Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 02:36 AM EDT

PDB ID	:	2GSZ
Title	:	Structure of A. aeolicus PilT with 6 monomers per asymmetric unit
Authors	:	Forest, K.T.; Satyshur, K.A.
Deposited on	:	2006-04-27
Resolution	:	4.20 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 (i) 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 (i)) were used in the production of this report:

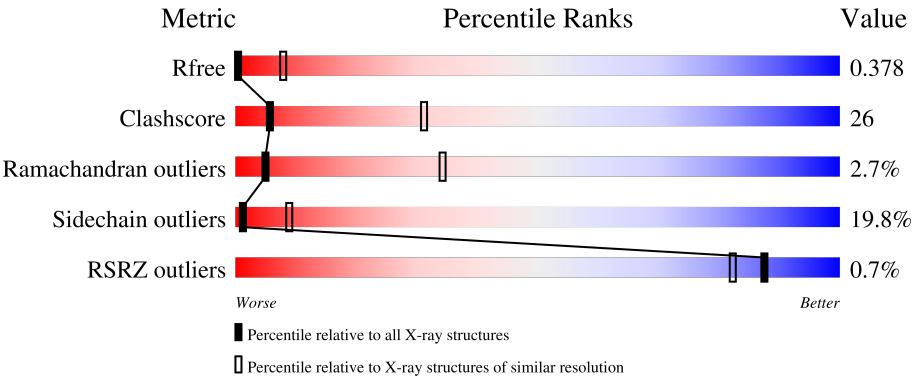
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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}	130704	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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 <=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	363	46% 37% 11% • 6%
1	B	363	44% 42% 9% 6%
1	C	363	% 46% 38% 10% 6%
1	D	363	43% 42% 9% 6%
1	E	363	% 42% 41% 10% • 6%

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Mol	Chain	Length	Quality of chain
1	F	363	43% 41% 10% • 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	375	-	-	X	-
2	SO4	C	375	-	-	X	-
2	SO4	E	375	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16344 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 twitching motility protein PilT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	Se	0	0	0
			2717	1731	471	505	1	9			
1	B	343	Total	C	N	O	S	Se	0	0	0
			2717	1731	471	505	1	9			
1	C	343	Total	C	N	O	S	Se	0	0	0
			2717	1731	471	505	1	9			
1	D	343	Total	C	N	O	S	Se	0	0	0
			2717	1731	471	505	1	9			
1	E	343	Total	C	N	O	S	Se	0	0	0
			2717	1731	471	505	1	9			
1	F	343	Total	C	N	O	S	Se	0	0	0
			2717	1731	471	505	1	9			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	MSE	MET	modified residue	GB 2983313
A	136	MSE	MET	modified residue	GB 2983313
A	156	MSE	MET	modified residue	GB 2983313
A	218	MSE	MET	modified residue	GB 2983313
A	318	MSE	MET	modified residue	GB 2983313
A	327	MSE	MET	modified residue	GB 2983313
A	330	MSE	MET	modified residue	GB 2983313
A	349	MSE	MET	modified residue	GB 2983313
A	361	MSE	MET	modified residue	GB 2983313
A	367	LEU	-	expression tag	GB 2983313
A	368	GLU	-	expression tag	GB 2983313
A	369	HIS	-	expression tag	GB 2983313
A	370	HIS	-	expression tag	GB 2983313
A	371	HIS	-	expression tag	GB 2983313
A	372	HIS	-	expression tag	GB 2983313
A	373	HIS	-	expression tag	GB 2983313
A	374	HIS	-	expression tag	GB 2983313

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Chain	Residue	Modelled	Actual	Comment	Reference
B	68	MSE	MET	modified residue	GB 2983313
B	136	MSE	MET	modified residue	GB 2983313
B	156	MSE	MET	modified residue	GB 2983313
B	218	MSE	MET	modified residue	GB 2983313
B	318	MSE	MET	modified residue	GB 2983313
B	327	MSE	MET	modified residue	GB 2983313
B	330	MSE	MET	modified residue	GB 2983313
B	349	MSE	MET	modified residue	GB 2983313
B	361	MSE	MET	modified residue	GB 2983313
B	367	LEU	-	expression tag	GB 2983313
B	368	GLU	-	expression tag	GB 2983313
B	369	HIS	-	expression tag	GB 2983313
B	370	HIS	-	expression tag	GB 2983313
B	371	HIS	-	expression tag	GB 2983313
B	372	HIS	-	expression tag	GB 2983313
B	373	HIS	-	expression tag	GB 2983313
B	374	HIS	-	expression tag	GB 2983313
C	68	MSE	MET	modified residue	GB 2983313
C	136	MSE	MET	modified residue	GB 2983313
C	156	MSE	MET	modified residue	GB 2983313
C	218	MSE	MET	modified residue	GB 2983313
C	318	MSE	MET	modified residue	GB 2983313
C	327	MSE	MET	modified residue	GB 2983313
C	330	MSE	MET	modified residue	GB 2983313
C	349	MSE	MET	modified residue	GB 2983313
C	361	MSE	MET	modified residue	GB 2983313
C	367	LEU	-	expression tag	GB 2983313
C	368	GLU	-	expression tag	GB 2983313
C	369	HIS	-	expression tag	GB 2983313
C	370	HIS	-	expression tag	GB 2983313
C	371	HIS	-	expression tag	GB 2983313
C	372	HIS	-	expression tag	GB 2983313
C	373	HIS	-	expression tag	GB 2983313
C	374	HIS	-	expression tag	GB 2983313
D	68	MSE	MET	modified residue	GB 2983313
D	136	MSE	MET	modified residue	GB 2983313
D	156	MSE	MET	modified residue	GB 2983313
D	218	MSE	MET	modified residue	GB 2983313
D	318	MSE	MET	modified residue	GB 2983313
D	327	MSE	MET	modified residue	GB 2983313
D	330	MSE	MET	modified residue	GB 2983313
D	349	MSE	MET	modified residue	GB 2983313

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Chain	Residue	Modelled	Actual	Comment	Reference
D	361	MSE	MET	modified residue	GB 2983313
D	367	LEU	-	expression tag	GB 2983313
D	368	GLU	-	expression tag	GB 2983313
D	369	HIS	-	expression tag	GB 2983313
D	370	HIS	-	expression tag	GB 2983313
D	371	HIS	-	expression tag	GB 2983313
D	372	HIS	-	expression tag	GB 2983313
D	373	HIS	-	expression tag	GB 2983313
D	374	HIS	-	expression tag	GB 2983313
E	68	MSE	MET	modified residue	GB 2983313
E	136	MSE	MET	modified residue	GB 2983313
E	156	MSE	MET	modified residue	GB 2983313
E	218	MSE	MET	modified residue	GB 2983313
E	318	MSE	MET	modified residue	GB 2983313
E	327	MSE	MET	modified residue	GB 2983313
E	330	MSE	MET	modified residue	GB 2983313
E	349	MSE	MET	modified residue	GB 2983313
E	361	MSE	MET	modified residue	GB 2983313
E	367	LEU	-	expression tag	GB 2983313
E	368	GLU	-	expression tag	GB 2983313
E	369	HIS	-	expression tag	GB 2983313
E	370	HIS	-	expression tag	GB 2983313
E	371	HIS	-	expression tag	GB 2983313
E	372	HIS	-	expression tag	GB 2983313
E	373	HIS	-	expression tag	GB 2983313
E	374	HIS	-	expression tag	GB 2983313
F	68	MSE	MET	modified residue	GB 2983313
F	136	MSE	MET	modified residue	GB 2983313
F	156	MSE	MET	modified residue	GB 2983313
F	218	MSE	MET	modified residue	GB 2983313
F	318	MSE	MET	modified residue	GB 2983313
F	327	MSE	MET	modified residue	GB 2983313
F	330	MSE	MET	modified residue	GB 2983313
F	349	MSE	MET	modified residue	GB 2983313
F	361	MSE	MET	modified residue	GB 2983313
F	367	LEU	-	expression tag	GB 2983313
F	368	GLU	-	expression tag	GB 2983313
F	369	HIS	-	expression tag	GB 2983313
F	370	HIS	-	expression tag	GB 2983313
F	371	HIS	-	expression tag	GB 2983313
F	372	HIS	-	expression tag	GB 2983313
F	373	HIS	-	expression tag	GB 2983313

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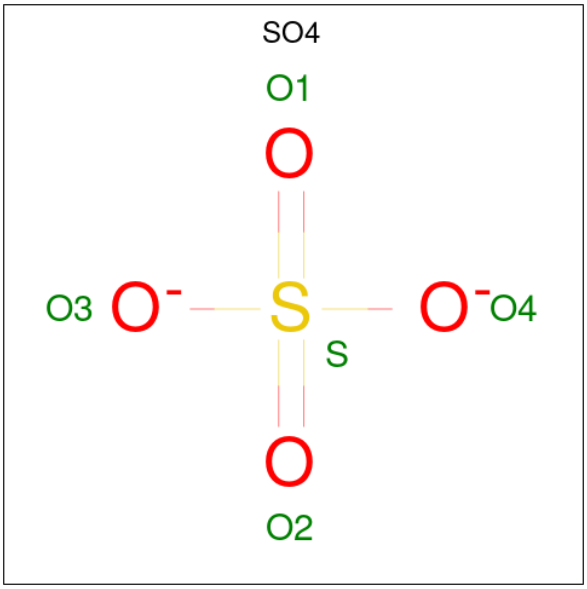
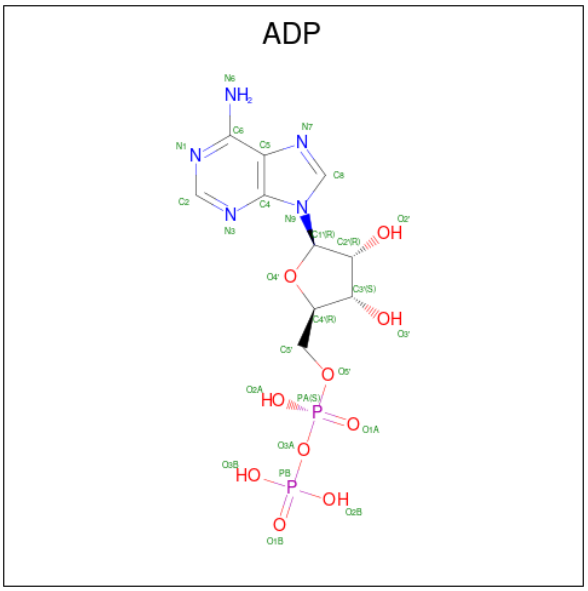
Chain	Residue	Modelled	Actual	Comment	Reference
F	374	HIS	-	expression tag	GB 2983313

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



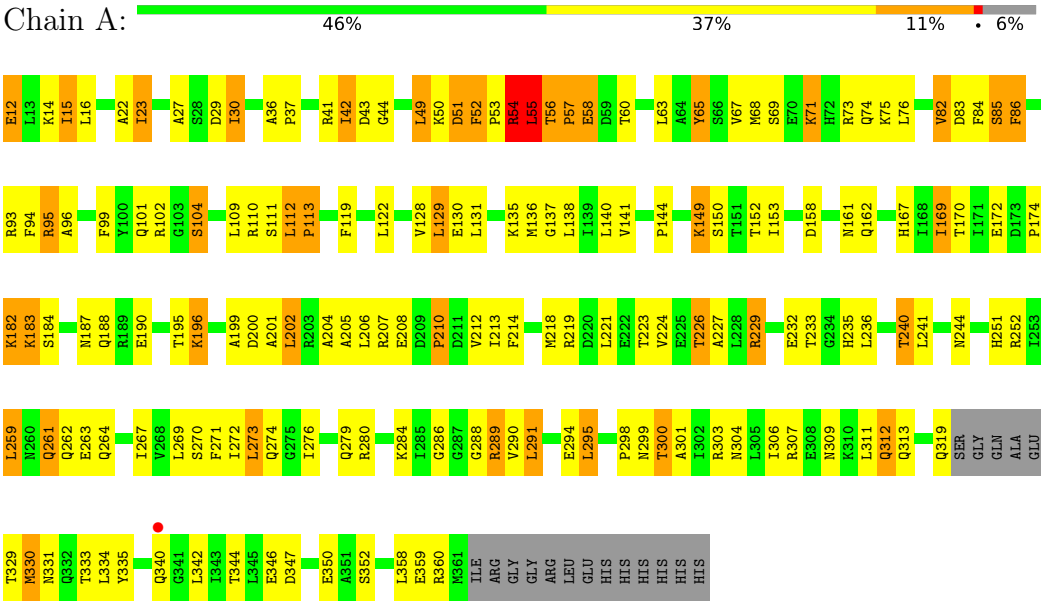
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots (i)

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.

