Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2024 – 08:54 pm GMT

PDB ID	:	5MG5
Title	:	A multi-component acyltransferase PhlABC from Pseudomonas protegens soaked with the monoacetylphloroglucinol (MAPG)
Authors	:	Pavkov-Keller, T.; Schmidt, N.G.; Kroutil, W.; Gruber, K.
Deposited on	:	2016-11-20
Resolution	:	3.44 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:

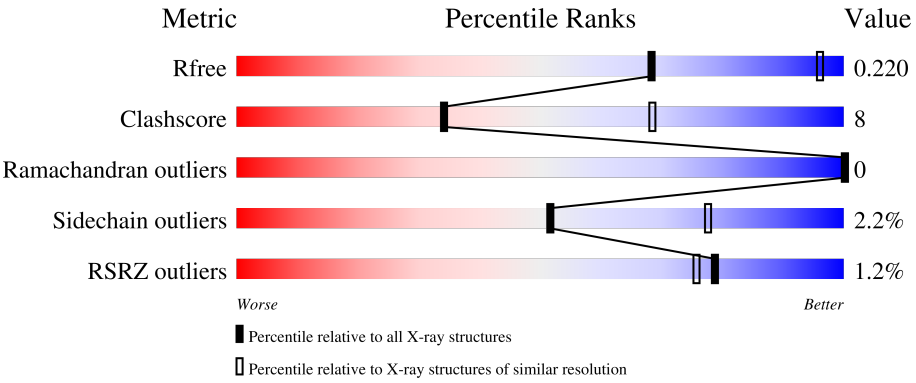
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.44 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	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (3.50-3.38)

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	362	81% 17%
1	D	362	81% 17%
1	G	362	% 80% 19%
1	J	362	83% 15%
1	M	362	78% 20%

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Mol	Chain	Length	Quality of chain
1	P	362	3% 78% 20%
1	S	362	78% 20%
1	V	362	81% 17%
2	B	146	3% 84% 16%
2	E	146	% 81% 18%
2	H	146	% 77% 22%
2	K	146	% 78% 21%
2	N	146	4% 80% 18%
2	Q	146	2% 86% 14%
2	T	146	5% 74% 24%
2	W	146	4% 73% 25%
3	C	398	% 83% 16%
3	F	398	% 76% 23%
3	I	398	% 73% 27%
3	L	398	76% 23%
3	O	398	2% 77% 22%
3	R	398	2% 74% 25%
3	U	398	2% 78% 22%
3	X	398	2% 81% 17%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 54522 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 Hydroxymethylglutaryl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2677	1687	452	529	9			
1	D	359	Total	C	N	O	S	0	0	0
			2686	1693	454	530	9			
1	G	359	Total	C	N	O	S	0	0	0
			2686	1693	454	530	9			
1	J	359	Total	C	N	O	S	0	0	0
			2686	1693	454	530	9			
1	M	359	Total	C	N	O	S	0	0	0
			2686	1693	454	530	9			
1	P	358	Total	C	N	O	S	0	0	0
			2677	1687	452	529	9			
1	S	358	Total	C	N	O	S	0	1	0
			2687	1693	455	530	9			
1	V	359	Total	C	N	O	S	0	0	0
			2686	1693	454	530	9			

- Molecule 2 is a protein called 2,4-diacetylphloroglucinol biosynthesis protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1150	721	208	207	14			
2	E	145	Total	C	N	O	S	0	0	0
			1150	721	208	207	14			
2	H	145	Total	C	N	O	S	0	0	0
			1150	721	208	207	14			
2	K	145	Total	C	N	O	S	0	0	0
			1150	721	208	207	14			
2	N	145	Total	C	N	O	S	0	0	0
			1150	721	208	207	14			
2	Q	145	Total	C	N	O	S	0	0	0
			1150	721	208	207	14			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	145	Total	C	N	O	S	0	0	0
			1150	721	208	207	14			
2	W	145	Total	C	N	O	S	0	0	0
			1150	721	208	207	14			

- Molecule 3 is a protein called 2,4-diacetylphloroglucinol biosynthesis protein PhlC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	395	Total	C	N	O	S	0	0	0
			2965	1862	512	571	20			
3	F	395	Total	C	N	O	S	0	0	0
			2965	1862	512	571	20			
3	I	396	Total	C	N	O	S	0	0	0
			2970	1865	513	572	20			
3	L	396	Total	C	N	O	S	0	0	0
			2970	1865	513	572	20			
3	O	396	Total	C	N	O	S	0	0	0
			2970	1865	513	572	20			
3	R	395	Total	C	N	O	S	0	0	0
			2965	1862	512	571	20			
3	U	396	Total	C	N	O	S	0	0	0
			2970	1865	513	572	20			
3	X	396	Total	C	N	O	S	0	0	0
			2970	1865	513	572	20			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	K	1	Total	Zn	0	0
			1	1		
4	N	1	Total	Zn	0	0
			1	1		
4	Q	1	Total	Zn	0	0
			1	1		
4	T	1	Total	Zn	0	0
			1	1		

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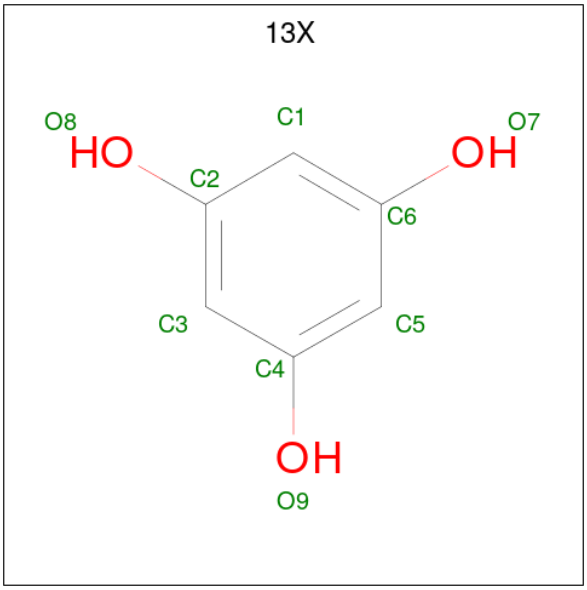
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	W	1	Total Zn 1 1	0	0

- Molecule 5 is benzene-1,3,5-triol (three-letter code: 13X) (formula: $C_6H_6O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 9 6 3	0	0
5	L	1	Total C O 9 6 3	0	0
5	O	1	Total C O 9 6 3	0	0
5	R	1	Total C O 9 6 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	5	Total O 5 5	0	0
6	B	3	Total O 3 3	0	0
6	C	5	Total O 5 5	0	0
6	D	3	Total O 3 3	0	0

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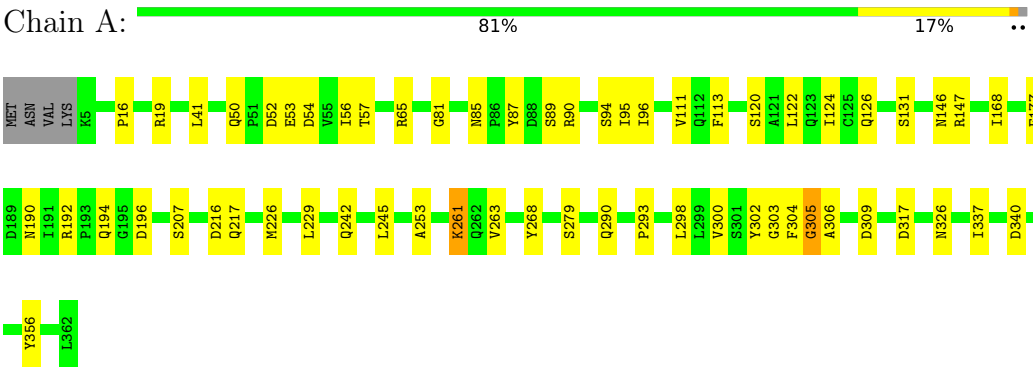
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	2	Total O 2 2	0	0
6	F	2	Total O 2 2	0	0
6	G	2	Total O 2 2	0	0
6	H	3	Total O 3 3	0	0
6	I	2	Total O 2 2	0	0
6	J	5	Total O 5 5	0	0
6	K	1	Total O 1 1	0	0
6	L	1	Total O 1 1	0	0
6	M	4	Total O 4 4	0	0
6	N	3	Total O 3 3	0	0
6	O	1	Total O 1 1	0	0
6	P	1	Total O 1 1	0	0
6	Q	2	Total O 2 2	0	0
6	R	3	Total O 3 3	0	0
6	S	2	Total O 2 2	0	0
6	T	1	Total O 1 1	0	0
6	U	1	Total O 1 1	0	0
6	V	6	Total O 6 6	0	0
6	X	4	Total O 4 4	0	0

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.

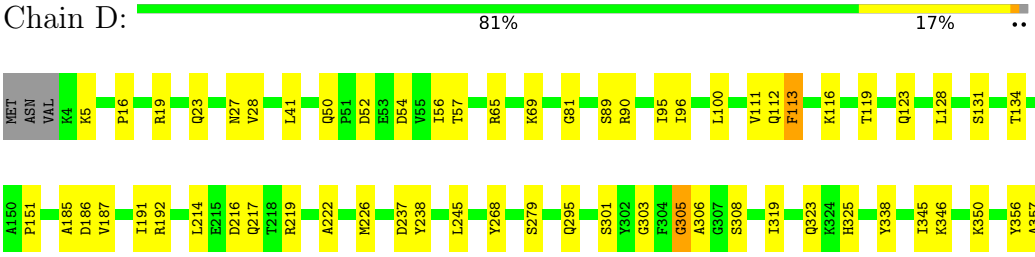
• Molecule 1: Hydroxymethylglutaryl-CoA synthase

Chain A:



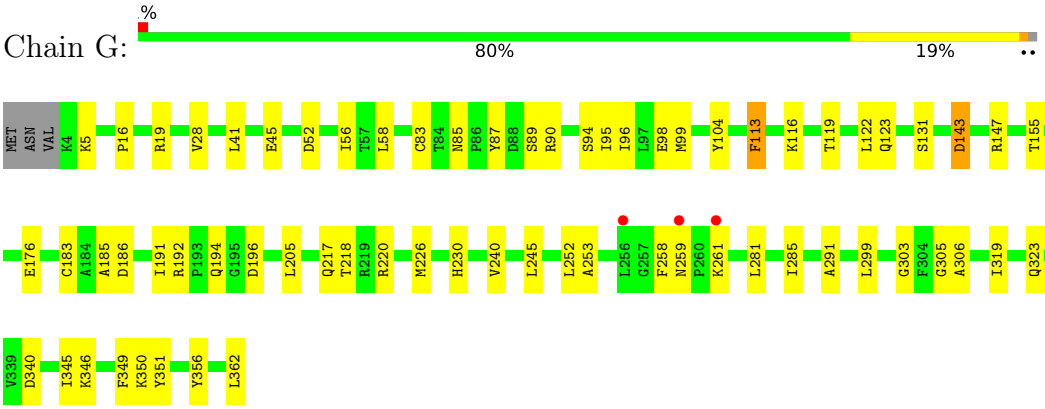
• Molecule 1: Hydroxymethylglutaryl-CoA synthase

Chain D:



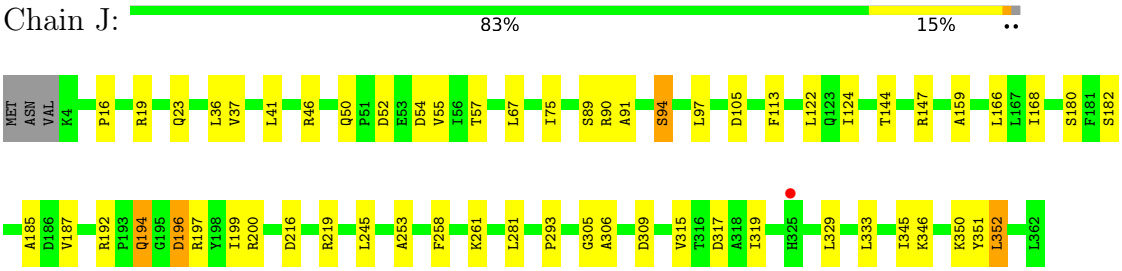
• Molecule 1: Hydroxymethylglutaryl-CoA synthase

Chain G:



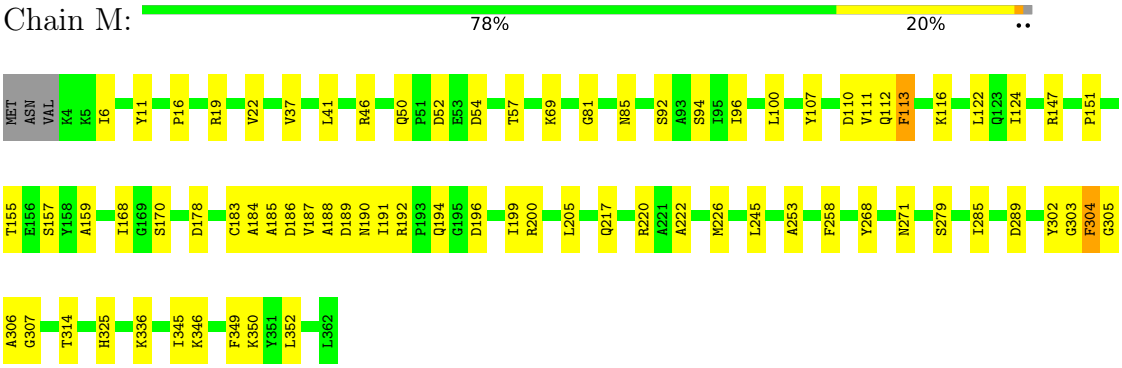
• Molecule 1: Hydroxymethylglutaryl-CoA synthase

Chain J:



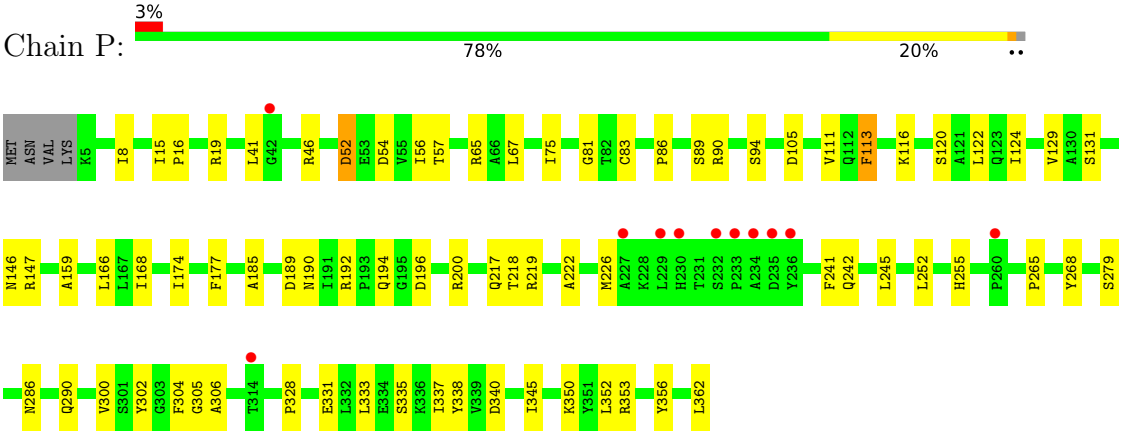
• Molecule 1: Hydroxymethylglutaryl-CoA synthase

