



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 07:42 AM EST

PDB ID : 2Z2S
Title : Crystal Structure of Rhodobacter sphaeroides SigE in complex with the anti-sigma ChrR
Authors : Darst, S.A.; Campbell, E.A.
Deposited on : 2007-05-26
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

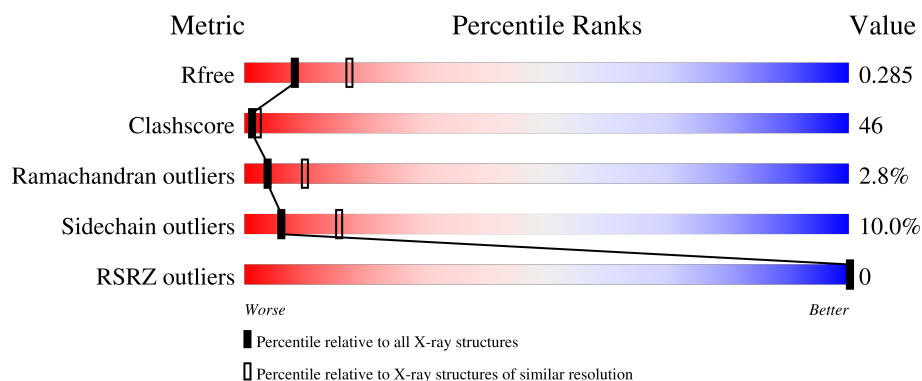
1 Overall quality at a glance

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))
R_{free}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (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 $\leq 5\%$. 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	184	
1	C	184	
1	E	184	
1	G	184	
2	B	203	

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Mol	Chain	Length	Quality of chain
2	D	203	
2	F	203	
2	H	203	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	D	204	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10379 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 RpoE, ECF SigE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	Se	0	0	0
			1317	827	248	236	1	5			
1	C	172	Total	C	N	O	S	Se	0	0	0
			1333	839	253	235	1	5			
1	E	155	Total	C	N	O	S	Se	0	0	0
			1238	777	235	221	1	4			
1	G	160	Total	C	N	O	S	Se	0	0	0
			1269	799	239	226	1	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q3IYV6
A	-1	PRO	-	expression tag	UNP Q3IYV6
A	0	HIS	-	expression tag	UNP Q3IYV6
C	-2	GLY	-	expression tag	UNP Q3IYV6
C	-1	PRO	-	expression tag	UNP Q3IYV6
C	0	HIS	-	expression tag	UNP Q3IYV6
E	-2	GLY	-	expression tag	UNP Q3IYV6
E	-1	PRO	-	expression tag	UNP Q3IYV6
E	0	HIS	-	expression tag	UNP Q3IYV6
G	-2	GLY	-	expression tag	UNP Q3IYV6
G	-1	PRO	-	expression tag	UNP Q3IYV6
G	0	HIS	-	expression tag	UNP Q3IYV6

- Molecule 2 is a protein called Anti-Sigma factor ChrR, transcriptional activator ChrR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	182	Total	C	N	O	S	Se	0	0	0
			1258	788	225	239	4	2			
2	D	169	Total	C	N	O	S	Se	0	0	0
			1186	746	210	224	4	2			

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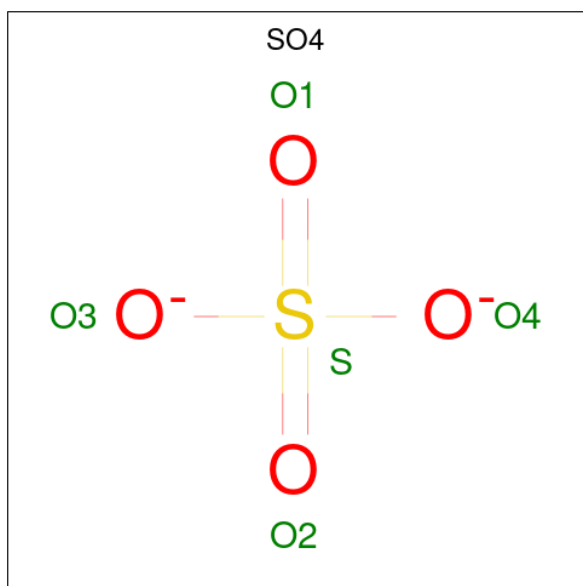
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	F	169	Total	C	N	O	S	Se	0	0	0
			1161	732	202	221	4	2			
2	H	175	Total	C	N	O	S	Se	0	0	0
			1222	767	210	239	4	2			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		
3	H	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		

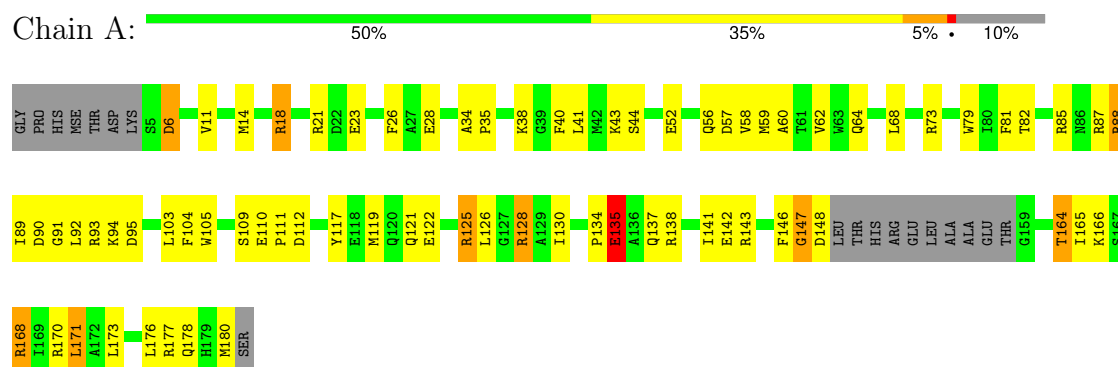
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	52	Total 52	O 52	0	0
5	B	47	Total 47	O 47	0	0
5	C	59	Total 59	O 59	0	0
5	D	38	Total 38	O 38	0	0
5	E	56	Total 56	O 56	0	0
5	F	39	Total 39	O 39	0	0
5	G	56	Total 56	O 56	0	0
5	H	34	Total 34	O 34	0	0

3 Residue-property plots

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

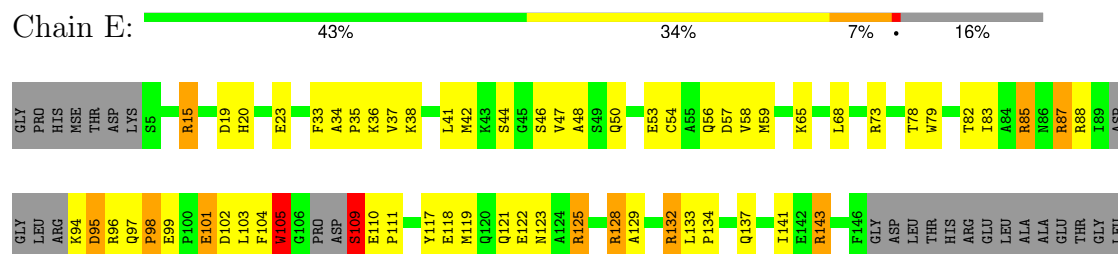
• Molecule 1: RpoE, ECF SigE



• Molecule 1: RpoE, ECF SigE



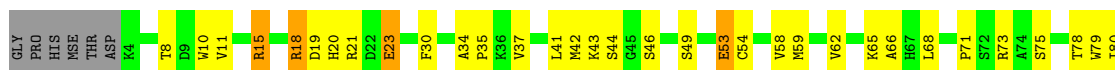
• Molecule 1: RpoE, ECF SigE





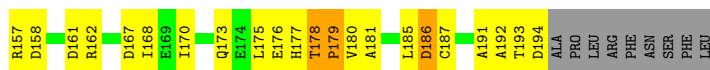
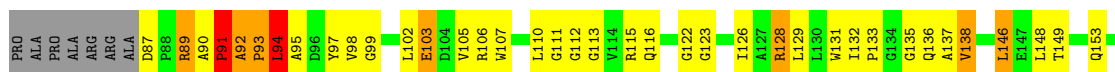
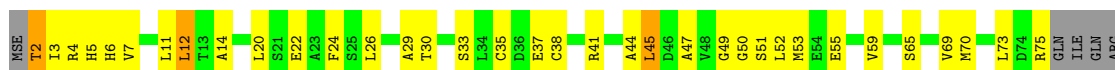
• Molecule 1: RpoE, ECF SigE

Chain G: 41% 38% 8% 13%



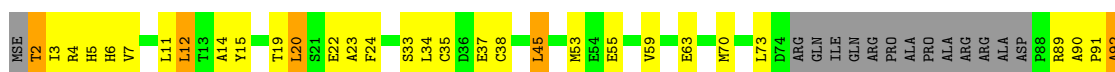
• Molecule 2: Anti-Sigma factor ChrR, transcriptional activator ChrR

Chain B: 43% 39% 6% 10%



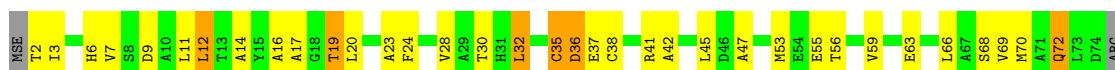
• Molecule 2: Anti-Sigma factor ChrR, transcriptional activator ChrR