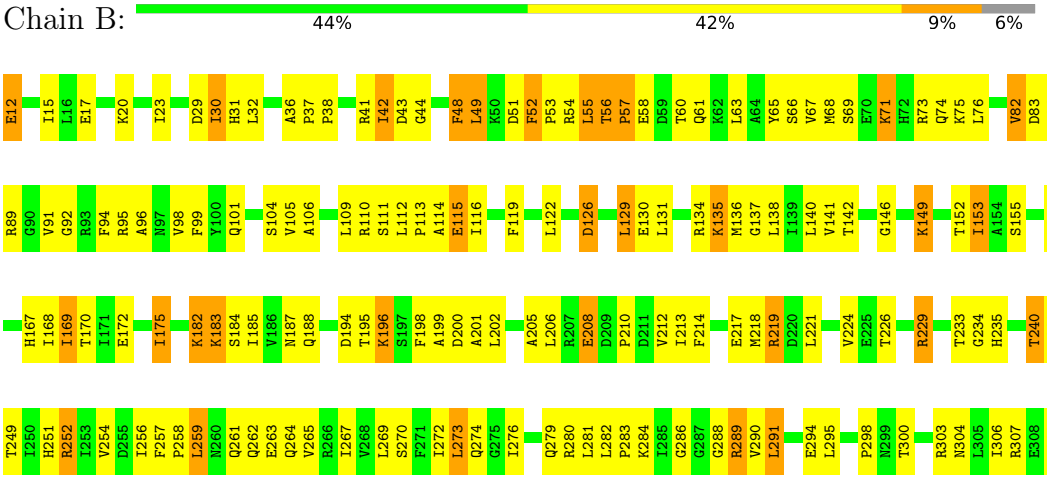
• Molecule 1: twitching motility protein PilT

Chain A:



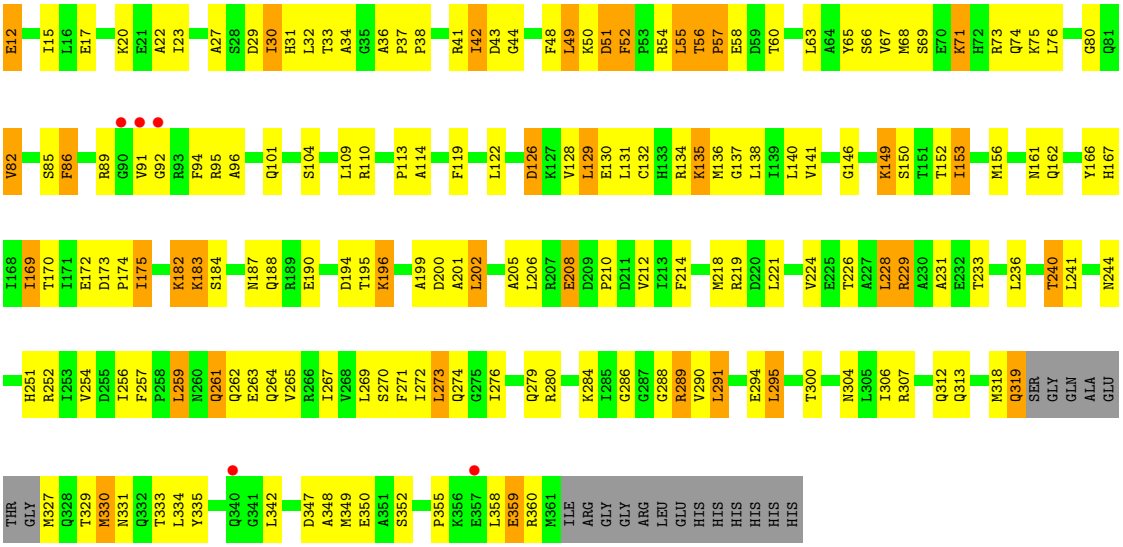
• Molecule 1: twitching motility protein PilT

Chain B:



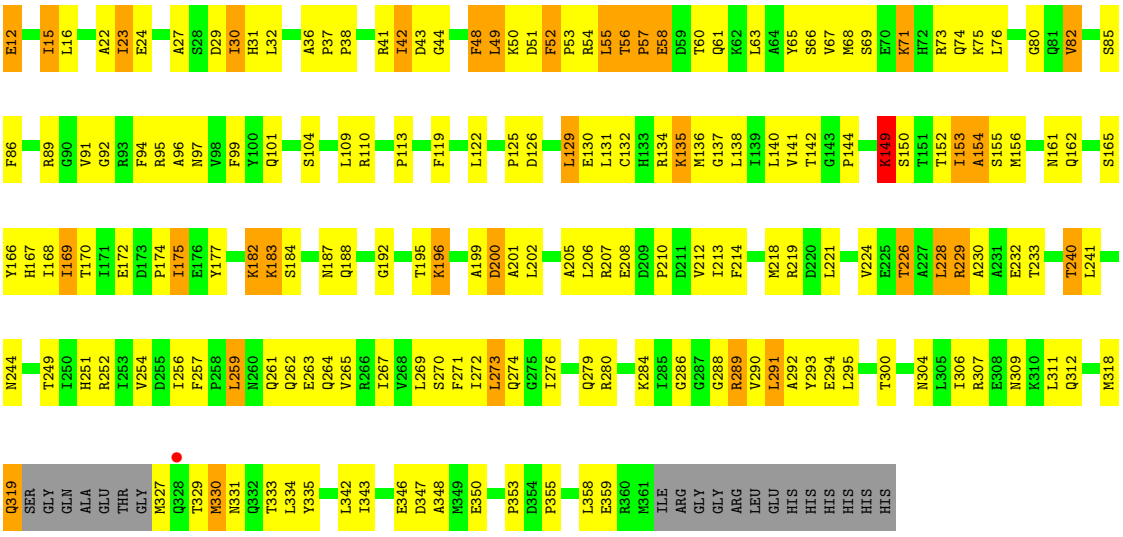
• Molecule 1: twitching motility protein PilT

Chain C:



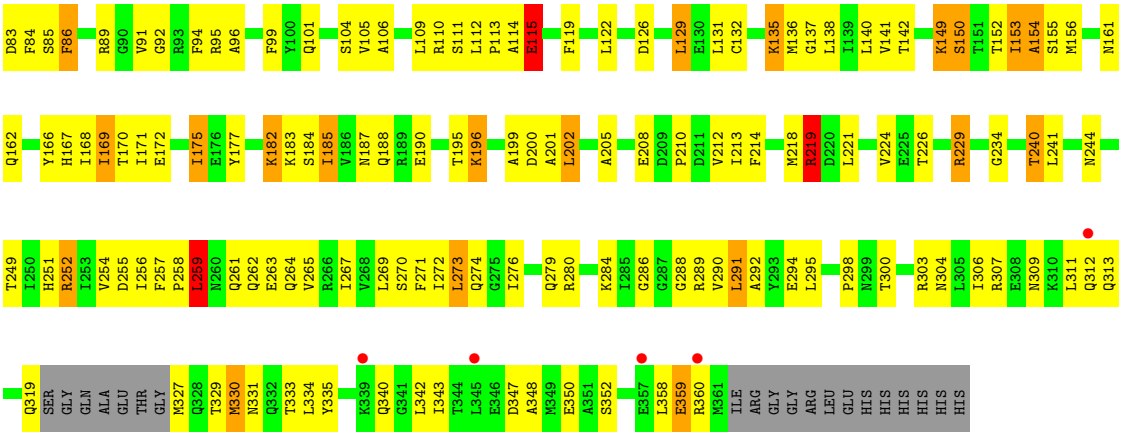
• Molecule 1: twitching motility protein PilT

Chain D:



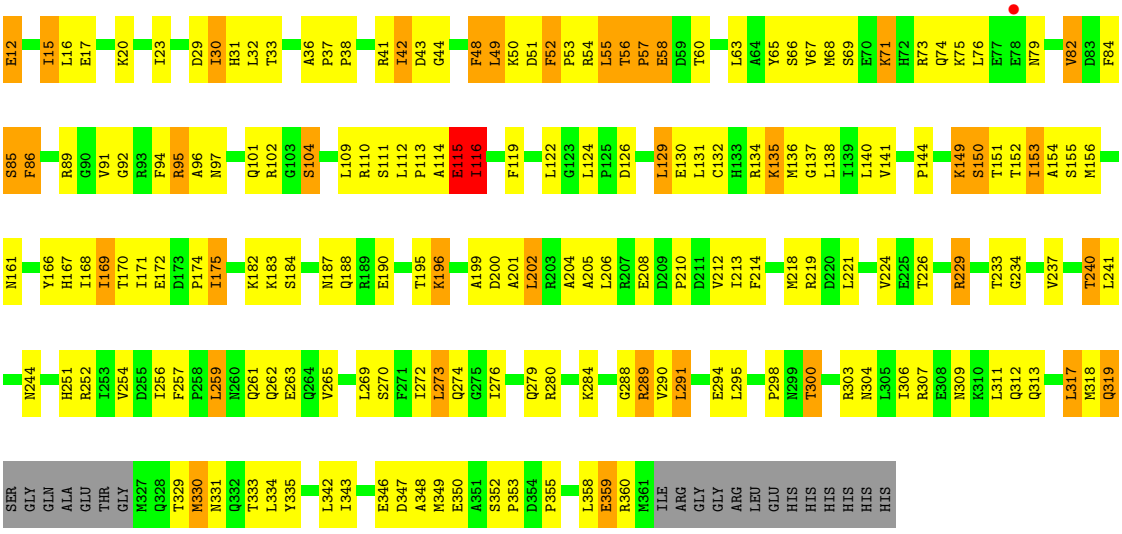
• Molecule 1: twitching motility protein PilT

Chain E:



• Molecule 1: twitching motility protein PilT

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	206.11Å 105.24Å 123.02Å 90.00° 111.06° 90.00°	Depositor
Resolution (Å)	25.00 – 4.20 32.48 – 4.20	Depositor EDS
% Data completeness (in resolution range)	94.8 (25.00-4.20) 94.7 (32.48-4.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	6.91 (at 4.27Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.343 , 0.406 0.321 , 0.378	Depositor DCC
R_{free} test set	859 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	115.0	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 9.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	16344	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, ADP

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	0.83	0/2753	0.83	3/3702 (0.1%)
1	B	0.88	3/2753 (0.1%)	0.83	1/3702 (0.0%)
1	C	0.80	0/2753	0.82	2/3702 (0.1%)
1	D	0.80	0/2753	0.90	5/3702 (0.1%)
1	E	0.83	1/2753 (0.0%)	0.91	9/3702 (0.2%)
1	F	0.83	1/2753 (0.0%)	0.85	7/3702 (0.2%)
All	All	0.83	5/16518 (0.0%)	0.86	27/22212 (0.1%)

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	F	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	115	GLU	CD-OE1	13.20	1.40	1.25
1	B	115	GLU	CD-OE2	11.11	1.37	1.25
1	F	115	GLU	CD-OE2	6.81	1.33	1.25
1	E	115	GLU	CG-CD	5.85	1.60	1.51
1	B	115	GLU	CG-CD	5.22	1.59	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	289	ARG	NE-CZ-NH1	-15.71	112.44	120.30
1	D	289	ARG	NE-CZ-NH2	15.63	128.12	120.30
1	E	219	ARG	CG-CD-NE	12.56	138.18	111.80
1	E	219	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	D	289	ARG	CD-NE-CZ	8.79	135.91	123.60
1	E	219	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	A	55	LEU	CA-CB-CG	7.10	131.64	115.30
1	E	219	ARG	CD-NE-CZ	6.95	133.33	123.60
1	F	55	LEU	CA-CB-CG	6.76	130.85	115.30
1	E	55	LEU	CA-CB-CG	6.63	130.54	115.30
1	F	115	GLU	C-N-CA	6.61	138.22	121.70
1	D	55	LEU	CA-CB-CG	6.49	130.23	115.30
1	E	89	ARG	CB-CG-CD	6.36	128.12	111.60
1	A	289	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	F	115	GLU	N-CA-C	-6.23	94.19	111.00
1	E	89	ARG	CG-CD-NE	6.19	124.80	111.80
1	E	89	ARG	NE-CZ-NH2	6.13	123.36	120.30
1	C	55	LEU	CA-CB-CG	5.96	129.02	115.30
1	F	317	LEU	CA-CB-CG	5.46	127.86	115.30
1	F	116	ILE	N-CA-C	5.33	125.40	111.00
1	F	289	ARG	CG-CD-NE	5.33	122.99	111.80
1	C	289	ARG	CG-CD-NE	5.28	122.89	111.80
1	B	55	LEU	CA-CB-CG	5.16	127.17	115.30
1	F	124	LEU	CA-CB-CG	5.16	127.16	115.30
1	E	259	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	D	149	LYS	CD-CE-NZ	-5.02	100.15	111.70
1	A	54	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	115	GLU	Peptide
1	F	114	ALA	Peptide
1	F	115	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2717	0	2798	162	2
1	B	2717	0	2798	152	4
1	C	2717	0	2798	136	0
1	D	2717	0	2797	162	3
1	E	2717	0	2798	180	0
1	F	2717	0	2798	154	0
2	B	5	0	0	6	0
2	C	5	0	0	4	0
2	E	5	0	0	2	0
3	F	27	0	12	7	0
All	All	16344	0	16799	845	5

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 26.