Chain M:



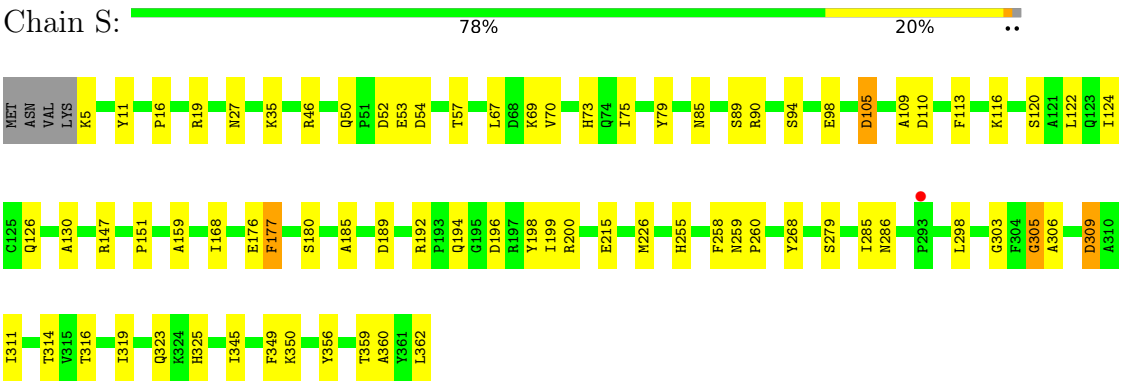
• Molecule 1: Hydroxymethylglutaryl-CoA synthase

Chain P:



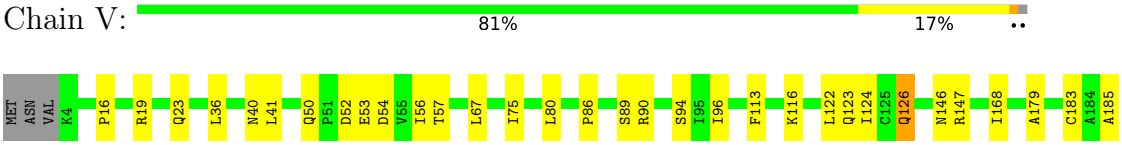
• Molecule 1: Hydroxymethylglutaryl-CoA synthase

Chain S:



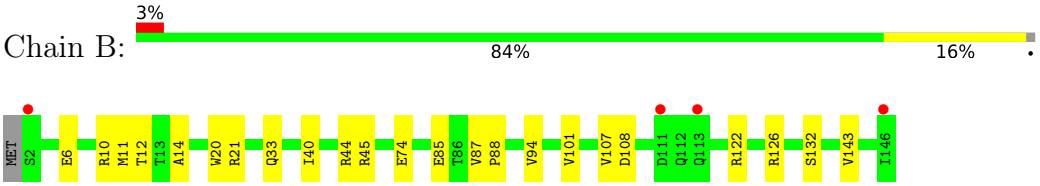
• Molecule 1: Hydroxymethylglutaryl-CoA synthase

Chain V:



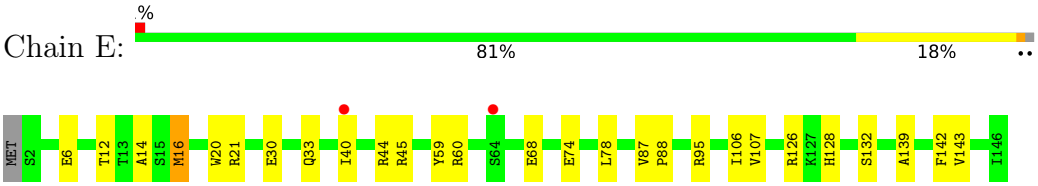
• Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein

Chain B:



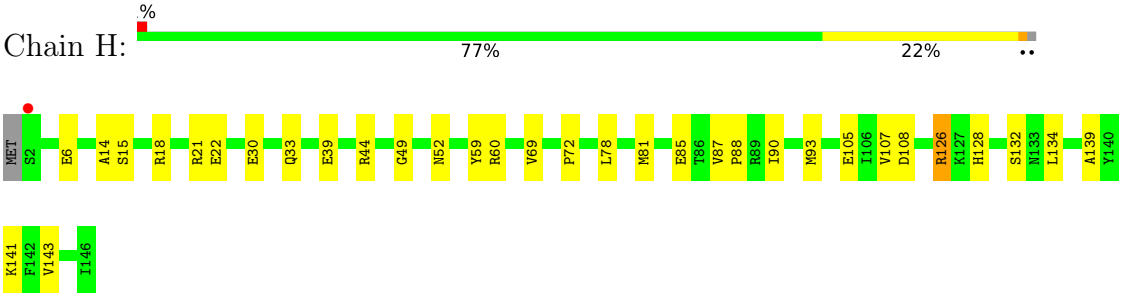
• Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein

Chain E:



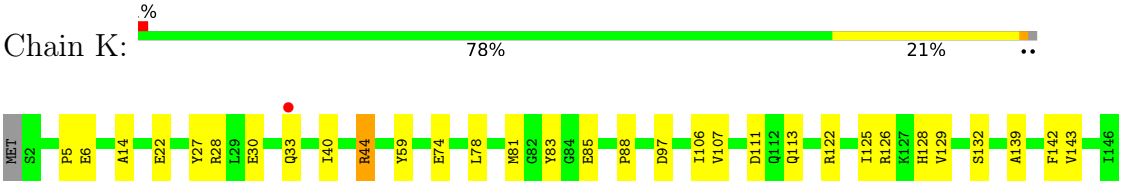
• Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein

Chain H:



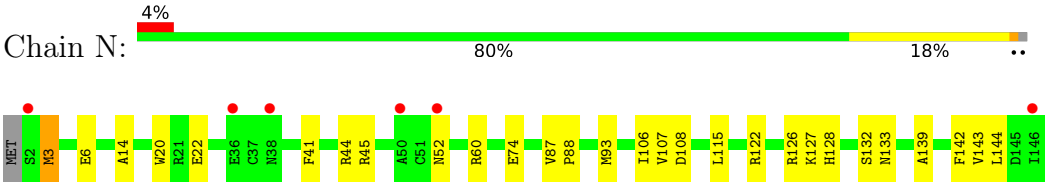
• Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein

Chain K:



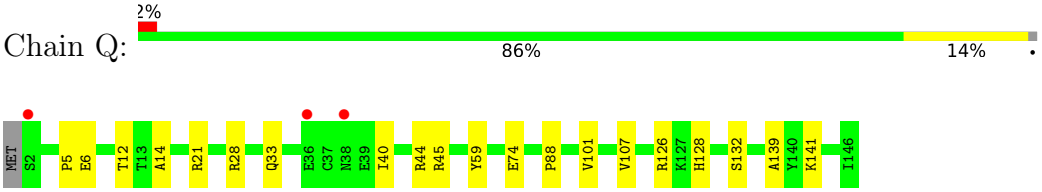
• Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein

Chain N:



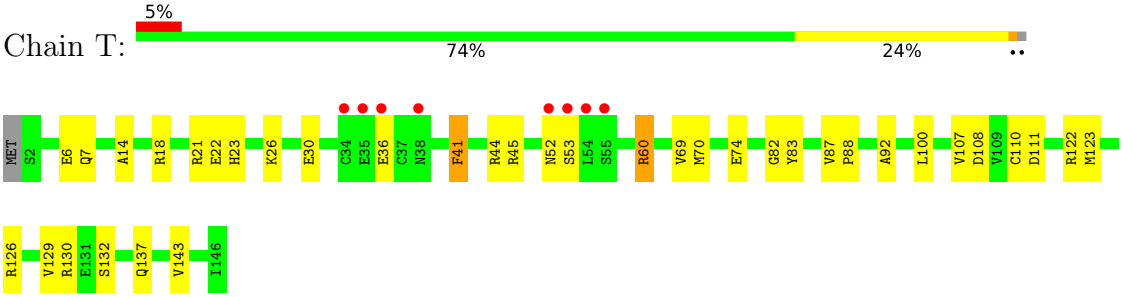
• Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein

Chain Q:



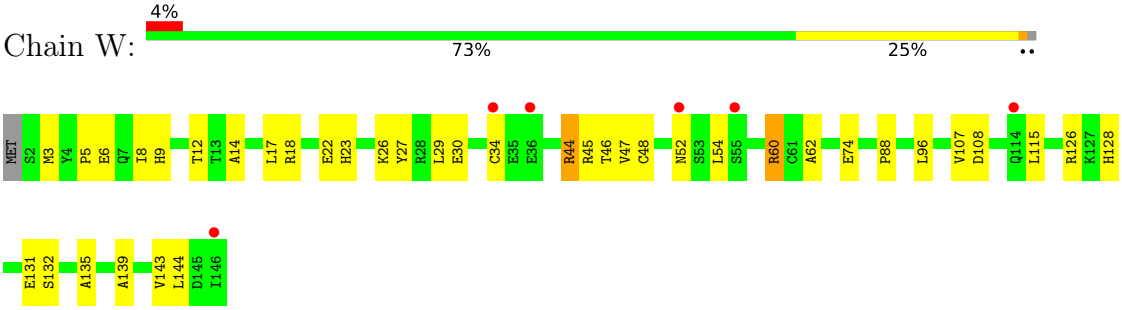
• Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein

Chain T:



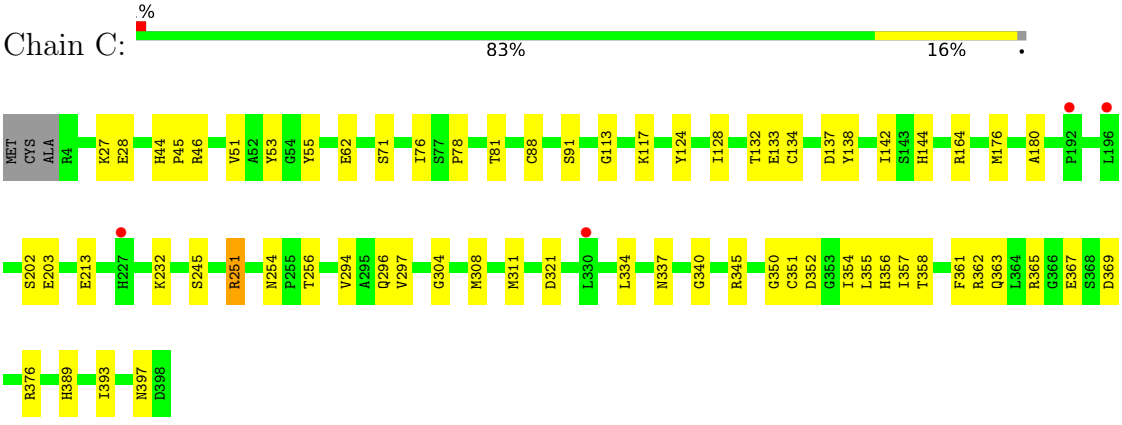
• Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein

Chain W:



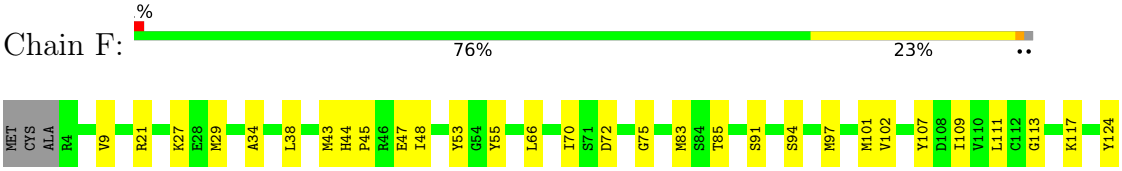
• Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein PhlC

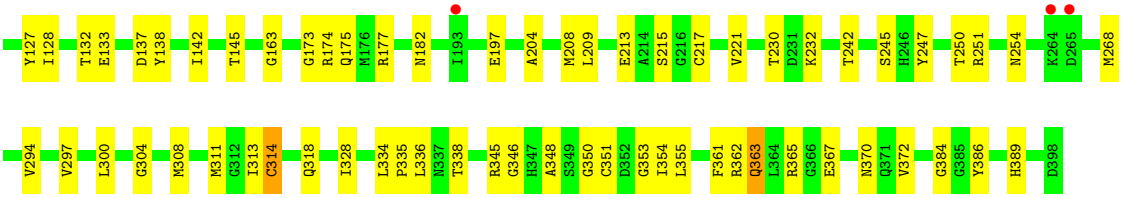
Chain C:



• Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein PhlC

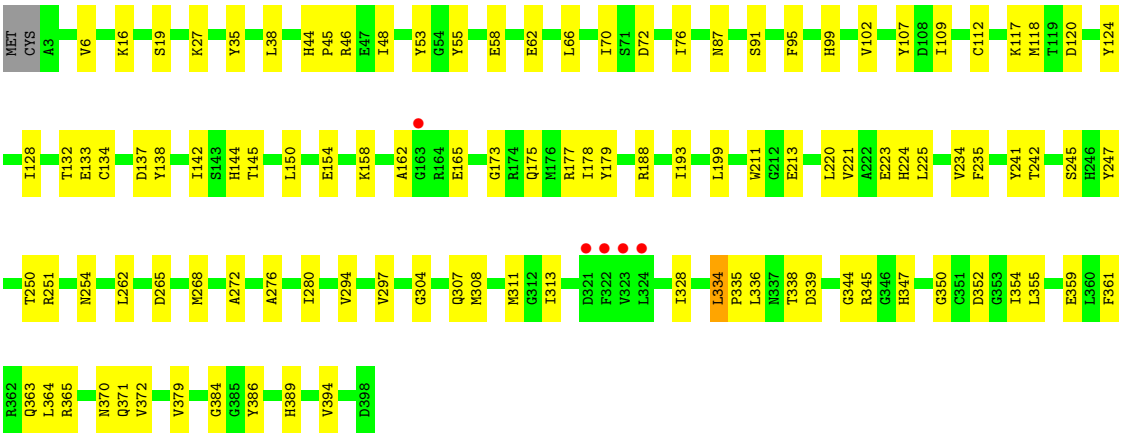
Chain F:





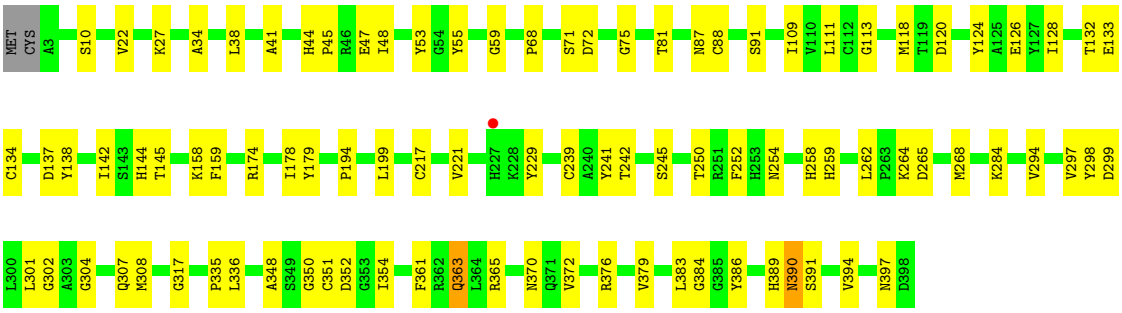
• Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein PhlC