Chain D: 38% 34% 8% 17%



• Molecule 2: Anti-Sigma factor ChrR, transcriptional activator ChrR

Chain F: 40% 35% 6% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.14Å 46.45Å 141.70Å 90.00° 91.63° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70 25.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	75.2 (25.00-2.70) 69.4 (25.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.286 0.247 , 0.285	Depositor DCC
R_{free} test set	1629 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.772	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.155 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10379	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.45	0/1340	0.66	0/1800
1	C	0.44	0/1356	0.68	1/1824 (0.1%)
1	E	0.89	3/1259 (0.2%)	0.92	5/1689 (0.3%)
1	G	0.55	0/1292	0.76	1/1738 (0.1%)
2	B	0.52	1/1276 (0.1%)	0.85	5/1741 (0.3%)
2	D	2.27	20/1202 (1.7%)	1.51	26/1635 (1.6%)
2	F	0.65	3/1173 (0.3%)	1.02	11/1598 (0.7%)
2	H	0.47	0/1237	0.75	1/1687 (0.1%)
All	All	0.95	27/10135 (0.3%)	0.92	50/13712 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	2
2	F	0	1
All	All	0	3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	170	ILE	CA-CB	38.69	2.43	1.54
2	D	179	PRO	CA-C	32.82	2.18	1.52
2	D	170	ILE	CA-C	27.23	2.23	1.52
2	D	180	VAL	N-CA	20.70	1.87	1.46
1	E	105	TRP	C-N	-19.66	0.97	1.33
2	D	179	PRO	N-CA	19.46	1.80	1.47
2	D	179	PRO	CB-CG	17.41	2.37	1.50
2	D	170	ILE	C-N	17.04	1.66	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	180	VAL	CA-CB	16.90	1.90	1.54
1	E	109	SER	CB-OG	13.12	1.59	1.42
2	D	179	PRO	C-N	11.31	1.60	1.34
2	D	179	PRO	CA-CB	-11.20	1.31	1.53
1	E	109	SER	C-N	-11.04	1.08	1.34
2	D	180	VAL	CA-C	10.21	1.79	1.52
2	D	180	VAL	CB-CG1	9.37	1.72	1.52
2	D	179	PRO	CG-CD	8.69	1.79	1.50
2	D	170	ILE	CG1-CD1	8.42	2.08	1.50
2	F	173	GLN	C-N	7.59	1.51	1.34
2	D	170	ILE	CB-CG1	7.11	1.74	1.54
2	D	179	PRO	C-O	5.93	1.35	1.23
2	F	172	ASP	C-N	5.92	1.47	1.34
2	F	180	VAL	N-CA	5.79	1.57	1.46
2	D	179	PRO	N-CD	5.50	1.55	1.47
2	D	170	ILE	N-CA	5.37	1.57	1.46
2	D	181	ALA	N-CA	5.23	1.56	1.46
2	D	169	GLU	CG-CD	-5.12	1.44	1.51
2	B	138	VAL	CB-CG2	-5.01	1.42	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	179	PRO	CA-CB-CG	-18.86	68.17	104.00
1	E	105	TRP	O-C-N	-16.71	94.80	123.20
2	D	180	VAL	CB-CA-C	-16.03	80.94	111.40
2	D	170	ILE	CG1-CB-CG2	-15.55	77.19	111.40
2	D	170	ILE	N-CA-CB	-14.38	77.72	110.80
2	F	173	GLN	O-C-N	13.32	144.02	122.70
2	D	179	PRO	N-CA-C	13.21	146.46	112.10
2	D	170	ILE	CB-CA-C	11.58	134.76	111.60
2	D	170	ILE	C-N-CD	-10.86	96.70	120.60
2	F	173	GLN	C-N-CA	-10.56	95.30	121.70
1	E	95	ASP	CB-CG-OD2	10.55	127.80	118.30
2	D	179	PRO	CB-CA-C	-10.27	86.33	112.00
1	E	109	SER	O-C-N	-10.14	106.47	122.70
2	D	179	PRO	CA-N-CD	-9.29	98.50	111.50
2	D	181	ALA	N-CA-C	8.79	134.73	111.00
2	B	158	ASP	N-CA-C	-8.76	87.36	111.00
2	D	170	ILE	C-N-CA	8.62	158.20	122.00
2	D	180	VAL	CG1-CB-CG2	-8.53	97.25	110.90
2	D	122	GLY	N-CA-C	-8.50	91.85	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	179	PRO	C-N-CA	8.49	142.93	121.70
2	F	173	GLN	CA-C-N	-8.24	99.07	117.20
2	D	112	GLY	N-CA-C	-7.66	93.96	113.10
2	F	90	ALA	C-N-CD	-7.54	104.02	120.60
2	D	180	VAL	N-CA-CB	7.35	127.67	111.50
2	H	110	LEU	N-CA-C	7.16	130.33	111.00
2	F	175	LEU	CA-C-O	7.11	135.02	120.10
2	D	170	ILE	CA-C-N	7.00	136.70	117.10
2	F	161	ASP	N-CA-C	6.90	129.62	111.00
2	D	170	ILE	CA-CB-CG2	6.76	124.42	110.90
2	D	180	VAL	O-C-N	-6.36	112.53	122.70
1	G	15	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	96	ARG	NE-CZ-NH1	-5.97	117.31	120.30
2	D	169	GLU	O-C-N	5.97	132.25	122.70
2	B	91	PRO	N-CA-C	5.89	127.43	112.10
2	D	170	ILE	CB-CG1-CD1	5.89	130.40	113.90
1	E	95	ASP	CB-CG-OD1	-5.86	113.03	118.30
2	D	180	VAL	CA-CB-CG2	5.72	119.48	110.90
1	E	105	TRP	CA-C-N	5.64	127.47	116.20
2	F	172	ASP	CA-C-O	5.54	131.74	120.10
2	B	175	LEU	N-CA-C	5.49	125.83	111.00
2	F	179	PRO	O-C-N	5.46	131.44	122.70
2	D	170	ILE	CA-CB-CG1	5.37	121.20	111.00
2	F	179	PRO	N-CA-C	5.36	126.03	112.10
2	B	179	PRO	N-CA-C	5.36	126.02	112.10
2	F	180	VAL	CB-CA-C	-5.25	101.42	111.40
2	D	194	ASP	N-CA-C	5.25	125.16	111.00
2	D	169	GLU	CB-CA-C	-5.20	100.00	110.40
2	F	179	PRO	CA-C-N	-5.13	105.91	117.20
2	D	110	LEU	CA-CB-CG	5.12	127.07	115.30
2	B	138	VAL	CB-CA-C	-5.10	101.71	111.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	105	TRP	Mainchain
1	E	109	SER	Mainchain
2	F	90	ALA	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1317	0	1275	89	0
1	C	1333	0	1279	118	0
1	E	1238	0	1194	131	0
1	G	1269	0	1225	119	0
2	B	1258	0	1189	130	0
2	D	1186	0	1156	180	0
2	F	1161	0	1102	116	0
2	H	1222	0	1167	107	0
3	B	1	0	0	0	0
3	D	1	0	0	2	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
4	E	5	0	0	1	0
4	G	5	0	0	1	0
5	A	52	0	0	19	0
5	B	47	0	0	33	0
5	C	59	0	0	32	0
5	D	38	0	0	16	0
5	E	56	0	0	26	0
5	F	39	0	0	22	0
5	G	56	0	0	32	0
5	H	34	0	0	18	0
All	All	10379	0	9587	899	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 46.