All (845) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:MSE:SE	1:E:136:MSE:CE	2.14	1.44
1:B:136:MSE:SE	1:B:136:MSE:CE	2.14	1.44
1:A:136:MSE:CE	1:A:136:MSE:SE	2.18	1.42
1:A:218:MSE:CE	1:A:218:MSE:SE	2.18	1.41
1:C:136:MSE:SE	1:C:136:MSE:CE	2.19	1.41
1:D:136:MSE:SE	1:D:136:MSE:CE	2.23	1.35
1:A:304:ASN:OD1	1:B:259:LEU:HD21	1.29	1.26
1:A:71:LYS:NZ	1:A:196:LYS:HE2	1.53	1.24
1:E:229:ARG:NH1	1:F:144:PRO:HB2	1.52	1.22
1:C:264:GLN:HE22	1:D:353:PRO:HA	1.09	1.17
1:D:307:ARG:HD3	1:E:258:PRO:CA	1.77	1.15
1:C:264:GLN:NE2	1:D:353:PRO:HA	1.62	1.13
1:A:149:LYS:H	1:A:149:LYS:HD3	1.06	1.12
1:F:259:LEU:HA	1:F:262:GLN:HB2	1.31	1.12
1:B:149:LYS:HD3	1:B:149:LYS:H	1.12	1.11
1:D:307:ARG:CD	1:E:258:PRO:HA	1.81	1.10
1:A:232:GLU:O	1:B:219:ARG:HG3	1.52	1.09
1:E:149:LYS:HD3	1:E:149:LYS:H	1.12	1.09
1:B:259:LEU:HA	1:B:262:GLN:HB2	1.38	1.06
1:E:259:LEU:HA	1:E:262:GLN:HB2	1.36	1.06
1:D:149:LYS:H	1:D:149:LYS:HD3	1.18	1.06
1:A:136:MSE:SE	1:B:252:ARG:HH22	1.89	1.04
1:A:136:MSE:SE	1:B:252:ARG:NH2	2.41	1.04
1:A:71:LYS:HZ2	1:A:196:LYS:HE2	1.06	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LYS:H	1:C:149:LYS:HD3	1.17	1.03
1:B:149:LYS:NZ	2:B:375:SO4:S	2.31	1.03
1:D:307:ARG:HD3	1:E:258:PRO:HA	1.08	1.02
1:B:43:ASP:OD1	1:B:281:LEU:O	1.78	1.02
1:D:259:LEU:HA	1:D:262:GLN:HB2	1.36	1.01
1:C:259:LEU:HA	1:C:262:GLN:HB2	1.41	0.98
1:D:233:THR:CB	1:E:219:ARG:HD2	1.92	0.97
1:C:331:ASN:HA	1:C:334:LEU:HD12	1.46	0.97
1:E:94:PHE:CD2	1:E:111:SER:HA	1.98	0.97
1:A:259:LEU:HA	1:A:262:GLN:HB2	1.43	0.97
1:E:267:ILE:HD13	1:F:355:PRO:HG2	1.44	0.96
1:A:331:ASN:HA	1:A:334:LEU:HD12	1.50	0.94
1:A:304:ASN:OD1	1:B:259:LEU:CD2	2.15	0.93
1:F:71:LYS:HZ2	1:F:196:LYS:HE2	1.32	0.93
1:B:331:ASN:HA	1:B:334:LEU:HD12	1.47	0.93
1:A:307:ARG:HD3	1:B:258:PRO:HG3	1.49	0.92
1:E:196:LYS:HE3	1:E:196:LYS:HA	1.53	0.91
1:A:271:PHE:CE1	1:B:256:ILE:HG22	2.06	0.91
1:F:71:LYS:NZ	1:F:196:LYS:HE2	1.83	0.90
1:E:331:ASN:HA	1:E:334:LEU:HD12	1.54	0.90
1:F:149:LYS:H	1:F:149:LYS:HD3	1.34	0.89
1:C:196:LYS:HE3	1:C:196:LYS:HA	1.52	0.89
1:D:331:ASN:HA	1:D:334:LEU:HD12	1.53	0.89
1:F:149:LYS:H	1:F:149:LYS:CD	1.88	0.87
1:D:136:MSE:SE	1:E:252:ARG:NH2	2.58	0.86
1:C:149:LYS:H	1:C:149:LYS:CD	1.89	0.86
1:D:233:THR:HB	1:E:219:ARG:HD2	1.56	0.86
1:F:331:ASN:HA	1:F:334:LEU:HD12	1.58	0.85
1:D:149:LYS:H	1:D:149:LYS:CD	1.89	0.85
1:E:271:PHE:CE2	1:F:350:GLU:OE1	2.29	0.85
1:A:149:LYS:H	1:A:149:LYS:CD	1.89	0.84
1:A:149:LYS:HD3	1:A:149:LYS:N	1.88	0.84
1:D:94:PHE:HD2	1:D:110:ARG:O	1.60	0.84
1:F:196:LYS:HE3	1:F:196:LYS:HA	1.59	0.84
1:A:271:PHE:CZ	1:B:256:ILE:HG22	2.12	0.84
1:C:42:ILE:O	1:C:43:ASP:HB2	1.77	0.84
1:F:149:LYS:NZ	3:F:500:ADP:PB	2.51	0.84
1:E:149:LYS:HD3	1:E:149:LYS:N	1.93	0.83
1:C:267:ILE:CD1	1:D:355:PRO:HG2	2.08	0.83
1:E:38:PRO:HD3	1:E:56:THR:OG1	1.79	0.82
1:B:149:LYS:HD3	1:B:149:LYS:N	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:LYS:HA	1:D:196:LYS:HE3	1.61	0.82
1:F:149:LYS:HZ2	3:F:500:ADP:PB	2.02	0.82
1:E:94:PHE:HD2	1:E:111:SER:HA	1.42	0.82
1:A:122:LEU:O	1:A:291:LEU:HD23	1.80	0.81
1:A:304:ASN:HD21	1:B:259:LEU:HD23	1.44	0.81
1:F:85:SER:OG	1:F:190:GLU:OE1	1.98	0.81
1:A:71:LYS:HZ3	1:A:196:LYS:HE2	1.46	0.80
1:A:94:PHE:HD2	1:A:110:ARG:O	1.64	0.80
1:F:170:THR:OG1	1:F:188:GLN:HG2	1.81	0.80
1:B:161:ASN:HA	1:B:184:SER:OG	1.82	0.80
1:C:149:LYS:HD3	1:C:149:LYS:N	1.95	0.80
1:D:38:PRO:HD3	1:D:56:THR:OG1	1.82	0.80
1:E:229:ARG:HH12	1:F:144:PRO:HB2	1.46	0.80
1:E:149:LYS:H	1:E:149:LYS:CD	1.94	0.79
1:D:167:HIS:CE1	1:D:169:ILE:HD12	2.17	0.79
1:E:269:LEU:O	1:E:273:LEU:HB2	1.81	0.79
1:D:170:THR:HG22	1:D:214:PHE:HB3	1.65	0.79
1:B:94:PHE:HD2	1:B:110:ARG:O	1.66	0.79
1:D:170:THR:OG1	1:D:188:GLN:HG2	1.83	0.79
1:D:60:THR:HA	1:D:63:LEU:HD12	1.65	0.79
1:A:304:ASN:CG	1:B:259:LEU:HD21	2.02	0.78
1:F:138:LEU:HD22	1:F:140:LEU:HD21	1.65	0.78
1:C:149:LYS:NZ	2:C:375:SO4:S	2.56	0.78
1:D:42:ILE:O	1:D:43:ASP:HB2	1.82	0.78
1:B:60:THR:HA	1:B:63:LEU:HD12	1.66	0.78
1:C:149:LYS:NZ	2:C:375:SO4:O1	2.16	0.78
1:C:170:THR:HG22	1:C:214:PHE:HB3	1.66	0.77
1:E:229:ARG:NH1	1:F:144:PRO:CB	2.43	0.77
1:B:149:LYS:H	1:B:149:LYS:CD	1.93	0.77
1:E:267:ILE:HD13	1:F:355:PRO:CG	2.15	0.77
1:E:335:TYR:HB2	1:E:358:LEU:HD11	1.67	0.77
1:C:170:THR:OG1	1:C:188:GLN:HG2	1.85	0.77
1:E:94:PHE:HE2	1:E:111:SER:HG	1.28	0.77
1:B:42:ILE:O	1:B:43:ASP:HB2	1.85	0.77
1:B:170:THR:OG1	1:B:188:GLN:HG2	1.85	0.76
1:A:60:THR:HA	1:A:63:LEU:HD12	1.67	0.76
1:C:60:THR:HA	1:C:63:LEU:HD12	1.66	0.76
1:A:307:ARG:HD3	1:B:258:PRO:CG	2.14	0.76
1:C:38:PRO:HD3	1:C:56:THR:OG1	1.86	0.76
1:B:284:LYS:HE3	1:B:342:LEU:HD23	1.67	0.76
1:B:335:TYR:HB2	1:B:358:LEU:HD11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LYS:HE3	1:A:196:LYS:HA	1.68	0.76
1:A:161:ASN:HA	1:A:184:SER:OG	1.86	0.76
1:E:170:THR:OG1	1:E:188:GLN:HG2	1.87	0.75
1:A:91:VAL:HG13	1:A:92:GLY:H	1.52	0.75
1:C:264:GLN:NE2	1:D:353:PRO:CA	2.46	0.75
1:F:42:ILE:O	1:F:43:ASP:HB2	1.86	0.75
1:F:122:LEU:O	1:F:291:LEU:HD23	1.86	0.75
1:A:42:ILE:O	1:A:43:ASP:HB2	1.86	0.75
1:B:122:LEU:O	1:B:291:LEU:HD23	1.87	0.74
1:C:94:PHE:HD2	1:C:110:ARG:O	1.70	0.74
1:E:172:GLU:HG2	1:E:214:PHE:HE2	1.52	0.74
1:C:335:TYR:HB2	1:C:358:LEU:HD11	1.69	0.74
1:E:94:PHE:HD2	1:E:110:ARG:O	1.71	0.74
1:F:141:VAL:HG12	1:F:141:VAL:O	1.88	0.74
1:F:149:LYS:NZ	3:F:500:ADP:O1B	2.20	0.74
1:D:271:PHE:HE1	1:E:255:ASP:HB3	1.52	0.74
1:F:161:ASN:HA	1:F:184:SER:OG	1.87	0.74
1:C:138:LEU:HD22	1:C:140:LEU:HD21	1.70	0.74
1:D:136:MSE:SE	1:E:252:ARG:HH21	2.20	0.74
1:A:58:GLU:O	1:A:58:GLU:HG2	1.88	0.73
1:C:161:ASN:HA	1:C:184:SER:OG	1.87	0.73
1:C:267:ILE:HD13	1:D:355:PRO:HG2	1.70	0.73
1:A:170:THR:OG1	1:A:188:GLN:HG2	1.87	0.73
1:E:91:VAL:HG13	1:E:92:GLY:H	1.53	0.73
1:C:267:ILE:HD13	1:D:355:PRO:CG	2.18	0.73
1:C:205:ALA:HA	1:C:208:GLU:OE2	1.88	0.73
1:E:12:GLU:HA	1:E:52:PHE:CE1	2.23	0.73
1:D:149:LYS:HD3	1:D:149:LYS:N	1.94	0.73
1:D:172:GLU:HG2	1:D:214:PHE:HE2	1.53	0.73
1:F:269:LEU:O	1:F:273:LEU:HB2	1.89	0.73
1:E:94:PHE:HE2	1:E:111:SER:OG	1.72	0.72
1:C:271:PHE:CD1	1:D:346:GLU:HG3	2.23	0.72
1:F:38:PRO:HD3	1:F:56:THR:OG1	1.88	0.72
1:E:161:ASN:HA	1:E:184:SER:OG	1.88	0.72
1:C:122:LEU:O	1:C:291:LEU:HD23	1.90	0.72
1:C:63:LEU:O	1:C:66:SER:OG	2.08	0.72
1:D:30:ILE:CD1	1:D:32:LEU:HD21	2.20	0.71
1:D:161:ASN:HA	1:D:184:SER:OG	1.89	0.71
1:F:335:TYR:HB2	1:F:358:LEU:HD11	1.72	0.71
1:E:170:THR:HG22	1:E:214:PHE:HB3	1.72	0.71
1:D:269:LEU:O	1:D:273:LEU:HB2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:PHE:CE2	1:E:111:SER:HA	2.25	0.70
1:B:76:LEU:HG	1:B:76:LEU:O	1.91	0.70
1:B:269:LEU:O	1:B:273:LEU:HB2	1.92	0.70
1:A:71:LYS:NZ	1:A:196:LYS:CE	2.45	0.70
1:F:119:PHE:CD1	1:F:129:LEU:HG	2.26	0.70
1:B:138:LEU:HD22	1:B:140:LEU:HD21	1.74	0.70
1:E:42:ILE:O	1:E:43:ASP:HB2	1.90	0.70
1:F:218:MSE:HE3	1:F:224:VAL:HG22	1.74	0.69
1:F:284:LYS:HE3	1:F:342:LEU:HD23	1.73	0.69
1:B:91:VAL:HG13	1:B:92:GLY:H	1.56	0.69
1:E:122:LEU:O	1:E:291:LEU:HD23	1.92	0.69
1:E:60:THR:HA	1:E:63:LEU:HD12	1.75	0.69
1:A:279:GLN:O	1:A:280:ARG:HG3	1.93	0.69
1:D:94:PHE:CD2	1:D:110:ARG:O	2.45	0.69
1:E:229:ARG:CZ	1:F:144:PRO:HB2	2.22	0.69
1:A:271:PHE:CZ	1:B:256:ILE:CG2	2.76	0.68
1:A:138:LEU:HD22	1:A:140:LEU:HD21	1.76	0.68
1:D:307:ARG:HD3	1:E:258:PRO:CB	2.22	0.68
1:C:172:GLU:HG2	1:C:214:PHE:HE2	1.58	0.68
1:C:284:LYS:HE3	1:C:342:LEU:HD23	1.75	0.68
1:A:170:THR:HG22	1:A:214:PHE:HB3	1.75	0.68
1:A:195:THR:HG21	1:A:201:ALA:HB2	1.75	0.68
1:D:233:THR:HA	1:E:219:ARG:NE	2.09	0.68
1:E:172:GLU:HG2	1:E:214:PHE:CE2	2.28	0.68
1:E:96:ALA:HA	1:E:109:LEU:HD23	1.76	0.67
1:A:137:GLY:HA2	1:A:272:ILE:HG13	1.74	0.67
1:C:218:MSE:HE3	1:C:224:VAL:HG22	1.74	0.67
1:F:149:LYS:CD	1:F:149:LYS:N	2.58	0.67
1:A:188:GLN:H	1:B:101:GLN:HE21	1.41	0.67
1:B:218:MSE:HE3	1:B:224:VAL:HG22	1.76	0.67
1:F:12:GLU:HA	1:F:52:PHE:CE1	2.30	0.67
1:D:30:ILE:HD13	1:D:32:LEU:HD21	1.76	0.67
1:F:60:THR:HA	1:F:63:LEU:HD12	1.74	0.67
1:E:137:GLY:HA2	1:E:272:ILE:HG13	1.76	0.67
1:C:49:LEU:C	1:C:51:ASP:H	1.97	0.67
1:D:119:PHE:CD1	1:D:129:LEU:HG	2.30	0.67
1:D:335:TYR:HB2	1:D:358:LEU:HD11	1.76	0.67
1:D:122:LEU:O	1:D:291:LEU:HD23	1.95	0.66
1:D:284:LYS:HE3	1:D:342:LEU:HD23	1.76	0.66
1:C:208:GLU:HG2	1:D:99:PHE:CE1	2.30	0.66
1:A:335:TYR:HB2	1:A:358:LEU:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:LEU:HD11	1:C:276:ILE:HG13	1.76	0.66
1:B:12:GLU:HA	1:B:52:PHE:CE1	2.30	0.66
1:D:91:VAL:HG13	1:D:92:GLY:H	1.61	0.66
1:D:218:MSE:HE3	1:D:224:VAL:HG22	1.77	0.66
1:D:172:GLU:HG2	1:D:214:PHE:CE2	2.30	0.66
1:D:233:THR:HA	1:E:219:ARG:HE	1.60	0.66
1:B:149:LYS:O	1:B:153:ILE:HG12	1.96	0.66
1:D:149:LYS:CD	1:D:149:LYS:N	2.52	0.65
1:A:269:LEU:O	1:A:273:LEU:HB2	1.97	0.65
1:E:138:LEU:HD22	1:E:140:LEU:HD21	1.77	0.65
1:B:38:PRO:HD3	1:B:56:THR:OG1	1.97	0.65
1:B:149:LYS:HD3	2:B:375:SO4:O4	1.96	0.65
1:F:91:VAL:HG13	1:F:92:GLY:H	1.62	0.65
1:F:137:GLY:HA2	1:F:272:ILE:HG13	1.77	0.65
1:A:307:ARG:HD3	1:B:258:PRO:CB	2.26	0.65
1:D:273:LEU:HD11	1:D:276:ILE:HG13	1.79	0.65
1:A:271:PHE:CE1	1:B:256:ILE:CG2	2.79	0.65
1:A:12:GLU:HA	1:A:52:PHE:CE1	2.32	0.65
1:A:85:SER:OG	1:A:190:GLU:OE1	2.12	0.65
1:B:172:GLU:HG2	1:B:214:PHE:HE2	1.62	0.65
1:B:196:LYS:HE3	1:B:196:LYS:HA	1.77	0.65