Chain I:



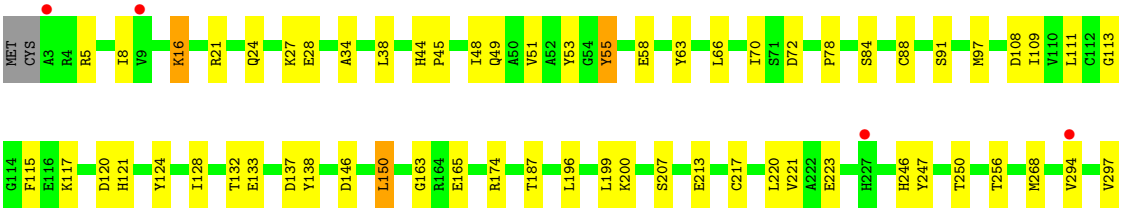
• Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein PhlC

Chain L:



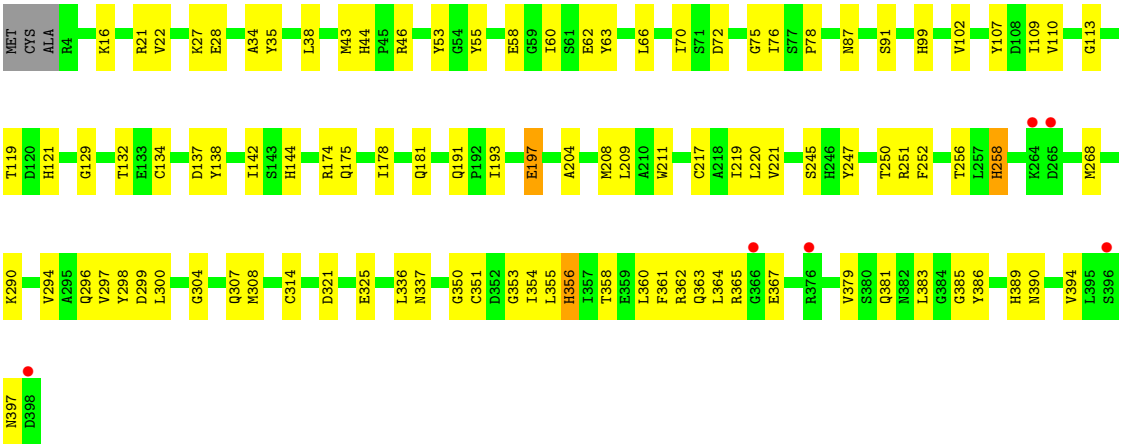
• Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein PhlC

Chain O:



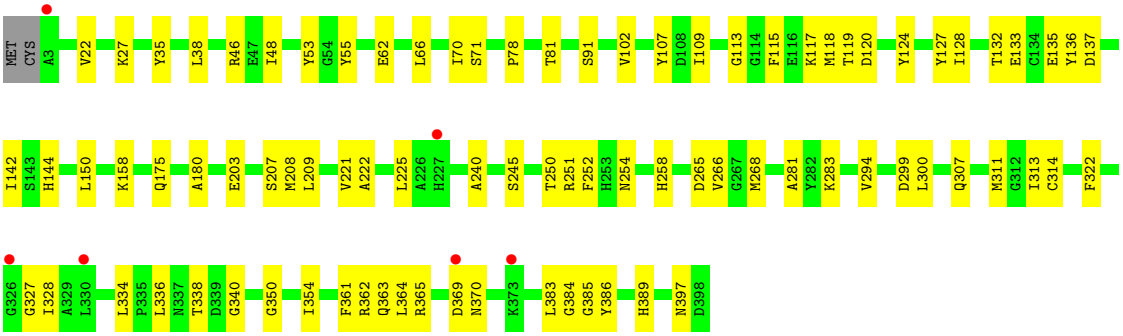
• Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein PhlC

Chain R:



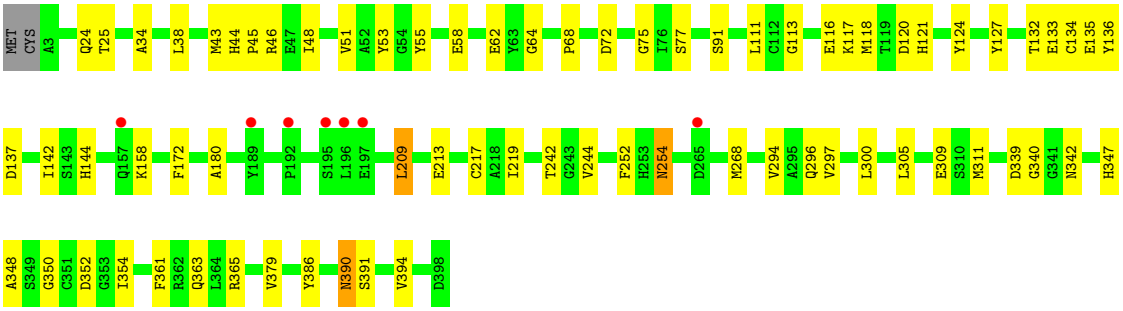
• Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein PhlC

Chain U:



• Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein PhlC

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.79Å 229.78Å 311.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 3.44 49.72 – 3.44	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.73-3.44) 99.2 (49.72-3.44)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.165 , 0.221 0.165 , 0.220	Depositor DCC
R_{free} test set	4986 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	53.9	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	54522	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 13X, SCY

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	0.25	0/2721	0.46	0/3695
1	D	0.25	0/2730	0.45	0/3706
1	G	0.26	0/2730	0.47	0/3706
1	J	0.25	0/2730	0.45	0/3706
1	M	0.25	0/2730	0.47	0/3706
1	P	0.25	0/2721	0.46	0/3695
1	S	0.25	0/2732	0.46	0/3710
1	V	0.25	0/2730	0.48	0/3706
2	B	0.25	0/1172	0.46	0/1580
2	E	0.25	0/1172	0.44	0/1580
2	H	0.24	0/1172	0.45	0/1580
2	K	0.25	0/1172	0.45	0/1580
2	N	0.24	0/1172	0.44	0/1580
2	Q	0.26	0/1172	0.46	0/1580
2	T	0.25	0/1172	0.45	0/1580
2	W	0.25	0/1172	0.46	0/1580
3	C	0.26	0/3019	0.45	0/4082
3	F	0.25	0/3019	0.44	0/4082
3	I	0.26	0/3024	0.44	0/4089
3	L	0.26	0/3024	0.45	0/4089
3	O	0.26	0/3024	0.45	0/4089
3	R	0.26	0/3019	0.45	0/4082
3	U	0.26	0/3024	0.44	0/4089
3	X	0.26	0/3024	0.47	0/4089
All	All	0.26	0/55377	0.45	0/74961

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	G	0	1
1	M	0	1
1	P	0	1
1	S	0	1
1	V	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	GLY	Peptide
1	D	305	GLY	Peptide
1	G	305	GLY	Peptide
1	M	305	GLY	Peptide
1	P	305	GLY	Peptide
1	S	305	GLY	Peptide
1	V	305	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2677	0	2662	46	0
1	D	2686	0	2675	51	0
1	G	2686	0	2675	50	0
1	J	2686	0	2675	45	0
1	M	2686	0	2675	57	0
1	P	2677	0	2662	55	0
1	S	2687	0	2668	57	0
1	V	2686	0	2675	49	0
2	B	1150	0	1149	21	0
2	E	1150	0	1149	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1150	0	1149	24	0
2	K	1150	0	1149	22	0
2	N	1150	0	1149	19	0
2	Q	1150	0	1149	16	0
2	T	1150	0	1149	30	0
2	W	1150	0	1149	30	0
3	C	2965	0	2869	46	0
3	F	2965	0	2869	65	0
3	I	2970	0	2874	79	0
3	L	2970	0	2874	67	0
3	O	2970	0	2874	59	0
3	R	2965	0	2869	65	0
3	U	2970	0	2874	59	0
3	X	2970	0	2874	50	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
4	N	1	0	0	0	0
4	Q	1	0	0	0	0
4	T	1	0	0	0	0
4	W	1	0	0	0	0
5	C	9	0	6	2	0
5	L	9	0	6	2	0
5	O	9	0	6	1	0
5	R	9	0	6	0	0
6	A	5	0	0	0	0
6	B	3	0	0	0	0
6	C	5	0	0	0	0
6	D	3	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	3	0	0	0	0
6	I	2	0	0	0	0
6	J	5	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	M	4	0	0	0	0
6	N	3	0	0	0	0
6	O	1	0	0	1	0
6	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Q	2	0	0	0	0
6	R	3	0	0	0	0
6	S	2	0	0	0	0
6	T	1	0	0	0	0
6	U	1	0	0	0	0
6	V	6	0	0	0	0
6	X	4	0	0	0	0
All	All	54522	0	53560	902	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 8.

