A:260:PRO:HG2	1.81	0.79
1:D:22:ARG:HH12	1:D:148:GLN:HE22	1.28	0.78
1:D:172:SER:OG	1:D:175:LEU:HB2	1.83	0.78
1:B:179:ARG:NH2	1:B:243:GLU:OE1	2.18	0.77
1:C:87:TRP:HZ3	1:C:144:LEU:HB3	1.49	0.77
1:D:316:GLN:HA	1:D:316:GLN:NE2	1.98	0.77
1:D:356:TYR:CZ	1:D:363:LYS:HD3	2.20	0.76
1:A:107:PRO:HB2	1:A:112:LEU:CD1	2.16	0.75
1:B:45:THR:HB	1:B:97:GLU:HG2	1.69	0.75
1:A:22:ARG:CG	1:A:24:ASN:O	2.36	0.74
1:B:22:ARG:NH2	1:B:148:GLN:HE21	1.82	0.73
1:B:347:MSE:HA	1:B:350:ARG:HD2	1.70	0.73
1:D:185[A]:THR:HG21	1:D:194:ARG:NH2	2.03	0.73
1:D:98:ARG:HG2	1:D:100:ASP:OD1	1.88	0.73
1:A:6:VAL:HA	1:A:11:TRP:CD1	2.24	0.73
1:B:21:GLN:NE2	1:B:22:ARG:H	1.87	0.73
1:D:107:PRO:HB3	1:D:111:GLU:CD	2.14	0.72
1:A:317:GLN:NE2	1:B:137:LEU:HG	2.03	0.72
1:B:322:LEU:HD23	1:B:358:GLN:HG3	1.70	0.72
1:A:313:ARG:HD2	1:B:313:ARG:HA	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:TYR:HA	1:B:57:THR:HG21	1.69	0.72
1:A:139:HIS:HE1	2:A:419:HOH:O	1.71	0.72
1:B:12:TRP:CZ2	1:B:76:VAL:HG22	2.23	0.72
1:D:101:ILE:HG21	1:D:119:LEU:HD21	1.72	0.71
1:D:157:CYS:N	1:D:158:PRO:HD3	2.05	0.71
1:D:167:GLU:OE1	1:D:180:ARG:HD2	1.90	0.71
1:A:193:GLU:HB3	1:A:269:SER:CB	2.19	0.71
1:C:47:LYS:HG2	1:C:99:ASP:OD1	1.90	0.71
1:C:347:MSE:SE	1:D:313:ARG:NH1	2.73	0.71
1:B:360:HIS:HA	1:B:363:LYS:HG3	1.72	0.71
1:C:45:THR:HG22	1:C:97:GLU:HB3	1.70	0.71
1:C:53:ILE:HB	1:C:56:VAL:HB	1.73	0.71
1:B:33:TRP:HH2	2:B:463:HOH:O	1.74	0.70
1:B:57:THR:O	1:B:58:ASP:C	2.33	0.70
1:C:236:ASP:CG	1:C:239:HIS:HD1	2.00	0.70
1:C:244:LEU:CB	1:C:245:PRO:HD3	2.17	0.70
1:C:38:GLN:HE21	1:C:45:THR:H	1.37	0.70
1:C:188:ASP:O	1:C:189:VAL:HB	1.90	0.70
1:A:23:LEU:HD11	1:A:29:GLU:HB2	1.74	0.70
1:A:107:PRO:HB2	1:A:112:LEU:HD11	1.72	0.70
1:A:110:LEU:HD22	1:A:110:LEU:H	1.56	0.69
1:A:152:GLN:HG2	2:A:418:HOH:O	1.91	0.69
1:B:244:LEU:O	1:B:286:SER:HB2	1.90	0.69
1:C:22:ARG:HG2	1:C:24:ASN:O	1.92	0.69
1:C:337:ILE:HD11	1:C:339:LEU:HG	1.74	0.69
1:C:360:HIS:N	1:C:361:PRO:CD	2.55	0.69
1:C:38:GLN:HE22	1:C:45:THR:CB	2.06	0.69
1:B:340:GLU:HB2	1:B:369:ARG:HB2	1.73	0.69
1:C:256:GLN:O	1:C:260:PRO:HG2	1.93	0.69
1:C:244:LEU:O	1:C:286:SER:HB2	1.92	0.69
1:A:48:ARG:NH2	1:A:99:ASP:HB2	2.08	0.68
1:B:187:GLY:HA2	2:B:420:HOH:O	1.91	0.68
1:A:313:ARG:HG2	1:B:313:ARG:HB2	1.76	0.68
1:C:20:TRP:CE3	1:C:146:MSE:HE1	2.29	0.68
1:A:170:TRP:CE3	1:A:179:ARG:HD3	2.29	0.68
1:C:313:ARG:HG2	1:D:313:ARG:HH21	1.59	0.67
1:B:185:THR:HG22	1:B:187:GLY:H	1.60	0.67
1:D:125:ALA:O	1:D:127:PRO:HD3	1.94	0.67
1:C:50:TRP:CH2	1:C:102:PHE:HB2	2.29	0.67
1:C:193:GLU:HB3	1:C:269:SER:HB2	1.77	0.67
1:D:224:LEU:CD2	1:D:389:ILE:HG13	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ARG:NH1	1:B:148:GLN:NE2	2.42	0.67
1:D:162:GLU:HB2	1:D:163:ILE:HD12	1.77	0.67
1:C:182:TRP:HB2	1:C:231:LEU:HB2	1.76	0.67
1:C:359:LEU:HB3	1:C:362:ILE:CD1	2.25	0.67
1:D:22:ARG:NH1	1:D:148:GLN:NE2	2.42	0.67
1:D:369:ARG:NH2	1:D:390:ASP:OD1	2.29	0.66
1:A:105:PRO:HG3	1:C:174:ARG:HH22	1.61	0.66
1:B:165:ALA:HB2	1:B:184:PHE:CD2	2.30	0.66
1:D:134:LYS:HE3	1:D:138:GLY:O	1.95	0.66
1:B:22:ARG:NH1	1:B:148:GLN:HE22	1.84	0.66
1:A:215:LEU:O	1:A:219:THR:HG23	1.95	0.66
1:C:110:LEU:HG	1:D:350:ARG:HH12	1.59	0.66
1:A:317:GLN:NE2	1:B:137:LEU:CG	2.59	0.66
1:D:53:ILE:H	1:D:57:THR:HB	1.60	0.66
1:A:211:VAL:CG2	1:A:385:MSE:HE1	2.26	0.66
1:D:203:GLU:HG2	1:D:233:ASP:OD2	1.96	0.66
1:A:212:TRP:HB2	1:A:213:PRO:HD3	1.78	0.65
1:A:360:HIS:N	1:A:361:PRO:CD	2.60	0.65
1:D:316:GLN:HE21	1:D:316:GLN:CA	2.01	0.65
1:C:360:HIS:HA	1:C:363:LYS:HG3	1.78	0.65
1:A:203:GLU:HG2	1:A:233:ASP:OD2	1.96	0.65
1:C:127:PRO:HD3	2:C:466:HOH:O	1.96	0.65
1:B:281:SER:OG	1:B:282:PHE:N	2.30	0.65
1:D:68:MSE:HE2	1:D:78:GLN:HA	1.77	0.64
1:A:194:ARG:HH11	1:A:194:ARG:HB2	1.62	0.64
1:B:340:GLU:CB	1:B:369:ARG:HB2	2.27	0.64
1:C:92:CYS:HB2	1:C:124:ILE:O	1.97	0.64
1:C:187:GLY:CA	1:C:226:PRO:HB3	2.27	0.64
1:D:246:CYS:SG	1:D:321:LEU:HD13	2.37	0.64
1:C:113:ARG:HH21	1:D:350:ARG:HD3	1.62	0.64
1:B:24:ASN:HD21	1:B:27:MSE:HB2	1.62	0.63
1:D:288:LEU:CD1	1:D:292:LEU:HD11	2.28	0.63
1:C:57:THR:O	1:C:57:THR:CG2	2.40	0.63
1:C:345:GLU:HG3	1:C:375:HIS:HB2	1.80	0.63
1:A:23:LEU:HD21	1:A:29:GLU:HB2	1.79	0.63
1:B:47:LYS:HB3	1:B:99:ASP:HB3	1.81	0.63
1:B:101:ILE:HG21	1:B:119:LEU:HD11	1.81	0.63