1:C:264:GLN:NE2	1:D:353:PRO:O	2.29	0.64
1:D:188:GLN:H	1:E:101:GLN:HE21	1.45	0.64
1:F:49:LEU:C	1:F:51:ASP:H	2.00	0.64
1:D:224:VAL:HG21	1:D:256:ILE:HD11	1.80	0.64
1:E:69:SER:O	1:E:73:ARG:HG3	1.97	0.64
1:B:119:PHE:CD1	1:B:129:LEU:HG	2.33	0.64
1:F:94:PHE:HD2	1:F:110:ARG:O	1.80	0.64
1:D:138:LEU:HD22	1:D:140:LEU:HD21	1.80	0.64
1:D:304:ASN:OD1	1:E:259:LEU:HD11	1.98	0.64
1:C:149:LYS:CD	1:C:149:LYS:N	2.55	0.64
1:F:132:CYS:SG	1:F:156:MSE:HB3	2.37	0.64
1:F:269:LEU:HG	1:F:273:LEU:HD23	1.80	0.64
1:A:240:THR:C	1:A:241:LEU:HD12	2.19	0.64
1:C:12:GLU:HA	1:C:52:PHE:CE1	2.33	0.63
1:D:71:LYS:HD3	1:D:192:GLY:O	1.98	0.63
1:E:150:SER:OG	2:E:375:SO4:O2	2.16	0.63
1:E:271:PHE:HE1	1:F:346:GLU:HG3	1.64	0.63
1:E:136:MSE:HE2	1:E:234:GLY:HA2	1.81	0.63
1:F:273:LEU:HD11	1:F:276:ILE:HG13	1.79	0.63
1:E:284:LYS:H	1:E:288:GLY:HA2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:PHE:CD1	1:E:129:LEU:HG	2.33	0.63
1:A:167:HIS:ND1	1:A:210:PRO:HA	2.14	0.63
1:B:167:HIS:ND1	1:B:210:PRO:HA	2.13	0.63
1:D:167:HIS:HE1	1:D:169:ILE:HD12	1.62	0.63
1:F:76:LEU:O	1:F:76:LEU:HG	1.99	0.63
1:B:273:LEU:HD11	1:B:276:ILE:HG13	1.81	0.62
1:E:30:ILE:CD1	1:E:32:LEU:HD21	2.30	0.62
1:A:273:LEU:HD11	1:A:276:ILE:HG13	1.82	0.62
1:A:269:LEU:HG	1:A:273:LEU:HD23	1.80	0.62
1:A:284:LYS:HE3	1:A:342:LEU:HD23	1.82	0.62
1:B:94:PHE:CD2	1:B:110:ARG:O	2.50	0.62
1:F:195:THR:HG22	1:F:196:LYS:H	1.65	0.62
1:A:119:PHE:CD1	1:A:129:LEU:HG	2.35	0.62
1:B:170:THR:HG22	1:B:214:PHE:HB3	1.80	0.62
1:F:149:LYS:O	1:F:153:ILE:HG12	2.00	0.62
1:C:195:THR:HG21	1:C:201:ALA:HB2	1.82	0.62
1:E:36:ALA:HB1	1:E:37:PRO:HD2	1.82	0.61
1:A:71:LYS:HD2	1:A:196:LYS:HZ3	1.63	0.61
1:C:187:ASN:HA	1:D:101:GLN:HE21	1.65	0.61
1:C:269:LEU:O	1:C:273:LEU:HB2	1.99	0.61
1:F:294:GLU:HB2	1:F:330:MSE:HG2	1.82	0.61
1:B:137:GLY:HA2	1:B:272:ILE:HG13	1.82	0.61
1:C:172:GLU:HG2	1:C:214:PHE:CE2	2.36	0.61
1:D:195:THR:HG22	1:D:196:LYS:H	1.66	0.61
1:F:149:LYS:HD3	1:F:149:LYS:N	2.10	0.61
1:E:264:GLN:HE21	1:F:353:PRO:HA	1.66	0.61
1:F:149:LYS:HZ3	3:F:500:ADP:PB	2.23	0.61
1:C:141:VAL:HG12	1:C:141:VAL:O	2.01	0.60
1:B:205:ALA:HA	1:B:208:GLU:OE2	2.00	0.60
1:D:67:VAL:HG13	1:D:86:PHE:CD1	2.35	0.60
1:D:137:GLY:HA2	1:D:272:ILE:HG13	1.83	0.60
1:A:99:PHE:CE1	1:F:208:GLU:HG2	2.36	0.60
1:A:49:LEU:C	1:A:51:ASP:H	2.05	0.60
1:B:149:LYS:N	1:B:149:LYS:CD	2.61	0.60
1:A:218:MSE:HE3	1:A:224:VAL:HG22	1.83	0.60
1:F:67:VAL:HG13	1:F:86:PHE:CD1	2.36	0.60
1:F:150:SER:OG	3:F:500:ADP:O3B	2.20	0.59
1:E:49:LEU:C	1:E:51:ASP:H	2.06	0.59
1:B:172:GLU:HG2	1:B:214:PHE:CE2	2.37	0.59
1:C:284:LYS:H	1:C:288:GLY:HA2	1.67	0.59
1:D:195:THR:HG21	1:D:201:ALA:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:VAL:HG21	1:E:256:ILE:HD11	1.84	0.59
1:D:233:THR:OG1	1:E:219:ARG:HD2	2.02	0.59
1:B:96:ALA:HA	1:B:109:LEU:HD23	1.84	0.59
1:D:12:GLU:HA	1:D:52:PHE:CE1	2.38	0.59
1:E:264:GLN:NE2	1:F:353:PRO:HA	2.17	0.59
1:F:141:VAL:HG12	1:F:149:LYS:HB3	1.84	0.59
1:A:271:PHE:CD1	1:B:256:ILE:HG22	2.38	0.58
1:A:304:ASN:HD21	1:B:259:LEU:CD2	2.13	0.58
1:E:114:ALA:O	1:E:115:GLU:HB3	2.01	0.58
1:A:71:LYS:CD	1:A:196:LYS:NZ	2.67	0.58
1:A:195:THR:HG22	1:A:196:LYS:H	1.68	0.58
1:B:162:GLN:HG2	1:B:182:LYS:HG2	1.85	0.58
1:C:69:SER:O	1:C:73:ARG:HG3	2.03	0.58
1:C:162:GLN:HG2	1:C:182:LYS:HG2	1.85	0.58
1:E:304:ASN:HD22	1:E:307:ARG:HH11	1.49	0.58
1:F:167:HIS:ND1	1:F:210:PRO:HA	2.19	0.58
1:D:205:ALA:HA	1:D:208:GLU:OE2	2.02	0.58
1:D:63:LEU:O	1:D:66:SER:OG	2.20	0.58
1:F:224:VAL:HG21	1:F:256:ILE:HD11	1.85	0.58
1:D:208:GLU:HG2	1:E:99:PHE:CE1	2.38	0.58
1:E:273:LEU:HD11	1:E:276:ILE:HG13	1.85	0.58
1:E:141:VAL:O	1:E:141:VAL:HG12	2.03	0.58
1:F:131:LEU:HD21	1:F:274:GLN:O	2.04	0.58
1:A:94:PHE:CD2	1:A:110:ARG:O	2.53	0.58
1:A:136:MSE:SE	1:B:252:ARG:HH21	2.34	0.58
1:A:101:GLN:HE21	1:F:187:ASN:HA	1.69	0.58
1:D:259:LEU:CA	1:D:262:GLN:HB2	2.24	0.58
1:E:94:PHE:HE2	1:E:111:SER:CB	2.16	0.58
1:E:166:TYR:O	1:E:184:SER:HB2	2.04	0.58
1:A:71:LYS:HD3	1:A:196:LYS:HZ1	1.69	0.57
1:A:304:ASN:ND2	1:B:259:LEU:CD2	2.67	0.57
1:E:271:PHE:CE1	1:F:346:GLU:HG3	2.40	0.57
1:F:349:MSE:SE	1:F:355:PRO:HA	2.54	0.57
1:C:304:ASN:HD22	1:C:307:ARG:HH11	1.52	0.57
1:C:56:THR:HG22	1:C:57:PRO:HD2	1.86	0.57
1:D:141:VAL:HG12	1:D:149:LYS:HB3	1.87	0.57
1:E:94:PHE:CD2	1:E:110:ARG:O	2.54	0.57
1:F:304:ASN:HD22	1:F:307:ARG:HH11	1.52	0.57
1:A:172:GLU:HG2	1:A:214:PHE:CE2	2.39	0.57
1:B:304:ASN:HD22	1:B:307:ARG:HH11	1.52	0.57
1:E:284:LYS:HE3	1:E:342:LEU:HD23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:VAL:HG13	1:B:86:PHE:CD1	2.40	0.57
1:C:170:THR:HG1	1:C:188:GLN:HG2	1.69	0.57
1:A:304:ASN:ND2	1:B:259:LEU:HD23	2.18	0.56
1:B:224:VAL:HG21	1:B:256:ILE:HD11	1.86	0.56
1:E:131:LEU:HD21	1:E:274:GLN:O	2.06	0.56
1:E:294:GLU:HB2	1:E:330:MSE:HG2	1.87	0.56
1:C:279:GLN:O	1:C:280:ARG:HG3	2.05	0.56
1:C:91:VAL:HG13	1:C:92:GLY:H	1.70	0.56
1:D:167:HIS:ND1	1:D:210:PRO:HA	2.20	0.56
1:D:233:THR:HA	1:E:219:ARG:CD	2.36	0.56
1:E:67:VAL:HG13	1:E:86:PHE:CD1	2.40	0.56
1:E:218:MSE:HE3	1:E:224:VAL:HG22	1.86	0.56
1:A:205:ALA:HA	1:A:208:GLU:OE2	2.06	0.56
1:B:169:ILE:HG13	1:B:187:ASN:HB2	1.87	0.55
1:B:63:LEU:O	1:B:66:SER:OG	2.23	0.55
1:B:194:ASP:O	1:C:80:GLY:HA3	2.04	0.55
1:C:264:GLN:CD	1:D:353:PRO:O	2.44	0.55
1:D:132:CYS:SG	1:D:156:MSE:HB3	2.47	0.55
1:C:94:PHE:CD2	1:C:110:ARG:O	2.55	0.55
1:D:96:ALA:HA	1:D:109:LEU:HD23	1.88	0.55
1:E:68:MSE:HE3	1:E:82:VAL:HG21	1.88	0.55
1:B:284:LYS:H	1:B:288:GLY:HA2	1.71	0.55
1:C:67:VAL:HG13	1:C:86:PHE:CD1	2.41	0.55
1:D:36:ALA:HB1	1:D:37:PRO:HD2	1.89	0.55
1:F:95:ARG:NH1	1:F:174:PRO:HD3	2.21	0.55
1:D:294:GLU:HB2	1:D:330:MSE:HG2	1.89	0.55
1:A:307:ARG:HD3	1:B:258:PRO:HB3	1.86	0.55
1:B:149:LYS:NZ	2:B:375:SO4:O4	2.29	0.55
1:B:195:THR:HG21	1:B:201:ALA:HB2	1.89	0.55
1:C:141:VAL:HG12	1:C:149:LYS:HB3	1.88	0.55
1:E:270:SER:HB3	1:E:306:ILE:HB	1.88	0.55
1:F:318:MSE:C	1:F:319:GLN:HG3	2.26	0.55
1:B:269:LEU:HG	1:B:273:LEU:HD23	1.89	0.55
1:B:279:GLN:O	1:B:280:ARG:HG3	2.07	0.55
1:D:162:GLN:HG2	1:D:182:LYS:HG2	1.89	0.55
1:D:56:THR:HG22	1:D:57:PRO:HD2	1.89	0.55
1:F:279:GLN:O	1:F:280:ARG:HG3	2.07	0.55
1:A:76:LEU:O	1:A:76:LEU:HG	2.07	0.54
1:C:267:ILE:CD1	1:D:355:PRO:CG	2.81	0.54
1:A:141:VAL:HG12	1:A:141:VAL:O	2.06	0.54
1:D:229:ARG:O	1:D:233:THR:HG22	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:LYS:O	1:E:153:ILE:HG12	2.06	0.54
1:E:271:PHE:CD2	1:F:350:GLU:OE1	2.59	0.54
1:F:170:THR:HG22	1:F:214:PHE:HB3	1.89	0.54
1:A:67:VAL:HG13	1:A:86:PHE:CD1	2.41	0.54
1:B:131:LEU:HD21	1:B:274:GLN:O	2.07	0.54
1:D:207:ARG:HD2	1:E:83:ASP:OD1	2.07	0.54
1:E:269:LEU:HG	1:E:273:LEU:HD23	1.90	0.54
1:F:169:ILE:HG13	1:F:187:ASN:HB2	1.89	0.54
1:A:71:LYS:HZ3	1:A:196:LYS:CE	2.14	0.54
1:D:49:LEU:C	1:D:51:ASP:H	2.10	0.54
1:E:56:THR:HG22	1:E:57:PRO:HD2	1.90	0.54
1:C:196:LYS:HE3	1:C:196:LYS:CA	2.32	0.54
1:D:122:LEU:HD21	1:D:152:THR:HA	1.89	0.54
1:A:131:LEU:HD21	1:A:274:GLN:O	2.08	0.54
1:E:187:ASN:HA	1:F:101:GLN:HE21	1.72	0.54
1:E:309:ASN:O	1:E:311:LEU:HG	2.08	0.54
1:A:56:THR:HG22	1:A:57:PRO:HD2	1.90	0.54
1:B:259:LEU:CA	1:B:262:GLN:HB2	2.25	0.54
1:E:15:ILE:HG23	1:E:16:LEU:H	1.73	0.54
1:E:168:ILE:HG23	1:E:212:VAL:HB	1.90	0.54
1:F:119:PHE:CE1	1:F:129:LEU:HG	2.43	0.54
1:B:210:PRO:HG2	1:B:213:ILE:HD11	1.89	0.54
1:C:22:ALA:O	1:C:27:ALA:CB	2.56	0.54
1:D:232:GLU:O	1:E:219:ARG:HD3	2.08	0.54
1:D:233:THR:CA	1:E:219:ARG:HD2	2.37	0.54
1:F:195:THR:HG21	1:F:201:ALA:HB2	1.89	0.54
1:A:71:LYS:HD2	1:A:196:LYS:NZ	2.22	0.54
1:A:270:SER:HB3	1:A:306:ILE:HB	1.89	0.54
1:C:137:GLY:HA2	1:C:272:ILE:HG13	1.89	0.54
1:F:138:LEU:HD22	1:F:140:LEU:CD2	2.36	0.54
1:D:304:ASN:HD22	1:D:307:ARG:HH11	1.57	0.53
1:E:259:LEU:HD23	1:E:259:LEU:H	1.71	0.53
1:F:205:ALA:HA	1:F:208:GLU:OE2	2.07	0.53
1:A:169:ILE:HG13	1:A:187:ASN:HB2	1.90	0.53
1:B:52:PHE:HB3	1:B:53:PRO:HD3	1.88	0.53
1:F:170:THR:HG1	1:F:188:GLN:HG2	1.71	0.53
1:F:202:LEU:O	1:F:205:ALA:N	2.42	0.53
1:C:149:LYS:HD3	2:C:375:SO4:O3	2.08	0.53
1:D:271:PHE:CE1	1:E:255:ASP:HB3	2.40	0.53
1:E:167:HIS:ND1	1:E:210:PRO:HA	2.24	0.53
1:A:96:ALA:HA	1:A:109:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ASN:CG	1:B:259:LEU:CD2	2.72	0.53
1:B:65:TYR:HD1	1:B:73:ARG:NH1	2.07	0.53
1:C:270:SER:HB3	1:C:306:ILE:HB	1.90	0.53
1:A:172:GLU:HG2	1:A:214:PHE:HE2	1.71	0.53
1:E:170:THR:HG1	1:E:188:GLN:HG2	1.72	0.53
1:E:149:LYS:N	1:E:149:LYS:CD	2.62	0.53
1:F:71:LYS:HZ2	1:F:196:LYS:CE	2.15	0.53
1:F:136:MSE:HE2	1:F:234:GLY:HA2	1.90	0.53
1:C:42:ILE:O	1:C:43:ASP:CB	2.53	0.53
1:C:119:PHE:CD1	1:C:129:LEU:HG	2.43	0.53
1:F:71:LYS:NZ	1:F:196:LYS:CE	2.64	0.53
1:E:149:LYS:NZ	2:E:375:SO4:O1	2.42	0.53
1:F:151:THR:OG1	3:F:500:ADP:O1A	2.24	0.53
1:F:166:TYR:O	1:F:184:SER:HB2	2.09	0.53
1:C:122:LEU:HD21	1:C:152:THR:HA	1.90	0.53
1:E:169:ILE:HG13	1:E:187:ASN:HB2	1.90	0.53
1:F:63:LEU:O	1:F:66:SER:OG	2.27	0.53
1:F:86:PHE:H	1:F:86:PHE:HD2	1.56	0.53
1:D:304:ASN:OD1	1:E:259:LEU:CD1	2.56	0.53
1:B:146:GLY:N	2:B:375:SO4:O3	2.38	0.52
1:D:131:LEU:HD21	1:D:274:GLN:O	2.09	0.52
1:E:30:ILE:HD13	1:E:32:LEU:HD21	1.89	0.52
1:A:65:TYR:CD1	1:A:73:ARG:HD2	2.43	0.52
1:A:122:LEU:HD21	1:A:152:THR:HA	1.91	0.52
1:D:76:LEU:HG	1:D:76:LEU:O	2.09	0.52
1:E:132:CYS:SG	1:E:156:MSE:HB3	2.49	0.52