All (902) 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)
3:U:132:THR:HG22	3:U:133:GLU:H	1.21	1.04
1:D:238:TYR:OH	1:D:295:GLN:OE1	1.76	1.03
3:L:132:THR:HG22	3:L:133:GLU:H	1.24	1.02
3:C:132:THR:HG22	3:C:133:GLU:H	1.25	0.99
3:X:132:THR:HG22	3:X:133:GLU:H	1.27	0.98
3:I:133:GLU:OE2	3:U:27:LYS:NZ	2.00	0.94
1:D:238:TYR:CZ	1:D:295:GLN:OE1	2.21	0.92
1:G:192:ARG:HB3	1:P:89:SER:HB2	1.53	0.91
1:P:200:ARG:NH1	1:S:356:TYR:O	2.04	0.91
2:H:18:ARG:NH1	3:U:62:GLU:OE1	2.06	0.88
1:G:356:TYR:O	1:V:200:ARG:NH1	2.07	0.86
3:X:46:ARG:NH1	3:X:75:GLY:O	2.11	0.83
3:I:87:ASN:HB2	3:I:389:HIS:HE2	1.44	0.83
3:I:158:LYS:NZ	3:I:265:ASP:OD2	2.11	0.82
1:A:89:SER:HB2	1:D:192:ARG:HB3	1.58	0.82
3:C:132:THR:OG1	3:C:144:HIS:NE2	2.13	0.82
1:P:52:ASP:OD1	2:T:126:ARG:NH1	2.11	0.82
1:A:192:ARG:HB3	1:D:89:SER:HB2	1.62	0.81
3:I:46:ARG:HH12	3:U:258:HIS:CG	1.99	0.81
1:J:192:ARG:NH2	1:J:196:ASP:O	2.14	0.81
3:O:294:VAL:HG11	3:O:363:GLN:HG2	1.63	0.81
3:X:294:VAL:HG11	3:X:363:GLN:HG2	1.64	0.80
3:X:209:LEU:HD22	3:X:300:LEU:HD13	1.64	0.80
1:P:356:TYR:O	1:S:200:ARG:NH1	2.14	0.79
3:I:27:LYS:NZ	3:U:133:GLU:OE2	2.16	0.77
1:G:147:ARG:NH2	2:Q:6:GLU:OE2	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:TYR:CE2	1:D:295:GLN:OE1	2.38	0.76
1:G:194:GLN:OE1	1:P:147:ARG:NH1	2.19	0.76
3:L:132:THR:OG1	3:L:144:HIS:NE2	2.18	0.76
1:D:52:ASP:OD1	2:K:126:ARG:NH1	2.17	0.75
3:X:51:VAL:HG22	3:X:111:LEU:HB3	1.69	0.75
1:G:28:VAL:O	1:V:346:LYS:NZ	2.19	0.74
3:R:43:MET:HE1	3:R:219:ILE:HG21	1.69	0.74
3:U:384:GLY:HA3	3:U:389:HIS:HD2	1.51	0.74
1:M:192:ARG:NH2	1:M:196:ASP:O	2.21	0.74
3:C:245:SER:O	3:C:251:ARG:NH1	2.20	0.74
1:S:69:LYS:NZ	1:S:325:HIS:O	2.21	0.73
2:H:14:ALA:H	2:H:132:SER:HB2	1.53	0.73
3:O:109:ILE:HG12	3:O:221:VAL:HG23	1.70	0.73
3:F:27:LYS:NZ	3:O:133:GLU:OE2	2.20	0.73
2:B:126:ARG:NH1	1:M:52:ASP:OD1	2.21	0.73
2:E:126:ARG:NH1	1:J:52:ASP:OD1	2.20	0.73
3:C:27:LYS:NZ	3:L:133:GLU:OE2	2.21	0.73
1:G:52:ASP:OD1	2:W:126:ARG:NH1	2.19	0.73
1:V:123:GLN:NE2	1:V:309:ASP:OD1	2.21	0.73
2:T:6:GLU:OE2	1:V:147:ARG:NH2	2.21	0.72
1:S:147:ARG:NH2	2:W:6:GLU:OE2	2.22	0.72
3:L:239:CYS:O	3:L:284:LYS:NZ	2.23	0.72
2:W:30:GLU:OE2	2:W:60:ARG:NH1	2.23	0.71
1:J:105:ASP:HA	1:M:183:CYS:HA	1.71	0.71
3:U:132:THR:HG22	3:U:133:GLU:N	2.00	0.71
3:R:91:SER:OG	3:R:350:GLY:O	2.06	0.71
3:C:132:THR:HG22	3:C:133:GLU:N	2.04	0.71
1:S:349:PHE:HB3	2:W:5:PRO:HD2	1.72	0.71
3:I:338:THR:OG1	3:I:359:GLU:OE2	2.09	0.70
2:T:82:GLY:HA3	2:T:129:VAL:HG12	1.71	0.70
2:T:30:GLU:OE2	2:T:60:ARG:NH1	2.24	0.70
2:B:74:GLU:HG2	2:B:88:PRO:HB3	1.74	0.70
1:S:345:ILE:HG23	1:S:350:LYS:HB2	1.73	0.70
1:D:16:PRO:O	1:D:19:ARG:NH1	2.25	0.70
3:F:132:THR:OG1	3:F:137:ASP:OD1	2.10	0.70
1:G:186:ASP:OD1	2:T:23:HIS:NE2	2.24	0.70
3:F:294:VAL:HG21	3:F:363:GLN:HE21	1.57	0.70
2:K:113:GLN:NE2	3:R:175:GLN:OE1	2.25	0.69
3:F:91:SER:OG	3:F:350:GLY:O	2.10	0.69
3:O:16:LYS:HG3	3:O:187:THR:HA	1.73	0.69
2:W:74:GLU:HG2	2:W:88:PRO:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:178:ILE:HG12	3:I:193:ILE:HD13	1.73	0.69
1:D:23:GLN:O	1:D:27:ASN:ND2	2.22	0.69
3:O:91:SER:OG	3:O:350:GLY:O	2.09	0.69
1:P:217:GLN:HG3	1:P:306:ALA:HB1	1.74	0.69
3:I:179:TYR:HD1	3:I:370:ASN:HD22	1.40	0.69
3:L:384:GLY:HA3	3:L:389:HIS:HD2	1.58	0.69
3:U:294:VAL:HG11	3:U:363:GLN:HG2	1.75	0.69
3:C:91:SER:OG	3:C:350:GLY:O	2.10	0.68
2:W:9:HIS:NE2	3:X:62:GLU:OE2	2.23	0.68
1:S:194:GLN:OE1	1:V:147:ARG:NH1	2.26	0.68
2:H:6:GLU:OE2	1:P:147:ARG:NH2	2.27	0.68
2:E:45:ARG:NH2	3:O:72:ASP:O	2.24	0.68
3:I:241:TYR:HE1	3:I:389:HIS:HB2	1.57	0.68
3:F:362:ARG:NH2	3:F:367:GLU:O	2.27	0.68
3:I:268:MET:O	3:I:386:TYR:OH	2.11	0.68
2:Q:14:ALA:H	2:Q:132:SER:HB2	1.59	0.68
1:J:315:VAL:HG13	1:J:319:ILE:HG13	1.74	0.68
2:Q:126:ARG:NH1	1:S:52:ASP:OD1	2.26	0.68
3:L:132:THR:HG22	3:L:133:GLU:N	2.04	0.68
1:J:46:ARG:NH1	1:J:159:ALA:O	2.27	0.67
3:I:38:LEU:HD21	3:I:48:ILE:HD11	1.75	0.67
3:I:91:SER:OG	3:I:350:GLY:O	2.12	0.67
2:K:14:ALA:H	2:K:132:SER:HB2	1.59	0.67
3:L:297:VAL:HG22	3:L:336:LEU:HD11	1.76	0.67
3:O:38:LEU:HD21	3:O:48:ILE:HD11	1.75	0.67
2:B:21:ARG:NH2	3:L:120:ASP:OD1	2.27	0.67
2:B:85:GLU:O	1:M:346:LYS:NZ	2.25	0.67
3:X:91:SER:OG	3:X:350:GLY:O	2.13	0.67
2:K:6:GLU:OE2	1:M:147:ARG:NH2	2.24	0.66
1:V:217:GLN:HG3	1:V:306:ALA:HB1	1.77	0.66
1:A:305:GLY:HA3	1:D:90:ARG:HG3	1.74	0.66
2:H:108:ASP:CG	2:H:126:ARG:HH12	1.97	0.66
1:M:22:VAL:HG13	1:M:157:SER:HB2	1.77	0.66
1:D:217:GLN:HG3	1:D:306:ALA:HB1	1.78	0.66
3:L:124:TYR:CZ	3:L:128:ILE:HD11	2.31	0.66
3:X:132:THR:HG22	3:X:133:GLU:N	2.04	0.66
1:A:52:ASP:OD1	2:N:126:ARG:NH1	2.29	0.66
1:P:83:CYS:O	1:P:192:ARG:NH1	2.28	0.66
1:S:124:ILE:HD13	1:V:124:ILE:HD13	1.75	0.66
3:C:133:GLU:OE2	3:L:27:LYS:NZ	2.29	0.65
1:D:28:VAL:O	1:J:346:LYS:NZ	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:NH2	2:E:6:GLU:OE2	2.29	0.65
1:G:89:SER:HB2	1:P:192:ARG:HB3	1.78	0.65
1:G:217:GLN:HG3	1:G:306:ALA:HB1	1.77	0.65
1:G:185:ALA:O	1:P:94:SER:OG	2.14	0.65
1:M:192:ARG:HD3	1:M:199:ILE:HG12	1.76	0.65
3:R:137:ASP:HB2	3:R:142:ILE:HB	1.76	0.65
2:T:74:GLU:HG3	2:T:88:PRO:HB3	1.77	0.65
3:O:174:ARG:NH2	6:O:601:HOH:O	2.29	0.65
3:R:268:MET:O	3:R:386:TYR:OH	2.15	0.64
3:O:362:ARG:NH2	3:O:367:GLU:O	2.31	0.64
3:U:91:SER:HB3	3:U:354:ILE:HG12	1.78	0.64
3:R:109:ILE:HG12	3:R:221:VAL:HG23	1.79	0.64
2:T:26:LYS:NZ	2:T:137:GLN:OE1	2.29	0.64
3:X:117:LYS:NZ	3:X:213:GLU:OE1	2.30	0.64
2:N:93:MET:HG2	3:O:150:LEU:HD22	1.78	0.64
1:P:362:LEU:O	1:S:200:ARG:NH2	2.31	0.64
1:S:16:PRO:O	1:S:19:ARG:NH1	2.31	0.64
1:G:83:CYS:HG	1:P:89:SER:HG	1.45	0.64
1:A:85:ASN:ND2	1:A:87:TYR:O	2.31	0.63
3:F:297:VAL:HG12	3:F:311:MET:HE1	1.81	0.63
3:L:38:LEU:HD21	3:L:48:ILE:HD11	1.81	0.63
3:R:209:LEU:HD23	3:R:300:LEU:HB2	1.81	0.63
2:Q:74:GLU:HB3	2:Q:88:PRO:HB3	1.80	0.63
1:D:216:ASP:OD1	1:D:219:ARG:NH1	2.31	0.63
1:D:149:THR:O	1:D:350:LYS:NZ	2.32	0.63
3:L:109:ILE:HG12	3:L:221:VAL:HG23	1.81	0.63
2:K:74:GLU:HG2	2:K:88:PRO:HB3	1.81	0.62
3:R:245:SER:O	3:R:251:ARG:NH1	2.32	0.62
3:I:46:ARG:HE	3:I:76:ILE:HA	1.63	0.62
3:F:21:ARG:O	3:F:117:LYS:NZ	2.32	0.62
2:H:30:GLU:OE2	2:H:60:ARG:NH1	2.32	0.62
1:V:216:ASP:OD1	1:V:219:ARG:NH1	2.31	0.62
3:I:124:TYR:CZ	3:I:128:ILE:HD11	2.35	0.62
3:F:72:ASP:O	2:N:45:ARG:NH2	2.30	0.62
1:G:83:CYS:HB3	1:G:143:ASP:OD2	1.99	0.62
2:H:49:GLY:O	3:U:46:ARG:NH2	2.33	0.62
2:B:14:ALA:H	2:B:132:SER:HB2	1.65	0.62
3:L:88:SCY:OCD	5:L:500:13X:O7	2.15	0.62
2:B:6:GLU:OE2	1:D:147:ARG:NH2	2.33	0.62
1:J:147:ARG:NH1	1:M:194:GLN:OE1	2.33	0.62
1:J:185:ALA:O	1:M:94:SER:OG	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:137:ASP:OD1	3:L:138:TYR:N	2.32	0.62
2:Q:45:ARG:NH2	3:X:72:ASP:O	2.32	0.62
3:R:27:LYS:NZ	3:X:133:GLU:OE2	2.32	0.61
3:U:268:MET:O	3:U:386:TYR:OH	2.17	0.61
1:G:345:ILE:HG23	1:G:350:LYS:HB2	1.82	0.61
1:P:242:GLN:NE2	1:P:279:SER:OG	2.33	0.61
3:I:72:ASP:OD1	2:T:45:ARG:NH1	2.23	0.61
2:K:111:ASP:OD1	3:R:174:ARG:NH2	2.33	0.61
1:J:90:ARG:NH1	1:M:186:ASP:OD1	2.33	0.61
1:V:41:LEU:HB3	1:V:245:LEU:HD22	1.82	0.61
3:X:58:GLU:OE1	3:X:64:GLY:HA3	2.01	0.61
3:I:294:VAL:HG11	3:I:363:GLN:HG2	1.81	0.61
1:S:185:ALA:O	1:V:94:SER:OG	2.19	0.61
3:F:268:MET:O	3:F:386:TYR:OH	2.19	0.61
1:P:16:PRO:O	1:P:19:ARG:NH1	2.33	0.61
3:I:363:GLN:HE22	3:I:371:GLN:HA	1.66	0.61
1:P:219:ARG:HH22	1:P:255:HIS:CD2	2.18	0.61
1:J:41:LEU:HD12	1:J:245:LEU:HD22	1.83	0.61
3:L:91:SER:OG	3:L:350:GLY:O	2.18	0.61
1:M:69:LYS:NZ	1:M:325:HIS:O	2.34	0.60
1:S:89:SER:HB2	1:V:192:ARG:HB3	1.83	0.60
1:V:226:MET:HE3	1:V:298:LEU:HD22	1.83	0.60
3:L:91:SER:HB3	3:L:354:ILE:HG12	1.84	0.60
3:X:268:MET:O	3:X:386:TYR:OH	2.17	0.60
1:V:16:PRO:O	1:V:19:ARG:NH1	2.34	0.60
3:O:137:ASP:OD1	3:O:138:TYR:N	2.34	0.60
3:C:124:TYR:CZ	3:C:128:ILE:HD11	2.36	0.60
1:S:192:ARG:NH2	1:S:196:ASP:O	2.35	0.60
1:A:89:SER:O	1:A:90:ARG:HB3	2.02	0.60
3:U:328:ILE:HB	3:U:336:LEU:HB2	1.83	0.60
3:F:94:SER:HA	3:F:97:MET:HE2	1.84	0.60
1:M:16:PRO:O	1:M:19:ARG:NH1	2.35	0.59
1:S:105:ASP:HA	1:V:183:CYS:HA	1.84	0.59
1:J:147:ARG:NH2	2:N:6:GLU:OE2	2.35	0.59
1:M:345:ILE:HG23	1:M:350:LYS:HB2	1.85	0.59
3:U:91:SER:OG	3:U:350:GLY:O	2.19	0.59
2:Q:28:ARG:NH1	1:S:98:GLU:O	2.35	0.59
1:G:94:SER:OG	1:P:185:ALA:O	2.21	0.59
2:K:5:PRO:HD2	1:M:349:PHE:HB3	1.84	0.59
1:A:90:ARG:HD2	1:D:191:ILE:HG22	1.85	0.59
3:X:44:HIS:CD2	3:X:45:PRO:HD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:105:ASP:OD1	1:M:220:ARG:NH2	2.34	0.58
3:L:390:ASN:HD22	3:L:391:SER:N	2.01	0.58
2:T:107:VAL:HG23	2:T:143:VAL:HG12	1.85	0.58
3:F:245:SER:O	3:F:251:ARG:NH1	2.33	0.58
3:I:72:ASP:O	2:T:45:ARG:NH2	2.27	0.58
3:I:162:ALA:HA	3:I:165:GLU:OE2	2.03	0.58
3:U:338:THR:O	3:U:370:ASN:ND2	2.35	0.58
1:A:90:ARG:HG3	1:D:305:GLY:HA3	1.84	0.58
1:A:179:ALA:HB3	1:A:229:LEU:HD21	1.85	0.58
1:J:197:ARG:HB2	2:N:3:MET:HE2	1.84	0.58
2:W:14:ALA:H	2:W:132:SER:HB2	1.68	0.58
3:I:137:ASP:HB2	3:I:142:ILE:HB	1.85	0.58
3:I:223:GLU:HG3	3:I:235:PHE:HE1	1.69	0.58
3:L:259:HIS:HB3	3:L:262:LEU:HD11	1.85	0.58
3:I:58:GLU:OE2	3:U:127:TYR:OH	2.18	0.58
1:D:89:SER:O	1:D:90:ARG:HB3	2.03	0.58
3:I:46:ARG:NH1	3:U:258:HIS:CG	2.71	0.58
3:R:379:VAL:HG22	3:R:394:VAL:HG22	1.85	0.58
1:A:356:TYR:O	1:M:200:ARG:NH2	2.31	0.57
3:C:294:VAL:HG11	3:C:363:GLN:HG2	1.85	0.57
3:R:62:GLU:OE2	2:W:18:ARG:NH1	2.20	0.57
3:I:117:LYS:NZ	3:I:213:GLU:OE1	2.34	0.57
3:C:164:ARG:NH2	3:C:321:ASP:OD1	2.37	0.57
2:N:74:GLU:HG2	2:N:88:PRO:HB3	1.85	0.57
2:Q:21:ARG:HD2	3:X:25:THR:HG22	1.87	0.57
1:S:90:ARG:HD2	1:V:191:ILE:HG22	1.87	0.57
1:V:191:ILE:HD12	1:V:193:PRO:HD3	1.85	0.57
1:J:16:PRO:O	1:J:19:ARG:NH1	2.38	0.57
1:J:305:GLY:N	1:J:306:ALA:HA	2.20	0.57
2:W:22:GLU:OE2	2:W:44:ARG:NH1	2.37	0.57
1:D:54:ASP:H	1:D:57:THR:HB	1.69	0.57
2:N:107:VAL:HG23	2:N:143:VAL:HG12	1.86	0.57
1:S:215:GLU:OE1	1:S:255[B]:HIS:ND1	2.35	0.57
2:T:14:ALA:H	2:T:132:SER:HB2	1.70	0.57
3:F:101:MET:HB3	3:F:107:TYR:HD2	1.69	0.57
1:P:345:ILE:HG23	1:P:350:LYS:HB2	1.86	0.56
3:L:294:VAL:HG11	3:L:363:GLN:HG2	1.87	0.56
3:U:124:TYR:CZ	3:U:128:ILE:HD11	2.39	0.56
3:C:46:ARG:HH12	3:L:258:HIS:CG	2.23	0.56
3:O:297:VAL:HG22	3:O:336:LEU:HD11	1.87	0.56
1:A:90:ARG:HH11	1:A:95:ILE:HG12	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:113:GLY:HA2	3:O:354:ILE:HG13	1.86	0.56
1:P:52:ASP:HB2	2:T:126:ARG:HB3	1.88	0.56
3:C:137:ASP:HB2	3:C:142:ILE:HB	1.88	0.56
3:I:276:ALA:O	3:I:280:ILE:HG12	2.04	0.56
3:C:78:PRO:HB2	3:L:242:THR:HB	1.88	0.56
1:P:46:ARG:NH1	1:P:159:ALA:O	2.35	0.56
3:R:134:CYS:HA	3:R:138:TYR:HB3	1.86	0.56
1:J:90:ARG:HD2	1:M:191:ILE:HG22	1.87	0.56
3:R:247:TYR:HB3	3:R:250:THR:HG23	1.88	0.56
1:A:16:PRO:O	1:A:19:ARG:NH1	2.39	0.56
1:M:217:GLN:HG3	1:M:306:ALA:HB1	1.88	0.56
1:J:182:SER:OG	1:J:309:ASP:OD1	2.15	0.55
1:M:178:ASP:OD2	1:M:314:THR:OG1	2.24	0.55
2:B:10:ARG:NH1	1:D:357:ALA:O	2.40	0.55
3:F:294:VAL:HG11	3:F:363:GLN:HG2	1.88	0.55
1:S:192:ARG:HB3	1:V:89:SER:HB2	1.87	0.55
1:G:253:ALA:HB1	1:G:258:PHE:HB2	1.88	0.55
2:Q:101:VAL:HG21	3:R:252:PHE:HB2	1.88	0.55
3:U:117:LYS:NZ	3:U:119:THR:OG1	2.40	0.55
1:A:131:SER:HB3	1:D:131:SER:HB3	1.87	0.55
1:A:226:MET:HE3	1:A:298:LEU:HD22	1.87	0.55
2:E:14:ALA:H	2:E:132:SER:HB2	1.71	0.55
1:P:189:ASP:OD2	1:P:302:TYR:OH	2.23	0.55
1:S:359:THR:OG1	1:S:360:ALA:N	2.40	0.55
3:U:209:LEU:HD23	3:U:300:LEU:HB2	1.88	0.55
2:H:22:GLU:OE2	2:H:44:ARG:NH2	2.40	0.55
1:S:67:LEU:HD11	1:S:75:ILE:HD11	1.89	0.55
2:H:85:GLU:O	1:V:346:LYS:HE3	2.06	0.55
1:J:89:SER:HB2	1:M:192:ARG:HE	1.71	0.55
3:L:241:TYR:HE1	3:L:389:HIS:HB3	1.72	0.55
1:P:328:PRO:HG2	1:P:331:GLU:HB2	1.88	0.55
2:Q:33:GLN:HG3	2:Q:40:ILE:HG22	1.88	0.55
3:C:345:ARG:HD3	3:C:355:LEU:HD13	1.88	0.55
2:E:74:GLU:HG2	2:E:88:PRO:HB3	1.88	0.55
2:N:14:ALA:H	2:N:132:SER:HB2	1.70	0.55
3:O:335:PRO:HG2	3:O:372:VAL:HG22	1.88	0.55
3:C:389:HIS:CE1	3:L:68:PRO:HD3	2.42	0.55
3:F:209:LEU:HG	3:F:300:LEU:HD13	1.88	0.55
1:G:16:PRO:O	1:G:19:ARG:NH1	2.40	0.54
1:M:85:ASN:OD1	1:M:92:SER:OG	2.25	0.54
1:S:151:PRO:HG3	1:S:350:LYS:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:46:ARG:NH1	3:R:76:ILE:HA	2.23	0.54
3:L:47:GLU:OE2	3:L:229:TYR:OH	2.21	0.54
3:O:298:TYR:O	3:O:307:GLN:NE2	2.37	0.54
1:G:41:LEU:HD12	1:G:245:LEU:HD22	1.90	0.54
3:I:120:ASP:OD1	2:T:21:ARG:NH2	2.40	0.54
3:O:21:ARG:O	3:O:117:LYS:NZ	2.41	0.54
1:P:129:VAL:HG21	1:P:168:ILE:HG22	1.90	0.54
1:D:338:TYR:HB2	3:R:197:GLU:HG3	1.88	0.54
1:D:356:TYR:O	1:J:200:ARG:NH2	2.30	0.54
1:D:113:PHE:CD1	1:D:116:LYS:HE2	2.43	0.54
2:E:33:GLN:HB2	2:E:59:TYR:HB2	1.90	0.54
1:M:113:PHE:CD1	1:M:116:LYS:HE2	2.43	0.53
2:Q:21:ARG:NH2	3:X:120:ASP:OD1	2.38	0.53
1:D:90:ARG:HH11	1:D:95:ILE:HG12	1.74	0.53
3:U:113:GLY:HA2	3:U:354:ILE:HG13	1.89	0.53
1:M:271:ASN:HD21	1:M:336:LYS:HE2	1.72	0.53
1:V:345:ILE:HG23	1:V:350:LYS:HB2	1.90	0.53
1:A:120:SER:O	1:A:124:ILE:HG12	2.09	0.53
3:I:224:HIS:CD2	3:I:225:LEU:HG	2.43	0.53
1:M:155:THR:HG22	1:M:205:LEU:HD21	1.91	0.53
1:S:54:ASP:H	1:S:57:THR:HB	1.73	0.53
1:V:189:ASP:OD1	1:V:189:ASP:N	2.39	0.53
3:X:34:ALA:HA	3:X:217:CYS:SG	2.48	0.53
3:U:35:TYR:HA	3:U:38:LEU:HD12	1.89	0.53
3:U:124:TYR:OH	3:U:128:ILE:HD11	2.09	0.53
3:F:109:ILE:HG12	3:F:221:VAL:HG23	1.90	0.53
3:L:179:TYR:HD1	3:L:370:ASN:HD22	1.56	0.53
1:M:41:LEU:HD12	1:M:245:LEU:HD22	1.91	0.53