1:D:113:ARG:O	1:D:117:ARG:HB2	1.97	0.63
1:D:51:VAL:O	1:D:57:THR:HG21	1.97	0.63
1:B:98:ARG:HG2	1:B:100:ASP:OD1	1.99	0.63
1:D:34:TRP:CZ2	1:D:37:PRO:HD3	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:C	1:A:121:PRO:HD2	2.23	0.63
1:A:205:TRP:HE1	1:A:280:GLN:HE22	1.47	0.63
1:A:337:ILE:HD12	1:A:338:VAL:C	2.24	0.63
1:C:313:ARG:CG	1:D:313:ARG:HB2	2.26	0.63
1:A:188:ASP:O	1:A:189:VAL:HB	1.99	0.62
1:D:269:SER:OG	1:D:271:ARG:HG3	1.99	0.62
1:B:154:GLY:HA3	1:B:214:VAL:HG13	1.80	0.62
1:A:244:LEU:HB2	1:A:245:PRO:HD3	1.80	0.62
1:A:110:LEU:HB3	1:B:350:ARG:HH22	1.65	0.62
1:A:234:ALA:O	1:A:235:ILE:HB	1.99	0.62
1:B:30:VAL:HG21	1:B:83:LEU:HD12	1.81	0.62
1:B:250:PHE:O	1:B:254:VAL:HG13	2.00	0.62
1:D:360:HIS:HB3	1:D:361:PRO:HD3	1.80	0.62
1:C:313:ARG:HG2	1:D:313:ARG:NH2	2.15	0.62
1:B:88:ARG:HG3	1:B:145:GLU:HG2	1.81	0.61
1:B:113:ARG:O	1:B:117:ARG:HB2	1.99	0.61
1:A:316:GLN:NE2	2:A:427:HOH:O	2.32	0.61
1:A:317:GLN:CD	1:B:137:LEU:HG	2.25	0.61
1:C:312:HIS:CG	1:C:317:GLN:HB2	2.34	0.61
1:D:119:LEU:C	1:D:121:PRO:HD2	2.25	0.61
1:C:288:LEU:HD13	1:C:321:LEU:HD11	1.81	0.61
1:D:57:THR:O	1:D:58:ASP:C	2.43	0.61
1:B:53:ILE:N	1:B:57:THR:HB	2.08	0.61
1:B:362:ILE:HG22	1:B:362:ILE:O	1.99	0.61
1:C:288:LEU:HD22	1:C:292:LEU:HD22	1.80	0.61
1:D:326:LYS:HG2	1:D:358:GLN:OE1	2.00	0.61
1:C:23:LEU:HD21	1:C:29:GLU:HB2	1.82	0.61
1:C:113:ARG:HD2	1:D:314:GLY:O	2.01	0.61
1:C:119:LEU:C	1:C:121:PRO:HD2	2.26	0.61
1:C:349:MSE:O	1:C:353:GLN:HG2	2.00	0.61
1:D:293:HIS:CE1	1:D:330:VAL:HG11	2.36	0.61
1:B:185:THR:CG2	1:B:194:ARG:HH21	2.09	0.61
1:D:347:MSE:HA	1:D:350:ARG:CD	2.30	0.61
1:D:107:PRO:HB3	1:D:111:GLU:OE1	2.01	0.61
1:B:107:PRO:HB2	1:B:111:GLU:CD	2.26	0.60
1:B:108:ASP:O	1:B:112:LEU:HD13	2.01	0.60
1:A:179:ARG:HD2	2:A:435:HOH:O	2.02	0.60
1:C:309:TRP:CE2	1:D:313:ARG:HD3	2.36	0.60
1:D:288:LEU:HD13	1:D:292:LEU:CD1	2.30	0.60
1:A:78:GLN:OE1	1:C:264:VAL:HG22	2.01	0.60
1:A:321:LEU:HD23	2:A:453:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:VAL:HG12	1:A:56:VAL:O	2.00	0.60
1:B:203:GLU:HG3	1:B:233:ASP:HA	1.83	0.60
1:C:316:GLN:HG2	1:C:317:GLN:H	1.66	0.60
1:C:360:HIS:O	1:C:363:LYS:HG3	2.02	0.60
1:B:155:TRP:CE2	1:B:381:ARG:HB2	2.37	0.59
1:A:314:GLY:O	1:B:113:ARG:HG2	2.03	0.59
1:B:302:LEU:HD13	1:B:338:VAL:HB	1.83	0.59
1:D:68:MSE:HE2	1:D:78:GLN:CA	2.31	0.59
1:D:203:GLU:HG3	1:D:233:ASP:HA	1.85	0.59
1:B:293:HIS:CE1	1:B:330:VAL:HG11	2.37	0.59
1:C:79:TRP:CH2	1:C:81:THR:HB	2.37	0.59
1:B:163:ILE:H	1:B:163:ILE:HD12	1.68	0.59
1:C:203:GLU:HG2	1:C:233:ASP:OD2	2.03	0.59
1:A:349:MSE:O	1:A:353:GLN:HG2	2.03	0.59
1:B:72:ALA:HB3	2:B:476:HOH:O	2.03	0.59
1:C:23:LEU:HD11	1:C:29:GLU:HB2	1.85	0.59
1:D:27:MSE:HG2	1:D:82:GLN:HB3	1.84	0.59
1:A:113:ARG:HD2	1:B:314:GLY:O	2.03	0.58
1:B:107:PRO:HG2	1:B:112:LEU:CD1	2.31	0.58
1:C:195:PRO:HD2	1:C:226:PRO:O	2.03	0.58
1:D:108:ASP:O	1:D:112:LEU:HD13	2.03	0.58
1:B:19:GLU:HB2	1:B:33:TRP:HZ3	1.68	0.58
1:C:205:TRP:HE1	1:C:280:GLN:HE22	1.49	0.58
1:B:57:THR:HG22	1:B:58:ASP:N	2.19	0.58
1:B:194:ARG:HB3	1:B:227:ALA:HA	1.86	0.58
1:B:200:LEU:HD12	1:B:283:GLY:O	2.02	0.58
1:B:212:TRP:HB2	1:B:213:PRO:CD	2.30	0.58
1:C:315:GLY:HA2	2:C:490:HOH:O	2.03	0.58
1:C:154:GLY:C	1:C:214:VAL:HG13	2.29	0.58
1:C:244:LEU:N	1:C:245:PRO:CD	2.67	0.58
1:D:276:VAL:HG22	1:D:300:CYS:HB2	1.86	0.57
1:B:339:LEU:HD13	1:B:368:TRP:HZ3	1.69	0.57
1:D:224:LEU:HD23	1:D:389:ILE:HA	1.86	0.57
1:A:38:GLN:HE21	1:A:45:THR:H	1.50	0.57
1:A:360:HIS:HA	1:A:363:LYS:HE2	1.87	0.57
1:D:133:TRP:CE2	1:D:209:MSE:HE3	2.40	0.57
1:A:188:ASP:O	1:A:189:VAL:CB	2.52	0.57
1:C:313:ARG:HG3	1:D:313:ARG:CB	2.30	0.57
1:D:360:HIS:HA	1:D:363:LYS:HG3	1.86	0.57
1:A:28:PHE:CZ	1:A:147:PRO:HG2	2.39	0.57
1:A:317:GLN:NE2	1:B:137:LEU:HD21	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:TRP:CZ3	1:C:144:LEU:HB3	2.36	0.57
1:D:12:TRP:CZ2	1:D:76:VAL:HG22	2.40	0.57
1:D:109:ARG:NH2	2:D:444:HOH:O	2.36	0.57
1:D:185[A]:THR:HG22	1:D:187:GLY:H	1.70	0.57
1:D:52:TYR:CE1	1:D:58:ASP:HA	2.40	0.56
1:A:65:PRO:HB3	1:A:116:TRP:CZ2	2.40	0.56
1:A:120:LEU:N	1:A:121:PRO:HD2	2.19	0.56
1:A:138:GLY:N	2:A:479:HOH:O	2.28	0.56
1:A:194:ARG:HB2	1:A:194:ARG:NH1	2.21	0.56
1:B:22:ARG:NH2	1:B:148:GLN:NE2	2.49	0.56
1:C:234:ALA:O	1:C:235:ILE:HB	2.05	0.56
1:D:393:GLN:HB3	1:D:394:PRO:HD3	1.86	0.56