1:F:94:PHE:CD2	1:F:111:SER:HA	2.44	0.52
1:F:358:LEU:C	1:F:360:ARG:H	2.13	0.52
1:B:69:SER:O	1:B:73:ARG:HG3	2.09	0.52
1:B:185:ILE:HD11	1:C:33:THR:HB	1.91	0.52
1:D:269:LEU:HG	1:D:273:LEU:HD23	1.91	0.52
1:C:229:ARG:O	1:C:233:THR:HG22	2.08	0.52
1:F:96:ALA:HA	1:F:109:LEU:HD23	1.92	0.52
1:C:49:LEU:C	1:C:51:ASP:N	2.62	0.52
1:C:138:LEU:HD22	1:C:140:LEU:CD2	2.39	0.52
1:C:294:GLU:HB2	1:C:330:MSE:HG2	1.92	0.52
1:E:240:THR:C	1:E:241:LEU:HD12	2.30	0.52
1:F:49:LEU:C	1:F:51:ASP:N	2.63	0.52
1:F:153:ILE:O	1:F:155:SER:N	2.43	0.52
1:A:195:THR:HG22	1:A:196:LYS:N	2.24	0.52
1:A:207:ARG:HD2	1:B:83:ASP:OD1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:MSE:SE	1:B:98:VAL:HG21	2.60	0.52
1:C:131:LEU:HD21	1:C:274:GLN:O	2.10	0.52
1:D:169:ILE:HG13	1:D:187:ASN:HB2	1.90	0.52
1:D:200:ASP:HB2	1:E:81:GLN:HE22	1.74	0.52
1:E:205:ALA:HA	1:E:208:GLU:OE2	2.10	0.52
1:A:86:PHE:H	1:A:86:PHE:HD2	1.57	0.52
1:D:149:LYS:O	1:D:153:ILE:HG12	2.09	0.52
1:A:170:THR:HG1	1:A:188:GLN:HG2	1.75	0.52
1:A:208:GLU:HG2	1:B:99:PHE:CE1	2.45	0.52
1:B:56:THR:HG22	1:B:57:PRO:HD2	1.90	0.52
1:E:22:ALA:O	1:E:27:ALA:CB	2.58	0.52
1:F:270:SER:HB3	1:F:306:ILE:HB	1.92	0.52
1:C:76:LEU:O	1:C:76:LEU:HG	2.10	0.52
1:C:170:THR:HB	1:C:214:PHE:HD2	1.75	0.52
1:F:331:ASN:ND2	1:F:352:SER:OG	2.43	0.51
1:B:105:VAL:HG12	1:B:106:ALA:N	2.25	0.51
1:B:264:GLN:HA	1:B:267:ILE:HD12	1.90	0.51
1:B:149:LYS:NZ	2:B:375:SO4:O3	2.38	0.51
1:F:196:LYS:HE3	1:F:196:LYS:CA	2.38	0.51
1:A:309:ASN:O	1:A:311:LEU:HG	2.10	0.51
1:C:271:PHE:CD1	1:D:346:GLU:CG	2.91	0.51
1:D:85:SER:OG	1:D:174:PRO:HB2	2.11	0.51
1:C:224:VAL:HG21	1:C:256:ILE:HD11	1.93	0.51
1:F:68:MSE:HE3	1:F:82:VAL:HG21	1.92	0.51
1:A:85:SER:OG	1:A:174:PRO:HB2	2.10	0.51
1:D:30:ILE:CD1	1:D:32:LEU:CD2	2.87	0.51
1:A:84:PHE:CE2	1:A:96:ALA:HB3	2.46	0.51
1:F:204:ALA:O	1:F:205:ALA:C	2.49	0.51
1:C:169:ILE:HG13	1:C:187:ASN:HB2	1.91	0.51
1:A:187:ASN:HA	1:B:101:GLN:HE21	1.76	0.50
1:E:267:ILE:CD1	1:F:355:PRO:HG2	2.29	0.50
1:B:187:ASN:HA	1:C:101:GLN:HE21	1.76	0.50
1:C:167:HIS:CE1	1:C:169:ILE:HD12	2.47	0.50
1:F:172:GLU:HG2	1:F:214:PHE:CE2	2.46	0.50
1:A:144:PRO:HB2	1:F:229:ARG:NH1	2.27	0.50
1:D:69:SER:O	1:D:73:ARG:HG3	2.11	0.50
1:D:200:ASP:HB2	1:E:81:GLN:NE2	2.26	0.50
1:D:347:ASP:O	1:D:350:GLU:HB3	2.11	0.50
1:E:279:GLN:O	1:E:280:ARG:HG3	2.10	0.50
1:E:122:LEU:HD21	1:E:152:THR:HA	1.92	0.50
1:C:130:GLU:HG2	1:C:134:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:PRO:HB2	1:D:177:TYR:CE1	2.46	0.50
1:E:52:PHE:HB3	1:E:53:PRO:HD3	1.93	0.50
1:B:294:GLU:HB2	1:B:330:MSE:HG2	1.92	0.50
1:C:264:GLN:HA	1:C:267:ILE:HD12	1.93	0.50
1:D:195:THR:HG22	1:D:196:LYS:N	2.24	0.50
1:E:15:ILE:HG23	1:E:16:LEU:N	2.27	0.50
1:B:94:PHE:CD2	1:B:111:SER:HA	2.47	0.50
1:C:175:ILE:HD11	1:C:190:GLU:HB2	1.92	0.50
1:D:279:GLN:O	1:D:280:ARG:HG3	2.11	0.50
1:E:105:VAL:HG12	1:E:106:ALA:N	2.27	0.50
1:E:171:ILE:HD11	1:E:202:LEU:HA	1.93	0.50
1:F:149:LYS:HD3	3:F:500:ADP:O3B	2.12	0.50
1:F:168:ILE:HG23	1:F:212:VAL:HB	1.93	0.50
1:B:142:THR:HG21	1:B:249:THR:OG1	2.12	0.50
1:D:31:HIS:C	1:D:32:LEU:HD23	2.32	0.50
1:E:48:PHE:CD1	1:E:48:PHE:N	2.80	0.50
1:E:49:LEU:C	1:E:51:ASP:N	2.65	0.50
1:E:284:LYS:HG2	1:E:286:GLY:H	1.76	0.50
1:F:135:LYS:HD3	1:F:135:LYS:H	1.77	0.50
1:F:240:THR:C	1:F:241:LEU:HD12	2.31	0.50
1:A:41:ARG:HD3	1:A:44:GLY:HA2	1.94	0.50
1:B:195:THR:HG22	1:B:196:LYS:H	1.76	0.50
1:B:240:THR:C	1:B:241:LEU:HD12	2.32	0.50
1:C:166:TYR:O	1:C:184:SER:HB2	2.12	0.50
1:D:168:ILE:HG23	1:D:212:VAL:HB	1.94	0.50
1:E:167:HIS:CE1	1:E:169:ILE:HD12	2.47	0.50
1:A:294:GLU:HB2	1:A:330:MSE:HG2	1.93	0.49
1:B:49:LEU:C	1:B:51:ASP:H	2.14	0.49
1:A:158:ASP:O	1:A:161:ASN:HB3	2.13	0.49
1:D:229:ARG:O	1:D:233:THR:CG2	2.60	0.49
1:E:36:ALA:HB1	1:E:37:PRO:CD	2.41	0.49
1:F:122:LEU:HD21	1:F:152:THR:HA	1.94	0.49
1:A:36:ALA:HB1	1:A:37:PRO:HD2	1.94	0.49
1:D:41:ARG:HD3	1:D:44:GLY:HA2	1.94	0.49
1:A:233:THR:HB	1:B:219:ARG:HG2	1.94	0.49
1:A:331:ASN:ND2	1:A:352:SER:OG	2.46	0.49
1:C:194:ASP:O	1:D:80:GLY:HA3	2.12	0.49
1:E:195:THR:HG22	1:E:196:LYS:H	1.78	0.49
1:B:135:LYS:H	1:B:135:LYS:HD3	1.78	0.49
1:B:167:HIS:CE1	1:B:169:ILE:HD12	2.48	0.49
1:D:240:THR:C	1:D:241:LEU:HD12	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LEU:HD21	1:B:152:THR:HA	1.94	0.49
1:B:218:MSE:HE2	1:B:241:LEU:HD11	1.94	0.49
1:E:210:PRO:HG2	1:E:213:ILE:HD11	1.93	0.49
1:F:210:PRO:HG2	1:F:213:ILE:HD11	1.94	0.49
1:A:22:ALA:O	1:A:27:ALA:CB	2.60	0.49
1:E:284:LYS:N	1:E:288:GLY:HA2	2.28	0.49
1:A:299:ASN:O	1:A:301:ALA:N	2.46	0.48
1:A:224:VAL:HG21	1:A:256:ILE:HD11	1.95	0.48
1:B:94:PHE:HD2	1:B:111:SER:HA	1.77	0.48
1:C:22:ALA:O	1:C:27:ALA:HB3	2.13	0.48
1:C:349:MSE:SE	1:C:355:PRO:HA	2.63	0.48
1:F:52:PHE:HB3	1:F:53:PRO:HD3	1.94	0.48
1:A:284:LYS:H	1:A:288:GLY:HA2	1.78	0.48
1:B:36:ALA:HB1	1:B:37:PRO:HD2	1.95	0.48
1:B:331:ASN:ND2	1:B:352:SER:OG	2.47	0.48
1:E:347:ASP:O	1:E:350:GLU:HB3	2.14	0.48
1:F:153:ILE:O	1:F:154:ALA:C	2.52	0.48
1:F:254:VAL:HG12	1:F:262:GLN:HG2	1.94	0.48
1:A:202:LEU:O	1:A:205:ALA:N	2.46	0.48
1:E:195:THR:HG21	1:E:201:ALA:HB2	1.95	0.48
1:E:254:VAL:HG12	1:E:262:GLN:HG2	1.95	0.48
1:F:172:GLU:HG2	1:F:214:PHE:HE2	1.77	0.48
1:A:240:THR:O	1:A:241:LEU:HD12	2.12	0.48
1:A:284:LYS:HG2	1:A:286:GLY:H	1.79	0.48
1:C:96:ALA:HA	1:C:109:LEU:HD23	1.96	0.48
1:C:132:CYS:SG	1:C:156:MSE:HB3	2.54	0.48
1:D:38:PRO:HD3	1:D:56:THR:HG1	1.79	0.48
1:D:119:PHE:CE1	1:D:129:LEU:HG	2.48	0.48
1:E:264:GLN:HA	1:E:267:ILE:HD12	1.95	0.48
1:F:229:ARG:O	1:F:233:THR:HG22	2.13	0.48
1:A:52:PHE:HB3	1:A:53:PRO:HD3	1.96	0.48
1:B:168:ILE:HG23	1:B:212:VAL:HB	1.95	0.48
1:C:218:MSE:HE2	1:C:241:LEU:HD11	1.95	0.48
1:F:36:ALA:HB1	1:F:37:PRO:HD2	1.94	0.48
1:F:69:SER:O	1:F:73:ARG:HG3	2.14	0.48
1:B:86:PHE:CE2	1:B:94:PHE:HB2	2.49	0.48
1:C:86:PHE:H	1:C:86:PHE:HD2	1.62	0.48
1:E:63:LEU:O	1:E:66:SER:OG	2.29	0.48
1:F:171:ILE:HD11	1:F:202:LEU:HA	1.95	0.48
1:A:358:LEU:C	1:A:360:ARG:H	2.17	0.47
1:E:129:LEU:HD23	1:E:129:LEU:HA	1.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:CZ	1:A:178:VAL:HG23	2.45	0.47
1:B:284:LYS:HG2	1:B:286:GLY:H	1.78	0.47
1:D:257:PHE:CZ	1:D:265:VAL:HG21	2.49	0.47
1:E:196:LYS:HA	1:E:196:LYS:CE	2.36	0.47
1:D:42:ILE:O	1:D:43:ASP:CB	2.56	0.47
1:E:358:LEU:C	1:E:360:ARG:H	2.18	0.47
1:A:254:VAL:HG12	1:A:262:GLN:HG2	1.96	0.47
1:A:271:PHE:CE2	1:B:256:ILE:HG22	2.49	0.47
1:D:175:ILE:H	1:D:175:ILE:HG13	1.53	0.47
1:E:333:THR:O	1:E:333:THR:HG22	2.14	0.47
1:B:343:ILE:HD12	1:B:348:ALA:HB2	1.96	0.47
1:C:149:LYS:O	1:C:153:ILE:HG12	2.14	0.47
1:C:267:ILE:HD13	1:D:355:PRO:HG3	1.94	0.47
1:A:182:LYS:HB3	1:A:183:LYS:H	1.58	0.47
1:A:229:ARG:O	1:A:233:THR:CG2	2.62	0.47
1:B:136:MSE:HE2	1:B:234:GLY:HA2	1.96	0.47
1:D:49:LEU:C	1:D:51:ASP:N	2.68	0.47
1:D:52:PHE:HB3	1:D:53:PRO:HD3	1.95	0.47
1:D:271:PHE:CE2	1:E:252:ARG:NH1	2.82	0.47
1:E:265:VAL:O	1:E:269:LEU:HB2	2.15	0.47
1:B:48:PHE:CD1	1:B:48:PHE:N	2.82	0.47
1:C:188:GLN:H	1:D:101:GLN:HE21	1.62	0.47
1:D:86:PHE:CE2	1:D:94:PHE:HB2	2.49	0.47
1:D:210:PRO:HG2	1:D:213:ILE:HD11	1.95	0.47
1:E:162:GLN:HG2	1:E:182:LYS:HG2	1.97	0.47
1:F:56:THR:HG22	1:F:57:PRO:HD2	1.96	0.47
1:F:94:PHE:HD2	1:F:111:SER:HA	1.78	0.47
1:B:130:GLU:HG2	1:B:134:ARG:HH21	1.79	0.47
1:E:41:ARG:HD3	1:E:44:GLY:HA2	1.96	0.47
1:A:304:ASN:HD22	1:A:307:ARG:HH11	1.61	0.47
1:C:135:LYS:H	1:C:135:LYS:HD3	1.79	0.47
1:D:22:ALA:O	1:D:27:ALA:CB	2.63	0.47
1:E:196:LYS:HE3	1:E:196:LYS:CA	2.37	0.47
1:B:270:SER:HB3	1:B:306:ILE:HB	1.96	0.47
1:F:86:PHE:CE2	1:F:94:PHE:HB2	2.49	0.47
1:F:95:ARG:HB2	1:F:112:LEU:HG	1.96	0.47
1:F:229:ARG:O	1:F:233:THR:CG2	2.63	0.47
1:B:304:ASN:ND2	1:B:307:ARG:HH11	2.12	0.46
1:C:41:ARG:HD3	1:C:44:GLY:HA2	1.97	0.46
1:A:202:LEU:O	1:A:205:ALA:HB3	2.14	0.46
1:B:141:VAL:HG12	1:B:141:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:ILE:CD1	1:C:32:LEU:HD21	2.45	0.46
1:B:229:ARG:CZ	1:B:229:ARG:HB3	2.46	0.46
1:C:182:LYS:HB3	1:C:183:LYS:H	1.51	0.46
1:C:240:THR:C	1:C:241:LEU:HD12	2.35	0.46
1:D:86:PHE:H	1:D:86:PHE:HD2	1.63	0.46
1:D:141:VAL:HG12	1:D:141:VAL:O	2.15	0.46
1:A:229:ARG:O	1:A:233:THR:HG22	2.15	0.46
1:F:94:PHE:CD2	1:F:110:ARG:O	2.66	0.46
1:B:141:VAL:HB	1:B:153:ILE:HD11	1.97	0.46
1:A:340:GLN:HB3	1:A:342:LEU:HD12	1.97	0.46
1:E:331:ASN:ND2	1:E:352:SER:OG	2.49	0.46
1:F:284:LYS:H	1:F:288:GLY:HA2	1.80	0.46
1:B:138:LEU:HD22	1:B:140:LEU:CD2	2.44	0.46
1:C:36:ALA:HB1	1:C:37:PRO:HD2	1.98	0.46
1:D:343:ILE:HD12	1:D:348:ALA:HB2	1.98	0.46
1:F:102:ARG:C	1:F:104:SER:H	2.19	0.46
1:A:15:ILE:HG23	1:A:16:LEU:N	2.30	0.46
1:B:254:VAL:HG12	1:B:262:GLN:HG2	1.97	0.46
1:C:267:ILE:HD11	1:D:355:PRO:HG2	1.92	0.46
1:E:257:PHE:CZ	1:E:265:VAL:HG21	2.50	0.46
1:E:304:ASN:ND2	1:E:307:ARG:HH11	2.13	0.46
1:A:149:LYS:O	1:A:153:ILE:HG12	2.16	0.46
1:C:229:ARG:O	1:C:233:THR:CG2	2.64	0.45
1:C:257:PHE:CZ	1:C:265:VAL:HG21	2.51	0.45
1:D:154:ALA:HB2	1:D:177:TYR:CD2	2.52	0.45
1:F:257:PHE:CZ	1:F:265:VAL:HG21	2.51	0.45
1:B:182:LYS:HB3	1:B:183:LYS:H	1.52	0.45
1:C:331:ASN:ND2	1:C:352:SER:OG	2.49	0.45
1:D:15:ILE:HG23	1:D:16:LEU:H	1.80	0.45
1:E:218:MSE:HE2	1:E:241:LEU:HD11	1.98	0.45
1:A:54:ARG:O	1:A:55:LEU:C	2.53	0.45
1:D:136:MSE:SE	1:E:252:ARG:HH22	2.42	0.45
1:E:42:ILE:O	1:E:43:ASP:CB	2.57	0.45