3:O:313:ILE:HG22	3:O:322:PHE:HE1	1.73	0.53
1:S:147:ARG:NH1	1:V:194:GLN:OE1	2.42	0.53
1:V:54:ASP:H	1:V:57:THR:HB	1.73	0.53
1:D:345:ILE:HG23	1:D:350:LYS:HB2	1.90	0.53
1:G:85:ASN:ND2	1:G:87:TYR:O	2.42	0.52
3:L:158:LYS:NZ	3:L:265:ASP:OD2	2.42	0.52
2:B:107:VAL:HG23	2:B:143:VAL:HG12	1.91	0.52
1:G:259:ASN:ND2	1:G:261:LYS:HB2	2.24	0.52
3:I:124:TYR:OH	3:I:128:ILE:HD11	2.09	0.52
1:G:319:ILE:HG13	1:G:323:GLN:HE21	1.75	0.52
3:U:362:ARG:NH1	3:U:369:ASP:OD2	2.42	0.52
2:E:107:VAL:HG23	2:E:143:VAL:HG12	1.90	0.52
3:R:258:HIS:CE1	3:X:46:ARG:HH21	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:126:GLN:HE21	1:S:130:ALA:HB2	1.74	0.52
1:D:346:LYS:NZ	2:K:85:GLU:O	2.31	0.52
1:G:281:LEU:O	1:G:285:ILE:HG12	2.10	0.52
1:G:362:LEU:O	1:V:200:ARG:NH2	2.43	0.52
3:C:297:VAL:HG12	3:C:311:MET:HE1	1.91	0.52
1:G:147:ARG:NH1	1:P:194:GLN:OE1	2.43	0.52
3:R:144:HIS:CD2	3:R:385:GLY:HA2	2.44	0.52
2:W:107:VAL:HG23	2:W:143:VAL:HG12	1.90	0.52
1:A:94:SER:OG	1:D:185:ALA:O	2.28	0.52
3:F:137:ASP:HB2	3:F:142:ILE:HB	1.92	0.52
3:O:5:ARG:NE	3:O:223:GLU:OE2	2.42	0.52
3:O:299:ASP:OD1	3:O:299:ASP:N	2.41	0.52
3:U:158:LYS:NZ	3:U:265:ASP:OD2	2.25	0.52
3:F:308:MET:HG2	3:F:336:LEU:HD11	1.92	0.52
1:G:5:LYS:HD3	1:G:176:GLU:OE2	2.10	0.51
3:I:87:ASN:HB2	3:I:389:HIS:NE2	2.19	0.51
3:I:188:ARG:HG3	3:I:344:GLY:HA2	1.92	0.51
3:L:361:PHE:O	3:L:365:ARG:HG3	2.10	0.51
3:R:297:VAL:HG22	3:R:336:LEU:HD11	1.91	0.51
3:R:321:ASP:O	3:R:325:GLU:HG3	2.10	0.51
1:G:98:GLU:OE2	1:G:104:TYR:OH	2.21	0.51
3:X:379:VAL:HG22	3:X:394:VAL:HG22	1.92	0.51
3:F:175:GLN:HG2	3:F:328:ILE:HG13	1.91	0.51
3:F:250:THR:O	3:F:254:ASN:HB2	2.11	0.51
3:C:117:LYS:NZ	3:C:213:GLU:OE1	2.27	0.51
1:V:187:VAL:O	1:V:305:GLY:HA2	2.10	0.51
3:L:87:ASN:OD1	3:L:389:HIS:NE2	2.27	0.51
3:O:322:PHE:CE2	3:O:327:GLY:HA3	2.45	0.51
3:C:88:SCY:HE2	5:C:500:13X:C1	2.41	0.51
3:F:124:TYR:CZ	3:F:128:ILE:HD11	2.45	0.51
3:O:375:ALA:O	3:O:397:ASN:ND2	2.44	0.51
3:R:299:ASP:OD1	3:R:299:ASP:N	2.44	0.51
3:U:175:GLN:HG2	3:U:328:ILE:HG13	1.92	0.51
3:U:299:ASP:OD1	3:U:299:ASP:N	2.41	0.51
3:X:390:ASN:HD22	3:X:391:SER:N	2.08	0.51
3:F:111:LEU:HD11	3:F:217:CYS:HB2	1.92	0.51
3:I:313:ILE:HD12	3:I:334:LEU:HD13	1.93	0.51
3:L:137:ASP:HB2	3:L:142:ILE:HB	1.92	0.51
1:M:253:ALA:HB1	1:M:258:PHE:HB2	1.93	0.51
3:U:144:HIS:CD2	3:U:385:GLY:HA2	2.46	0.51
1:V:67:LEU:HD11	1:V:75:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:ILE:O	1:D:323:GLN:HG2	2.11	0.51
3:I:361:PHE:O	3:I:365:ARG:HG3	2.11	0.51
2:B:21:ARG:NH1	3:L:22:VAL:O	2.44	0.50
1:D:301:SER:O	1:D:308:SER:OG	2.19	0.50
3:U:313:ILE:HD13	3:U:334:LEU:HD22	1.92	0.50
3:F:247:TYR:HB3	3:F:250:THR:HG23	1.92	0.50
3:C:132:THR:CG2	3:C:133:GLU:H	2.08	0.50
3:F:113:GLY:HA2	3:F:354:ILE:HG13	1.92	0.50
2:T:22:GLU:OE2	2:T:44:ARG:NH1	2.44	0.50
3:F:328:ILE:HB	3:F:336:LEU:HB2	1.92	0.50
3:I:46:ARG:NH1	3:U:258:HIS:ND1	2.53	0.50
2:K:85:GLU:OE1	2:K:85:GLU:N	2.44	0.50
1:V:340:ASP:OD1	1:V:340:ASP:N	2.44	0.50
3:C:46:ARG:HE	3:C:76:ILE:HA	1.77	0.50
1:P:268:TYR:OH	1:P:279:SER:HA	2.12	0.50
3:F:38:LEU:HD21	3:F:48:ILE:HD11	1.94	0.50
3:F:242:THR:HB	3:O:78:PRO:HB2	1.93	0.50
1:J:124:ILE:HD13	1:M:124:ILE:HD13	1.92	0.50
2:H:107:VAL:HG23	2:H:143:VAL:HG12	1.94	0.50
3:I:95:PHE:CE1	3:I:220:LEU:HD11	2.46	0.50
3:I:35:TYR:OH	2:T:52:ASN:OD1	2.30	0.50
1:M:46:ARG:HD2	1:M:159:ALA:O	2.12	0.50
2:B:108:ASP:OD2	2:B:126:ARG:NH2	2.45	0.49
3:I:134:CYS:HA	3:I:138:TYR:HB3	1.94	0.49
1:J:94:SER:OG	1:M:185:ALA:O	2.29	0.49
2:Q:33:GLN:HB2	2:Q:59:TYR:HB2	1.94	0.49
2:B:45:ARG:NH2	3:L:72:ASP:O	2.42	0.49
3:C:28:GLU:OE2	2:K:44:ARG:NH2	2.45	0.49
3:F:209:LEU:HD23	3:F:300:LEU:HB2	1.92	0.49
3:I:16:LYS:HB3	3:I:19:SER:HB2	1.95	0.49
3:I:234:VAL:HG13	3:I:364:LEU:HD12	1.93	0.49
1:P:56:ILE:HG13	1:P:86:PRO:HG2	1.92	0.49
3:R:60:ILE:O	2:W:18:ARG:NH2	2.45	0.49
3:R:35:TYR:HA	3:R:38:LEU:HD12	1.92	0.49
3:R:361:PHE:O	3:R:365:ARG:HG3	2.11	0.49
1:S:215:GLU:OE1	1:S:255[A]:HIS:ND1	2.45	0.49
1:J:122:LEU:HD13	1:J:166:LEU:HD12	1.93	0.49
1:V:189:ASP:HB2	1:V:209:LYS:HE2	1.93	0.49
3:F:163:GLY:HA3	1:S:27:ASN:ND2	2.27	0.49
1:J:37:VAL:HA	1:J:41:LEU:HB2	1.95	0.49
1:S:305:GLY:HA3	1:V:90:ARG:HH21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:22:GLU:OE1	3:U:136:TYR:OH	2.18	0.49
3:X:297:VAL:HG12	3:X:311:MET:HE1	1.94	0.49
3:C:71:SER:OG	3:C:81:THR:OG1	2.27	0.49
3:C:88:SCY:HE2	5:C:500:13X:C2	2.43	0.49
3:F:133:GLU:OE2	3:O:27:LYS:NZ	2.46	0.49
1:G:56:ILE:HG23	1:G:96:ILE:HG12	1.95	0.49
2:H:78:LEU:HD13	3:I:145:THR:HG21	1.94	0.49
3:I:250:THR:O	3:I:254:ASN:HB2	2.12	0.49
3:I:173:GLY:O	3:I:177:ARG:HG2	2.13	0.49
3:O:84:SER:HB3	3:O:97:MET:HE1	1.94	0.49
1:P:113:PHE:CD1	1:P:116:LYS:HE2	2.48	0.49
3:R:46:ARG:NH1	3:R:75:GLY:O	2.46	0.49
3:R:258:HIS:CG	3:X:46:ARG:HH21	2.30	0.49
2:T:108:ASP:OD2	2:T:126:ARG:NH2	2.46	0.49
1:M:54:ASP:H	1:M:57:THR:HB	1.76	0.49
2:N:115:LEU:HB2	2:N:144:LEU:HD11	1.95	0.49
2:H:134:LEU:HD21	1:P:356:TYR:HD2	1.77	0.49
3:O:34:ALA:HA	3:O:217:CYS:SG	2.53	0.49
3:R:297:VAL:HG13	3:R:336:LEU:HD21	1.94	0.49
3:U:222:ALA:HB3	3:U:225:LEU:HD12	1.95	0.49
3:X:252:PHE:CZ	3:X:268:MET:HG3	2.48	0.49
2:E:21:ARG:NH2	3:O:120:ASP:OD1	2.44	0.49
2:W:128:HIS:CD2	2:W:139:ALA:HB3	2.48	0.49
2:E:16:MET:HE2	1:M:189:ASP:HA	1.95	0.48
1:G:83:CYS:SG	1:P:89:SER:OG	2.58	0.48
1:M:41:LEU:HD12	1:M:245:LEU:HD13	1.95	0.48
2:N:128:HIS:CD2	2:N:139:ALA:HB3	2.48	0.48
3:U:245:SER:O	3:U:251:ARG:NH1	2.45	0.48
1:G:113:PHE:CD1	1:G:116:LYS:HE3	2.48	0.48
2:H:85:GLU:OE2	2:H:85:GLU:N	2.46	0.48
2:K:107:VAL:HG23	2:K:143:VAL:HG12	1.94	0.48
1:M:19:ARG:HE	1:M:271:ASN:ND2	2.10	0.48
3:U:118:MET:HB2	3:U:124:TYR:CG	2.48	0.48
3:X:43:MET:HE1	3:X:219:ILE:HG21	1.95	0.48
1:A:90:ARG:HH21	1:D:191:ILE:HG21	1.78	0.48
1:D:303:GLY:O	1:D:306:ALA:HA	2.13	0.48
2:H:21:ARG:NH2	3:U:120:ASP:OD1	2.47	0.48
2:K:78:LEU:HD13	3:L:145:THR:HG21	1.96	0.48
3:C:91:SER:HB3	3:C:354:ILE:HG12	1.96	0.48
1:S:94:SER:OG	1:V:185:ALA:O	2.31	0.48
3:C:113:GLY:HA2	3:C:354:ILE:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:240:VAL:HB	1:G:299:LEU:HD23	1.96	0.48
3:R:34:ALA:HA	3:R:217:CYS:SG	2.53	0.48
3:U:384:GLY:HA3	3:U:389:HIS:CD2	2.40	0.48
3:L:111:LEU:HD21	3:L:217:CYS:HB2	1.94	0.48
1:V:123:GLN:HA	1:V:126:GLN:HB3	1.95	0.48
3:L:113:GLY:HA2	3:L:354:ILE:HG13	1.94	0.48
2:N:22:GLU:OE2	2:N:44:ARG:NH1	2.47	0.48
3:F:338:THR:HG21	3:F:363:GLN:HE22	1.78	0.48
1:G:340:ASP:N	1:G:340:ASP:OD1	2.47	0.48
3:L:71:SER:OG	3:L:81:THR:OG1	2.25	0.48
1:S:226:MET:HE3	1:S:298:LEU:HD22	1.95	0.48
3:X:113:GLY:HA2	3:X:354:ILE:HG13	1.96	0.48
1:A:345:ILE:HG23	1:A:350:LYS:HB2	1.95	0.48
1:D:237:ASP:OD1	1:D:295:GLN:NE2	2.47	0.48
3:L:348:ALA:HB3	3:L:351:CYS:HB3	1.96	0.48
3:O:247:TYR:HB3	3:O:250:THR:HG23	1.95	0.48
3:R:258:HIS:CD2	3:X:46:ARG:HE	2.32	0.48
3:I:363:GLN:NE2	3:I:371:GLN:HA	2.29	0.47
3:O:268:MET:O	3:O:386:TYR:OH	2.32	0.47
3:R:78:PRO:HB2	3:X:242:THR:HB	1.94	0.47
3:R:87:ASN:HD22	3:R:385:GLY:N	2.12	0.47
3:R:181:GLN:NE2	3:R:191:GLN:O	2.42	0.47
3:R:294:VAL:HG11	3:R:363:GLN:HG2	1.96	0.47
1:A:90:ARG:NH1	1:D:186:ASP:OD1	2.48	0.47
3:C:297:VAL:CG1	3:C:311:MET:HE1	2.44	0.47
3:I:44:HIS:CD2	3:I:45:PRO:HD2	2.49	0.47
1:P:54:ASP:H	1:P:57:THR:HB	1.77	0.47
3:R:46:ARG:NH1	2:W:52:ASN:HD21	2.11	0.47
3:U:207:SER:OG	3:U:207:SER:O	2.30	0.47
1:V:56:ILE:HG13	1:V:86:PRO:HG2	1.97	0.47
3:X:137:ASP:HB2	3:X:142:ILE:HB	1.96	0.47
3:I:72:ASP:OD2	3:U:245:SER:HB2	2.13	0.47
3:L:44:HIS:CG	3:L:45:PRO:HD2	2.50	0.47
1:V:50:GLN:HB2	1:V:53:GLU:HG3	1.96	0.47
1:A:217:GLN:HG3	1:A:306:ALA:HB1	1.96	0.47
3:C:304:GLY:O	3:C:308:MET:HG3	2.15	0.47
3:I:132:THR:HG23	3:I:144:HIS:NE2	2.29	0.47
3:L:297:VAL:HG13	3:L:336:LEU:HD21	1.95	0.47
3:L:335:PRO:HG2	3:L:372:VAL:HG22	1.96	0.47
3:O:51:VAL:HG22	3:O:111:LEU:HB3	1.95	0.47
1:J:55:VAL:HG23	1:J:144:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:85:THR:O	3:F:85:THR:OG1	2.33	0.47
1:A:122:LEU:HD11	1:A:168:ILE:HD11	1.97	0.47
2:B:33:GLN:HG3	2:B:40:ILE:HG22	1.97	0.47
3:C:361:PHE:O	3:C:365:ARG:HG3	2.15	0.47
3:F:29:MET:HE2	3:F:215:SER:HB3	1.97	0.47
3:L:118:MET:HB2	3:L:124:TYR:CG	2.49	0.47
3:L:134:CYS:HA	3:L:138:TYR:HB3	1.97	0.47
3:L:252:PHE:CZ	3:L:268:MET:HG3	2.50	0.47
3:L:299:ASP:OD1	3:L:299:ASP:N	2.45	0.47
1:P:67:LEU:HD11	1:P:75:ILE:HD11	1.96	0.47
1:P:340:ASP:OD1	1:P:340:ASP:N	2.43	0.47
1:S:11:TYR:CE1	1:S:285:ILE:HG23	2.50	0.47
1:S:122:LEU:HD11	1:S:168:ILE:HD11	1.97	0.47
3:X:361:PHE:O	3:X:365:ARG:HG3	2.14	0.47
3:F:44:HIS:CD2	3:F:45:PRO:HD2	2.49	0.47
3:I:6:VAL:HG21	3:I:99:HIS:CD2	2.50	0.47
3:R:46:ARG:NH2	3:R:75:GLY:O	2.47	0.47
1:A:268:TYR:OH	1:A:279:SER:HA	2.14	0.47
3:F:361:PHE:O	3:F:365:ARG:HG3	2.13	0.47
2:H:105:GLU:OE2	2:H:141:LYS:HE2	2.15	0.47
3:O:364:LEU:HB3	3:O:397:ASN:HB3	1.96	0.47
3:R:204:ALA:HB3	3:R:208:MET:HB2	1.97	0.47
1:V:214:LEU:HD21	1:V:248:THR:HG23	1.97	0.47
3:F:102:VAL:HA	3:F:107:TYR:O	2.15	0.47
1:J:194:GLN:OE1	1:M:147:ARG:NH1	2.48	0.47
1:S:90:ARG:NH1	1:V:186:ASP:OD1	2.46	0.47
3:U:322:PHE:CE1	3:U:327:GLY:HA3	2.50	0.47
2:B:10:ARG:NH2	1:D:356:TYR:OH	2.48	0.46
3:I:247:TYR:HB3	3:I:250:THR:HG23	1.96	0.46
2:K:33:GLN:HB3	2:K:59:TYR:HB2	1.96	0.46
3:R:121:HIS:NE2	2:W:12:THR:HA	2.30	0.46
1:P:189:ASP:OD1	1:P:189:ASP:N	2.47	0.46
1:S:192:ARG:HD3	1:S:199:ILE:HG12	1.97	0.46
1:D:41:LEU:HB3	1:D:245:LEU:HD22	1.98	0.46
3:F:294:VAL:HG21	3:F:363:GLN:NE2	2.25	0.46
1:P:89:SER:O	1:P:90:ARG:HG2	2.15	0.46
3:U:252:PHE:CZ	3:U:268:MET:HG3	2.50	0.46
3:U:361:PHE:O	3:U:365:ARG:HG3	2.15	0.46
3:F:335:PRO:HG2	3:F:372:VAL:HG22	1.97	0.46
1:M:37:VAL:HA	1:M:41:LEU:HB2	1.97	0.46
1:P:265:PRO:O	1:P:286:ASN:ND2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ASP:HA	2:N:127:LYS:HB3	1.98	0.46
2:B:85:GLU:N	2:B:85:GLU:OE1	2.49	0.46
1:S:177:PHE:CZ	1:S:311:ILE:HG12	2.50	0.46
3:X:132:THR:CG2	3:X:137:ASP:OD2	2.62	0.46
1:G:191:ILE:HG22	1:P:90:ARG:HD2	1.98	0.46
3:I:335:PRO:HG2	3:I:372:VAL:HG22	1.98	0.46
1:J:90:ARG:NH1	1:M:188:ALA:HB2	2.30	0.46
1:S:105:ASP:OD1	1:V:220:ARG:NH2	2.42	0.46
1:S:268:TYR:OH	1:S:279:SER:HA	2.16	0.46
1:J:253:ALA:HB1	1:J:258:PHE:HB2	1.98	0.46
2:K:33:GLN:HB2	2:K:40:ILE:HG22	1.98	0.46
3:O:124:TYR:CE2	3:O:128:ILE:HD11	2.51	0.46
2:H:33:GLN:HB2	2:H:59:TYR:HB2	1.97	0.46
3:L:250:THR:O	3:L:254:ASN:HB2	2.16	0.46
3:O:345:ARG:NH1	3:O:346:GLY:O	2.49	0.46
1:P:122:LEU:HD13	1:P:166:LEU:HD12	1.97	0.46
1:S:116:LYS:HE3	1:S:309:ASP:HB2	1.98	0.46
1:V:179:ALA:HB3	1:V:229:LEU:HD21	1.97	0.46
1:A:50:GLN:HB2	1:A:53:GLU:HG3	1.98	0.46
2:E:68:GLU:OE2	2:E:95:ARG:NH2	2.49	0.46
1:J:54:ASP:H	1:J:57:THR:HB	1.81	0.46
3:L:304:GLY:O	3:L:308:MET:HG3	2.15	0.46
3:O:146:ASP:O	3:O:150:LEU:HD12	2.16	0.46
3:R:364:LEU:HB3	3:R:397:ASN:HB3	1.98	0.46
3:R:365:ARG:HB2	3:R:367:GLU:HG3	1.97	0.46
1:S:46:ARG:HD3	1:S:159:ALA:O	2.16	0.46
3:U:38:LEU:HD21	3:U:48:ILE:HD11	1.97	0.46
2:W:34:CYS:SG	2:W:48:CYS:HB2	2.56	0.46
2:E:33:GLN:HG3	2:E:40:ILE:HG22	1.99	0.45
3:F:314:CYS:HB2	3:F:318:GLN:HB2	1.98	0.45
3:U:180:ALA:HB2	3:U:340:GLY:HA3	1.98	0.45
3:I:46:ARG:HA	3:I:46:ARG:HD3	1.62	0.45
1:M:268:TYR:OH	1:M:279:SER:HA	2.16	0.45
3:R:121:HIS:HE2	2:W:12:THR:HA	1.81	0.45
1:D:338:TYR:CB	3:R:197:GLU:HG3	2.46	0.45
1:G:226:MET:O	1:G:230:HIS:N	2.49	0.45
3:I:384:GLY:HA3	3:I:389:HIS:CD2	2.51	0.45
1:J:67:LEU:HD11	1:J:75:ILE:HD11	1.98	0.45
1:M:190:ASN:HB2	1:M:304:PHE:CG	2.51	0.45
3:R:58:GLU:OE2	3:X:127:TYR:OH	2.14	0.45
3:R:381:GLN:OE1	3:R:390:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:THR:HG22	3:L:59:GLY:O	2.16	0.45
3:C:134:CYS:HA	3:C:138:TYR:HB3	1.97	0.45
3:F:197:GLU:HG3	1:P:338:TYR:HB2	1.97	0.45
3:L:88:SCY:OCD	5:L:500:13X:C6	2.64	0.45
2:N:108:ASP:CG	2:N:126:ARG:HH22	2.19	0.45
3:O:361:PHE:O	3:O:365:ARG:HG3	2.16	0.45
1:P:81:GLY:HA2	1:P:111:VAL:O	2.17	0.45
1:S:176:GLU:N	1:S:314:THR:O	2.41	0.45
2:T:83:TYR:CE2	2:T:129:VAL:HG13	2.52	0.45
3:F:9:VAL:HG12	3:F:230:THR:HG22	1.99	0.45
1:J:122:LEU:HD11	1:J:168:ILE:HD11	1.98	0.45
2:K:22:GLU:OE2	2:K:44:ARG:NH1	2.49	0.45
1:V:41:LEU:HD22	1:V:245:LEU:HD13	1.99	0.45
1:A:188:ALA:HB2	1:D:90:ARG:HH22	1.81	0.45
1:G:303:GLY:O	1:G:306:ALA:HA	2.17	0.45
3:O:66:LEU:O	3:O:70:ILE:HG12	2.16	0.45
1:D:146:ASN:N	1:D:146:ASN:OD1	2.49	0.45
1:G:346:LYS:HB2	1:G:351:TYR:HE2	1.82	0.45
3:I:175:GLN:HG2	3:I:328:ILE:HG13	1.98	0.45
1:J:180:SER:OG	1:M:107:TYR:OH	2.34	0.45
3:R:132:THR:HG23	3:R:144:HIS:NE2	2.31	0.45
1:M:85:ASN:ND2	1:M:110:ASP:OD2	2.45	0.45
3:F:44:HIS:N	3:F:47:GLU:OE1	2.47	0.45
1:J:261:LYS:HD3	1:J:261:LYS:O	2.17	0.45
2:K:128:HIS:CD2	2:K:139:ALA:HB3	2.52	0.45
1:A:253:ALA:HB2	1:A:263:VAL:HG21	1.99	0.44
2:B:108:ASP:CG	2:B:126:ARG:HH22	2.21	0.44
1:D:187:VAL:HG22	2:N:20:TRP:NE1	2.32	0.44
2:E:12:THR:HA	3:O:121:HIS:HE2	1.81	0.44
3:F:336:LEU:HD23	3:F:336:LEU:HA	1.78	0.44
3:O:24:GLN:HB2	3:O:28:GLU:HB2	1.99	0.44
3:R:389:HIS:CE1	3:X:68:PRO:HD3	2.52	0.44
1:S:85:ASN:ND2	1:S:110:ASP:OD2	2.41	0.44
3:U:137:ASP:HB2	3:U:142:ILE:HB	1.99	0.44
3:X:116:GLU:HB3	3:X:348:ALA:HB1	1.98	0.44
3:F:313:ILE:HD13	3:F:334:LEU:HD22	1.98	0.44
1:G:218:THR:HG21	1:G:252:LEU:HD13	1.97	0.44
1:J:293:PRO:HB3	1:J:317:ASP:HA	2.00	0.44
1:M:271:ASN:ND2	1:M:336:LYS:HE2	2.32	0.44
2:N:106:ILE:HA	2:N:142:PHE:O	2.18	0.44
1:S:189:ASP:OD1	1:S:189:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:232:LYS:O	3:C:365:ARG:HD2	2.18	0.44