1:C:203:GLU:HG3	1:C:233:ASP:HA	1.87	0.56
1:C:233:ASP:OD2	1:C:234:ALA:N	2.38	0.56
1:C:251:TRP:O	1:C:255:GLN:HG3	2.05	0.56
1:A:139:HIS:CE1	2:A:419:HOH:O	2.51	0.56
1:A:203:GLU:CG	1:A:233:ASP:OD2	2.52	0.56
1:C:393:GLN:N	1:C:394:PRO:CD	2.69	0.56
1:A:105:PRO:CG	1:C:174:ARG:HH22	2.18	0.56
1:A:69:GLN:HB3	1:C:264:VAL:CG2	2.33	0.56
1:C:189:VAL:HG13	1:C:189:VAL:O	2.06	0.56
1:A:10:SER:HA	1:A:13:GLN:HE21	1.70	0.56
1:B:199:LEU:HD22	1:B:231:LEU:HD11	1.88	0.56
1:C:338:VAL:HG22	1:C:367:PHE:HB2	1.87	0.56
1:D:155:TRP:CE2	1:D:381:ARG:HB2	2.41	0.55
1:D:340:GLU:HB2	1:D:369:ARG:HB2	1.88	0.55
1:C:345:GLU:HG2	1:C:348:ILE:HD13	1.88	0.55
1:A:259:LEU:HB2	1:A:260:PRO:HD3	1.87	0.55
1:D:107:PRO:HB2	1:D:112:LEU:CD1	2.36	0.55
1:D:212:TRP:HB2	1:D:213:PRO:HD3	1.88	0.55
1:D:94:ILE:HG21	1:D:119:LEU:HB3	1.89	0.55
1:B:24:ASN:ND2	1:B:27:MSE:HB2	2.21	0.55
1:A:101:ILE:HA	2:A:415:HOH:O	2.07	0.55
1:D:107:PRO:HB2	1:D:112:LEU:HD11	1.88	0.55
1:B:318:GLU:HG2	1:B:326:LYS:HZ3	1.72	0.55
1:D:170:TRP:CE3	1:D:179:ARG:HD3	2.42	0.55
1:A:263:LYS:HG3	1:A:268:PHE:CE1	2.42	0.55
1:B:269:SER:OG	1:B:271:ARG:HG3	2.07	0.55
1:D:347:MSE:O	1:D:350:ARG:HG2	2.07	0.55
1:A:65:PRO:HB3	1:A:116:TRP:HZ2	1.72	0.55
1:B:281:SER:HA	1:B:305:SER:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:LYS:HG2	1:B:358:GLN:OE1	2.06	0.55
1:C:24:ASN:OD1	1:C:27:MSE:CB	2.51	0.55
1:D:45:THR:HB	1:D:97:GLU:HG2	1.89	0.55
1:A:105:PRO:HD2	2:A:476:HOH:O	2.07	0.54
1:B:165:ALA:HB2	1:B:184:PHE:HB2	1.87	0.54
1:D:291:GLY:O	1:D:335:LEU:HD21	2.08	0.54
1:D:343:ILE:HG23	1:D:371:VAL:O	2.07	0.54
1:D:48:ARG:NH2	2:D:417:HOH:O	2.39	0.54
1:D:211:VAL:HG22	1:D:385:MSE:HE1	1.89	0.54
1:D:259:LEU:HB2	1:D:260:PRO:HD3	1.88	0.54
1:D:371:VAL:CG1	1:D:372:ASP:N	2.70	0.54
1:A:30:VAL:HG21	1:A:83:LEU:HD12	1.90	0.54
1:A:105:PRO:HG3	1:C:174:ARG:NH2	2.22	0.54
1:A:310:TRP:CE2	1:A:311:PRO:HB3	2.43	0.54
1:D:6:VAL:HA	1:D:11:TRP:CD2	2.43	0.54
1:D:94:ILE:HD12	1:D:116:TRP:HZ3	1.73	0.54
1:A:316:GLN:CG	1:A:317:GLN:H	2.20	0.54
1:A:337:ILE:HD11	1:A:339:LEU:CG	2.36	0.54
1:B:318:GLU:HG2	1:B:326:LYS:NZ	2.21	0.54
1:D:22:ARG:NH1	1:D:148:GLN:HE22	2.01	0.54
1:A:12:TRP:CZ2	1:A:76:VAL:HG22	2.43	0.54
1:A:320:VAL:CG1	1:A:321:LEU:N	2.71	0.54
1:A:112:LEU:HB2	2:A:422:HOH:O	2.08	0.54
1:C:211:VAL:CG2	1:C:385:MSE:HE1	2.38	0.53
1:C:211:VAL:HG22	1:C:385:MSE:HE1	1.90	0.53
1:D:203:GLU:CG	1:D:233:ASP:OD2	2.55	0.53
1:D:300:CYS:HB3	1:D:391:LEU:HG	1.90	0.53
1:B:125:ALA:O	1:B:127:PRO:HD3	2.08	0.53
1:C:10:SER:HA	1:C:13:GLN:NE2	2.23	0.53
1:D:47:LYS:CB	1:D:99:ASP:HB3	2.39	0.53
1:D:276:VAL:HG22	1:D:300:CYS:CB	2.38	0.53
1:A:120:LEU:N	1:A:121:PRO:CD	2.71	0.53
1:B:69:GLN:NE2	2:B:482:HOH:O	2.41	0.53
1:D:53:ILE:CG2	1:D:56:VAL:HB	2.38	0.53
1:D:343:ILE:HG12	1:D:372:ASP:HA	1.90	0.53
1:A:317:GLN:NE2	1:B:137:LEU:CD2	2.72	0.53
1:C:12:TRP:HZ2	1:C:76:VAL:HG22	1.66	0.53
1:C:369:ARG:NH2	1:C:387:GLY:HA2	2.23	0.53
1:D:212:TRP:CH2	1:D:231:LEU:HD22	2.44	0.53
1:D:196:LEU:HD22	1:D:268:PHE:CE2	2.43	0.53
1:B:11:TRP:CZ2	1:B:15:LYS:HE3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:SER:HA	1:C:257:GLU:OE2	2.09	0.53
1:D:92:CYS:HB2	1:D:124:ILE:O	2.09	0.53
1:D:396:PHE:HE2	2:D:446:HOH:O	1.92	0.53
1:B:212:TRP:CB	1:B:213:PRO:HD3	2.30	0.53
1:D:34:TRP:CH2	1:D:36:ASP:HA	2.43	0.53
1:D:47:LYS:HB3	1:D:99:ASP:HB3	1.91	0.53
1:D:135:GLY:HA2	2:D:427:HOH:O	2.09	0.53
1:D:155:TRP:CZ2	1:D:381:ARG:HB2	2.44	0.53
1:B:165:ALA:CB	1:B:184:PHE:HB2	2.39	0.53
1:A:389:ILE:HA	2:A:411:HOH:O	2.08	0.52
1:D:131:GLN:HB3	1:D:143:ALA:HB3	1.90	0.52
1:D:196:LEU:HB2	1:D:268:PHE:CD2	2.44	0.52
1:D:201:ASP:HA	1:D:203:GLU:OE2	2.08	0.52
1:A:38:GLN:HE22	1:A:45:THR:HB	1.73	0.52
1:C:241:ALA:O	1:C:245:PRO:HG2	2.09	0.52
1:B:339:LEU:HD13	1:B:368:TRP:CZ3	2.44	0.52
1:C:316:GLN:HG2	1:C:317:GLN:N	2.25	0.52
1:C:6:VAL:HA	1:C:11:TRP:CD1	2.44	0.52
1:C:30:VAL:HG21	1:C:83:LEU:HD12	1.92	0.52
1:C:221:ARG:NH2	2:C:417:HOH:O	2.42	0.52
1:C:10:SER:HA	1:C:13:GLN:HE21	1.74	0.52
1:D:362:ILE:HG22	1:D:362:ILE:O	2.09	0.52
1:A:362:ILE:HG12	1:A:362:ILE:O	2.09	0.52
1:B:99:ASP:C	1:B:99:ASP:OD2	2.52	0.52
1:C:350:ARG:NH1	1:C:353:GLN:NE2	2.58	0.52
1:A:79:TRP:CH2	1:A:81:THR:HB	2.45	0.52
1:C:219:THR:HG22	1:C:224:LEU:HB2	1.90	0.52
1:C:321:LEU:HD22	1:C:321:LEU:O	2.10	0.52