All (899) 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)
2:D:179:PRO:CD	2:D:179:PRO:CG	1.79	1.54
2:D:180:VAL:C	2:D:180:VAL:CA	1.79	1.50
2:D:180:VAL:CA	2:D:180:VAL:CB	1.90	1.48
2:D:156:PHE:HE2	2:D:179:PRO:CB	1.28	1.45
2:D:179:PRO:CA	2:D:179:PRO:N	1.80	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:156:PHE:CE2	2:D:179:PRO:CB	2.06	1.39
2:D:180:VAL:CA	2:D:180:VAL:N	1.87	1.37
2:D:170:ILE:CD1	2:D:170:ILE:CG1	2.08	1.31
2:F:172:ASP:O	5:F:237:HOH:O	1.53	1.26
2:D:169:GLU:O	2:D:170:ILE:CG1	1.86	1.21
2:D:169:GLU:CG	2:D:170:ILE:H	1.40	1.19
2:D:179:PRO:CG	2:D:179:PRO:CA	2.24	1.16
2:D:169:GLU:C	2:D:170:ILE:CG1	2.15	1.16
1:A:18:ARG:HG3	1:A:18:ARG:HH11	1.06	1.14
2:D:169:GLU:O	2:D:170:ILE:HG12	0.97	1.13
2:F:175:LEU:N	5:F:237:HOH:O	1.78	1.13
2:D:2:THR:HG23	2:D:4:ARG:HH12	0.98	1.12
2:D:169:GLU:CG	2:D:170:ILE:N	2.00	1.12
2:D:179:PRO:CA	2:D:179:PRO:C	2.18	1.12
1:G:119:MSE:HE1	1:G:165:ILE:HD11	1.24	1.11
2:D:169:GLU:HG2	2:D:170:ILE:N	1.62	1.11
1:E:94:LYS:O	2:F:122:GLY:HA3	1.51	1.10
2:D:156:PHE:HE2	2:D:179:PRO:HB3	0.94	1.10
2:D:92:ALA:HB1	2:D:93:PRO:HD3	1.29	1.09
2:F:137:ALA:HB2	2:F:180:VAL:HG22	1.18	1.09
1:G:18:ARG:HG3	1:G:18:ARG:HH11	1.13	1.08
2:D:133:PRO:HA	2:D:186:ASP:OD2	1.52	1.07
1:E:170:ARG:NH1	2:F:37:GLU:HA	1.69	1.07
2:D:169:GLU:C	2:D:170:ILE:HG12	1.73	1.06
2:H:131:TRP:HA	5:H:222:HOH:O	1.52	1.06
2:B:92:ALA:CB	2:B:93:PRO:HD3	1.84	1.06
2:D:170:ILE:C	2:D:170:ILE:CA	2.23	1.06
1:G:15:ARG:HH22	1:G:110:GLU:CD	1.57	1.05
2:D:2:THR:CG2	2:D:4:ARG:HH12	1.69	1.05
2:D:113:GLY:O	2:D:133:PRO:HD3	1.55	1.05
2:H:37:GLU:HG3	5:H:207:HOH:O	1.56	1.04
2:F:172:ASP:OD2	2:F:173:GLN:N	1.91	1.03
2:H:98:VAL:HG12	5:H:210:HOH:O	1.59	1.02
2:B:33:SER:OG	2:B:92:ALA:HB2	1.60	1.01
2:F:91:PRO:HD2	2:F:94:LEU:HB3	1.39	1.01
2:D:179:PRO:CG	2:D:179:PRO:CB	2.37	1.01
2:B:92:ALA:HB3	2:B:93:PRO:HD3	1.40	1.00
2:D:2:THR:HG23	2:D:4:ARG:NH1	1.76	1.00
1:C:87:ARG:HG2	1:C:87:ARG:HH11	1.24	1.00
2:B:132:ILE:HD11	2:B:138:VAL:HG22	1.42	0.99
2:D:156:PHE:CE2	2:D:179:PRO:HB3	1.86	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:161:PRO:O	1:G:162:LEU:HD23	1.65	0.96
2:D:170:ILE:CA	2:D:170:ILE:CB	2.43	0.95
2:F:175:LEU:HB2	5:F:237:HOH:O	1.65	0.95
2:D:98:VAL:HG12	2:D:99:GLY:N	1.81	0.95
2:D:106:ARG:HG2	2:D:106:ARG:HH11	1.32	0.95
1:G:94:LYS:CB	2:H:122:GLY:HA3	1.96	0.94
2:H:14:ALA:HB1	5:H:237:HOH:O	1.64	0.94
2:F:70:MSE:HE1	2:H:66:LEU:HD23	1.50	0.93
2:D:92:ALA:CB	2:D:93:PRO:HD3	1.99	0.93
1:C:4:LYS:HA	5:C:220:HOH:O	1.67	0.92
2:B:2:THR:HG23	2:B:4:ARG:NH1	1.84	0.92
1:E:128:ARG:HG2	1:E:128:ARG:HH11	1.35	0.92
2:B:89:ARG:HG2	2:B:89:ARG:HH11	1.35	0.92
2:H:30:THR:HB	5:H:214:HOH:O	1.69	0.92
2:H:92:ALA:HB1	2:H:93:PRO:CD	1.99	0.92
2:B:132:ILE:CD1	2:B:138:VAL:CG2	2.47	0.91
1:E:170:ARG:NH1	2:F:37:GLU:CA	2.32	0.91
2:D:20:LEU:HD23	2:D:24:PHE:CB	1.99	0.91
2:F:165:ALA:HA	5:F:241:HOH:O	1.69	0.91
2:D:180:VAL:C	2:D:180:VAL:CB	2.40	0.90
2:D:98:VAL:HG12	2:D:99:GLY:H	1.36	0.90
1:G:15:ARG:NH2	1:G:110:GLU:CD	2.23	0.90
1:A:18:ARG:HG3	1:A:18:ARG:NH1	1.85	0.89
2:D:165:ALA:HA	5:D:235:HOH:O	1.70	0.89
1:E:101:GLU:OE1	1:E:102:ASP:N	2.05	0.89
2:H:92:ALA:CB	2:H:93:PRO:CD	2.50	0.89
1:E:87:ARG:HB2	5:E:222:HOH:O	1.72	0.89
2:B:132:ILE:HD11	2:B:138:VAL:CG2	2.02	0.89
2:B:92:ALA:HB3	2:B:93:PRO:CD	2.04	0.88
2:D:116:GLN:HB2	2:D:130:LEU:CD2	2.03	0.88
2:F:90:ALA:HB2	2:F:102:LEU:HD21	1.55	0.88
1:G:88:ARG:HD3	5:G:205:HOH:O	1.75	0.87
2:F:172:ASP:O	2:F:175:LEU:N	2.07	0.87
2:D:169:GLU:HG3	2:D:170:ILE:H	1.39	0.87
2:B:89:ARG:HH11	2:B:89:ARG:CG	1.88	0.87
1:C:132:ARG:HH12	2:F:72:GLN:CD	1.78	0.87
2:H:90:ALA:HB2	2:H:102:LEU:HD13	1.57	0.87
2:D:20:LEU:CD2	2:D:24:PHE:HB3	2.05	0.87
1:G:94:LYS:CB	2:H:123:GLY:H	1.87	0.86
1:E:44:SER:HB2	5:E:193:HOH:O	1.75	0.86
1:G:119:MSE:CE	1:G:165:ILE:HD11	2.03	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:LEU:HD23	1:G:160:LEU:N	1.90	0.86
1:E:44:SER:CB	1:E:88:ARG:HH22	1.89	0.85
2:F:6:HIS:HB3	2:F:38:CYS:SG	2.16	0.85
2:D:179:PRO:CD	2:D:179:PRO:CA	2.54	0.85
1:G:80:ILE:HG22	2:H:53:MSE:CE	2.05	0.85
2:D:113:GLY:O	2:D:133:PRO:CD	2.23	0.85
1:E:170:ARG:HH12	2:F:37:GLU:CA	1.90	0.85
2:F:137:ALA:CB	2:F:180:VAL:HG22	2.06	0.85
1:A:89:ILE:HD12	1:A:93:ARG:NH2	1.91	0.85
2:D:92:ALA:HB1	2:D:93:PRO:CD	2.07	0.85
1:E:166:LYS:HD2	2:F:41:ARG:HG3	1.59	0.84
2:D:179:PRO:CB	2:D:179:PRO:N	2.40	0.84
2:B:157:ARG:HA	5:B:229:HOH:O	1.77	0.83
1:C:114:ALA:HB3	5:C:237:HOH:O	1.78	0.83
1:A:18:ARG:HH11	1:A:18:ARG:CG	1.90	0.83
1:G:18:ARG:HG3	1:G:18:ARG:NH1	1.87	0.83
2:D:38:CYS:HG	3:D:204:ZN:ZN	0.90	0.82
1:G:173:LEU:HD23	5:G:212:HOH:O	1.79	0.82
2:D:179:PRO:CB	2:D:179:PRO:C	2.47	0.82
1:E:128:ARG:NH1	4:E:182:SO4:O2	2.11	0.82
2:B:132:ILE:CD1	2:B:138:VAL:HG22	2.05	0.82
2:D:106:ARG:HG2	2:D:106:ARG:NH1	1.93	0.82
1:C:125:ARG:HG3	1:C:125:ARG:HH11	1.45	0.81
2:B:51:SER:O	2:B:55:GLU:HG2	1.80	0.81
2:B:162:ARG:HA	5:B:229:HOH:O	1.80	0.81
2:D:116:GLN:HB2	2:D:130:LEU:HD22	1.61	0.81
1:C:112:ASP:HB3	5:C:237:HOH:O	1.80	0.81
2:D:165:ALA:HB2	5:D:226:HOH:O	1.79	0.81
2:F:175:LEU:CB	5:F:237:HOH:O	2.24	0.81
2:D:169:GLU:C	2:D:170:ILE:HG13	2.00	0.81
2:H:30:THR:HG23	2:H:150:LEU:CD2	2.11	0.80
2:D:180:VAL:C	2:D:180:VAL:CG1	2.50	0.80
1:A:178:GLN:HE21	2:H:105:VAL:HA	1.44	0.80
2:B:132:ILE:HD13	2:B:138:VAL:HG23	1.62	0.80
2:D:20:LEU:HD23	2:D:24:PHE:HB3	1.61	0.80
1:E:134:PRO:HG2	1:E:137:GLN:OE1	1.82	0.80
1:A:6:ASP:HB2	5:A:206:HOH:O	1.82	0.79
1:G:132:ARG:O	1:G:132:ARG:HG2	1.83	0.79
1:E:143:ARG:HA	1:E:143:ARG:HH11	1.46	0.79
2:H:30:THR:HG23	2:H:150:LEU:HD22	1.64	0.79
1:E:119:MSE:HB2	5:E:205:HOH:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:92:ALA:HB1	2:H:93:PRO:HD3	1.65	0.78
2:B:92:ALA:CB	2:B:93:PRO:CD	2.58	0.78
1:E:170:ARG:HH11	2:F:37:GLU:HA	1.47	0.78
2:B:132:ILE:HD13	2:B:138:VAL:CG2	2.13	0.78
2:D:126:ILE:HA	5:D:237:HOH:O	1.82	0.78
2:D:20:LEU:HD23	2:D:24:PHE:HB2	1.62	0.78
2:D:106:ARG:HH11	2:D:106:ARG:CG	1.96	0.78
1:G:79:TRP:O	1:G:82:THR:HB	1.83	0.78
1:E:170:ARG:HH12	2:F:37:GLU:N	1.81	0.78
2:B:6:HIS:HB3	2:B:38:CYS:SG	2.24	0.77
1:E:54:CYS:SG	5:E:222:HOH:O	2.42	0.77
1:C:31:GLN:HB2	5:C:226:HOH:O	1.84	0.77
2:H:92:ALA:CB	2:H:93:PRO:HD2	2.14	0.77
2:D:179:PRO:O	2:D:179:PRO:HG2	1.85	0.77
2:D:92:ALA:CB	2:D:93:PRO:CD	2.59	0.77
2:D:114:VAL:HG12	2:D:114:VAL:O	1.84	0.77
1:G:143:ARG:HA	1:G:143:ARG:HH11	1.49	0.77
1:G:174:ASP:O	1:G:177:ARG:HB2	1.83	0.77
2:H:92:ALA:HB3	2:H:93:PRO:HD2	1.67	0.77
2:H:188:ILE:HA	5:H:222:HOH:O	1.85	0.77
1:E:41:LEU:HD23	1:E:88:ARG:HH21	1.50	0.77
1:E:33:PHE:HB3	5:E:235:HOH:O	1.85	0.77
1:C:138:ARG:HH21	2:D:55:GLU:CD	1.88	0.76
1:G:138:ARG:HH22	2:H:55:GLU:CD	1.87	0.76
2:D:180:VAL:N	2:D:180:VAL:HA	1.96	0.76
1:A:103:LEU:HA	5:A:199:HOH:O	1.84	0.76
1:C:34:ALA:HB3	1:C:35:PRO:HD3	1.68	0.76
1:C:166:LYS:HD2	1:E:94:LYS:CB	2.16	0.76
2:B:128:ARG:NH1	2:B:191:ALA:HB3	2.01	0.76
2:B:33:SER:CB	2:B:92:ALA:HB2	2.15	0.76
2:D:163:PHE:CE2	2:D:169:GLU:HB3	2.20	0.76
2:B:37:GLU:HG3	5:B:231:HOH:O	1.85	0.76
2:D:153:GLN:HA	5:D:226:HOH:O	1.86	0.76
1:A:128:ARG:HG2	1:A:128:ARG:HH11	1.51	0.75
1:C:71:PRO:HD2	5:C:190:HOH:O	1.86	0.75
1:E:134:PRO:CG	1:E:137:GLN:OE1	2.34	0.75
2:D:156:PHE:CE2	2:D:179:PRO:HB2	2.17	0.75
2:B:2:THR:HG23	2:B:4:ARG:HH11	1.51	0.75
2:B:93:PRO:HD2	2:B:94:LEU:H	1.50	0.75
1:E:59:MSE:HE3	5:E:235:HOH:O	1.87	0.75
2:D:34:LEU:HA	5:D:214:HOH:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:128:ARG:NH1	4:G:182:SO4:O2	2.19	0.75
1:C:154:LEU:CB	2:D:45:LEU:HD11	2.16	0.74
1:E:44:SER:HB2	1:E:88:ARG:HH22	1.51	0.74
2:B:116:GLN:HB3	5:B:208:HOH:O	1.88	0.74
1:E:47:VAL:HB	5:E:215:HOH:O	1.87	0.74
2:B:93:PRO:HB2	5:B:211:HOH:O	1.86	0.74
2:D:169:GLU:C	2:D:170:ILE:CB	2.55	0.74
2:F:14:ALA:HB1	5:F:236:HOH:O	1.86	0.74
2:D:179:PRO:CG	2:D:179:PRO:C	2.56	0.74
2:F:66:LEU:HD23	2:H:70:MSE:HE1	1.68	0.74
2:D:156:PHE:CD2	2:D:179:PRO:CB	2.69	0.74
2:F:105:VAL:HA	5:F:230:HOH:O	1.88	0.73
2:H:89:ARG:O	2:H:91:PRO:HD3	1.88	0.73
2:H:6:HIS:HB3	2:H:38:CYS:SG	2.29	0.73
1:C:99:GLU:HB3	5:D:216:HOH:O	1.89	0.73
2:D:169:GLU:HA	2:D:170:ILE:HG13	1.70	0.73
2:B:170:ILE:HG13	5:B:248:HOH:O	1.89	0.73
1:A:43:LYS:HD2	5:B:235:HOH:O	1.88	0.72
1:G:135:GLU:HA	1:G:135:GLU:OE1	1.88	0.72
1:C:101:GLU:HB2	2:D:33:SER:HB2	1.71	0.72
2:F:68:SER:O	2:F:72:GLN:NE2	2.22	0.72
1:A:103:LEU:HD11	1:A:177:ARG:NH2	2.05	0.72
1:C:50:GLN:OE1	1:C:50:GLN:HA	1.88	0.72
1:G:88:ARG:HD2	5:G:221:HOH:O	1.90	0.72
1:A:134:PRO:HD2	5:A:200:HOH:O	1.87	0.72
2:B:14:ALA:HB1	2:B:20:LEU:HD13	1.72	0.72
2:H:27:VAL:O	2:H:30:THR:HG22	1.90	0.72
2:B:53:MSE:HA	5:B:247:HOH:O	1.87	0.72
2:D:134:GLY:O	2:D:183:ARG:HA	1.90	0.72
1:G:177:ARG:NH2	2:H:36:ASP:OD2	2.23	0.72
1:G:176:LEU:HB3	5:G:212:HOH:O	1.88	0.71
1:G:160:LEU:N	1:G:160:LEU:CD2	2.53	0.71
1:E:174:ASP:O	1:E:177:ARG:HB2	1.90	0.71
2:B:93:PRO:CD	2:B:94:LEU:H	2.04	0.71
2:D:169:GLU:CA	2:D:170:ILE:HG13	2.21	0.71
1:E:41:LEU:CD2	1:E:88:ARG:HE	2.03	0.71
1:C:160:LEU:HG	5:C:197:HOH:O	1.90	0.71
1:C:125:ARG:HD2	5:E:236:HOH:O	1.90	0.71
1:C:110:GLU:CG	1:C:111:PRO:HD2	2.22	0.70
1:C:128:ARG:HG2	1:C:128:ARG:HH11	1.57	0.70
1:E:128:ARG:HH11	1:E:128:ARG:CG	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:89:ARG:HH11	2:F:89:ARG:HG2	1.56	0.70
1:E:125:ARG:HD3	5:E:217:HOH:O	1.91	0.70
1:E:166:LYS:HD2	2:F:41:ARG:CG	2.20	0.70
1:G:94:LYS:CB	2:H:122:GLY:CA	2.68	0.70
2:D:180:VAL:HG12	2:D:180:VAL:O	1.92	0.70
1:C:101:GLU:HG3	2:D:92:ALA:HA	1.74	0.69
1:C:117:TYR:O	1:C:121:GLN:HG2	1.91	0.69
2:D:180:VAL:C	2:D:180:VAL:HG12	2.12	0.69
1:G:83:ILE:HG13	5:G:209:HOH:O	1.90	0.69
1:C:99:GLU:O	2:D:93:PRO:HG3	1.92	0.69
2:B:162:ARG:HG3	5:B:229:HOH:O	1.90	0.69
1:G:18:ARG:HG2	1:G:19:ASP:OD1	1.91	0.69
1:G:85:ARG:HA	5:G:205:HOH:O	1.92	0.69
2:D:113:GLY:O	2:D:133:PRO:CG	2.41	0.69