1:F:52:PHE:O	1:F:53:PRO:C	2.55	0.45
1:F:141:VAL:O	1:F:141:VAL:CG1	2.59	0.45
1:A:69:SER:O	1:A:73:ARG:HG3	2.16	0.45
1:B:17:GLU:HA	1:B:20:LYS:HB2	1.99	0.45
1:B:58:GLU:O	1:B:58:GLU:HG2	2.17	0.45
1:E:61:GLN:O	1:E:65:TYR:HB2	2.17	0.45
1:A:71:LYS:CD	1:A:196:LYS:HZ1	2.29	0.45
1:A:259:LEU:CA	1:A:262:GLN:HB2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:PHE:HD2	1:B:86:PHE:H	1.63	0.45
1:B:126:ASP:N	1:B:126:ASP:OD2	2.49	0.45
1:A:167:HIS:CE1	1:A:169:ILE:HD12	2.52	0.45
1:E:58:GLU:O	1:E:58:GLU:HG2	2.17	0.45
1:E:68:MSE:HB3	1:E:72:HIS:HB2	1.98	0.45
1:E:343:ILE:HD12	1:E:348:ALA:HB2	1.99	0.45
1:A:102:ARG:C	1:A:104:SER:H	2.19	0.45
1:C:196:LYS:HA	1:C:196:LYS:CE	2.37	0.45
1:E:94:PHE:CE2	1:E:111:SER:OG	2.53	0.45
1:F:65:TYR:CD1	1:F:73:ARG:HD2	2.52	0.45
1:F:195:THR:HG22	1:F:196:LYS:N	2.30	0.45
1:E:54:ARG:O	1:E:56:THR:N	2.50	0.45
1:E:340:GLN:HB3	1:E:342:LEU:HD12	1.99	0.45
1:F:84:PHE:CE2	1:F:96:ALA:HB3	2.52	0.45
1:D:271:PHE:HE2	1:E:252:ARG:NH1	2.15	0.44
1:E:22:ALA:O	1:E:27:ALA:HB3	2.16	0.44
1:E:142:THR:HG21	1:E:249:THR:OG1	2.17	0.44
1:E:259:LEU:CA	1:E:262:GLN:HB2	2.25	0.44
1:E:358:LEU:O	1:E:360:ARG:N	2.41	0.44
1:A:101:GLN:HE21	1:F:188:GLN:H	1.64	0.44
1:C:284:LYS:HG2	1:C:286:GLY:H	1.82	0.44
1:D:23:ILE:H	1:D:23:ILE:HG13	1.61	0.44
1:D:135:LYS:H	1:D:135:LYS:HD3	1.82	0.44
1:D:284:LYS:H	1:D:288:GLY:HA2	1.81	0.44
1:F:167:HIS:CE1	1:F:169:ILE:HD12	2.51	0.44
1:A:86:PHE:CD2	1:A:86:PHE:N	2.85	0.44
1:A:307:ARG:CD	1:B:258:PRO:HB3	2.48	0.44
1:A:347:ASP:O	1:A:350:GLU:HB3	2.17	0.44
1:C:68:MSE:HE3	1:C:82:VAL:HG21	1.99	0.44
1:C:212:VAL:HG13	1:C:236:LEU:HB3	1.99	0.44
1:D:264:GLN:HA	1:D:267:ILE:HD12	2.00	0.44
1:A:42:ILE:O	1:A:43:ASP:CB	2.59	0.44
1:B:309:ASN:O	1:B:311:LEU:HG	2.17	0.44
1:E:31:HIS:C	1:E:32:LEU:HD23	2.38	0.44
1:A:49:LEU:C	1:A:51:ASP:N	2.68	0.44
1:A:129:LEU:HA	1:A:129:LEU:HD23	1.55	0.44
1:D:15:ILE:HG23	1:D:16:LEU:N	2.33	0.44
1:A:54:ARG:O	1:A:56:THR:N	2.50	0.44
1:C:146:GLY:N	2:C:375:SO4:O1	2.35	0.44
1:D:68:MSE:HE3	1:D:82:VAL:HG21	1.99	0.44
1:D:142:THR:HG21	1:D:249:THR:OG1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:THR:HB	1:E:214:PHE:HD2	1.83	0.44
1:F:298:PRO:HB2	1:F:303:ARG:HH11	1.82	0.44
1:B:31:HIS:C	1:B:32:LEU:HD23	2.38	0.44
1:C:34:ALA:O	1:C:56:THR:O	2.36	0.44
1:E:135:LYS:H	1:E:135:LYS:HD3	1.83	0.44
1:C:229:ARG:NH1	1:D:144:PRO:HB2	2.33	0.44
1:D:165:SER:HB3	1:E:46:ILE:H	1.82	0.44
1:A:264:GLN:HA	1:A:267:ILE:HD12	2.00	0.43
1:B:158:ASP:O	1:B:161:ASN:HB3	2.18	0.43
1:B:175:ILE:H	1:B:175:ILE:HG13	1.56	0.43
1:C:167:HIS:ND1	1:C:210:PRO:HA	2.31	0.43
1:D:182:LYS:HB3	1:D:183:LYS:H	1.46	0.43
1:C:358:LEU:C	1:C:360:ARG:H	2.19	0.43
1:D:333:THR:HG22	1:D:333:THR:O	2.19	0.43
1:B:119:PHE:CE1	1:B:129:LEU:HG	2.53	0.43
1:C:71:LYS:NZ	1:C:196:LYS:HE2	2.33	0.43
1:D:30:ILE:HD12	1:D:32:LEU:CD2	2.48	0.43
1:E:30:ILE:CD1	1:E:32:LEU:CD2	2.94	0.43
1:E:154:ALA:HB2	1:E:177:TYR:CD2	2.52	0.43
1:E:171:ILE:CD1	1:E:202:LEU:HA	2.48	0.43
1:F:31:HIS:C	1:F:32:LEU:HD23	2.39	0.43
1:A:312:GLN:CD	1:A:312:GLN:H	2.21	0.43
1:C:195:THR:HG21	1:C:201:ALA:CB	2.48	0.43
1:D:284:LYS:HG2	1:D:286:GLY:H	1.83	0.43
1:F:86:PHE:N	1:F:86:PHE:CD2	2.86	0.43
1:F:171:ILE:CD1	1:F:202:LEU:HA	2.49	0.43
1:B:112:LEU:HA	1:B:113:PRO:HD3	1.84	0.43
1:F:175:ILE:H	1:F:175:ILE:HG13	1.66	0.43
1:F:259:LEU:CA	1:F:262:GLN:HB2	2.22	0.43
1:A:86:PHE:CE2	1:A:94:PHE:HB2	2.54	0.43
1:B:84:PHE:CE2	1:B:96:ALA:HB3	2.53	0.43
1:B:284:LYS:N	1:B:288:GLY:HA2	2.34	0.43
1:B:358:LEU:O	1:B:360:ARG:N	2.42	0.43
1:C:17:GLU:HA	1:C:20:LYS:HB2	2.00	0.43
1:C:269:LEU:HG	1:C:273:LEU:HD23	2.00	0.43
1:E:52:PHE:O	1:E:53:PRO:C	2.57	0.43
1:A:218:MSE:HE2	1:A:241:LEU:HD11	1.99	0.43
1:A:261:GLN:O	1:A:262:GLN:C	2.57	0.43
1:B:65:TYR:CD1	1:B:73:ARG:HD2	2.54	0.43
1:C:333:THR:HG22	1:C:333:THR:O	2.19	0.43
1:D:233:THR:CA	1:E:219:ARG:CD	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:ILE:CD1	1:F:32:LEU:HD21	2.48	0.43
1:F:343:ILE:HD12	1:F:348:ALA:HB2	2.00	0.43
1:C:173:ASP:HA	1:C:174:PRO:HA	1.86	0.43
1:F:42:ILE:O	1:F:43:ASP:CB	2.62	0.43
1:A:212:VAL:HG13	1:A:236:LEU:HB3	2.01	0.42
1:B:30:ILE:CD1	1:B:32:LEU:HD21	2.49	0.42
1:C:228:LEU:O	1:C:231:ALA:N	2.52	0.42
1:C:264:GLN:NE2	1:D:353:PRO:C	2.72	0.42
1:D:48:PHE:CD1	1:D:48:PHE:N	2.87	0.42
1:E:12:GLU:HB3	1:E:52:PHE:CZ	2.54	0.42
1:A:22:ALA:O	1:A:27:ALA:HB3	2.19	0.42
1:D:309:ASN:O	1:D:311:LEU:HG	2.18	0.42
1:F:237:VAL:O	1:F:237:VAL:HG12	2.19	0.42
1:E:138:LEU:HD22	1:E:140:LEU:CD2	2.47	0.42
1:F:333:THR:HG22	1:F:333:THR:O	2.19	0.42
1:A:128:VAL:C	1:A:130:GLU:N	2.71	0.42
1:A:204:ALA:O	1:A:205:ALA:C	2.55	0.42
1:B:68:MSE:HE3	1:B:82:VAL:HG21	2.01	0.42
1:F:309:ASN:O	1:F:311:LEU:HG	2.20	0.42
1:A:15:ILE:HG23	1:A:16:LEU:H	1.84	0.42
1:A:30:ILE:HG13	1:A:109:LEU:HB2	2.01	0.42
1:A:333:THR:HG22	1:A:333:THR:O	2.19	0.42
1:B:195:THR:HG22	1:B:196:LYS:N	2.34	0.42
1:C:202:LEU:O	1:C:205:ALA:HB3	2.20	0.42
1:E:84:PHE:CE2	1:E:96:ALA:HB3	2.54	0.42
1:F:58:GLU:HG2	1:F:58:GLU:O	2.18	0.42
1:A:112:LEU:HA	1:A:113:PRO:HD2	1.74	0.42
1:A:195:THR:HG21	1:A:201:ALA:CB	2.46	0.42
1:D:254:VAL:HG12	1:D:262:GLN:HG2	2.01	0.42
1:A:162:GLN:HG2	1:A:182:LYS:HG2	2.01	0.42
1:A:272:ILE:HD12	1:A:272:ILE:HA	1.91	0.42
1:B:282:LEU:HB3	1:B:283:PRO:HD2	2.02	0.42
1:C:254:VAL:HG12	1:C:262:GLN:HG2	2.02	0.42
1:D:61:GLN:O	1:D:65:TYR:HB2	2.20	0.42
1:B:41:ARG:HD3	1:B:44:GLY:HA2	2.02	0.42
1:D:58:GLU:O	1:D:58:GLU:HG2	2.20	0.42
1:E:153:ILE:O	1:E:155:SER:N	2.53	0.42
1:A:210:PRO:HG2	1:A:213:ILE:HD11	2.01	0.42
1:C:175:ILE:H	1:C:175:ILE:HG13	1.53	0.42
1:D:291:LEU:HD12	1:D:292:ALA:N	2.35	0.42
1:F:130:GLU:HG2	1:F:134:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:THR:C	1:A:346:GLU:H	2.23	0.42
1:D:270:SER:HB3	1:D:306:ILE:HB	2.01	0.42
1:E:229:ARG:CZ	1:E:229:ARG:HB3	2.49	0.42
1:F:15:ILE:HG23	1:F:16:LEU:H	1.85	0.42
1:C:229:ARG:CZ	1:C:229:ARG:HB3	2.50	0.41
1:E:86:PHE:CE2	1:E:94:PHE:HB2	2.55	0.41
1:E:94:PHE:CE2	1:E:111:SER:CA	2.99	0.41
1:E:152:THR:O	1:E:155:SER:HB2	2.20	0.41
1:E:169:ILE:O	1:E:169:ILE:CG2	2.68	0.41
1:F:17:GLU:HA	1:F:20:LYS:HB2	2.02	0.41
1:F:129:LEU:HD23	1:F:129:LEU:HA	1.79	0.41
1:C:86:PHE:CE2	1:C:94:PHE:HB2	2.55	0.41
1:C:269:LEU:HD12	1:C:269:LEU:HA	1.96	0.41
1:C:284:LYS:N	1:C:288:GLY:HA2	2.32	0.41
1:F:214:PHE:O	1:F:214:PHE:CG	2.71	0.41
1:A:233:THR:HA	1:B:219:ARG:HE	1.85	0.41
1:B:152:THR:O	1:B:155:SER:HB2	2.20	0.41
1:C:49:LEU:O	1:C:51:ASP:N	2.53	0.41
1:F:49:LEU:O	1:F:51:ASP:N	2.53	0.41
1:B:161:ASN:HA	1:B:184:SER:HG	1.81	0.41
1:D:187:ASN:HA	1:E:101:GLN:HE21	1.86	0.41
1:E:105:VAL:CG1	1:E:106:ALA:N	2.83	0.41
1:E:291:LEU:HD12	1:E:292:ALA:N	2.34	0.41
1:B:42:ILE:O	1:B:43:ASP:CB	2.59	0.41
1:B:71:LYS:HB3	1:B:71:LYS:HE2	1.81	0.41
1:B:149:LYS:NZ	2:B:375:SO4:O2	2.53	0.41
1:C:128:VAL:CG2	1:C:295:LEU:HD11	2.51	0.41
1:D:166:TYR:O	1:D:184:SER:HB2	2.21	0.41
1:A:14:LYS:O	1:A:15:ILE:C	2.58	0.41
1:A:149:LYS:CD	1:A:149:LYS:N	2.59	0.41
1:D:125:PRO:HD3	1:D:293:TYR:OH	2.21	0.41
1:E:40:VAL:HG12	1:E:42:ILE:HG13	2.03	0.41
1:E:269:LEU:HD12	1:E:269:LEU:HA	1.82	0.41
1:E:298:PRO:HB2	1:E:303:ARG:HH11	1.86	0.41
1:F:102:ARG:C	1:F:104:SER:N	2.73	0.41
1:D:153:ILE:O	1:D:155:SER:N	2.54	0.41
1:F:358:LEU:C	1:F:360:ARG:N	2.73	0.41
1:A:101:GLN:NE2	1:F:187:ASN:HA	2.35	0.41
1:A:188:GLN:H	1:B:101:GLN:NE2	2.13	0.41
1:A:298:PRO:HB2	1:A:303:ARG:HH11	1.86	0.41
1:B:233:THR:HG23	1:B:235:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ARG:HA	1:B:289:ARG:HD3	1.68	0.41
1:D:318:MSE:C	1:D:319:GLN:HG3	2.41	0.41
1:F:12:GLU:HB3	1:F:52:PHE:CZ	2.56	0.41
1:F:15:ILE:HG23	1:F:16:LEU:N	2.36	0.41
1:A:226:THR:O	1:A:227:ALA:C	2.58	0.41
1:B:358:LEU:C	1:B:360:ARG:H	2.20	0.41
1:D:130:GLU:HG2	1:D:134:ARG:HH21	1.86	0.41
1:D:153:ILE:O	1:D:154:ALA:C	2.60	0.41
1:D:226:THR:HA	1:D:229:ARG:HB2	2.03	0.41
1:D:257:PHE:CE1	1:D:265:VAL:HG21	2.56	0.41
1:E:112:LEU:HA	1:E:113:PRO:HD3	1.79	0.41
1:E:175:ILE:HD11	1:E:190:GLU:HB2	2.02	0.41
1:E:195:THR:HG22	1:E:196:LYS:N	2.36	0.41
1:F:36:ALA:HB1	1:F:37:PRO:CD	2.51	0.41
1:A:223:THR:O	1:A:224:VAL:C	2.57	0.41
1:B:49:LEU:C	1:B:51:ASP:N	2.74	0.41
1:B:298:PRO:HB2	1:B:303:ARG:HH11	1.86	0.41
1:C:68:MSE:HB2	1:C:73:ARG:HG2	2.03	0.41
1:C:86:PHE:N	1:C:86:PHE:CD2	2.89	0.41
1:A:68:MSE:HE3	1:A:82:VAL:HG21	2.03	0.40
1:A:233:THR:HG23	1:A:235:HIS:CE1	2.55	0.40
1:C:205:ALA:O	1:C:210:PRO:HG3	2.21	0.40
1:C:318:MSE:C	1:C:319:GLN:HG3	2.41	0.40
1:D:230:ALA:HA	1:D:233:THR:HG22	2.03	0.40
1:E:185:ILE:HD11	1:F:33:THR:HB	2.02	0.40
1:F:48:PHE:CD1	1:F:48:PHE:N	2.89	0.40
1:B:52:PHE:O	1:B:53:PRO:C	2.59	0.40
1:B:257:PHE:CZ	1:B:265:VAL:HG21	2.56	0.40
1:C:31:HIS:C	1:C:32:LEU:HD23	2.42	0.40
1:F:41:ARG:HD3	1:F:44:GLY:HA2	2.03	0.40
1:F:95:ARG:CZ	1:F:174:PRO:HG3	2.52	0.40
1:F:318:MSE:O	1:F:319:GLN:HG3	2.19	0.40
1:F:347:ASP:O	1:F:350:GLU:HB3	2.21	0.40
1:A:128:VAL:CG2	1:A:295:LEU:HD11	2.51	0.40
1:D:228:LEU:O	1:D:232:GLU:HG2	2.20	0.40
1:A:95:ARG:HB2	1:A:112:LEU:HG	2.02	0.40
1:C:347:ASP:O	1:C:350:GLU:HB3	2.21	0.40
1:A:23:ILE:H	1:A:23:ILE:HG13	1.59	0.40
1:C:126:ASP:OD2	1:C:126:ASP:N	2.53	0.40
1:C:261:GLN:O	1:C:262:GLN:C	2.60	0.40
1:C:334:LEU:HD22	1:C:348:ALA:HB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:LEU:HD22	1:D:140:LEU:CD2	2.50	0.40