1:C:336:ARG:NH2	1:C:391:LEU:O	2.38	0.52
1:D:183:ILE:CD1	1:D:262:VAL:HG22	2.40	0.52
1:B:217:SER:O	1:B:221:ARG:HG3	2.10	0.52
1:C:68:MSE:HG2	1:C:79:TRP:HB2	1.91	0.52
1:C:203:GLU:CG	1:C:233:ASP:OD2	2.58	0.52
1:C:339:LEU:HD11	1:C:355:LEU:HD23	1.91	0.52
1:D:234:ALA:O	1:D:235:ILE:HB	2.10	0.52
1:C:331:SER:OG	1:C:333:GLU:HG3	2.09	0.51
1:D:174:ARG:NH2	1:D:256:GLN:HE22	2.09	0.51
1:B:52:TYR:CE1	1:B:58:ASP:HA	2.45	0.51
1:C:247:ASN:OD1	1:C:247:ASN:C	2.53	0.51
1:C:337:ILE:HD12	1:C:338:VAL:C	2.34	0.51
1:A:86:ASN:C	1:A:86:ASN:OD1	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:HIS:HB2	2:B:423:HOH:O	2.09	0.51
1:B:221:ARG:C	1:B:222:GLN:HG2	2.27	0.51
1:C:159:GLN:HE22	1:C:220:HIS:CG	2.28	0.51
1:C:188:ASP:O	1:C:189:VAL:CB	2.55	0.51
1:D:241:ALA:HB1	2:D:429:HOH:O	2.10	0.51
1:A:64:GLN:NE2	1:A:106:SER:HA	2.17	0.51
1:B:392:TRP:HD1	2:B:465:HOH:O	1.94	0.51
1:C:350:ARG:HB3	1:D:114:GLU:OE2	2.10	0.51
1:B:295:PRO:HD2	1:B:296:GLU:OE2	2.11	0.51
1:B:211:VAL:HG22	1:B:385:MSE:HE1	1.92	0.51
1:D:211:VAL:HG22	1:D:385:MSE:CE	2.40	0.51
1:B:346:PRO:O	1:B:350:ARG:HD2	2.10	0.51
1:A:275:THR:O	1:A:300:CYS:HB2	2.11	0.51
1:B:47:LYS:CB	1:B:99:ASP:HB3	2.41	0.51
1:B:221:ARG:O	1:B:222:GLN:CG	2.39	0.51
1:C:68:MSE:HE2	1:C:78:GLN:HA	1.93	0.51
1:C:184:PHE:HB2	1:C:212:TRP:CZ3	2.46	0.51
1:A:110:LEU:HB3	1:B:350:ARG:NH2	2.25	0.50
1:D:154:GLY:HA3	1:D:214:VAL:HG13	1.92	0.50
1:B:211:VAL:HG22	1:B:385:MSE:CE	2.41	0.50
1:A:177:ASN:C	1:A:177:ASN:HD22	2.20	0.50
1:B:288:LEU:HD13	1:B:292:LEU:HD11	1.92	0.50
1:B:347:MSE:HA	1:B:350:ARG:CD	2.41	0.50
1:A:279:GLY:HA3	1:A:283:GLY:C	2.36	0.50
1:C:20:TRP:CD2	1:C:146:MSE:HE1	2.46	0.50
1:C:369:ARG:HH22	1:C:387:GLY:N	2.08	0.50
1:A:114:GLU:O	1:A:118:LYS:HD3	2.11	0.50
1:D:183:ILE:HD11	1:D:262:VAL:HG22	1.93	0.50
1:B:172:SER:OG	1:B:175:LEU:HB2	2.12	0.50
1:C:110:LEU:HB3	1:D:350:ARG:NH2	2.27	0.50
1:A:20:TRP:CE3	1:A:146:MSE:HE1	2.46	0.50
1:A:313:ARG:HG2	1:B:313:ARG:CB	2.42	0.50
1:D:36:ASP:OD1	1:D:37:PRO:HD2	2.12	0.50
1:A:293:HIS:HB2	1:A:294:TRP:CE3	2.46	0.49
1:B:179:ARG:O	1:B:179:ARG:HG2	2.12	0.49
1:C:120:LEU:N	1:C:121:PRO:HD2	2.26	0.49
1:C:217:SER:O	1:C:221:ARG:HG3	2.12	0.49
1:A:87:TRP:HZ3	1:A:144:LEU:HB3	1.77	0.49
1:A:145:GLU:O	1:A:146:MSE:HE2	2.12	0.49
1:B:203:GLU:CG	1:B:233:ASP:OD2	2.60	0.49
1:B:240:ARG:NH2	1:B:282:PHE:HB2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:LEU:O	1:D:113:ARG:C	2.55	0.49
1:D:340:GLU:CB	1:D:369:ARG:HB2	2.43	0.49
1:A:211:VAL:O	1:A:215:LEU:HG	2.11	0.49
1:B:52:TYR:HA	1:B:57:THR:CG2	2.42	0.49
1:B:70:ARG:HG2	1:B:71:ILE:O	2.12	0.49
1:D:68:MSE:HE2	1:D:78:GLN:C	2.37	0.49
1:B:51:VAL:O	1:B:57:THR:HG21	2.13	0.49
1:C:41:GLU:OE1	1:C:41:GLU:N	2.29	0.49
1:D:120:LEU:N	1:D:121:PRO:CD	2.75	0.49
1:D:195:PRO:HB3	1:D:274:ARG:HD3	1.95	0.49
1:D:260:PRO:O	1:D:264:VAL:HG23	2.12	0.49
1:A:246:CYS:O	1:B:242:HIS:HE1	1.95	0.49
1:A:259:LEU:N	1:A:260:PRO:CD	2.75	0.49
1:B:12:TRP:CE2	1:B:76:VAL:HG22	2.47	0.49
1:B:101:ILE:HD11	1:B:115:GLY:HA2	1.95	0.49
1:B:107:PRO:CB	1:B:111:GLU:CD	2.85	0.49
1:B:377:ALA:HA	1:B:380:TRP:HB2	1.94	0.49
1:C:49:VAL:HB	1:C:68:MSE:HB2	1.93	0.49
1:D:199:LEU:HD23	1:D:205:TRP:CD1	2.47	0.49
1:B:87:TRP:CH2	1:B:89:GLY:HA3	2.48	0.49
1:B:152:GLN:HB3	1:B:382:GLY:CA	2.37	0.49
1:B:359:LEU:HB3	1:B:366:ILE:HD11	1.95	0.49
1:C:264:VAL:HG12	1:C:265:ILE:CD1	2.37	0.49
1:C:378:LEU:O	1:C:378:LEU:HG	2.11	0.49
1:D:281:SER:OG	1:D:282:PHE:N	2.46	0.49
1:A:38:GLN:HE22	1:A:45:THR:CB	2.26	0.48
1:C:302:LEU:HD13	1:C:338:VAL:HB	1.94	0.48
1:D:356:TYR:O	1:D:363:LYS:HE2	2.13	0.48
1:B:79:TRP:CH2	1:B:81:THR:HB	2.48	0.48
1:C:86:ASN:OD1	1:C:86:ASN:C	2.57	0.48
1:C:194:ARG:NH1	1:C:194:ARG:HB2	2.28	0.48
1:C:304:GLN:O	1:C:305:SER:HB2	2.12	0.48
1:C:360:HIS:N	1:C:361:PRO:HD2	2.28	0.48
1:D:22:ARG:HH22	1:D:148:GLN:HE21	1.61	0.48
1:D:92:CYS:SG	1:D:123:ALA:HB1	2.54	0.48
1:A:105:PRO:HB3	1:C:256:GLN:OE1	2.13	0.48
1:B:88:ARG:HD3	1:B:378:LEU:HG	1.95	0.48
1:C:109:ARG:HH21	1:C:110:LEU:HD11	1.77	0.48
1:B:196:LEU:HB2	1:B:268:PHE:CD2	2.48	0.48
1:A:251:TRP:O	1:A:255:GLN:HG3	2.13	0.48
1:D:308:TYR:HD1	2:D:443:HOH:O	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:HIS:ND1	1:C:363:LYS:HE2	2.28	0.48
1:D:97:GLU:HB2	2:D:406:HOH:O	2.12	0.48