2:E:87:VAL:HA	2:E:88:PRO:HA	1.78	0.44
2:H:126:ARG:NE	1:V:52:ASP:OD1	2.44	0.44
1:M:184:ALA:HA	1:M:307:GLY:HA2	1.99	0.44
3:U:252:PHE:HA	3:U:266:VAL:O	2.17	0.44
3:F:384:GLY:HA3	3:F:389:HIS:CD2	2.52	0.44
1:A:19:ARG:N	1:A:337:ILE:O	2.43	0.44
3:F:34:ALA:HA	3:F:217:CYS:SG	2.57	0.44
2:H:21:ARG:NH1	3:U:22:VAL:O	2.50	0.44
3:I:384:GLY:HA3	3:I:389:HIS:NE2	2.32	0.44
3:L:376:ARG:HA	3:L:397:ASN:ND2	2.32	0.44
1:S:126:GLN:NE2	1:S:130:ALA:HB2	2.33	0.44
1:S:359:THR:CG2	1:S:362:LEU:HB2	2.47	0.44
3:F:204:ALA:HB3	3:F:208:MET:HB2	2.00	0.44
3:F:304:GLY:O	3:F:308:MET:HG3	2.16	0.44
1:J:352:LEU:HD23	1:J:352:LEU:HA	1.87	0.44
3:R:113:GLY:HA2	3:R:354:ILE:HG13	2.00	0.44
3:U:240:ALA:HB3	3:U:281:ALA:HB2	2.00	0.44
3:U:364:LEU:HB3	3:U:397:ASN:HB3	2.00	0.44
3:X:43:MET:CE	3:X:219:ILE:HG21	2.47	0.44
1:A:300:VAL:HA	1:A:309:ASP:O	2.17	0.44
3:C:358:THR:O	3:C:362:ARG:HG3	2.18	0.44
3:F:351:CYS:O	3:F:355:LEU:HG	2.17	0.44
3:I:297:VAL:HG12	3:I:311:MET:HE1	1.99	0.44
1:J:90:ARG:HG2	1:J:91:ALA:N	2.32	0.44
3:L:132:THR:HG22	3:L:137:ASP:OD2	2.17	0.44
2:Q:28:ARG:HH12	1:S:98:GLU:HG3	1.82	0.44
2:Q:107:VAL:HG21	2:Q:141:LYS:HD3	1.99	0.44
3:R:110:VAL:HG12	3:R:220:LEU:HB2	1.99	0.44
1:A:41:LEU:HB3	1:A:245:LEU:HD22	2.00	0.44
2:E:128:HIS:CD2	2:E:139:ALA:HB3	2.53	0.44
3:I:46:ARG:HH11	3:I:46:ARG:HG3	1.83	0.44
3:I:379:VAL:HG22	3:I:394:VAL:HG22	2.00	0.44
2:Q:128:HIS:CD2	2:Q:139:ALA:HB3	2.53	0.44
3:R:66:LEU:O	3:R:70:ILE:HG12	2.18	0.44
2:E:78:LEU:HD13	3:F:145:THR:HG21	2.00	0.44
1:G:291:ALA:O	1:G:323:GLN:NE2	2.43	0.44
3:I:179:TYR:HD1	3:I:370:ASN:ND2	2.09	0.44
1:J:166:LEU:HD11	1:J:281:LEU:HD22	1.99	0.44
3:R:102:VAL:HA	3:R:107:TYR:O	2.18	0.44
3:U:250:THR:O	3:U:254:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:ALA:HB2	3:C:340:GLY:HA3	1.99	0.43
3:F:137:ASP:OD1	3:F:138:TYR:N	2.51	0.43
3:I:347:HIS:HD2	3:I:352:ASP:OD2	2.01	0.43
3:L:268:MET:O	3:L:386:TYR:OH	2.30	0.43
3:O:44:HIS:CG	3:O:45:PRO:HD2	2.53	0.43
2:T:41:PHE:HA	2:T:100:LEU:HD21	1.99	0.43
2:T:108:ASP:CG	2:T:126:ARG:HH22	2.21	0.43
2:W:26:LYS:HE3	3:X:135:GLU:O	2.18	0.43
1:A:302:TYR:HE1	1:A:306:ALA:HB1	1.83	0.43
2:B:21:ARG:H	2:B:21:ARG:HG2	1.65	0.43
1:D:222:ALA:O	1:D:226:MET:HG3	2.19	0.43
3:F:174:ARG:HH22	2:T:111:ASP:CG	2.21	0.43
1:G:89:SER:O	1:G:90:ARG:HG2	2.19	0.43
3:I:304:GLY:O	3:I:308:MET:HG3	2.18	0.43
3:I:339:ASP:OD2	3:I:345:ARG:NE	2.47	0.43
3:R:304:GLY:O	3:R:308:MET:HG3	2.18	0.43
1:S:5:LYS:HE2	1:S:316:THR:HG21	2.00	0.43
1:D:81:GLY:HA2	1:D:111:VAL:O	2.17	0.43
3:I:262:LEU:HD13	3:I:272:ALA:HB1	2.01	0.43
3:O:91:SER:HB3	3:O:354:ILE:HG12	2.01	0.43
3:R:22:VAL:HG12	3:R:119:THR:HG21	1.99	0.43
2:W:47:VAL:HG22	2:W:54:LEU:HD23	1.99	0.43
1:A:90:ARG:HH21	1:D:191:ILE:CG2	2.31	0.43
1:A:194:GLN:OE1	1:D:147:ARG:NH1	2.51	0.43
2:E:74:GLU:HG2	2:E:88:PRO:CB	2.48	0.43
3:F:348:ALA:HB3	3:F:351:CYS:HB3	2.00	0.43
2:H:108:ASP:OD1	2:H:126:ARG:NH1	2.51	0.43
3:I:242:THR:HB	3:U:78:PRO:HB2	1.99	0.43
3:I:347:HIS:CD2	3:I:352:ASP:OD2	2.71	0.43
3:U:71:SER:OG	3:U:81:THR:OG1	2.26	0.43
3:U:109:ILE:HG12	3:U:221:VAL:HG12	2.01	0.43
1:V:261:LYS:O	1:V:261:LYS:HD3	2.18	0.43
2:W:74:GLU:HG2	2:W:88:PRO:CB	2.46	0.43
3:X:118:MET:HB2	3:X:124:TYR:CG	2.54	0.43
1:A:54:ASP:H	1:A:57:THR:HB	1.83	0.43
3:C:44:HIS:CG	3:C:45:PRO:HD2	2.54	0.43
2:E:30:GLU:HG2	2:E:60:ARG:HD3	2.00	0.43
3:F:91:SER:HB2	3:F:353:GLY:HA3	2.01	0.43
3:I:44:HIS:CG	3:I:45:PRO:HD2	2.53	0.43
2:K:27:TYR:O	2:K:125:ILE:HD11	2.18	0.43
1:M:222:ALA:O	1:M:226:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:116:LYS:HE3	1:P:120:SER:OG	2.18	0.43
3:C:51:VAL:HG13	3:C:81:THR:HG23	2.01	0.43
3:C:357:ILE:HD11	3:C:393:ILE:HD12	2.01	0.43
2:E:44:ARG:NH2	3:O:28:GLU:OE2	2.52	0.43
2:H:72:PRO:HB3	2:H:90:ILE:HD13	2.01	0.43
3:I:354:ILE:HD13	3:I:354:ILE:HA	1.92	0.43
1:S:89:SER:O	1:S:90:ARG:HG2	2.18	0.43
1:V:254:LYS:HE3	1:V:254:LYS:HB2	1.74	0.43
2:E:20:TRP:NE1	1:M:187:VAL:HG22	2.34	0.43
2:H:87:VAL:HA	2:H:88:PRO:HA	1.78	0.43
3:I:308:MET:HG2	3:I:336:LEU:HD11	2.01	0.43
1:P:41:LEU:HB3	1:P:245:LEU:HD22	2.01	0.43
1:P:190:ASN:HB2	1:P:304:PHE:CG	2.53	0.43
3:U:66:LEU:O	3:U:70:ILE:HG12	2.18	0.43
2:W:115:LEU:HB2	2:W:144:LEU:HD11	2.01	0.43
3:X:132:THR:OG1	3:X:144:HIS:NE2	2.49	0.43
3:O:132:THR:HA	3:O:246:HIS:CG	2.54	0.43
3:C:296:GLN:NE2	3:C:337:ASN:HA	2.34	0.43
1:G:158:TYR:CG	1:G:245:LEU:HD21	2.54	0.43
3:O:382:ASN:O	3:O:390:ASN:ND2	2.52	0.43
1:P:19:ARG:N	1:P:337:ILE:O	2.37	0.43
3:R:28:GLU:HG2	2:W:46:THR:OG1	2.18	0.43
3:R:44:HIS:ND1	3:R:46:ARG:HB2	2.34	0.43
1:V:23:GLN:HE21	1:V:23:GLN:HB3	1.72	0.43
3:C:376:ARG:HA	3:C:397:ASN:OD1	2.19	0.43
1:D:69:LYS:NZ	1:D:325:HIS:O	2.52	0.43
3:F:44:HIS:CG	3:F:45:PRO:HD2	2.54	0.43
1:G:205:LEU:HD13	1:V:362:LEU:HD11	2.00	0.43
2:H:81:MET:HE3	2:T:7:GLN:HG2	2.01	0.43
1:M:122:LEU:HD11	1:M:168:ILE:HD11	2.01	0.43
2:N:74:GLU:HG2	2:N:88:PRO:CB	2.49	0.43
3:U:203:GLU:OE2	3:U:208:MET:HG2	2.18	0.43
1:A:303:GLY:O	1:A:306:ALA:HA	2.19	0.42
1:D:96:ILE:O	1:D:100:LEU:HG	2.19	0.42
3:I:46:ARG:NE	3:I:76:ILE:HA	2.33	0.42
3:L:132:THR:HG1	3:L:144:HIS:CD2	2.36	0.42
1:P:222:ALA:O	1:P:226:MET:HG3	2.19	0.42
1:P:335:SER:HB3	2:T:110:CYS:SG	2.58	0.42
1:S:70:VAL:HG12	1:S:73:HIS:HB2	2.00	0.42
1:S:303:GLY:O	1:S:306:ALA:HA	2.18	0.42
1:A:81:GLY:HA2	1:A:111:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:44:HIS:CD2	3:C:45:PRO:HD2	2.54	0.42
3:F:124:TYR:OH	3:F:128:ILE:HD11	2.19	0.42
3:I:62:GLU:OE1	2:T:18:ARG:NH1	2.26	0.42
2:K:83:TYR:CE2	2:K:129:VAL:HB	2.54	0.42
3:L:298:TYR:O	3:L:307:GLN:NE2	2.46	0.42
1:P:241:PHE:HA	1:P:300:VAL:O	2.19	0.42
3:X:296:GLN:HE22	3:X:339:ASP:CG	2.23	0.42
3:I:102:VAL:HA	3:I:107:TYR:O	2.19	0.42
3:L:301:LEU:HB3	3:L:302:GLY:H	1.61	0.42
1:V:218:THR:HG21	1:V:252:LEU:HD13	2.00	0.42
1:A:242:GLN:NE2	1:A:279:SER:OG	2.52	0.42
3:C:245:SER:HB2	3:L:72:ASP:CG	2.39	0.42
2:E:68:GLU:OE1	2:E:95:ARG:NE	2.53	0.42
1:G:220:ARG:NH2	1:P:105:ASP:OD2	2.48	0.42
3:I:345:ARG:HH11	3:I:355:LEU:HD13	1.84	0.42
1:M:81:GLY:HA2	1:M:111:VAL:O	2.20	0.42
1:M:303:GLY:O	1:M:306:ALA:HA	2.20	0.42
3:O:297:VAL:HG13	3:O:336:LEU:HD21	2.00	0.42
1:S:177:PHE:CZ	1:S:180:SER:HB3	2.54	0.42
1:G:131:SER:HB3	1:P:131:SER:HB3	2.02	0.42
3:I:245:SER:O	3:I:251:ARG:NH1	2.51	0.42
3:F:75:GLY:HA2	3:O:256:THR:HG23	2.01	0.42
3:L:159:PHE:CD1	3:L:317:GLY:HA3	2.54	0.42
1:P:352:LEU:HD23	1:S:198:TYR:OH	2.20	0.42
2:W:22:GLU:OE1	3:X:136:TYR:OH	2.20	0.42
1:A:293:PRO:HB3	1:A:317:ASP:HA	2.01	0.42
2:B:20:TRP:NE1	1:J:187:VAL:HG22	2.35	0.42
3:I:307:GLN:O	3:I:311:MET:HB2	2.19	0.42
3:L:194:PRO:HB2	3:L:199:LEU:HG	2.01	0.42
2:T:69:VAL:HG13	3:U:150:LEU:HD22	2.01	0.42
3:X:180:ALA:HB2	3:X:340:GLY:HA3	2.02	0.42
3:X:297:VAL:CG1	3:X:311:MET:HE1	2.50	0.42
2:H:93:MET:HG2	3:I:150:LEU:HD13	2.02	0.42
3:I:109:ILE:HG12	3:I:221:VAL:HG13	2.01	0.42
2:K:106:ILE:HA	2:K:142:PHE:O	2.19	0.42
3:L:128:ILE:HD13	3:L:128:ILE:HA	1.79	0.42
3:O:351:CYS:O	3:O:355:LEU:HG	2.20	0.42
3:U:307:GLN:O	3:U:311:MET:HB2	2.20	0.42
1:D:151:PRO:HG3	1:D:350:LYS:HD3	2.00	0.42
3:F:345:ARG:NH1	3:F:346:GLY:O	2.52	0.42
1:G:183:CYS:SG	1:G:220:ARG:HG2	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:118:MET:HB2	3:I:124:TYR:CG	2.55	0.42
1:J:346:LYS:HB2	1:J:351:TYR:HE2	1.85	0.42
1:M:11:TYR:OH	1:M:289:ASP:OD1	2.27	0.42
2:N:87:VAL:HA	2:N:88:PRO:HA	1.85	0.42
3:O:207:SER:OG	3:O:301:LEU:HA	2.19	0.42
3:C:44:HIS:ND1	3:C:46:ARG:HB2	2.35	0.42
3:C:46:ARG:HA	3:C:46:ARG:HD3	1.75	0.42
3:C:202:SER:OG	3:C:203:GLU:N	2.52	0.42
3:C:354:ILE:HD13	3:C:354:ILE:HA	1.90	0.42
1:G:356:TYR:CE1	2:W:8:ILE:HD13	2.55	0.42
1:M:19:ARG:HE	1:M:271:ASN:HD22	1.67	0.42
3:O:91:SER:HB2	3:O:353:GLY:HA3	2.01	0.42
3:O:163:GLY:N	3:O:165:GLU:OE1	2.53	0.42
1:P:265:PRO:HB3	1:P:290:GLN:NE2	2.35	0.42
3:R:358:THR:O	3:R:362:ARG:HG3	2.20	0.42
1:S:226:MET:HE1	1:S:258:PHE:CZ	2.55	0.42
2:T:36:GLU:OE2	2:T:53:SER:OG	2.26	0.42
1:A:351:TYR:CE1	1:M:345:ILE:HD12	2.55	0.41
3:R:129:GLY:O	3:R:132:THR:OG1	2.38	0.41
3:R:298:TYR:O	3:R:307:GLN:NE2	2.48	0.41
1:A:190:ASN:HB2	1:A:304:PHE:CG	2.55	0.41
1:A:340:ASP:OD1	1:A:340:ASP:N	2.52	0.41
1:D:128:LEU:HD12	1:D:134:THR:HG23	2.03	0.41
3:F:91:SER:HB2	3:F:353:GLY:CA	2.50	0.41
1:G:119:THR:O	1:G:123:GLN:HG3	2.21	0.41
3:L:379:VAL:HG22	3:L:394:VAL:HG22	2.02	0.41
1:M:189:ASP:OD1	1:M:189:ASP:N	2.53	0.41
1:M:302:TYR:HE1	1:M:306:ALA:HB1	1.85	0.41
1:P:8:ILE:O	1:P:174:ILE:HG22	2.20	0.41
2:T:87:VAL:HA	2:T:88:PRO:HA	1.76	0.41
2:W:108:ASP:OD2	2:W:126:ARG:NH2	2.52	0.41
2:W:131:GLU:HB2	2:W:135:ALA:O	2.20	0.41
1:D:65:ARG:HH21	2:K:122:ARG:NH2	2.17	0.41
3:F:365:ARG:HB2	3:F:367:GLU:HG3	2.03	0.41
1:G:155:THR:HA	1:G:158:TYR:CZ	2.56	0.41
3:I:66:LEU:O	3:I:70:ILE:HG12	2.20	0.41
1:J:305:GLY:N	1:J:306:ALA:CA	2.83	0.41
3:O:117:LYS:HD3	3:O:213:GLU:OE2	2.19	0.41
1:P:15:ILE:HD13	1:P:333:LEU:HD21	2.02	0.41
1:P:46:ARG:HH12	1:P:146:ASN:CB	2.32	0.41
3:R:256:THR:O	3:X:46:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:296:GLN:NE2	3:R:337:ASN:HA	2.36	0.41
3:C:365:ARG:NE	3:C:367:GLU:OE1	2.52	0.41
1:D:56:ILE:HG23	1:D:96:ILE:HG12	2.02	0.41
3:F:127:TYR:OH	3:O:58:GLU:OE2	2.27	0.41
1:M:6:ILE:HG12	1:M:170:SER:HB3	2.03	0.41
1:M:151:PRO:HG3	1:M:350:LYS:HD2	2.03	0.41
2:T:70:MET:HA	2:T:92:ALA:HA	2.01	0.41
3:X:209:LEU:HD12	3:X:342:ASN:HB3	2.02	0.41
1:A:65:ARG:HH21	2:N:122:ARG:NH2	2.17	0.41
2:B:87:VAL:HA	2:B:88:PRO:HA	1.86	0.41
3:C:128:ILE:HA	3:C:128:ILE:HD13	1.78	0.41
3:I:199:LEU:HA	3:I:199:LEU:HD23	1.87	0.41
1:J:36:LEU:HG	1:J:41:LEU:HD23	2.03	0.41
1:J:91:ALA:HB2	1:M:113:PHE:CG	2.56	0.41
3:L:10:SER:HB3	3:L:41:ALA:HB2	2.03	0.41
2:N:14:ALA:O	2:N:133:ASN:ND2	2.50	0.41
3:O:313:ILE:HD12	3:O:334:LEU:HD13	2.03	0.41
2:Q:12:THR:HA	3:X:121:HIS:HE2	1.85	0.41
3:U:55:TYR:HB3	3:U:115:PHE:CE2	2.56	0.41
3:U:66:LEU:HD12	3:U:66:LEU:HA	1.85	0.41
2:W:3:MET:HE3	2:W:3:MET:HB2	1.97	0.41
1:G:45:GLU:OE2	1:G:338:TYR:HE1	2.04	0.41
3:L:174:ARG:O	3:L:178:ILE:HG13	2.21	0.41
3:L:199:LEU:HD23	3:L:199:LEU:HA	1.95	0.41
3:L:264:LYS:HD3	3:L:264:LYS:HA	1.87	0.41
3:L:363:GLN:OE1	3:L:372:VAL:HG23	2.21	0.41
3:O:88:SCY:HE2	5:O:500:13X:C6	2.51	0.41
2:T:26:LYS:HE3	3:U:135:GLU:O	2.21	0.41
1:V:36:LEU:HD12	1:V:40:ASN:HB2	2.03	0.41
1:V:56:ILE:HG23	1:V:96:ILE:HG12	2.03	0.41
1:A:56:ILE:HG23	1:A:96:ILE:HG12	2.03	0.41
1:A:261:LYS:H	1:A:261:LYS:HD2	1.84	0.41
1:D:119:THR:O	1:D:123:GLN:HG3	2.20	0.41
3:F:21:ARG:HG3	3:F:213:GLU:HG3	2.03	0.41
1:G:349:PHE:HB3	2:Q:5:PRO:HD2	2.03	0.41
1:M:11:TYR:CE1	1:M:285:ILE:HG23	2.55	0.41
1:P:111:VAL:HG21	1:P:124:ILE:HD12	2.03	0.41
3:R:72:ASP:O	2:W:45:ARG:NH2	2.23	0.41
1:V:122:LEU:HD11	1:V:168:ILE:HD11	2.01	0.41
2:B:11:MET:HE3	2:B:12:THR:HG23	2.03	0.41
3:C:256:THR:HG23	3:L:75:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:128:HIS:CD2	2:H:139:ALA:HB3	2.56	0.41
3:I:112:CYS:SG	3:I:220:LEU:HD13	2.61	0.41
1:J:192:ARG:HD3	1:J:199:ILE:HG12	2.03	0.41
2:K:81:MET:HG3	3:L:126:GLU:OE1	2.21	0.41
3:L:384:GLY:HA3	3:L:389:HIS:CD2	2.46	0.41
3:O:55:TYR:HB3	3:O:115:PHE:CE2	2.56	0.41
3:R:63:TYR:CE2	3:X:134:CYS:HB2	2.56	0.41
1:S:120:SER:O	1:S:124:ILE:HG13	2.19	0.41
1:V:226:MET:HB3	1:V:231:THR:O	2.20	0.41
3:X:38:LEU:HD21	3:X:48:ILE:HD11	2.02	0.41
1:D:268:TYR:OH	1:D:279:SER:HA	2.21	0.41
3:I:347:HIS:CD2	3:I:352:ASP:OD1	2.74	0.41
1:J:216:ASP:OD1	1:J:219:ARG:NH1	2.54	0.41
3:R:91:SER:HB2	3:R:353:GLY:HA3	2.02	0.41
3:R:351:CYS:O	3:R:355:LEU:HG	2.20	0.41
1:S:79:TYR:CE1	1:S:109:ALA:HB3	2.56	0.41
1:V:146:ASN:OD1	1:V:146:ASN:N	2.53	0.41
3:X:24:GLN:O	3:X:117:LYS:HE2	2.20	0.41
3:R:356:HIS:O	3:R:360:LEU:HD12	2.21	0.41
3:X:244:VAL:HG11	3:X:254:ASN:OD1	2.21	0.41
3:X:305:LEU:O	3:X:309:GLU:HG3	2.21	0.41
1:A:126:GLN:HG2	1:A:177:PHE:CE1	2.56	0.40
3:F:66:LEU:O	3:F:70:ILE:HG12	2.21	0.40
1:J:329:LEU:HG	1:J:333:LEU:HD13	2.03	0.40
3:O:49:GLN:OE1	3:O:108:ASP:N	2.38	0.40
3:U:102:VAL:HA	3:U:107:TYR:O	2.21	0.40
1:V:80:LEU:HD13	1:V:96:ILE:HD12	2.02	0.40
2:W:23:HIS:O	2:W:27:TYR:HB2	2.21	0.40
2:W:62:ALA:O	2:W:96:LEU:HD13	2.21	0.40
2:B:94:VAL:O	2:B:101:VAL:HA	2.21	0.40
3:F:173:GLY:O	3:F:177:ARG:HG2	2.20	0.40
2:H:69:VAL:HG11	3:I:154:GLU:HB2	2.04	0.40
1:J:345:ILE:HG23	1:J:350:LYS:CB	2.51	0.40
3:O:8:ILE:HG12	3:O:220:LEU:CD2	2.51	0.40
1:P:65:ARG:HH21	2:T:122:ARG:NH2	2.19	0.40
2:E:106:ILE:HA	2:E:142:PHE:O	2.21	0.40
3:F:97:MET:O	3:F:101:MET:HG3	2.21	0.40
1:G:16:PRO:HG3	1:G:58:LEU:HD11	2.04	0.40
1:G:122:LEU:HD11	1:G:168:ILE:HD11	2.02	0.40
3:L:34:ALA:HA	3:L:217:CYS:SG	2.61	0.40
3:O:132:THR:HB	3:O:133:GLU:H	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:196:LEU:HD23	3:O:200:LYS:HE2	2.02	0.40
3:O:199:LEU:HD23	3:O:199:LEU:HA	1.87	0.40
1:S:319:ILE:HG13	1:S:323:GLN:NE2	2.37	0.40
2:K:28:ARG:HB2	2:K:30:GLU:HG3	2.02	0.40
1:M:96:ILE:O	1:M:100:LEU:HG	2.22	0.40
3:O:84:SER:HB3	3:O:97:MET:CE	2.51	0.40
1:P:218:THR:HG21	1:P:252:LEU:HD22	2.04	0.40
1:A:146:ASN:OD1	1:A:146:ASN:N	2.53	0.40
3:F:182:ASN:ND2	3:F:370:ASN:OD1	2.47	0.40
1:G:95:ILE:O	1:G:99:MET:HG3	2.21	0.40
3:R:178:ILE:HG13	3:R:193:ILE:HD12	2.03	0.40
1:S:50:GLN:HB2	1:S:53:GLU:HG3	2.03	0.40
1:S:259:ASN:HB2	1:S:260:PRO:HD2	2.03	0.40
2:W:29:LEU:HD12	2:W:29:LEU:HA	1.95	0.40
3:X:132:THR:HG21	3:X:137:ASP:OD2	2.21	0.40