2:D:156:PHE:CD2	2:D:179:PRO:HB2	2.26	0.69
2:F:90:ALA:HB2	2:F:102:LEU:CD2	2.22	0.69
2:F:157:ARG:O	2:F:179:PRO:HA	1.91	0.69
1:C:138:ARG:NH2	2:D:55:GLU:CD	2.45	0.68
1:E:164:THR:HG23	5:E:208:HOH:O	1.93	0.68
2:F:172:ASP:CG	2:F:173:GLN:N	2.45	0.68
2:H:89:ARG:C	2:H:91:PRO:HD3	2.12	0.68
1:E:19:ASP:HB2	1:E:20:HIS:HD2	1.58	0.68
2:F:151:VAL:HG12	5:F:241:HOH:O	1.93	0.68
2:B:41:ARG:HD2	5:B:221:HOH:O	1.93	0.68
2:F:115:ARG:NH2	2:F:131:TRP:CD2	2.62	0.68
1:C:89:ILE:HD12	1:C:93:ARG:NH2	2.08	0.68
5:C:203:HOH:O	2:D:53:MSE:HE3	1.92	0.68
2:D:116:GLN:HB2	2:D:130:LEU:HD21	1.76	0.68
2:D:179:PRO:CG	2:D:179:PRO:N	2.57	0.68
2:D:137:ALA:HB1	2:D:180:VAL:HG22	1.75	0.68
1:C:79:TRP:O	1:C:82:THR:HB	1.94	0.68
2:D:53:MSE:HA	5:D:242:HOH:O	1.92	0.68
1:C:87:ARG:HG2	1:C:87:ARG:NH1	2.01	0.67
1:E:58:VAL:HG12	1:E:59:MSE:HE2	1.76	0.67
2:D:179:PRO:C	2:D:179:PRO:HG2	2.15	0.67
2:D:20:LEU:CD2	2:D:24:PHE:CB	2.68	0.67
2:D:155:ALA:HB2	2:D:164:GLY:HA2	1.75	0.67
1:E:41:LEU:HD22	1:E:88:ARG:HE	1.59	0.67
2:F:89:ARG:HG3	5:F:213:HOH:O	1.94	0.67
5:E:238:HOH:O	2:F:55:GLU:HB2	1.95	0.67
2:H:121:THR:HA	5:H:236:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:ARG:C	1:E:98:PRO:HD3	2.14	0.67
2:H:5:HIS:HB2	2:H:167:ASP:OD1	1.94	0.67
2:B:176:GLU:HA	5:B:219:HOH:O	1.94	0.66
2:D:14:ALA:HA	5:D:221:HOH:O	1.94	0.66
2:D:179:PRO:N	2:D:179:PRO:HA	2.03	0.66
2:F:30:THR:HG23	2:F:91:PRO:HG2	1.77	0.66
1:E:101:GLU:OE2	1:E:103:LEU:HD23	1.96	0.66
1:G:128:ARG:HH11	1:G:128:ARG:HG2	1.59	0.66
1:C:43:LYS:HB3	1:C:146:PHE:CE2	2.31	0.66
1:G:170:ARG:HG3	1:G:170:ARG:HH11	1.60	0.66
1:G:132:ARG:O	1:G:132:ARG:CG	2.44	0.66
2:B:14:ALA:CB	2:B:20:LEU:HD13	2.26	0.65
1:C:142:GLU:O	1:C:146:PHE:HD1	1.77	0.65
1:C:83:ILE:O	5:C:215:HOH:O	2.14	0.65
2:D:98:VAL:CG1	2:D:99:GLY:H	2.00	0.65
1:C:132:ARG:NE	1:E:56:GLN:HE22	1.94	0.65
2:D:170:ILE:N	2:D:170:ILE:CB	2.60	0.65
2:F:119:LEU:HD21	2:F:129:LEU:CD1	2.25	0.65
1:C:103:LEU:HD22	1:C:180:MSE:SE	2.46	0.65
1:C:168:ARG:NH2	1:C:171:LEU:HD12	2.11	0.65
1:G:37:VAL:HG22	2:H:53:MSE:HE1	1.79	0.65
1:G:94:LYS:CB	2:H:123:GLY:N	2.60	0.65
2:B:92:ALA:HB1	2:B:93:PRO:HD3	1.73	0.65
1:C:118:GLU:HG2	5:C:214:HOH:O	1.94	0.65
2:D:89:ARG:C	2:D:91:PRO:HD3	2.16	0.65
2:H:94:LEU:O	2:H:94:LEU:HD22	1.97	0.65
1:A:79:TRP:NE1	5:A:201:HOH:O	2.29	0.65
2:B:91:PRO:HG2	5:B:209:HOH:O	1.97	0.64
2:B:178:THR:N	2:B:179:PRO:CD	2.61	0.64
1:E:44:SER:CB	1:E:88:ARG:NH2	2.59	0.64
1:E:101:GLU:HA	2:F:92:ALA:CB	2.27	0.64
2:D:110:LEU:O	2:D:114:VAL:HB	1.96	0.64
1:A:170:ARG:HH12	1:G:94:LYS:HA	1.63	0.64
1:A:60:ALA:HB1	5:A:210:HOH:O	1.97	0.64
2:D:128:ARG:HD3	2:D:130:LEU:CD2	2.28	0.64
2:F:69:VAL:HA	2:F:72:GLN:NE2	2.13	0.64
1:G:41:LEU:HB3	5:G:224:HOH:O	1.98	0.64
2:D:34:LEU:HD21	2:D:91:PRO:HG3	1.80	0.64
1:E:15:ARG:HH21	1:E:110:GLU:CB	2.11	0.64
1:E:57:ASP:OD1	1:E:87:ARG:HD3	1.97	0.64
1:E:85:ARG:NH1	2:F:16:ALA:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:CYS:SG	3:D:204:ZN:ZN	1.86	0.63
2:F:178:THR:N	2:F:179:PRO:CD	2.61	0.63
1:A:117:TYR:O	1:A:121:GLN:HG2	1.97	0.63
5:C:200:HOH:O	2:D:120:PRO:HG2	1.99	0.63
2:B:157:ARG:HG2	5:B:229:HOH:O	1.98	0.63
2:F:87:ASP:HB2	2:F:100:ARG:O	1.99	0.63
1:G:95:ASP:O	1:G:96:ARG:HB2	1.97	0.63
2:H:5:HIS:N	2:H:167:ASP:OD1	2.32	0.63
1:G:173:LEU:O	1:G:177:ARG:HG2	1.98	0.63
2:H:110:LEU:HG	2:H:110:LEU:O	1.98	0.63
2:B:112:GLY:HA3	2:B:136:GLN:HE22	1.64	0.63
1:G:101:GLU:HA	5:G:210:HOH:O	1.99	0.63
1:A:89:ILE:CD1	1:A:93:ARG:NH2	2.62	0.63
2:B:98:VAL:HG12	2:B:99:GLY:N	2.14	0.63
2:F:172:ASP:CG	2:F:174:GLU:H	2.03	0.62
1:C:87:ARG:HH11	1:C:87:ARG:CG	2.04	0.62
1:C:96:ARG:NH1	5:C:215:HOH:O	2.20	0.62
5:C:199:HOH:O	2:D:19:THR:HG21	1.98	0.62
2:B:103:GLU:HB2	5:B:236:HOH:O	1.99	0.62
2:F:153:GLN:N	5:F:241:HOH:O	2.33	0.62
1:A:40:PHE:HB2	5:B:247:HOH:O	2.00	0.62
1:C:40:PHE:HB2	5:D:242:HOH:O	1.99	0.62
1:E:164:THR:HB	5:E:199:HOH:O	1.99	0.62
1:C:73:ARG:HD3	1:C:173:LEU:HG	1.82	0.62
2:D:6:HIS:HB3	2:D:38:CYS:SG	2.39	0.62
1:E:170:ARG:NH1	2:F:37:GLU:N	2.45	0.62
1:C:67:HIS:O	5:C:221:HOH:O	2.16	0.62
1:A:125:ARG:HD2	5:G:185:HOH:O	1.99	0.61
1:G:80:ILE:HG22	2:H:53:MSE:HE3	1.81	0.61
1:A:79:TRP:O	1:A:82:THR:HB	2.01	0.61
2:H:133:PRO:HA	2:H:186:ASP:OD2	2.00	0.61
1:A:125:ARG:HG3	1:A:125:ARG:HH11	1.64	0.61
2:B:137:ALA:HB1	2:B:179:PRO:O	2.00	0.61
1:C:80:ILE:HG22	5:C:203:HOH:O	2.01	0.61
1:C:132:ARG:NE	1:E:56:GLN:NE2	2.48	0.61
1:C:176:LEU:HD23	1:C:176:LEU:O	2.01	0.61
1:E:117:TYR:O	1:E:121:GLN:HG2	2.00	0.61
1:E:132:ARG:HD2	5:E:237:HOH:O	2.00	0.61
2:F:14:ALA:HB1	2:F:20:LEU:HD13	1.83	0.61
2:B:29:ALA:HB3	5:B:226:HOH:O	2.00	0.60
1:E:87:ARG:NH2	5:E:236:HOH:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:24:PHE:CE1	2:H:148:LEU:HG	2.36	0.60
2:D:33:SER:CB	2:D:92:ALA:HB2	2.31	0.60
1:G:44:SER:HB3	5:G:221:HOH:O	2.01	0.60
1:G:117:TYR:O	1:G:121:GLN:HG2	2.01	0.60
2:D:107:TRP:HZ3	2:D:129:LEU:O	1.84	0.60
1:E:97:GLN:O	1:E:97:GLN:HG3	2.01	0.60
1:A:68:LEU:CB	5:A:201:HOH:O	2.48	0.60
1:G:170:ARG:HG3	1:G:170:ARG:NH1	2.14	0.60
1:A:88:ARG:HD2	5:A:209:HOH:O	2.00	0.60
1:G:105:TRP:HA	5:G:232:HOH:O	2.00	0.60
1:A:176:LEU:HD23	1:A:176:LEU:O	2.02	0.60
1:C:84:ALA:O	1:C:87:ARG:HG2	2.01	0.60
1:C:110:GLU:HG3	1:C:111:PRO:HD2	1.84	0.60
1:C:167:SER:HB2	5:E:201:HOH:O	2.01	0.60
1:E:101:GLU:CA	2:F:92:ALA:CB	2.80	0.60
2:F:133:PRO:HB3	5:F:239:HOH:O	2.02	0.59
2:H:3:ILE:HD13	2:H:35:CYS:HB2	1.85	0.59
1:E:134:PRO:HB2	1:E:137:GLN:OE1	2.02	0.59
1:C:170:ARG:NH2	2:D:37:GLU:OE2	2.35	0.59
1:G:44:SER:HB3	5:G:228:HOH:O	2.00	0.59
1:E:23:GLU:HB3	2:F:70:MSE:HE3	1.83	0.59
1:E:41:LEU:HD22	1:E:88:ARG:NE	2.18	0.59
2:H:33:SER:CB	2:H:92:ALA:HB2	2.33	0.59
1:C:110:GLU:HG2	1:C:111:PRO:HD2	1.85	0.59
1:C:138:ARG:NH2	2:D:55:GLU:OE1	2.35	0.59
1:E:15:ARG:NH2	1:E:110:GLU:CB	2.65	0.59
2:F:3:ILE:HD13	2:F:35:CYS:HB2	1.84	0.59
1:G:101:GLU:HB3	5:G:222:HOH:O	2.02	0.59
1:A:58:VAL:HG12	1:A:59:MSE:HE2	1.85	0.58
1:E:101:GLU:OE2	1:E:103:LEU:CD2	2.51	0.58
1:E:161:PRO:O	1:E:163:GLY:N	2.36	0.58
1:G:122:GLU:HG2	5:G:183:HOH:O	2.03	0.58
2:H:30:THR:CG2	2:H:150:LEU:CD2	2.81	0.58
1:A:34:ALA:HB3	1:A:35:PRO:HD3	1.84	0.58
2:H:11:LEU:HD11	2:H:148:LEU:HD21	1.84	0.58
1:A:166:LYS:HE2	5:A:205:HOH:O	2.02	0.58
2:H:159:GLU:HA	5:H:238:HOH:O	2.03	0.58
1:G:109:SER:C	1:G:110:GLU:HG3	2.22	0.58
2:D:92:ALA:HA	5:D:233:HOH:O	2.03	0.58
2:D:101:ARG:O	2:D:103:GLU:N	2.35	0.58
1:E:79:TRP:O	1:E:82:THR:HB	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:14:ALA:CB	2:F:20:LEU:HD13	2.33	0.58
2:F:28:VAL:O	2:F:32:LEU:HD23	2.03	0.57
1:A:81:PHE:HA	2:B:53:MSE:HE3	1.86	0.57
2:B:11:LEU:HD11	2:B:148:LEU:HD21	1.86	0.57
1:C:81:PHE:HA	2:D:53:MSE:CE	2.34	0.57
2:D:3:ILE:HD13	2:D:35:CYS:HB2	1.87	0.57
2:D:170:ILE:CD1	2:D:170:ILE:HG21	2.34	0.57
1:E:134:PRO:CB	1:E:137:GLN:OE1	2.52	0.57
1:G:58:VAL:HG12	1:G:59:MSE:HE2	1.86	0.57
1:C:18:ARG:CZ	5:C:221:HOH:O	2.52	0.57
1:A:21:ARG:NE	2:B:75:ARG:O	2.37	0.57
1:A:94:LYS:HG3	1:A:95:ASP:N	2.19	0.57
1:G:138:ARG:NH2	2:H:55:GLU:OE2	2.35	0.57
1:E:19:ASP:HB2	1:E:20:HIS:CD2	2.39	0.57
1:G:34:ALA:HB3	1:G:35:PRO:HD3	1.85	0.57
1:C:132:ARG:NH1	2:F:72:GLN:NE2	2.53	0.56
2:D:114:VAL:O	2:D:114:VAL:CG1	2.53	0.56
2:F:70:MSE:HE1	2:H:66:LEU:CD2	2.30	0.56
2:F:128:ARG:HH21	2:F:130:LEU:HD11	1.67	0.56
2:H:137:ALA:HA	2:H:180:VAL:HA	1.86	0.56
1:C:88:ARG:HG2	5:C:196:HOH:O	2.05	0.56
2:D:90:ALA:HB2	2:D:102:LEU:HD13	1.88	0.56
2:B:177:HIS:CD2	2:B:179:PRO:CD	2.89	0.56
2:D:4:ARG:HH11	2:D:4:ARG:HG2	1.70	0.56
2:H:98:VAL:HG11	2:H:102:LEU:HD12	1.87	0.56
1:C:63:TRP:CG	2:D:73:LEU:HD22	2.40	0.56
2:B:126:ILE:HD12	2:B:126:ILE:N	2.20	0.56
1:E:133:LEU:CD1	1:E:141:ILE:HD11	2.36	0.56
1:E:166:LYS:CD	2:F:41:ARG:HG3	2.33	0.56
2:F:119:LEU:HD21	2:F:129:LEU:HD11	1.86	0.56
1:G:161:PRO:O	1:G:162:LEU:CD2	2.48	0.56
2:B:89:ARG:CG	2:B:89:ARG:NH1	2.58	0.56
2:D:149:THR:HB	2:D:169:GLU:OE2	2.06	0.56
2:H:188:ILE:HG12	5:H:222:HOH:O	2.05	0.56
2:B:7:VAL:CG1	2:B:12:LEU:HD13	2.36	0.56
2:D:128:ARG:HD3	2:D:130:LEU:HD23	1.87	0.56
2:D:132:ILE:O	2:D:133:PRO:O	2.24	0.56
2:F:113:GLY:N	5:F:207:HOH:O	2.37	0.56
1:G:65:LYS:HB3	1:G:68:LEU:HD12	1.87	0.56
1:A:81:PHE:HA	2:B:53:MSE:CE	2.36	0.55
2:B:110:LEU:HD12	5:B:208:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:THR:CG2	2:F:91:PRO:HG2	2.34	0.55
2:F:35:CYS:SG	2:F:35:CYS:O	2.63	0.55
2:D:126:ILE:N	2:D:126:ILE:HD12	2.20	0.55
1:G:11:VAL:HG21	5:G:231:HOH:O	2.06	0.55
2:D:63:GLU:HG2	5:D:218:HOH:O	2.06	0.55
2:D:163:PHE:CE2	2:D:169:GLU:CB	2.90	0.55
1:G:104:PHE:C	5:G:197:HOH:O	2.44	0.55
1:E:50:GLN:HB2	5:E:215:HOH:O	2.06	0.55
1:C:87:ARG:NH1	1:C:87:ARG:CG	2.64	0.55
1:C:125:ARG:HH11	1:C:125:ARG:CG	2.19	0.55
1:G:176:LEU:O	1:G:176:LEU:HD23	2.07	0.55
2:H:57:ALA:HB3	5:H:211:HOH:O	2.06	0.55
1:C:154:LEU:O	1:C:158:THR:O	2.24	0.55
1:E:101:GLU:OE1	1:E:102:ASP:C	2.45	0.55
1:G:119:MSE:HE1	1:G:165:ILE:CD1	2.17	0.55
1:C:132:ARG:HH12	2:F:72:GLN:NE2	2.04	0.55
2:F:9:ASP:HA	5:F:221:HOH:O	2.06	0.55
2:F:133:PRO:HA	2:F:186:ASP:OD2	2.07	0.55
2:F:178:THR:HA	5:F:210:HOH:O	2.05	0.55
1:G:8:THR:HG22	1:G:8:THR:O	2.07	0.55
2:D:94:LEU:O	2:D:94:LEU:HD22	2.07	0.55
2:D:180:VAL:CA	2:D:180:VAL:HB	2.21	0.54
1:G:143:ARG:HH11	1:G:143:ARG:CA	2.20	0.54
2:H:55:GLU:O	2:H:55:GLU:HG3	2.06	0.54
2:B:98:VAL:O	2:B:99:GLY:O	2.26	0.54
1:C:168:ARG:HE	1:C:168:ARG:HA	1.72	0.54
2:B:93:PRO:CD	2:B:94:LEU:N	2.70	0.54
2:D:97:TYR:HB3	2:D:119:LEU:HD22	1.90	0.54
2:F:119:LEU:HD21	2:F:129:LEU:HD12	1.88	0.54
2:F:115:ARG:NH2	2:F:131:TRP:CE3	2.75	0.54
1:A:18:ARG:HD3	5:A:203:HOH:O	2.06	0.54
1:A:68:LEU:HB2	5:A:201:HOH:O	2.08	0.54
1:C:119:MSE:HE3	1:C:119:MSE:O	2.07	0.54
2:D:89:ARG:HH11	2:D:89:ARG:HG2	1.72	0.54
1:G:85:ARG:NH1	2:H:16:ALA:O	2.41	0.54
1:A:125:ARG:HH11	1:A:125:ARG:CG	2.21	0.54
1:C:94:LYS:NZ	5:C:200:HOH:O	2.40	0.54
2:H:14:ALA:CB	2:H:20:LEU:HD13	2.37	0.54