1:D:99:ASP:OD2	1:D:99:ASP:C	2.55	0.48
1:D:272:ALA:HB2	1:D:296:GLU:O	2.13	0.48
1:C:34:TRP:CH2	1:C:95:PRO:HB3	2.49	0.48
1:C:113:ARG:HH22	1:D:350:ARG:HH11	1.61	0.48
1:C:369:ARG:HH22	1:C:387:GLY:CA	2.27	0.48
1:B:120:LEU:N	1:B:121:PRO:CD	2.77	0.47
1:A:271:ARG:HB2	1:A:274:ARG:HG2	1.95	0.47
1:D:101:ILE:CG2	1:D:119:LEU:HD11	2.44	0.47
1:D:133:TRP:CZ2	1:D:209:MSE:HE3	2.49	0.47
1:A:187:GLY:CA	1:A:226:PRO:HB3	2.32	0.47
1:A:313:ARG:CG	1:B:313:ARG:CB	2.92	0.47
1:C:314:GLY:O	1:D:113:ARG:HG2	2.14	0.47
1:A:209:MSE:O	1:A:210:PRO:C	2.57	0.47
1:A:313:ARG:HD2	1:B:313:ARG:CA	2.43	0.47
1:C:395:LEU:N	1:C:395:LEU:HD23	2.29	0.47
1:A:128:LEU:HD12	2:A:408:HOH:O	2.14	0.47
1:C:19:GLU:HG3	1:C:33:TRP:HZ3	1.78	0.47
1:C:68:MSE:HE2	1:C:78:GLN:CA	2.44	0.47
1:A:195:PRO:HB2	1:A:392:TRP:CZ2	2.49	0.47
1:B:165:ALA:CA	1:B:184:PHE:HD2	2.27	0.47
1:A:38:GLN:HE22	1:A:45:THR:H	1.59	0.47
1:A:350:ARG:HB3	1:B:114:GLU:OE2	2.15	0.47
1:C:195:PRO:HG2	1:C:227:ALA:HB2	1.97	0.47
1:A:293:HIS:HB2	1:A:294:TRP:CZ3	2.50	0.47
1:B:20:TRP:HA	1:B:29:GLU:O	2.14	0.47
1:C:293:HIS:C	1:C:295:PRO:HD3	2.40	0.47
1:C:318:GLU:H	1:C:318:GLU:HG3	1.48	0.47
1:C:177:ASN:C	1:C:177:ASN:HD22	2.23	0.47
1:C:209:MSE:O	1:C:210:PRO:C	2.58	0.47
1:B:271:ARG:HB3	1:B:273:ASP:OD1	2.14	0.47
1:C:314:GLY:O	1:D:113:ARG:CG	2.63	0.47
1:D:78:GLN:HG2	1:D:79:TRP:N	2.30	0.47
1:A:10:SER:HA	1:A:13:GLN:NE2	2.29	0.46
1:B:11:TRP:CH2	1:B:15:LYS:HE3	2.51	0.46
1:B:342:GLY:O	1:B:345:GLU:HG3	2.15	0.46
1:C:20:TRP:O	1:C:21:GLN:HG3	2.16	0.46
1:C:120:LEU:N	1:C:121:PRO:CD	2.78	0.46
1:C:152:GLN:HG2	1:C:382:GLY:HA3	1.98	0.46
1:C:251:TRP:CE2	1:C:290:ALA:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ILE:H	1:B:57:THR:CB	2.12	0.46
1:C:179:ARG:NH2	1:C:243:GLU:OE1	2.39	0.46
1:D:338:VAL:HG23	1:D:391:LEU:HD13	1.97	0.46
1:C:395:LEU:N	1:C:395:LEU:CD2	2.78	0.46
1:A:68:MSE:HG2	1:A:79:TRP:HB2	1.97	0.46
1:A:107:PRO:HB2	1:A:112:LEU:HD13	1.96	0.46
1:B:119:LEU:C	1:B:121:PRO:HD2	2.41	0.46
1:C:112:LEU:HD13	1:C:112:LEU:N	2.30	0.46
1:D:170:TRP:HE3	1:D:179:ARG:HD3	1.81	0.46
1:D:311:PRO:HD3	1:D:320:VAL:HB	1.97	0.46
1:C:97:GLU:OE1	1:C:122:GLN:NE2	2.47	0.46
1:C:240:ARG:HH22	1:C:281:SER:HB2	1.80	0.46
1:D:309:TRP:CE3	1:D:310:TRP:HA	2.50	0.46
1:A:206:ALA:HB2	1:A:231:LEU:HD22	1.98	0.46
1:C:179:ARG:HD2	2:C:447:HOH:O	2.15	0.46
1:C:308:TYR:CE2	1:C:355:LEU:HD22	2.51	0.46
1:D:49:VAL:O	1:D:68:MSE:HG3	2.15	0.46
1:A:316:GLN:HG2	1:A:317:GLN:H	1.81	0.46
1:A:360:HIS:HA	1:A:363:LYS:CE	2.46	0.46
1:B:12:TRP:CE2	1:B:35:ARG:HG3	2.51	0.46
1:B:203:GLU:HG2	1:B:233:ASP:OD2	2.15	0.46
1:C:40:SER:HB2	1:C:41:GLU:OE1	2.16	0.46
1:D:388:LEU:HD12	1:D:388:LEU:HA	1.60	0.45
1:A:170:TRP:CZ3	1:A:179:ARG:HD3	2.52	0.45
1:C:345:GLU:OE2	1:C:375:HIS:ND1	2.44	0.45
1:D:157:CYS:N	1:D:158:PRO:CD	2.77	0.45
1:A:189:VAL:O	1:A:189:VAL:HG13	2.15	0.45
1:B:163:ILE:HD12	1:B:163:ILE:N	2.30	0.45
1:C:109:ARG:HD3	1:D:109:ARG:HH21	1.81	0.45
1:C:167:GLU:HG3	1:C:182:TRP:NE1	2.31	0.45
1:C:219:THR:HG21	2:C:401:HOH:O	2.15	0.45
1:B:279:GLY:HA3	1:B:283:GLY:O	2.17	0.45
1:B:12:TRP:HZ2	1:B:76:VAL:HG22	1.78	0.45
1:B:345:GLU:HG2	1:B:374:GLY:HA2	1.98	0.45
1:C:104:ALA:HA	1:C:105:PRO:HD3	1.86	0.45
1:A:22:ARG:HD3	1:A:25:ASP:HA	1.98	0.45
1:C:166:LYS:NZ	1:C:168:ILE:HG22	2.32	0.45
1:C:324:LYS:CG	1:C:329:GLU:HB2	2.47	0.45
1:A:68:MSE:HE2	1:A:78:GLN:CA	2.46	0.45
1:A:88:ARG:HG3	1:A:145:GLU:HG2	1.99	0.45
1:D:6:VAL:HA	1:D:11:TRP:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:O	1:A:182:TRP:HA	2.17	0.45
1:A:203:GLU:HG3	1:A:233:ASP:HA	1.98	0.45
1:D:106:SER:HA	1:D:107:PRO:HD3	1.86	0.45
1:D:152:GLN:HB3	1:D:382:GLY:HA2	1.98	0.45
1:C:19:GLU:HG3	1:C:33:TRP:CZ3	2.52	0.45
1:C:339:LEU:HD13	1:C:368:TRP:HZ3	1.82	0.45
1:D:36:ASP:HA	1:D:37:PRO:HD3	1.88	0.45
1:A:240:ARG:CZ	1:A:282:PHE:HB2	2.47	0.45
1:A:324:LYS:HG2	1:A:330:VAL:HG23	1.99	0.45
1:B:162:GLU:HB2	1:B:163:ILE:HD12	1.98	0.45
1:C:342:GLY:HA2	1:C:371:VAL:HG22	1.98	0.45
1:D:170:TRP:CE3	1:D:179:ARG:CD	3.00	0.45
1:D:268:PHE:CD1	1:D:268:PHE:N	2.84	0.45
1:A:24:ASN:HB2	1:A:26:GLU:H	1.82	0.44
1:B:185:THR:HG21	1:B:194:ARG:NH2	2.09	0.44
1:A:393:GLN:N	1:A:394:PRO:CD	2.80	0.44
1:B:194:ARG:NH1	1:B:267:PRO:O	2.50	0.44
1:C:86:ASN:HA	1:C:148:GLN:C	2.43	0.44
1:B:24:ASN:C	1:B:26:GLU:N	2.75	0.44