There are no symmetry-related clashes.

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	356/362 (98%)	345 (97%)	11 (3%)	0	100	100
1	D	357/362 (99%)	345 (97%)	12 (3%)	0	100	100
1	G	357/362 (99%)	340 (95%)	17 (5%)	0	100	100
1	J	357/362 (99%)	347 (97%)	10 (3%)	0	100	100
1	M	357/362 (99%)	347 (97%)	10 (3%)	0	100	100
1	P	356/362 (98%)	345 (97%)	11 (3%)	0	100	100
1	S	357/362 (99%)	347 (97%)	10 (3%)	0	100	100
1	V	357/362 (99%)	346 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	143/146 (98%)	139 (97%)	4 (3%)	0	100	100
2	E	143/146 (98%)	138 (96%)	5 (4%)	0	100	100
2	H	143/146 (98%)	138 (96%)	5 (4%)	0	100	100
2	K	143/146 (98%)	140 (98%)	3 (2%)	0	100	100
2	N	143/146 (98%)	139 (97%)	4 (3%)	0	100	100
2	Q	143/146 (98%)	140 (98%)	3 (2%)	0	100	100
2	T	143/146 (98%)	140 (98%)	3 (2%)	0	100	100
2	W	143/146 (98%)	139 (97%)	4 (3%)	0	100	100
3	C	392/398 (98%)	376 (96%)	16 (4%)	0	100	100
3	F	392/398 (98%)	377 (96%)	15 (4%)	0	100	100
3	I	393/398 (99%)	380 (97%)	13 (3%)	0	100	100
3	L	393/398 (99%)	381 (97%)	12 (3%)	0	100	100
3	O	393/398 (99%)	382 (97%)	11 (3%)	0	100	100
3	R	392/398 (98%)	378 (96%)	14 (4%)	0	100	100
3	U	393/398 (99%)	378 (96%)	15 (4%)	0	100	100
3	X	393/398 (99%)	381 (97%)	12 (3%)	0	100	100
All	All	7139/7248 (98%)	6908 (97%)	231 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/283 (99%)	272 (98%)	7 (2%)	47	75
1	D	280/283 (99%)	275 (98%)	5 (2%)	59	81
1	G	280/283 (99%)	276 (99%)	4 (1%)	67	85
1	J	280/283 (99%)	272 (97%)	8 (3%)	42	71
1	M	280/283 (99%)	275 (98%)	5 (2%)	59	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	279/283 (99%)	274 (98%)	5 (2%)	59	81
1	S	280/283 (99%)	274 (98%)	6 (2%)	53	78
1	V	280/283 (99%)	276 (99%)	4 (1%)	67	85
2	B	124/125 (99%)	122 (98%)	2 (2%)	62	83
2	E	124/125 (99%)	123 (99%)	1 (1%)	81	92
2	H	124/125 (99%)	120 (97%)	4 (3%)	39	69
2	K	124/125 (99%)	122 (98%)	2 (2%)	62	83
2	N	124/125 (99%)	120 (97%)	4 (3%)	39	69
2	Q	124/125 (99%)	123 (99%)	1 (1%)	81	92
2	T	124/125 (99%)	120 (97%)	4 (3%)	39	69
2	W	124/125 (99%)	121 (98%)	3 (2%)	49	76
3	C	303/305 (99%)	292 (96%)	11 (4%)	35	66
3	F	303/305 (99%)	296 (98%)	7 (2%)	50	77
3	I	303/305 (99%)	299 (99%)	4 (1%)	69	86
3	L	303/305 (99%)	296 (98%)	7 (2%)	50	77
3	O	303/305 (99%)	296 (98%)	7 (2%)	50	77
3	R	303/305 (99%)	291 (96%)	12 (4%)	31	63
3	U	303/305 (99%)	299 (99%)	4 (1%)	69	86
3	X	303/305 (99%)	293 (97%)	10 (3%)	38	68
All	All	5654/5704 (99%)	5527 (98%)	127 (2%)	52	77