1:A:73:ARG:HD3	1:A:173:LEU:HG	1.90	0.54
2:D:155:ALA:CB	2:D:162:ARG:NH2	2.71	0.54
1:E:119:MSE:HE3	1:E:119:MSE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:SER:OG	1:E:88:ARG:NH1	2.28	0.53
1:A:137:GLN:NE2	5:A:200:HOH:O	2.40	0.53
2:B:133:PRO:HA	2:B:186:ASP:OD2	2.08	0.53
1:G:106:GLY:C	1:G:108:ASP:OD1	2.47	0.53
2:B:105:VAL:CG1	2:B:107:TRP:CE2	2.92	0.53
2:D:155:ALA:HA	2:D:163:PHE:O	2.08	0.53
2:F:91:PRO:O	2:F:95:ALA:HB2	2.09	0.53
1:G:108:ASP:OD1	1:G:108:ASP:N	2.34	0.53
1:E:87:ARG:HH11	1:E:87:ARG:HB3	1.72	0.53
1:A:68:LEU:HB3	5:A:201:HOH:O	2.08	0.53
1:C:130:ILE:O	1:C:133:LEU:HD12	2.09	0.53
2:D:98:VAL:CG1	2:D:99:GLY:N	2.51	0.53
2:H:90:ALA:CB	2:H:102:LEU:HD13	2.35	0.53
2:B:24:PHE:CE2	2:B:194:ASP:HB3	2.44	0.52
2:B:179:PRO:HD2	5:B:215:HOH:O	2.09	0.52
1:E:65:LYS:HB3	1:E:68:LEU:HD12	1.91	0.52
1:G:15:ARG:NH2	1:G:110:GLU:OE2	2.42	0.52
2:H:7:VAL:CG1	2:H:12:LEU:HD13	2.40	0.52
2:D:128:ARG:HD3	2:D:130:LEU:HD21	1.92	0.52
1:E:118:GLU:HB3	1:E:168:ARG:CZ	2.39	0.52
1:A:168:ARG:HG2	1:A:168:ARG:HH11	1.74	0.52
2:D:126:ILE:O	2:D:192:ALA:HA	2.08	0.52
2:D:138:VAL:HG13	2:D:139:PRO:HD2	1.90	0.52
1:E:73:ARG:NH2	1:E:103:LEU:O	2.43	0.52
1:E:176:LEU:O	1:E:176:LEU:HD23	2.09	0.52
1:G:86:ASN:HD22	1:G:97:GLN:HB3	1.74	0.52
1:C:18:ARG:NE	5:C:221:HOH:O	2.42	0.52
1:C:81:PHE:HA	2:D:53:MSE:HE3	1.92	0.52
1:C:130:ILE:HA	1:C:133:LEU:HD12	1.91	0.52
2:D:163:PHE:CD2	2:D:169:GLU:HB3	2.44	0.52
1:A:141:ILE:HG22	2:B:52:LEU:HD11	1.92	0.52
1:G:49:SER:O	1:G:53:GLU:HB3	2.09	0.52
1:C:89:ILE:HD12	1:C:93:ARG:HH22	1.74	0.52
1:E:104:PHE:CD1	1:E:104:PHE:C	2.84	0.52
2:H:5:HIS:CB	2:H:167:ASP:OD1	2.58	0.52
1:A:23:GLU:HB3	2:B:70:MSE:HE3	1.91	0.52
2:D:5:HIS:N	2:D:167:ASP:OD1	2.36	0.52
1:E:87:ARG:HH11	1:E:87:ARG:CG	2.23	0.52
1:E:143:ARG:HH11	1:E:143:ARG:CA	2.18	0.51
1:C:110:GLU:HG2	1:C:111:PRO:CD	2.40	0.51
2:D:155:ALA:HB3	2:D:162:ARG:NH2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:GLN:O	1:E:98:PRO:C	2.47	0.51
1:G:118:GLU:OE1	1:G:118:GLU:HA	2.10	0.51
2:H:153:GLN:O	2:H:187:CYS:HA	2.10	0.51
2:B:89:ARG:HG2	2:B:89:ARG:NH1	2.16	0.51
1:E:133:LEU:HD23	1:E:134:PRO:HD3	1.91	0.51
1:A:168:ARG:HG2	1:A:168:ARG:NH1	2.25	0.51
2:H:20:LEU:N	5:H:237:HOH:O	2.42	0.51
1:A:41:LEU:O	1:A:44:SER:HB2	2.10	0.51
1:A:90:ASP:OD1	1:A:91:GLY:N	2.38	0.51
2:B:98:VAL:CG1	2:B:99:GLY:N	2.74	0.51
1:C:23:GLU:HB3	2:D:70:MSE:HE3	1.93	0.51
2:B:50:GLY:O	2:B:53:MSE:HB3	2.11	0.51
2:B:91:PRO:C	5:B:242:HOH:O	2.49	0.51
1:E:143:ARG:HA	1:E:143:ARG:NH1	2.23	0.51
2:F:178:THR:O	5:F:210:HOH:O	2.19	0.51
1:A:26:PHE:CE2	2:B:73:LEU:HD11	2.46	0.51
2:B:98:VAL:HG21	2:B:129:LEU:HD11	1.93	0.51
2:F:102:LEU:H	2:F:102:LEU:HD23	1.75	0.51
1:G:146:PHE:O	1:G:147:GLY:C	2.49	0.51
2:F:24:PHE:CE2	2:F:194:ASP:HB3	2.46	0.51
1:A:21:ARG:HB2	5:A:198:HOH:O	2.10	0.51
1:C:168:ARG:HH21	1:C:171:LEU:HD12	1.74	0.51
1:A:38:LYS:HE2	2:B:59:VAL:HG12	1.93	0.51
1:C:132:ARG:NH1	2:F:72:GLN:CD	2.57	0.51
2:B:93:PRO:CG	5:B:226:HOH:O	2.59	0.50
1:E:42:MSE:HG2	1:E:46:SER:O	2.11	0.50
2:F:162:ARG:HG3	2:F:163:PHE:N	2.26	0.50
2:H:89:ARG:HG2	2:H:89:ARG:HH11	1.76	0.50
2:B:181:ALA:O	5:B:217:HOH:O	2.19	0.50
2:D:33:SER:OG	2:D:92:ALA:HB2	2.10	0.50
1:A:90:ASP:CG	1:A:91:GLY:N	2.65	0.50
2:D:89:ARG:HD2	2:D:153:GLN:HB2	1.94	0.50
1:G:44:SER:CB	5:G:221:HOH:O	2.58	0.50
1:G:175:ARG:HH11	1:G:175:ARG:HG3	1.76	0.50
2:H:23:ALA:HB3	2:H:125:ALA:HB3	1.93	0.50
2:B:113:GLY:H	2:B:136:GLN:HE22	1.59	0.50
2:B:122:GLY:N	5:B:207:HOH:O	2.45	0.50
2:B:126:ILE:O	2:B:192:ALA:HA	2.11	0.50
1:G:8:THR:O	1:G:8:THR:CG2	2.59	0.50
1:A:177:ARG:HA	1:A:180:MSE:HE2	1.93	0.50
1:C:48:ALA:HB2	5:C:208:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:GLU:HG3	2:D:92:ALA:CA	2.42	0.50
2:D:180:VAL:CG1	2:D:180:VAL:O	2.59	0.50
1:G:138:ARG:HG2	1:G:138:ARG:HH11	1.76	0.50
1:E:122:GLU:HG2	5:E:231:HOH:O	2.12	0.50
2:H:14:ALA:HB1	2:H:20:LEU:HD13	1.94	0.50
1:A:177:ARG:HD3	1:A:180:MSE:CE	2.41	0.50
1:C:132:ARG:NH1	2:F:72:GLN:OE1	2.29	0.50
1:C:132:ARG:HE	1:E:56:GLN:NE2	2.10	0.50
1:G:126:LEU:O	1:G:130:ILE:HG13	2.12	0.50
1:E:44:SER:HB3	1:E:88:ARG:NH2	2.27	0.50
1:G:119:MSE:O	1:G:119:MSE:HE3	2.12	0.50
1:A:28:GLU:OE2	1:A:28:GLU:HA	2.12	0.49
2:B:128:ARG:NH1	2:B:191:ALA:CB	2.75	0.49
1:C:134:PRO:HG2	5:E:227:HOH:O	2.11	0.49
2:D:3:ILE:CD1	2:D:35:CYS:HB2	2.41	0.49
2:B:136:GLN:O	5:B:217:HOH:O	2.20	0.49
1:E:42:MSE:SE	1:E:48:ALA:HA	2.62	0.49
2:H:136:GLN:HG3	2:H:137:ALA:N	2.27	0.49
1:E:128:ARG:HG2	1:E:128:ARG:NH1	2.14	0.49
1:G:66:ALA:N	5:G:191:HOH:O	2.44	0.49
1:G:95:ASP:N	5:G:195:HOH:O	2.45	0.49
2:D:90:ALA:N	2:D:91:PRO:HD3	2.27	0.49
2:B:41:ARG:CZ	5:B:231:HOH:O	2.61	0.49
1:C:8:THR:HG22	1:C:8:THR:O	2.11	0.49
2:F:107:TRP:HZ3	2:F:129:LEU:O	1.95	0.49
2:D:193:THR:HG22	2:D:194:ASP:N	2.28	0.49
2:F:180:VAL:HG23	5:F:223:HOH:O	2.11	0.49
1:G:107:PRO:HG2	5:G:219:HOH:O	2.11	0.49
1:E:37:VAL:HG23	5:E:235:HOH:O	2.12	0.49
2:F:153:GLN:O	2:F:187:CYS:HA	2.12	0.49
2:B:24:PHE:CZ	2:B:194:ASP:HB3	2.48	0.49
2:B:105:VAL:HG22	2:B:106:ARG:N	2.28	0.49
1:C:65:LYS:HE2	5:C:201:HOH:O	2.13	0.49
2:F:68:SER:C	2:F:72:GLN:NE2	2.66	0.49
2:F:66:LEU:CD2	2:H:70:MSE:HE1	2.41	0.49
2:D:151:VAL:C	5:D:235:HOH:O	2.51	0.49
1:E:87:ARG:HH11	1:E:87:ARG:CB	2.25	0.49
1:E:101:GLU:CB	2:F:92:ALA:HB2	2.43	0.49
1:E:128:ARG:NH1	1:E:128:ARG:CG	2.67	0.49
1:A:21:ARG:CD	2:B:75:ARG:O	2.60	0.48
5:C:223:HOH:O	1:E:87:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:GLN:O	2:D:187:CYS:HA	2.12	0.48
2:B:177:HIS:CD2	2:B:179:PRO:HG3	2.48	0.48
1:E:36:LYS:NZ	2:F:56:THR:O	2.46	0.48
2:H:41:ARG:NH1	5:H:207:HOH:O	2.20	0.48
1:A:81:PHE:CE2	2:B:49:GLY:HA3	2.47	0.48
1:C:32:HIS:HB2	5:C:224:HOH:O	2.12	0.48
1:E:44:SER:CB	1:E:88:ARG:HH12	2.26	0.48
1:E:73:ARG:HD3	1:E:173:LEU:HG	1.95	0.48
1:C:132:ARG:HE	1:E:56:GLN:HE22	1.59	0.48
2:D:156:PHE:CE2	2:D:179:PRO:CG	2.96	0.48
1:G:58:VAL:O	1:G:62:VAL:HG23	2.12	0.48
1:C:89:ILE:CD1	1:C:93:ARG:NH2	2.74	0.48
1:A:52:GLU:O	1:A:56:GLN:HG3	2.13	0.48
1:C:138:ARG:HG2	1:C:138:ARG:HH11	1.78	0.48
2:D:11:LEU:HD11	2:D:148:LEU:HD21	1.94	0.48
1:C:65:LYS:HB3	1:C:68:LEU:HD12	1.96	0.48
2:B:135:GLY:N	5:B:217:HOH:O	2.47	0.48
2:B:178:THR:H	2:B:179:PRO:HD3	1.79	0.48
1:E:78:THR:OG1	2:F:47:ALA:HA	2.13	0.48
1:E:88:ARG:HD3	5:E:210:HOH:O	2.13	0.48
1:E:101:GLU:N	2:F:92:ALA:HB3	2.28	0.48
1:A:128:ARG:HH11	1:A:128:ARG:CG	2.21	0.47
2:B:137:ALA:CB	2:B:180:VAL:HA	2.44	0.47
1:G:162:LEU:CD1	2:H:45:LEU:HD13	2.44	0.47
2:B:33:SER:HB3	2:B:92:ALA:HB2	1.93	0.47
1:C:84:ALA:O	1:C:87:ARG:NH1	2.45	0.47
1:E:161:PRO:C	1:E:163:GLY:N	2.67	0.47
1:A:90:ASP:CG	1:A:91:GLY:H	2.17	0.47
1:A:138:ARG:O	1:A:142:GLU:HG3	2.14	0.47
1:A:142:GLU:HB3	1:A:146:PHE:CE2	2.50	0.47
1:C:36:LYS:HE2	5:C:230:HOH:O	2.15	0.47
1:E:15:ARG:HG3	5:E:194:HOH:O	2.15	0.47
2:B:178:THR:H	2:B:179:PRO:CD	2.28	0.47
2:D:23:ALA:HB3	2:D:125:ALA:HB3	1.96	0.47
2:D:179:PRO:C	2:D:179:PRO:HB2	2.32	0.47
1:E:134:PRO:HD2	1:E:137:GLN:HB2	1.96	0.47
2:B:30:THR:HA	2:B:92:ALA:HB3	1.96	0.47
2:B:173:GLN:CB	5:B:246:HOH:O	2.63	0.47
2:F:167:ASP:CB	5:F:234:HOH:O	2.63	0.47
1:G:143:ARG:HA	1:G:143:ARG:NH1	2.25	0.47
2:H:24:PHE:HE2	2:H:194:ASP:OD1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:27:VAL:O	2:H:30:THR:CG2	2.62	0.47
1:E:101:GLU:OE1	1:E:101:GLU:C	2.53	0.47
1:C:8:THR:O	1:C:8:THR:CG2	2.62	0.47
1:C:15:ARG:NH2	1:C:110:GLU:OE1	2.48	0.47
2:F:149:THR:O	2:F:168:ILE:HG13	2.14	0.47
1:G:96:ARG:HG3	1:G:97:GLN:N	2.30	0.47
1:A:91:GLY:O	2:B:123:GLY:HA2	2.14	0.47
2:D:90:ALA:HA	2:D:94:LEU:HD12	1.97	0.47
2:F:63:GLU:HG3	5:F:229:HOH:O	2.14	0.47
1:E:88:ARG:NH2	5:E:193:HOH:O	2.47	0.46
2:F:152:LEU:C	5:F:241:HOH:O	2.52	0.46
2:F:172:ASP:O	2:F:174:GLU:N	2.48	0.46
2:B:2:THR:HG23	2:B:4:ARG:HH12	1.70	0.46
2:F:126:ILE:O	2:F:126:ILE:HG13	2.14	0.46
1:G:106:GLY:CA	1:G:108:ASP:OD1	2.63	0.46
1:A:104:PHE:CD1	1:A:104:PHE:C	2.88	0.46
2:B:5:HIS:N	2:B:167:ASP:OD1	2.46	0.46
1:C:93:ARG:HA	2:D:22:GLU:OE2	2.15	0.46
1:C:136:ALA:HB2	5:C:183:HOH:O	2.15	0.46
2:D:5:HIS:O	2:D:168:ILE:HG22	2.14	0.46
1:E:34:ALA:HB3	1:E:35:PRO:HD3	1.96	0.46
2:F:23:ALA:HB3	2:F:125:ALA:HB3	1.96	0.46
2:H:105:VAL:HG12	2:H:106:ARG:N	2.30	0.46
1:A:122:GLU:OE1	1:A:125:ARG:HD3	2.16	0.46
2:H:3:ILE:CD1	2:H:35:CYS:HB2	2.46	0.46
1:E:96:ARG:O	1:E:98:PRO:HD3	2.15	0.46
2:H:99:GLY:C	5:H:210:HOH:O	2.53	0.46
1:C:70:ASP:HA	5:C:190:HOH:O	2.16	0.46
1:C:128:ARG:HH11	1:C:128:ARG:CG	2.27	0.46
1:E:41:LEU:HD23	1:E:88:ARG:NH2	2.24	0.46
2:H:7:VAL:HG23	2:H:31:HIS:CD2	2.51	0.46
1:A:11:VAL:HG23	5:A:197:HOH:O	2.15	0.46
1:A:89:ILE:CD1	1:A:93:ARG:HH21	2.27	0.46
2:B:37:GLU:O	2:B:41:ARG:HG3	2.16	0.46
2:B:87:ASP:OD2	2:B:89:ARG:NH1	2.47	0.46
1:C:38:LYS:HE2	2:D:59:VAL:CG1	2.45	0.46
1:G:15:ARG:NH1	5:G:229:HOH:O	2.49	0.46
2:H:50:GLY:O	2:H:53:MSE:HB3	2.15	0.46
1:A:110:GLU:N	5:A:230:HOH:O	2.48	0.46
2:B:12:LEU:HD21	5:B:221:HOH:O	2.16	0.46
1:E:101:GLU:OE1	1:E:102:ASP:CA	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:CYS:HB2	5:G:225:HOH:O	2.15	0.46
1:E:170:ARG:NH1	2:F:36:ASP:C	2.69	0.46
1:G:80:ILE:CG2	2:H:53:MSE:HE3	2.46	0.46
2:D:2:THR:CG2	2:D:4:ARG:NH1	2.54	0.46
1:E:19:ASP:C	1:E:20:HIS:CD2	2.90	0.46
2:H:74:ASP:OD1	2:H:74:ASP:N	2.47	0.46
2:B:153:GLN:O	2:B:187:CYS:HA	2.17	0.45
1:C:171:LEU:HD11	2:F:96:ASP:O	2.16	0.45
2:F:89:ARG:HG2	2:F:89:ARG:NH1	2.26	0.45
1:E:101:GLU:OE1	1:E:102:ASP:O	2.34	0.45
2:F:102:LEU:HD21	5:F:213:HOH:O	2.16	0.45
2:H:107:TRP:HZ3	2:H:129:LEU:O	1.98	0.45
2:B:90:ALA:HA	2:B:94:LEU:HD12	1.98	0.45
2:D:119:LEU:HA	2:D:120:PRO:HD2	1.71	0.45
2:D:155:ALA:CB	2:D:164:GLY:HA2	2.44	0.45
1:E:87:ARG:CG	1:E:87:ARG:NH1	2.79	0.45
2:F:155:ALA:HB2	2:F:164:GLY:HA2	1.98	0.45
2:B:98:VAL:HG11	2:B:102:LEU:HD23	1.99	0.45
1:C:177:ARG:O	1:C:178:GLN:C	2.54	0.45
2:D:170:ILE:C	2:D:170:ILE:HA	2.29	0.45
1:G:174:ASP:O	1:G:177:ARG:CB	2.60	0.45