1:C:292:LEU:HD12	1:C:292:LEU:HA	1.63	0.44
1:D:170:TRP:O	1:D:178:SER:HA	2.17	0.44
1:D:172:SER:CB	1:D:175:LEU:HB2	2.47	0.44
1:A:360:HIS:HB3	1:A:361:PRO:HD3	1.98	0.44
1:A:212:TRP:CB	1:A:213:PRO:HD3	2.46	0.44
1:A:316:GLN:CG	1:A:317:GLN:N	2.79	0.44
1:B:259:LEU:O	1:B:260:PRO:C	2.60	0.44
1:D:143:ALA:HB1	1:D:378:LEU:HD21	1.99	0.44
1:B:157:CYS:N	1:B:158:PRO:HD3	2.33	0.44
1:C:250:PHE:O	1:C:254:VAL:HG23	2.16	0.44
1:D:107:PRO:HB3	1:D:111:GLU:OE2	2.17	0.44
1:A:107:PRO:HB3	1:A:111:GLU:HB2	2.00	0.44
1:C:288:LEU:HD12	1:C:308:TYR:CE1	2.53	0.44
1:A:318:GLU:H	1:A:318:GLU:HG3	1.44	0.44
1:C:30:VAL:O	1:C:80:THR:HA	2.17	0.44
1:D:113:ARG:HD2	2:D:436:HOH:O	2.17	0.44
1:D:356:TYR:CE2	1:D:363:LYS:HD3	2.53	0.44
1:A:126:ASP:HA	1:A:127:PRO:HD2	1.70	0.44
1:C:377:ALA:HA	1:C:380:TRP:CE3	2.53	0.44
1:A:135:GLY:O	2:A:479:HOH:O	2.20	0.43
1:D:241:ALA:HA	1:D:282:PHE:HE2	1.83	0.43
1:C:38:GLN:HE22	1:C:45:THR:H	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:TRP:HB3	1:D:120:LEU:HD11	2.00	0.43
1:D:196:LEU:HD12	1:D:197:ALA:H	1.83	0.43
1:A:276:VAL:HG22	1:A:300:CYS:CB	2.48	0.43
1:B:343:ILE:HA	1:B:349:MSE:HE2	1.99	0.43
1:C:294:TRP:N	1:C:295:PRO:HD3	2.33	0.43
1:A:194:ARG:HG3	1:A:226:PRO:O	2.18	0.43
1:B:247:ASN:OD1	1:B:247:ASN:C	2.61	0.43
1:C:27:MSE:HG3	1:C:28:PHE:H	1.84	0.43
1:C:64:GLN:NE2	1:C:105:PRO:O	2.49	0.43
1:B:199:LEU:HB2	1:B:231:LEU:HD12	2.00	0.43
1:C:246:CYS:O	1:D:242:HIS:HE1	2.01	0.43
1:D:101:ILE:HG21	1:D:119:LEU:HD11	2.00	0.43
1:D:347:MSE:CA	1:D:350:ARG:HD2	2.34	0.43
1:A:369:ARG:NH2	1:A:387:GLY:HA2	2.32	0.43
1:C:31:THR:HG21	1:C:33:TRP:CH2	2.54	0.43
1:A:52:TYR:HA	1:A:57:THR:HG21	2.01	0.43
1:A:157:CYS:SG	1:A:221:ARG:NH2	2.92	0.43
1:B:86:ASN:OD1	1:B:86:ASN:C	2.61	0.43
1:B:109:ARG:NH1	1:B:113:ARG:CZ	2.81	0.43
1:C:45:THR:O	1:C:97:GLU:HA	2.18	0.43
1:D:174:ARG:HH21	1:D:256:GLN:NE2	2.16	0.43
1:A:292:LEU:HD12	1:A:292:LEU:HA	1.89	0.43
1:B:39:GLY:HA2	1:B:75:ASP:HB3	2.01	0.43
1:B:41:GLU:H	1:B:41:GLU:CD	2.27	0.43
1:C:206:ALA:HB2	1:C:231:LEU:HD22	2.01	0.43
1:D:215:LEU:HD23	1:D:385:MSE:SE	2.68	0.43
1:B:197:ALA:HB2	1:B:392:TRP:CZ2	2.54	0.43
1:B:391:LEU:HD12	1:B:391:LEU:HA	1.90	0.43
1:C:159:GLN:HE22	1:C:220:HIS:CD2	2.37	0.43
1:A:200:LEU:HD13	1:A:244:LEU:HD22	2.00	0.42
1:B:24:ASN:C	1:B:26:GLU:H	2.27	0.42
1:B:152:GLN:HE22	1:B:381:ARG:HG3	1.84	0.42
1:C:113:ARG:O	1:C:117:ARG:HB2	2.19	0.42
1:C:292:LEU:HB3	1:C:330:VAL:HG11	2.01	0.42
1:D:211:VAL:HG13	1:D:215:LEU:CD1	2.49	0.42
1:A:85:ALA:O	1:A:148:GLN:N	2.48	0.42
1:B:356:TYR:CZ	1:B:363:LYS:HD3	2.53	0.42
1:B:388:LEU:HD12	1:B:388:LEU:HA	1.58	0.42
1:D:224:LEU:HD22	1:D:388:LEU:HB3	2.00	0.42
1:B:8:SER:OG	1:B:11:TRP:HB2	2.19	0.42
1:B:280:GLN:HE21	1:B:280:GLN:HB2	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:LEU:O	1:B:359:LEU:HG	2.19	0.42
1:C:70:ARG:HG2	1:C:71:ILE:O	2.19	0.42
1:D:112:LEU:N	1:D:112:LEU:HD12	2.32	0.42
1:A:240:ARG:NH1	1:A:282:PHE:CD2	2.87	0.42
1:C:113:ARG:NH2	1:D:350:ARG:HH11	2.17	0.42
1:A:310:TRP:HA	1:A:311:PRO:HA	1.68	0.42
1:B:157:CYS:SG	1:B:221:ARG:NH2	2.93	0.42
1:C:32:PHE:O	1:C:78:GLN:HA	2.18	0.42
1:C:280:GLN:HB2	2:C:461:HOH:O	2.18	0.42
1:D:71:ILE:HD12	1:D:76:VAL:CG1	2.49	0.42
1:B:101:ILE:CG2	1:B:119:LEU:HD11	2.48	0.42
1:B:302:LEU:C	1:B:302:LEU:HD12	2.45	0.42
1:B:320:VAL:CG1	1:B:321:LEU:N	2.81	0.42
1:B:369:ARG:HH22	1:B:387:GLY:HA2	1.85	0.42
1:C:27:MSE:HG3	1:C:28:PHE:N	2.35	0.42
1:C:291:GLY:O	1:C:295:PRO:HG3	2.20	0.42
1:A:236:ASP:C	1:A:236:ASP:OD1	2.63	0.42
1:A:359:LEU:HB3	1:A:362:ILE:HD11	2.02	0.42
1:C:350:ARG:NH1	1:C:353:GLN:HE21	2.17	0.42
1:A:280:GLN:C	1:A:281:SER:OG	2.63	0.42
1:B:269:SER:HB3	1:B:274:ARG:HD2	2.01	0.42
1:C:28:PHE:CZ	1:C:147:PRO:HG2	2.54	0.42
1:D:45:THR:HB	1:D:97:GLU:CG	2.49	0.42
1:D:165:ALA:HB2	1:D:184:PHE:HB2	2.02	0.42
1:A:359:LEU:HB3	1:A:362:ILE:CD1	2.50	0.42
1:C:66:GLN:HG2	2:C:463:HOH:O	2.20	0.42
1:C:203:GLU:HG2	1:C:233:ASP:CG	2.44	0.42
1:C:212:TRP:HB2	1:C:213:PRO:HD3	2.02	0.42
1:D:241:ALA:HA	1:D:282:PHE:CE2	2.54	0.42
1:D:281:SER:HA	1:D:305:SER:O	2.20	0.42
1:A:6:VAL:HA	1:A:11:TRP:CG	2.54	0.42
1:A:50:TRP:CZ2	1:A:102:PHE:HB2	2.55	0.42
1:A:188:ASP:O	1:A:189:VAL:HG12	2.19	0.42
1:A:212:TRP:HB2	1:A:213:PRO:CD	2.45	0.42
1:A:313:ARG:CG	1:B:313:ARG:HB2	2.46	0.42