All (5) 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:B:310:LYS:NZ	1:D:319:GLN:OE1[4_555]	1.37	0.83
1:A:73:ARG:NH2	1:A:73:ARG:NH2[2_554]	1.77	0.43
1:B:310:LYS:NZ	1:D:319:GLN:CD[4_555]	2.06	0.14
1:A:12:GLU:OE1	1:B:61:GLN:NE2[2_554]	2.07	0.13
1:B:345:LEU:CD2	1:D:24:GLU:O[1_565]	2.12	0.08

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	339/363 (93%)	279 (82%)	52 (15%)	8 (2%)	6	36
1	B	339/363 (93%)	276 (81%)	54 (16%)	9 (3%)	5	34
1	C	339/363 (93%)	278 (82%)	51 (15%)	10 (3%)	4	32
1	D	339/363 (93%)	277 (82%)	54 (16%)	8 (2%)	6	36
1	E	339/363 (93%)	280 (83%)	51 (15%)	8 (2%)	6	36
1	F	339/363 (93%)	279 (82%)	49 (14%)	11 (3%)	4	31
All	All	2034/2178 (93%)	1669 (82%)	311 (15%)	54 (3%)	5	34

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	ALA
1	A	199	ALA
1	C	50	LYS

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Mol	Chain	Res	Type
1	C	55	LEU
1	D	55	LEU
1	D	199	ALA
1	E	55	LEU
1	F	50	LYS
1	F	116	ILE
1	A	52	PHE
1	B	55	LEU
1	B	116	ILE
1	C	113	PRO
1	C	199	ALA
1	D	153	ILE
1	E	52	PHE
1	E	199	ALA
1	F	55	LEU
1	F	199	ALA
1	A	55	LEU
1	A	113	PRO
1	A	300	THR
1	B	52	PHE
1	B	198	PHE
1	B	199	ALA
1	C	52	PHE
1	C	114	ALA
1	C	208	GLU
1	D	50	LYS
1	D	52	PHE
1	D	97	ASN
1	D	154	ALA
1	E	154	ALA
1	E	359	GLU
1	F	52	PHE
1	F	97	ASN
1	A	57	PRO
1	C	153	ILE
1	C	359	GLU
1	E	50	LYS
1	F	57	PRO
1	F	300	THR
1	F	359	GLU
1	A	50	LYS
1	B	208	GLU

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Mol	Chain	Res	Type
1	C	57	PRO
1	B	153	ILE
1	D	57	PRO
1	F	113	PRO
1	E	57	PRO
1	E	153	ILE
1	B	57	PRO
1	A	210	PRO
1	F	153	ILE

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	297/303 (98%)	237 (80%)	60 (20%)	1 8
1	B	297/303 (98%)	241 (81%)	56 (19%)	1 10
1	C	297/303 (98%)	237 (80%)	60 (20%)	1 8
1	D	297/303 (98%)	242 (82%)	55 (18%)	1 11
1	E	297/303 (98%)	236 (80%)	61 (20%)	1 7
1	F	297/303 (98%)	237 (80%)	60 (20%)	1 8
All	All	1782/1818 (98%)	1430 (80%)	352 (20%)	1 9

All (352) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	15	ILE
1	A	23	ILE
1	A	29	ASP
1	A	30	ILE
1	A	42	ILE
1	A	49	LEU
1	A	51	ASP
1	A	54	ARG

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Mol	Chain	Res	Type
1	A	56	THR
1	A	58	GLU
1	A	65	TYR
1	A	71	LYS
1	A	74	GLN
1	A	75	LYS
1	A	82	VAL
1	A	83	ASP
1	A	85	SER
1	A	86	PHE
1	A	89	ARG
1	A	95	ARG
1	A	104	SER
1	A	111	SER
1	A	112	LEU
1	A	129	LEU
1	A	135	LYS
1	A	149	LYS
1	A	150	SER
1	A	169	ILE
1	A	175	ILE
1	A	182	LYS
1	A	183	LYS
1	A	196	LYS
1	A	200	ASP
1	A	202	LEU
1	A	206	LEU
1	A	219	ARG
1	A	221	LEU
1	A	226	THR
1	A	229	ARG
1	A	240	THR
1	A	244	ASN
1	A	251	HIS
1	A	252	ARG
1	A	259	LEU
1	A	261	GLN
1	A	263	GLU
1	A	273	LEU
1	A	289	ARG
1	A	290	VAL
1	A	291	LEU

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Mol	Chain	Res	Type
1	A	295	LEU
1	A	300	THR
1	A	312	GLN
1	A	313	GLN
1	A	319	GLN
1	A	327	MSE
1	A	329	THR
1	A	330	MSE
1	A	359	GLU
1	B	12	GLU
1	B	15	ILE
1	B	23	ILE
1	B	29	ASP
1	B	30	ILE
1	B	42	ILE
1	B	48	PHE
1	B	49	LEU
1	B	54	ARG
1	B	56	THR
1	B	71	LYS
1	B	74	GLN
1	B	75	LYS
1	B	82	VAL
1	B	85	SER
1	B	86	PHE
1	B	89	ARG
1	B	95	ARG
1	B	104	SER
1	B	126	ASP
1	B	129	LEU
1	B	135	LYS
1	B	149	LYS
1	B	169	ILE
1	B	175	ILE
1	B	182	LYS
1	B	183	LYS
1	B	196	LYS
1	B	200	ASP
1	B	202	LEU
1	B	206	LEU
1	B	217	GLU
1	B	219	ARG

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Mol	Chain	Res	Type
1	B	221	LEU
1	B	226	THR
1	B	229	ARG
1	B	240	THR
1	B	244	ASN
1	B	251	HIS
1	B	252	ARG
1	B	259	LEU
1	B	261	GLN
1	B	263	GLU
1	B	273	LEU
1	B	289	ARG
1	B	290	VAL
1	B	291	LEU
1	B	295	LEU
1	B	300	THR
1	B	312	GLN
1	B	313	GLN
1	B	319	GLN
1	B	327	MSE
1	B	329	THR
1	B	330	MSE
1	B	359	GLU
1	C	12	GLU
1	C	15	ILE
1	C	23	ILE
1	C	29	ASP
1	C	30	ILE
1	C	42	ILE
1	C	48	PHE
1	C	49	LEU
1	C	51	ASP
1	C	54	ARG
1	C	56	THR
1	C	58	GLU
1	C	65	TYR
1	C	71	LYS
1	C	74	GLN
1	C	75	LYS
1	C	82	VAL
1	C	85	SER
1	C	86	PHE