2:D:154:GLY:O	2:D:164:GLY:HA2	2.17	0.45
2:D:180:VAL:CG1	2:D:181:ALA:N	2.80	0.45
2:H:94:LEU:HB2	5:H:214:HOH:O	2.16	0.45
2:D:15:TYR:N	2:D:20:LEU:HD12	2.31	0.45
2:D:103:GLU:HA	2:D:107:TRP:HE1	1.81	0.45
1:E:104:PHE:CD1	1:E:104:PHE:O	2.70	0.45
1:A:87:ARG:HH11	1:A:87:ARG:HG2	1.81	0.45
1:A:125:ARG:NE	1:G:87:ARG:HH12	2.14	0.45
2:B:128:ARG:NH2	2:B:193:THR:OG1	2.48	0.45
1:C:22:ASP:O	1:C:25:ALA:HB3	2.17	0.45
2:D:121:THR:HG23	5:D:237:HOH:O	2.16	0.45
1:E:123:ASN:HA	1:E:165:ILE:HD11	1.99	0.45
2:H:102:LEU:HD12	2:H:102:LEU:HA	1.84	0.45
2:H:188:ILE:HG23	5:H:222:HOH:O	2.17	0.45
1:A:62:VAL:HG13	1:A:79:TRP:HZ3	1.82	0.45
1:A:110:GLU:OE1	1:A:111:PRO:HD2	2.17	0.45
1:C:106:GLY:C	1:C:108:ASP:N	2.71	0.45
1:E:20:HIS:CD2	1:E:20:HIS:N	2.85	0.45
1:E:129:ALA:O	1:E:132:ARG:HG2	2.17	0.45
2:B:45:LEU:HD12	2:B:45:LEU:HA	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:ALA:HB2	2:D:121:THR:HG21	1.99	0.45
2:F:11:LEU:HD11	2:F:148:LEU:HD21	1.99	0.45
2:F:178:THR:N	2:F:179:PRO:HD2	2.32	0.45
1:G:18:ARG:NE	5:G:226:HOH:O	2.49	0.45
1:G:73:ARG:NH2	1:G:103:LEU:O	2.49	0.45
1:G:126:LEU:HD11	1:G:130:ILE:HD11	1.99	0.45
2:D:169:GLU:O	2:D:170:ILE:CB	2.61	0.44
1:G:161:PRO:HG2	5:G:237:HOH:O	2.16	0.44
1:A:38:LYS:HE2	2:B:59:VAL:CG1	2.46	0.44
2:B:149:THR:O	2:B:168:ILE:HG13	2.17	0.44
2:D:7:VAL:HB	2:D:12:LEU:HD13	1.98	0.44
2:D:169:GLU:CA	2:D:170:ILE:CG1	2.84	0.44
1:A:128:ARG:HD2	2:H:72:GLN:HG3	1.99	0.44
2:B:161:ASP:N	5:B:234:HOH:O	2.50	0.44
1:C:125:ARG:CD	5:E:236:HOH:O	2.57	0.44
2:D:107:TRP:CZ3	2:D:129:LEU:O	2.67	0.44
2:H:132:ILE:HD13	2:H:138:VAL:CG2	2.47	0.44
1:A:135:GLU:HG3	5:A:215:HOH:O	2.17	0.44
2:B:2:THR:CG2	2:B:4:ARG:NH1	2.67	0.44
2:B:93:PRO:HG3	5:B:226:HOH:O	2.18	0.44
1:C:7:ARG:CZ	5:C:202:HOH:O	2.66	0.44
2:D:153:GLN:NE2	5:D:210:HOH:O	2.42	0.44
1:E:37:VAL:CG2	5:E:235:HOH:O	2.65	0.44
1:C:89:ILE:HG21	1:C:92:LEU:HD12	1.99	0.44
2:D:89:ARG:O	2:D:91:PRO:HD3	2.18	0.44
1:G:41:LEU:O	1:G:44:SER:HB2	2.18	0.44
1:G:94:LYS:CB	5:G:201:HOH:O	2.65	0.44
2:H:30:THR:CG2	2:H:150:LEU:HD23	2.47	0.44
1:E:19:ASP:CB	1:E:20:HIS:HD2	2.26	0.44
1:G:162:LEU:O	1:G:166:LYS:HB2	2.18	0.44
1:A:122:GLU:OE1	1:A:164:THR:HG21	2.17	0.44
2:B:146:LEU:N	2:B:194:ASP:OD1	2.44	0.44
2:D:116:GLN:CB	2:D:130:LEU:HD22	2.42	0.44
1:G:96:ARG:HB3	2:H:22:GLU:HG3	1.99	0.44
1:A:87:ARG:HG2	1:A:87:ARG:NH1	2.33	0.44
2:D:102:LEU:HD12	2:D:102:LEU:HA	1.84	0.44
2:H:12:LEU:HD12	2:H:12:LEU:HA	1.77	0.44
1:A:90:ASP:HA	5:A:209:HOH:O	2.18	0.43
1:A:128:ARG:CG	1:A:128:ARG:NH1	2.81	0.43
1:C:54:CYS:SG	1:C:87:ARG:HD3	2.58	0.43
2:D:130:LEU:HD22	2:D:130:LEU:HA	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:GLU:O	2:D:170:ILE:HG23	2.18	0.43
2:F:102:LEU:HG	5:F:213:HOH:O	2.18	0.43
1:G:135:GLU:OE1	1:G:135:GLU:CA	2.62	0.43
1:C:128:ARG:HG2	1:C:128:ARG:NH1	2.29	0.43
1:E:161:PRO:O	1:E:162:LEU:C	2.56	0.43
1:G:175:ARG:HG3	1:G:175:ARG:NH1	2.33	0.43
2:H:65:SER:O	2:H:69:VAL:HG23	2.18	0.43
2:B:115:ARG:HB2	2:B:131:TRP:HB3	2.00	0.43
2:B:115:ARG:HD2	5:B:212:HOH:O	2.17	0.43
1:C:58:VAL:HG12	1:C:59:MSE:HE2	1.99	0.43
2:F:68:SER:C	2:F:72:GLN:HE21	2.12	0.43
1:G:20:HIS:O	1:G:21:ARG:C	2.56	0.43
1:G:169:ILE:O	1:G:173:LEU:N	2.47	0.43
1:A:128:ARG:HG2	1:A:128:ARG:NH1	2.28	0.43
1:C:175:ARG:NE	5:C:188:HOH:O	2.43	0.43
1:G:41:LEU:HD22	1:G:88:ARG:HD2	1.99	0.43
2:H:164:GLY:O	2:H:167:ASP:HB2	2.18	0.43
1:A:94:LYS:CG	1:A:95:ASP:N	2.81	0.43
2:D:15:TYR:CA	2:D:20:LEU:HD12	2.49	0.43
2:D:180:VAL:CB	2:D:180:VAL:O	2.64	0.43
1:G:177:ARG:C	1:G:179:HIS:N	2.72	0.43
1:A:126:LEU:HD22	1:A:165:ILE:HD12	2.01	0.43
2:B:26:LEU:O	5:B:226:HOH:O	2.21	0.43
2:B:105:VAL:HG12	2:B:107:TRP:NE1	2.33	0.43
5:C:203:HOH:O	2:D:53:MSE:HG2	2.18	0.43
1:G:23:GLU:HB3	2:H:70:MSE:HE3	2.00	0.43
1:G:71:PRO:HB2	5:G:231:HOH:O	2.19	0.43
2:H:172:ASP:CG	2:H:173:GLN:N	2.72	0.43
2:B:93:PRO:O	2:B:95:ALA:N	2.51	0.43
1:E:87:ARG:O	1:E:88:ARG:C	2.55	0.43
2:F:17:ALA:HB3	2:F:19:THR:CG2	2.49	0.43
1:G:78:THR:OG1	2:H:47:ALA:HA	2.18	0.43
1:G:94:LYS:O	1:G:95:ASP:CB	2.66	0.43
1:A:18:ARG:NH2	1:A:105:TRP:O	2.52	0.43
2:B:112:GLY:HA3	2:B:136:GLN:NE2	2.33	0.43
1:C:118:GLU:HB3	1:C:168:ARG:HD2	2.01	0.43
1:G:104:PHE:C	1:G:104:PHE:CD1	2.92	0.43
2:B:178:THR:N	2:B:179:PRO:HD2	2.32	0.43
1:E:105:TRP:CZ2	1:E:111:PRO:HB3	2.54	0.43
2:H:162:ARG:HH11	2:H:162:ARG:HG2	1.84	0.43
2:B:7:VAL:HB	2:B:12:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:CYS:O	1:C:58:VAL:HG23	2.19	0.42
2:D:107:TRP:CZ2	2:D:131:TRP:HE3	2.37	0.42
1:E:41:LEU:CD2	1:E:88:ARG:NE	2.76	0.42
1:A:126:LEU:HD12	1:A:126:LEU:O	2.18	0.42
1:E:33:PHE:C	5:E:235:HOH:O	2.58	0.42
1:E:53:GLU:HG3	5:E:183:HOH:O	2.19	0.42
1:G:30:PHE:CD1	1:G:59:MSE:HG3	2.54	0.42
1:G:96:ARG:HG2	1:G:98:PRO:HG3	2.01	0.42
1:A:147:GLY:O	1:A:148:ASP:O	2.37	0.42
1:A:171:LEU:HD11	2:H:96:ASP:O	2.20	0.42
2:B:93:PRO:O	2:B:94:LEU:C	2.57	0.42
2:B:128:ARG:HH12	2:B:191:ALA:CB	2.31	0.42
1:C:133:LEU:HA	1:C:134:PRO:HD3	1.88	0.42
2:D:45:LEU:HD12	2:D:45:LEU:HA	1.86	0.42
2:D:180:VAL:HG12	2:D:181:ALA:N	2.34	0.42
2:F:17:ALA:HB3	2:F:19:THR:HG23	2.01	0.42
2:F:161:ASP:OD1	2:F:161:ASP:N	2.53	0.42
1:G:10:TRP:N	5:G:190:HOH:O	2.52	0.42
1:C:99:GLU:CB	5:D:216:HOH:O	2.60	0.42
2:D:89:ARG:HG2	2:D:89:ARG:NH1	2.34	0.42
1:G:42:MSE:HG2	1:G:46:SER:O	2.20	0.42
1:G:106:GLY:HA3	1:G:108:ASP:OD1	2.19	0.42
1:G:128:ARG:HH11	1:G:128:ARG:CG	2.26	0.42
2:H:24:PHE:CD1	2:H:148:LEU:HG	2.53	0.42
2:H:87:ASP:OD1	2:H:89:ARG:HG2	2.20	0.42
2:H:89:ARG:HH22	2:H:103:GLU:CD	2.23	0.42
1:C:138:ARG:O	1:C:142:GLU:HG3	2.19	0.42
1:E:105:TRP:HB3	1:E:109:SER:O	2.20	0.42
2:F:172:ASP:C	2:F:174:GLU:N	2.71	0.42
1:G:83:ILE:CD1	5:G:209:HOH:O	2.67	0.42
1:A:14:MSE:HE1	5:A:190:HOH:O	2.19	0.42
2:B:65:SER:O	2:B:69:VAL:HG23	2.20	0.42
1:C:50:GLN:OE1	1:C:50:GLN:CA	2.63	0.42
2:D:98:VAL:HG11	2:D:102:LEU:HD12	2.01	0.42
2:B:113:GLY:H	2:B:136:GLN:NE2	2.16	0.42
1:E:94:LYS:O	2:F:122:GLY:CA	2.44	0.42
2:F:87:ASP:HA	2:F:88:PRO:HD3	1.86	0.42
2:H:14:ALA:HB3	2:H:20:LEU:HD13	2.01	0.42
2:H:149:THR:O	2:H:168:ILE:HG13	2.20	0.42
1:E:38:LYS:HE2	2:F:59:VAL:CG1	2.50	0.42
1:G:162:LEU:HB3	2:H:44:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:89:ARG:NH2	2:H:103:GLU:OE2	2.53	0.42
2:B:3:ILE:CD1	2:B:35:CYS:HB2	2.50	0.42
2:F:12:LEU:HD12	2:F:12:LEU:HA	1.72	0.42
1:G:75:SER:HB2	5:G:213:HOH:O	2.19	0.42
2:H:110:LEU:O	2:H:110:LEU:CG	2.67	0.42
2:H:171:ALA:HA	2:H:175:LEU:HD23	2.01	0.42
1:A:138:ARG:HG2	1:A:138:ARG:HH11	1.85	0.41
2:B:87:ASP:OD1	2:B:89:ARG:HG2	2.20	0.41
1:C:43:LYS:CB	1:C:146:PHE:CE2	3.02	0.41
2:D:92:ALA:HB3	2:D:93:PRO:CD	2.47	0.41
1:E:87:ARG:NH1	1:E:87:ARG:HG2	2.34	0.41
2:H:159:GLU:CA	5:H:238:HOH:O	2.65	0.41
1:A:130:ILE:HG21	2:B:55:GLU:OE2	2.20	0.41
2:B:177:HIS:CD2	2:B:179:PRO:HD3	2.54	0.41
2:H:41:ARG:HD3	5:H:207:HOH:O	2.20	0.41
1:A:92:LEU:O	2:B:22:GLU:HB2	2.20	0.41
2:B:97:TYR:CD1	2:B:97:TYR:N	2.88	0.41
1:C:122:GLU:O	1:C:125:ARG:HB3	2.21	0.41
1:C:154:LEU:N	5:C:240:HOH:O	2.53	0.41
1:E:101:GLU:CA	2:F:92:ALA:HB2	2.50	0.41
2:H:2:THR:O	2:H:3:ILE:C	2.57	0.41
1:A:170:ARG:HG2	2:H:120:PRO:HB2	2.03	0.41
1:C:171:LEU:HD13	1:C:171:LEU:O	2.19	0.41
2:D:135:GLY:O	2:D:136:GLN:C	2.58	0.41
1:E:97:GLN:OE1	1:E:97:GLN:HA	2.20	0.41
1:E:133:LEU:CD1	1:E:141:ILE:CD1	2.98	0.41
2:B:87:ASP:OD1	2:B:89:ARG:NH1	2.53	0.41
1:C:95:ASP:HB3	1:C:96:ARG:H	1.53	0.41
2:D:115:ARG:HB2	2:D:131:TRP:HB3	2.03	0.41
1:E:38:LYS:HE2	2:F:59:VAL:HG12	2.02	0.41
1:E:47:VAL:O	1:E:48:ALA:C	2.58	0.41
2:H:23:ALA:HB3	2:H:125:ALA:CB	2.50	0.41
2:B:3:ILE:HD13	2:B:35:CYS:HB2	2.03	0.41
2:B:44:ALA:O	2:B:47:ALA:HB3	2.21	0.41
1:C:8:THR:HB	5:C:195:HOH:O	2.21	0.41
1:E:58:VAL:HG22	1:E:83:ILE:HG22	2.03	0.41
2:H:135:GLY:HA2	2:H:181:ALA:O	2.20	0.41
1:C:169:ILE:HG22	1:C:173:LEU:HD12	2.02	0.41
1:G:137:GLN:CG	5:G:194:HOH:O	2.69	0.41
2:H:179:PRO:HB2	5:H:220:HOH:O	2.20	0.41
2:B:157:ARG:CG	5:B:229:HOH:O	2.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:GLY:C	5:C:219:HOH:O	2.58	0.41
1:G:43:LYS:HG3	5:G:188:HOH:O	2.19	0.41
1:G:133:LEU:HD22	1:G:137:GLN:HB2	2.03	0.41
1:G:166:LYS:HB2	1:G:166:LYS:HE3	1.89	0.41
2:B:11:LEU:HD23	2:B:11:LEU:HA	1.89	0.41
2:B:105:VAL:HG22	2:B:106:ARG:H	1.85	0.41
1:C:107:PRO:HG2	5:C:210:HOH:O	2.20	0.41
1:C:130:ILE:HA	1:C:133:LEU:CD1	2.50	0.41
1:E:97:GLN:N	1:E:98:PRO:HD3	2.36	0.41
1:E:101:GLU:HB2	2:F:92:ALA:HB2	2.01	0.41
2:F:30:THR:HG23	2:F:91:PRO:CG	2.49	0.41
2:F:92:ALA:N	2:F:93:PRO:HD3	2.35	0.41
1:C:41:LEU:O	1:C:44:SER:HB2	2.21	0.41
2:D:154:GLY:N	5:D:226:HOH:O	2.49	0.41
2:H:136:GLN:HG3	2:H:137:ALA:O	2.21	0.41
1:A:64:GLN:NE2	5:A:210:HOH:O	2.54	0.40
1:G:41:LEU:HD22	1:G:88:ARG:CD	2.51	0.40
1:G:133:LEU:HD23	1:G:134:PRO:HD2	2.04	0.40
1:A:104:PHE:CD1	1:A:104:PHE:O	2.75	0.40
1:C:122:GLU:HG3	1:C:164:THR:HG22	2.04	0.40
1:E:99:GLU:O	2:F:93:PRO:HG3	2.20	0.40
2:F:7:VAL:CG1	2:F:12:LEU:HD13	2.51	0.40
2:F:32:LEU:HD11	2:F:42:ALA:HB2	2.02	0.40
2:F:91:PRO:O	2:F:95:ALA:CB	2.68	0.40
5:G:214:HOH:O	2:H:93:PRO:HB3	2.21	0.40
2:B:30:THR:N	5:B:226:HOH:O	2.54	0.40
2:B:132:ILE:HA	2:B:133:PRO:HD3	1.77	0.40
2:B:137:ALA:HB2	2:B:180:VAL:HA	2.03	0.40
2:F:178:THR:C	5:F:210:HOH:O	2.60	0.40
2:H:90:ALA:HA	2:H:94:LEU:HD12	2.03	0.40
1:A:109:SER:O	1:A:110:GLU:HG2	2.21	0.40
1:A:119:MSE:O	1:A:119:MSE:HE3	2.21	0.40
2:F:35:CYS:SG	2:F:37:GLU:HB3	2.62	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	162/184 (88%)	149 (92%)	11 (7%)	2 (1%)	11	28
1	C	168/184 (91%)	155 (92%)	11 (6%)	2 (1%)	11	28
1	E	147/184 (80%)	134 (91%)	10 (7%)	3 (2%)	6	16
1	G	154/184 (84%)	146 (95%)	4 (3%)	4 (3%)	4	11
2	B	178/203 (88%)	159 (89%)	13 (7%)	6 (3%)	3	7
2	D	163/203 (80%)	139 (85%)	13 (8%)	11 (7%)	1	1
2	F	159/203 (78%)	143 (90%)	13 (8%)	3 (2%)	6	17
2	H	169/203 (83%)	147 (87%)	17 (10%)	5 (3%)	3	9
All	All	1300/1548 (84%)	1172 (90%)	92 (7%)	36 (3%)	4	10