1:A:315:GLY:O	1:B:117:ARG:HG3	2.20	0.42
1:B:85:ALA:O	1:B:148:GLN:HB2	2.20	0.42
1:C:312:HIS:CD2	1:C:317:GLN:HB2	2.55	0.42
1:C:330:VAL:HG12	1:C:331:SER:N	2.35	0.42
1:D:119:LEU:C	1:D:121:PRO:CD	2.91	0.42
1:A:133:TRP:HZ3	1:A:143:ALA:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:C	1:A:346:PRO:HD3	2.45	0.41
1:A:360:HIS:N	1:A:361:PRO:HD2	2.35	0.41
1:C:315:GLY:N	1:C:347:MSE:HE3	2.35	0.41
1:D:302:LEU:HD13	1:D:338:VAL:HB	2.01	0.41
1:B:22:ARG:CZ	1:B:148:GLN:NE2	2.83	0.41
1:B:154:GLY:CA	1:B:214:VAL:HG13	2.48	0.41
1:B:193:GLU:N	2:B:430:HOH:O	2.53	0.41
1:C:31:THR:HG22	1:C:33:TRP:CZ3	2.55	0.41
1:A:114:GLU:OE2	1:A:114:GLU:HA	2.20	0.41
1:A:320:VAL:HG12	1:A:321:LEU:N	2.35	0.41
1:B:240:ARG:CZ	1:B:282:PHE:HB2	2.50	0.41
1:C:126:ASP:HA	1:C:127:PRO:HD2	1.75	0.41
1:C:152:GLN:HA	1:C:153:PRO:HD3	1.83	0.41
1:C:270:ASP:HA	1:C:297:ARG:HH22	1.85	0.41
1:C:308:TYR:O	1:C:319:GLY:HA3	2.20	0.41
1:D:12:TRP:CE2	1:D:35:ARG:HG3	2.55	0.41
1:B:271:ARG:HB2	1:B:274:ARG:HG2	2.02	0.41
1:D:53:ILE:HB	1:D:56:VAL:HB	2.02	0.41
1:D:244:LEU:N	1:D:245:PRO:CD	2.84	0.41
1:D:376:ASP:HB3	1:D:379:CYS:SG	2.60	0.41
1:A:302:LEU:HD22	1:A:387:GLY:HA3	2.03	0.41
1:C:19:GLU:CG	1:C:33:TRP:HZ3	2.33	0.41
1:C:42:GLU:O	1:C:42:GLU:HG3	2.19	0.41
1:C:240:ARG:NH1	1:C:282:PHE:CD2	2.88	0.41
1:D:118:LYS:O	1:D:121:PRO:HD2	2.20	0.41
1:D:177:ASN:OD1	1:D:179:ARG:NH1	2.52	0.41
1:D:325:LEU:O	1:D:328:GLY:N	2.53	0.41
1:B:52:TYR:CZ	1:B:58:ASP:HB3	2.55	0.41
1:B:167:GLU:OE1	1:B:180:ARG:HD2	2.20	0.41
1:C:68:MSE:HE2	1:C:77:TRP:C	2.45	0.41
1:D:343:ILE:CG1	1:D:372:ASP:O	2.68	0.41
1:A:22:ARG:HB2	1:A:28:PHE:CZ	2.55	0.41
1:A:314:GLY:O	1:B:113:ARG:CG	2.67	0.41
1:B:35:ARG:O	1:B:37:PRO:HD3	2.20	0.41
1:B:212:TRP:CB	1:B:213:PRO:CD	2.97	0.41
1:B:222:GLN:HG3	1:B:222:GLN:O	2.20	0.41
1:B:310:TRP:HA	1:B:311:PRO:HA	1.68	0.41
1:C:49:VAL:O	1:C:49:VAL:HG12	2.21	0.41
1:C:96:THR:OG1	1:C:98:ARG:HG2	2.20	0.41
1:C:203:GLU:CD	1:C:234:ALA:H	2.29	0.41
1:C:259:LEU:HD23	1:C:259:LEU:HA	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:GLU:HG3	1:C:333:GLU:H	1.57	0.41
1:A:144:LEU:HD22	1:A:146:MSE:HE3	2.02	0.41
1:A:194:ARG:NH1	1:A:267:PRO:O	2.53	0.41
1:B:203:GLU:CD	1:B:203:GLU:H	2.27	0.41
1:C:132:SER:HB3	1:C:141:VAL:O	2.21	0.41
1:C:279:GLY:HA3	1:C:283:GLY:C	2.45	0.41
1:D:8:SER:O	1:D:11:TRP:N	2.54	0.41
1:D:244:LEU:HA	1:D:244:LEU:HD23	1.74	0.41
1:A:45:THR:CG2	1:A:97:GLU:HB3	2.42	0.41
1:B:313:ARG:HB2	1:B:313:ARG:HH21	1.85	0.41
1:C:359:LEU:C	1:C:361:PRO:HD2	2.46	0.41
1:C:360:HIS:C	1:C:363:LYS:HG3	2.46	0.41
1:C:360:HIS:CA	1:C:363:LYS:HG3	2.47	0.41
1:A:66:GLN:HB3	2:A:429:HOH:O	2.20	0.40
1:B:194:ARG:HA	1:B:195:PRO:HD2	1.91	0.40
1:C:42:GLU:HG2	1:C:43:TYR:CZ	2.56	0.40
1:C:229:TYR:OH	1:C:392:TRP:HZ3	2.04	0.40
1:C:324:LYS:HG3	1:C:329:GLU:HB2	2.03	0.40
1:D:174:ARG:NH2	1:D:256:GLN:NE2	2.68	0.40
1:D:371:VAL:HG12	1:D:372:ASP:N	2.36	0.40
1:A:310:TRP:CG	1:A:311:PRO:HA	2.56	0.40
1:C:70:ARG:HG2	1:C:71:ILE:C	2.46	0.40
1:D:49:VAL:HG13	1:D:95:PRO:HG3	2.03	0.40
1:A:240:ARG:NH1	1:A:282:PHE:HB2	2.36	0.40
1:A:369:ARG:HH22	1:A:387:GLY:N	2.19	0.40
1:C:309:TRP:CZ2	1:D:313:ARG:HD3	2.56	0.40
1:A:144:LEU:HD22	1:A:146:MSE:CE	2.51	0.40
1:A:182:TRP:HB2	1:A:231:LEU:HB2	2.04	0.40
1:B:321:LEU:HB3	2:B:473:HOH:O	2.21	0.40
1:C:205:TRP:HE1	1:C:280:GLN:NE2	2.16	0.40
1:C:302:LEU:HD22	1:C:387:GLY:HA3	2.04	0.40
1:D:34:TRP:CH2	1:D:37:PRO:HD3	2.57	0.40
1:D:196:LEU:HD12	1:D:197:ALA:N	2.36	0.40
1:A:13:GLN:HE21	1:A:13:GLN:HB2	1.66	0.40
1:A:134:LYS:O	1:A:208:SER:OG	2.39	0.40
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.89	0.40
1:A:315:GLY:N	1:A:347:MSE:HE3	2.36	0.40
1:D:240:ARG:NH2	1:D:282:PHE:HB2	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:CYS:SG	1:C:157:CYS:SG[2_645]	1.87	0.33

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	377/403 (94%)	358 (95%)	18 (5%)	1 (0%)	36	53
1	B	377/403 (94%)	361 (96%)	15 (4%)	1 (0%)	36	53
1	C	377/403 (94%)	358 (95%)	18 (5%)	1 (0%)	36	53
1	D	379/403 (94%)	355 (94%)	22 (6%)	2 (0%)	24	40
All	All	1510/1612 (94%)	1432 (95%)	73 (5%)	5 (0%)	36	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	235	ILE
1	A	235	ILE
1	D	235	ILE
1	B	235	ILE