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Mol	Chain	Res	Type
1	C	89	ARG
1	C	95	ARG
1	C	104	SER
1	C	126	ASP
1	C	129	LEU
1	C	135	LYS
1	C	149	LYS
1	C	150	SER
1	C	169	ILE
1	C	175	ILE
1	C	182	LYS
1	C	183	LYS
1	C	196	LYS
1	C	200	ASP
1	C	202	LEU
1	C	206	LEU
1	C	219	ARG
1	C	221	LEU
1	C	226	THR
1	C	228	LEU
1	C	229	ARG
1	C	240	THR
1	C	244	ASN
1	C	251	HIS
1	C	252	ARG
1	C	259	LEU
1	C	261	GLN
1	C	263	GLU
1	C	273	LEU
1	C	289	ARG
1	C	290	VAL
1	C	291	LEU
1	C	295	LEU
1	C	300	THR
1	C	312	GLN
1	C	313	GLN
1	C	319	GLN
1	C	327	MSE
1	C	329	THR
1	C	330	MSE
1	C	359	GLU
1	D	12	GLU

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Mol	Chain	Res	Type
1	D	15	ILE
1	D	23	ILE
1	D	29	ASP
1	D	30	ILE
1	D	42	ILE
1	D	48	PHE
1	D	49	LEU
1	D	54	ARG
1	D	56	THR
1	D	58	GLU
1	D	71	LYS
1	D	74	GLN
1	D	75	LYS
1	D	82	VAL
1	D	89	ARG
1	D	95	ARG
1	D	104	SER
1	D	126	ASP
1	D	129	LEU
1	D	135	LYS
1	D	149	LYS
1	D	150	SER
1	D	169	ILE
1	D	175	ILE
1	D	182	LYS
1	D	183	LYS
1	D	196	LYS
1	D	200	ASP
1	D	202	LEU
1	D	206	LEU
1	D	219	ARG
1	D	221	LEU
1	D	226	THR
1	D	228	LEU
1	D	229	ARG
1	D	240	THR
1	D	244	ASN
1	D	251	HIS
1	D	252	ARG
1	D	259	LEU
1	D	261	GLN
1	D	263	GLU

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Mol	Chain	Res	Type
1	D	273	LEU
1	D	289	ARG
1	D	290	VAL
1	D	291	LEU
1	D	295	LEU
1	D	300	THR
1	D	312	GLN
1	D	319	GLN
1	D	327	MSE
1	D	329	THR
1	D	330	MSE
1	D	359	GLU
1	E	12	GLU
1	E	15	ILE
1	E	23	ILE
1	E	29	ASP
1	E	30	ILE
1	E	42	ILE
1	E	43	ASP
1	E	48	PHE
1	E	49	LEU
1	E	51	ASP
1	E	54	ARG
1	E	56	THR
1	E	58	GLU
1	E	65	TYR
1	E	71	LYS
1	E	74	GLN
1	E	75	LYS
1	E	79	ASN
1	E	82	VAL
1	E	85	SER
1	E	86	PHE
1	E	95	ARG
1	E	104	SER
1	E	115	GLU
1	E	126	ASP
1	E	129	LEU
1	E	135	LYS
1	E	149	LYS
1	E	150	SER
1	E	169	ILE

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Mol	Chain	Res	Type
1	E	175	ILE
1	E	182	LYS
1	E	183	LYS
1	E	185	ILE
1	E	196	LYS
1	E	200	ASP
1	E	202	LEU
1	E	219	ARG
1	E	221	LEU
1	E	226	THR
1	E	229	ARG
1	E	240	THR
1	E	244	ASN
1	E	251	HIS
1	E	252	ARG
1	E	259	LEU
1	E	261	GLN
1	E	263	GLU
1	E	273	LEU
1	E	289	ARG
1	E	290	VAL
1	E	291	LEU
1	E	295	LEU
1	E	300	THR
1	E	312	GLN
1	E	313	GLN
1	E	319	GLN
1	E	327	MSE
1	E	329	THR
1	E	330	MSE
1	E	359	GLU
1	F	12	GLU
1	F	15	ILE
1	F	23	ILE
1	F	29	ASP
1	F	30	ILE
1	F	42	ILE
1	F	48	PHE
1	F	49	LEU
1	F	54	ARG
1	F	56	THR
1	F	58	GLU

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Mol	Chain	Res	Type
1	F	71	LYS
1	F	74	GLN
1	F	75	LYS
1	F	79	ASN
1	F	82	VAL
1	F	85	SER
1	F	86	PHE
1	F	89	ARG
1	F	95	ARG
1	F	104	SER
1	F	115	GLU
1	F	116	ILE
1	F	126	ASP
1	F	129	LEU
1	F	135	LYS
1	F	149	LYS
1	F	150	SER
1	F	169	ILE
1	F	175	ILE
1	F	182	LYS
1	F	183	LYS
1	F	196	LYS
1	F	200	ASP
1	F	202	LEU
1	F	206	LEU
1	F	219	ARG
1	F	221	LEU
1	F	226	THR
1	F	229	ARG
1	F	240	THR
1	F	244	ASN
1	F	251	HIS
1	F	252	ARG
1	F	259	LEU
1	F	261	GLN
1	F	263	GLU
1	F	273	LEU
1	F	289	ARG
1	F	290	VAL
1	F	291	LEU
1	F	295	LEU
1	F	300	THR

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Mol	Chain	Res	Type
1	F	312	GLN
1	F	313	GLN
1	F	317	LEU
1	F	319	GLN
1	F	329	THR
1	F	330	MSE
1	F	359	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	187	ASN
1	A	242	HIS
1	A	261	GLN
1	A	331	ASN
1	B	74	GLN
1	B	101	GLN
1	B	187	ASN
1	B	261	GLN
1	B	304	ASN
1	B	331	ASN
1	C	74	GLN
1	C	187	ASN
1	C	261	GLN
1	C	264	GLN
1	C	304	ASN
1	D	74	GLN
1	D	251	HIS
1	D	261	GLN
1	E	74	GLN
1	E	187	ASN
1	E	242	HIS
1	E	261	GLN
1	E	264	GLN
1	E	304	ASN
1	E	331	ASN
1	F	74	GLN
1	F	161	ASN
1	F	181	HIS
1	F	187	ASN
1	F	261	GLN

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Mol	Chain	Res	Type
1	F	304	ASN
1	F	331	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	375	-	4,4,4	1.55	1 (25%)	6,6,6	1.56	1 (16%)
2	SO4	E	375	-	4,4,4	2.31	1 (25%)	6,6,6	0.68	0
2	SO4	C	375	-	4,4,4	0.24	0	6,6,6	0.59	0
3	ADP	F	500	-	24,29,29	1.55	5 (20%)	29,45,45	1.52	7 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	F	500	-	-	1/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	500	ADP	O4'-C1'	4.30	1.47	1.41
2	E	375	SO4	O2-S	4.07	1.68	1.46
3	F	500	ADP	C5-C4	3.45	1.50	1.40
3	F	500	ADP	C2-N3	2.51	1.36	1.32
2	B	375	SO4	O2-S	2.48	1.59	1.46
3	F	500	ADP	C4-N3	2.20	1.38	1.35
3	F	500	ADP	C6-C5	2.06	1.51	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	500	ADP	N3-C2-N1	-3.71	122.89	128.68
3	F	500	ADP	C4-C5-N7	-2.86	106.41	109.40
2	B	375	SO4	O4-S-O2	2.68	123.31	109.31
3	F	500	ADP	O3B-PB-O3A	2.67	113.59	104.64
3	F	500	ADP	C3'-C2'-C1'	2.45	104.67	100.98
3	F	500	ADP	C2-N1-C6	2.27	122.64	118.75
3	F	500	ADP	O3A-PB-O1B	-2.08	99.64	111.19
3	F	500	ADP	O4'-C1'-C2'	-2.01	103.99	106.93

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	500	ADP	PA-O3A-PB-O1B

There are no ring outliers.

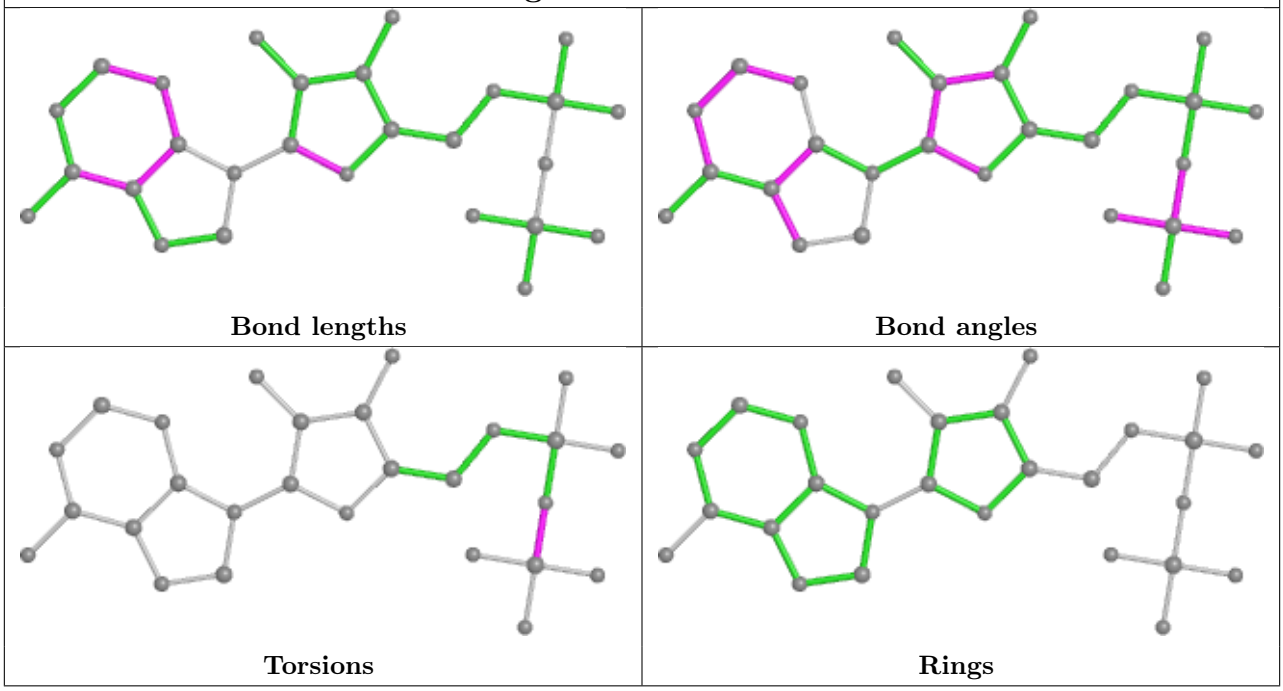
4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	375	SO4	6	0
2	E	375	SO4	2	0
2	C	375	SO4	4	0
3	F	500	ADP	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP F 500



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	334/363 (92%)	-0.23	1 (0%)	94	90	82, 118, 160, 176	0
1	B	334/363 (92%)	-0.25	1 (0%)	94	90	82, 118, 160, 176	0
1	C	334/363 (92%)	-0.23	5 (1%)	73	64	82, 118, 160, 176	0
1	D	334/363 (92%)	-0.16	1 (0%)	94	90	82, 118, 160, 176	0
1	E	334/363 (92%)	-0.13	5 (1%)	73	64	82, 118, 160, 176	0
1	F	334/363 (92%)	-0.20	1 (0%)	94	90	82, 118, 160, 176	0
All	All	2004/2178 (92%)	-0.20	14 (0%)	87	82	82, 118, 160, 176	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	339	LYS	3.0
1	C	90	GLY	2.8
1	C	91	VAL	2.7
1	E	345	LEU	2.5
1	C	92	GLY	2.4
1	E	360	ARG	2.2
1	B	357	GLU	2.2
1	D	328	GLN	2.1
1	A	340	GLN	2.1
1	F	78	GLU	2.1
1	E	357	GLU	2.1
1	C	357	GLU	2.0
1	C	340	GLN	2.0
1	E	312	GLN	2.0

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

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)

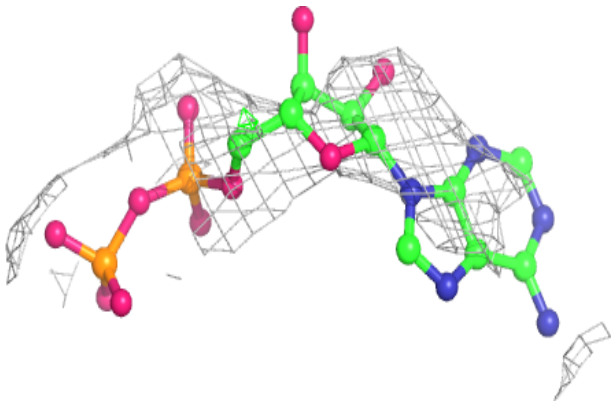
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

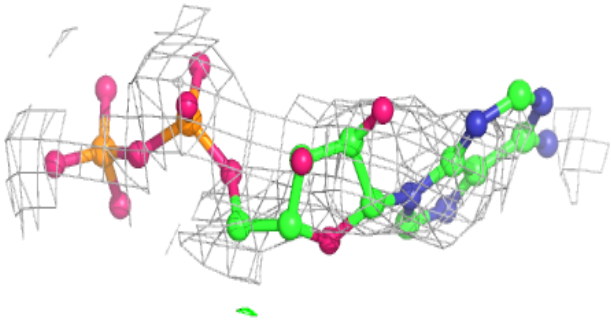
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	F	500	27/27	0.72	0.35	153,177,179,179	0
2	SO4	E	375	5/5	0.86	0.27	148,148,148,149	0
2	SO4	B	375	5/5	0.89	0.20	88,88,89,90	0
2	SO4	C	375	5/5	0.96	0.17	112,113,114,115	0

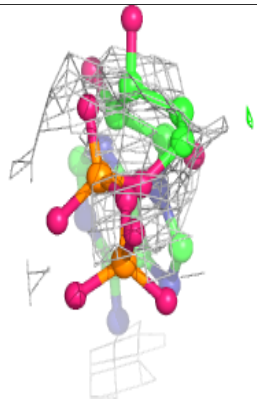
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP F 500:

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







6.5 Other polymers (i)

There are no such residues in this entry.