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	91	PRO
2	B	93	PRO
2	B	111	GLY
2	D	92	ALA
2	D	102	LEU
2	D	133	PRO
2	D	179	PRO
1	E	98	PRO
1	G	162	LEU
2	H	92	ALA
2	H	159	GLU
1	A	135	GLU
2	D	115	ARG
1	E	162	LEU
2	F	159	GLU
1	G	95	ASP
2	H	101	ARG

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Mol	Chain	Res	Type
2	B	92	ALA
2	B	94	LEU
2	B	178	THR
2	D	98	VAL
2	D	136	GLN
2	D	170	ILE
1	E	178	GLN
2	F	36	ASP
2	F	93	PRO
1	G	96	ARG
1	G	161	PRO
2	H	100	ARG
2	D	106	ARG
2	D	169	GLU
1	C	135	GLU
1	A	147	GLY
2	H	3	ILE
1	C	161	PRO
2	D	123	GLY

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	129/145 (89%)	116 (90%)	13 (10%)	6	15
1	C	125/145 (86%)	115 (92%)	10 (8%)	10	24
1	E	122/145 (84%)	110 (90%)	12 (10%)	6	16
1	G	124/145 (86%)	114 (92%)	10 (8%)	9	23
2	B	114/150 (76%)	103 (90%)	11 (10%)	7	17
2	D	112/150 (75%)	98 (88%)	14 (12%)	3	9
2	F	105/150 (70%)	92 (88%)	13 (12%)	4	9
2	H	115/150 (77%)	103 (90%)	12 (10%)	5	14
All	All	946/1180 (80%)	851 (90%)	95 (10%)	6	16