1	D	105	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/333 (97%)	286 (88%)	38 (12%)	5	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	324/333 (97%)	273 (84%)	51 (16%)	2	4
1	C	324/333 (97%)	274 (85%)	50 (15%)	2	4
1	D	326/333 (98%)	280 (86%)	46 (14%)	3	6
All	All	1298/1332 (97%)	1113 (86%)	185 (14%)	3	6

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	47	LYS
1	A	64	GLN
1	A	97	GLU
1	A	110	LEU
1	A	112	LEU
1	A	118	LYS
1	A	134	LYS
1	A	144	LEU
1	A	151	LEU
1	A	156	ASP
1	A	157	CYS
1	A	162	GLU
1	A	166	LYS
1	A	177	ASN
1	A	194	ARG
1	A	203	GLU
1	A	208	SER
1	A	220	HIS
1	A	223	GLN
1	A	265	ILE
1	A	273	ASP
1	A	277	VAL
1	A	281	SER
1	A	285	LEU
1	A	288	LEU
1	A	292	LEU
1	A	313	ARG
1	A	318	GLU
1	A	320	VAL
1	A	321	LEU
1	A	323	GLU
1	A	333	GLU

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Mol	Chain	Res	Type
1	A	337	ILE
1	A	339	LEU
1	A	362	ILE
1	A	369	ARG
1	A	395	LEU
1	B	13	GLN
1	B	19	GLU
1	B	21	GLN
1	B	27	MSE
1	B	38	GLN
1	B	45	THR
1	B	57	THR
1	B	66	GLN
1	B	101	ILE
1	B	111	GLU
1	B	113	ARG
1	B	114	GLU
1	B	118	LYS
1	B	131	GLN
1	B	134	LYS
1	B	137	LEU
1	B	144	LEU
1	B	159	GLN
1	B	163	ILE
1	B	168	ILE
1	B	175	LEU
1	B	179	ARG
1	B	188	ASP
1	B	189	VAL
1	B	193	GLU
1	B	194	ARG
1	B	203	GLU
1	B	207	GLN
1	B	211	VAL
1	B	221	ARG
1	B	254	VAL
1	B	277	VAL
1	B	280	GLN
1	B	282	PHE
1	B	288	LEU
1	B	302	LEU
1	B	305	SER

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Mol	Chain	Res	Type
1	B	313	ARG
1	B	316	GLN
1	B	320	VAL
1	B	322	LEU
1	B	323	GLU
1	B	337	ILE
1	B	339	LEU
1	B	344	ARG
1	B	347	MSE
1	B	348	ILE
1	B	381	ARG
1	B	388	LEU
1	B	391	LEU
1	B	393	GLN
1	C	13	GLN
1	C	14	SER
1	C	24	ASN
1	C	25	ASP
1	C	30	VAL
1	C	31	THR
1	C	42	GLU
1	C	47	LYS
1	C	64	GLN
1	C	66	GLN
1	C	78	GLN
1	C	83	LEU
1	C	97	GLU
1	C	109	ARG
1	C	110	LEU
1	C	112	LEU
1	C	118	LYS
1	C	134	LYS
1	C	137	LEU
1	C	144	LEU
1	C	162	GLU
1	C	166	LYS
1	C	177	ASN
1	C	194	ARG
1	C	203	GLU
1	C	208	SER
1	C	220	HIS
1	C	221	ARG

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Mol	Chain	Res	Type
1	C	223	GLN
1	C	244	LEU
1	C	264	VAL
1	C	273	ASP
1	C	277	VAL
1	C	281	SER
1	C	285	LEU
1	C	288	LEU
1	C	292	LEU
1	C	313	ARG
1	C	316	GLN
1	C	317	GLN
1	C	318	GLU
1	C	320	VAL
1	C	321	LEU
1	C	323	GLU
1	C	333	GLU
1	C	337	ILE
1	C	339	LEU
1	C	362	ILE
1	C	369	ARG
1	C	395	LEU
1	D	10	SER
1	D	13	GLN
1	D	21	GLN
1	D	24	ASN
1	D	25	ASP
1	D	27	MSE
1	D	57	THR
1	D	58	ASP
1	D	66	GLN
1	D	101	ILE
1	D	110	LEU
1	D	111	GLU
1	D	113	ARG
1	D	118	LYS
1	D	144	LEU
1	D	159	GLN
1	D	163	ILE
1	D	168	ILE
1	D	175	LEU
1	D	179	ARG

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Mol	Chain	Res	Type
1	D	189	VAL
1	D	193	GLU
1	D	194	ARG
1	D	203	GLU
1	D	211	VAL
1	D	222	GLN
1	D	254	VAL
1	D	277	VAL
1	D	288	LEU
1	D	302	LEU
1	D	313	ARG
1	D	316	GLN
1	D	318	GLU
1	D	320	VAL
1	D	322	LEU
1	D	323	GLU
1	D	337	ILE
1	D	339	LEU
1	D	340	GLU
1	D	344	ARG
1	D	347	MSE
1	D	348	ILE
1	D	350	ARG
1	D	388	LEU
1	D	391	LEU
1	D	393	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	24	ASN
1	A	38	GLN
1	A	64	GLN
1	A	139	HIS
1	A	148	GLN
1	A	159	GLN
1	A	177	ASN
1	A	220	HIS
1	A	222	GLN
1	A	255	GLN
1	A	256	GLN

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Mol	Chain	Res	Type
1	A	280	GLN
1	A	304	GLN
1	A	316	GLN
1	A	317	GLN
1	A	370	GLN
1	A	375	HIS
1	B	13	GLN
1	B	21	GLN
1	B	38	GLN
1	B	66	GLN
1	B	69	GLN
1	B	82	GLN
1	B	84	ASN
1	B	131	GLN
1	B	148	GLN
1	B	207	GLN
1	B	255	GLN
1	B	280	GLN
1	B	293	HIS
1	B	304	GLN
1	B	375	HIS
1	B	386	GLN
1	B	397	HIS
1	C	13	GLN
1	C	38	GLN
1	C	148	GLN
1	C	159	GLN
1	C	177	ASN
1	C	220	HIS
1	C	222	GLN
1	C	255	GLN
1	C	280	GLN
1	C	304	GLN
1	C	312	HIS
1	C	317	GLN
1	C	358	GLN
1	C	370	GLN
1	D	13	GLN
1	D	24	ASN
1	D	38	GLN
1	D	66	GLN
1	D	84	ASN

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Mol	Chain	Res	Type
1	D	148	GLN
1	D	222	GLN
1	D	242	HIS
1	D	255	GLN
1	D	256	GLN
1	D	293	HIS
1	D	316	GLN
1	D	317	GLN
1	D	352	ASN
1	D	386	GLN
1	D	397	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	376/403 (93%)	-0.92	0 100 100	19, 58, 98, 118	5 (1%)
1	B	376/403 (93%)	-0.92	0 100 100	15, 56, 94, 120	11 (2%)
1	C	376/403 (93%)	-1.01	0 100 100	12, 49, 85, 119	5 (1%)
1	D	376/403 (93%)	-0.99	0 100 100	9, 48, 93, 114	13 (3%)
All	All	1504/1612 (93%)	-0.96	0 100 100	9, 53, 95, 120	34 (2%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.