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	18	ARG
1	A	57	ASP
1	A	85	ARG
1	A	88	ARG
1	A	112	ASP
1	A	125	ARG
1	A	128	ARG
1	A	135	GLU
1	A	143	ARG
1	A	164	THR
1	A	168	ARG
1	A	171	LEU
2	B	2	THR
2	B	12	LEU
2	B	45	LEU
2	B	89	ARG
2	B	91	PRO
2	B	94	LEU
2	B	103	GLU
2	B	128	ARG
2	B	146	LEU
2	B	185	LEU
2	B	186	ASP
1	C	53	GLU
1	C	54	CYS
1	C	85	ARG
1	C	87	ARG
1	C	95	ASP
1	C	125	ARG
1	C	128	ARG
1	C	164	THR
1	C	168	ARG
1	C	171	LEU
2	D	2	THR
2	D	12	LEU
2	D	20	LEU
2	D	45	LEU
2	D	94	LEU
2	D	102	LEU
2	D	106	ARG
2	D	116	GLN

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Mol	Chain	Res	Type
2	D	130	LEU
2	D	136	GLN
2	D	143	HIS
2	D	170	ILE
2	D	179	PRO
2	D	186	ASP
1	E	15	ARG
1	E	85	ARG
1	E	87	ARG
1	E	95	ASP
1	E	101	GLU
1	E	109	SER
1	E	125	ARG
1	E	128	ARG
1	E	132	ARG
1	E	143	ARG
1	E	165	ILE
1	E	179	HIS
2	F	2	THR
2	F	12	LEU
2	F	19	THR
2	F	32	LEU
2	F	35	CYS
2	F	45	LEU
2	F	53	MSE
2	F	72	GLN
2	F	102	LEU
2	F	129	LEU
2	F	161	ASP
2	F	172	ASP
2	F	193	THR
1	G	18	ARG
1	G	23	GLU
1	G	53	GLU
1	G	85	ARG
1	G	128	ARG
1	G	133	LEU
1	G	143	ARG
1	G	160	LEU
1	G	164	THR
1	G	170	ARG
2	H	2	THR

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Mol	Chain	Res	Type
2	H	9	ASP
2	H	12	LEU
2	H	19	THR
2	H	45	LEU
2	H	53	MSE
2	H	94	LEU
2	H	126	ILE
2	H	147	GLU
2	H	167	ASP
2	H	186	ASP
2	H	194	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	56	GLN
1	A	178	GLN
2	B	5	HIS
2	B	153	GLN
2	B	177	HIS
1	C	32	HIS
1	E	20	HIS
1	E	56	GLN
1	E	123	ASN
1	G	86	ASN
2	H	177	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

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	G	182	-	4,4,4	0.28	0	6,6,6	0.10	0
4	SO4	E	182	-	4,4,4	0.27	0	6,6,6	0.32	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	182	SO4	1	0
4	E	182	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	109:SER	C	110:GLU	N	1.08
1	E	105:TRP	C	106:GLY	N	0.97

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	161/184 (87%)	-1.75	0 100 100	5, 33, 65, 75	0
1	C	167/184 (90%)	-1.71	0 100 100	9, 35, 70, 89	0
1	E	151/184 (82%)	-1.71	0 100 100	11, 38, 68, 83	0
1	G	156/184 (84%)	-1.69	0 100 100	12, 39, 68, 79	0
2	B	180/203 (88%)	-1.62	0 100 100	11, 48, 84, 91	0
2	D	167/203 (82%)	-1.53	0 100 100	21, 55, 88, 94	0
2	F	167/203 (82%)	-1.61	0 100 100	21, 44, 71, 85	0
2	H	173/203 (85%)	-1.67	0 100 100	19, 44, 72, 78	0
All	All	1322/1548 (85%)	-1.66	0 100 100	5, 43, 75, 94	0

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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	G	182	5/5	0.98	0.05	74,75,75,76	0
4	SO4	E	182	5/5	0.99	0.04	73,74,74,75	0
3	ZN	F	204	1/1	1.00	0.02	70,70,70,70	0
3	ZN	H	204	1/1	1.00	0.02	61,61,61,61	0
3	ZN	B	204	1/1	1.00	0.01	49,49,49,49	0
3	ZN	D	204	1/1	1.00	0.01	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.