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	PHE
1	A	196	ASP
1	A	207	SER
1	A	216	ASP
1	A	261	LYS
1	A	290	GLN
1	A	326	ASN
2	B	44	ARG
2	B	122	ARG
3	C	53	TYR
3	C	55	TYR

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Mol	Chain	Res	Type
3	C	62	GLU
3	C	176	MET
3	C	251	ARG
3	C	254	ASN
3	C	334	LEU
3	C	351	CYS
3	C	352	ASP
3	C	356	HIS
3	C	369	ASP
1	D	5	LYS
1	D	50	GLN
1	D	112	GLN
1	D	113	PHE
1	D	214	LEU
2	E	16	MET
3	F	43	MET
3	F	53	TYR
3	F	55	TYR
3	F	83	MET
3	F	232	LYS
3	F	314	CYS
3	F	363	GLN
1	G	113	PHE
1	G	143	ASP
1	G	196	ASP
1	G	326	ASN
2	H	15	SER
2	H	39	GLU
2	H	52	ASN
2	H	126	ARG
3	I	53	TYR
3	I	55	TYR
3	I	211	TRP
3	I	334	LEU
1	J	23	GLN
1	J	50	GLN
1	J	94	SER
1	J	97	LEU
1	J	113	PHE
1	J	194	GLN
1	J	196	ASP
1	J	352	LEU

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Mol	Chain	Res	Type
2	K	44	ARG
2	K	97	ASP
3	L	53	TYR
3	L	55	TYR
3	L	245	SER
3	L	352	ASP
3	L	363	GLN
3	L	383	LEU
3	L	390	ASN
1	M	50	GLN
1	M	112	GLN
1	M	113	PHE
1	M	304	PHE
1	M	352	LEU
2	N	3	MET
2	N	41	PHE
2	N	52	ASN
2	N	60	ARG
3	O	16	LYS
3	O	53	TYR
3	O	55	TYR
3	O	63	TYR
3	O	150	LEU
3	O	301	LEU
3	O	390	ASN
1	P	52	ASP
1	P	113	PHE
1	P	177	PHE
1	P	196	ASP
1	P	353	ARG
2	Q	44	ARG
3	R	16	LYS
3	R	21	ARG
3	R	53	TYR
3	R	55	TYR
3	R	99	HIS
3	R	197	GLU
3	R	211	TRP
3	R	258	HIS
3	R	290	LYS
3	R	314	CYS
3	R	356	HIS

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Mol	Chain	Res	Type
3	R	383	LEU
1	S	35	LYS
1	S	105	ASP
1	S	113	PHE
1	S	177	PHE
1	S	286	ASN
1	S	309	ASP
2	T	41	PHE
2	T	60	ARG
2	T	123	MET
2	T	130	ARG
3	U	53	TYR
3	U	283	LYS
3	U	314	CYS
3	U	383	LEU
1	V	113	PHE
1	V	116	LYS
1	V	126	GLN
1	V	309	ASP
2	W	17	LEU
2	W	44	ARG
2	W	60	ARG
3	X	53	TYR
3	X	55	TYR
3	X	77	SER
3	X	158	LYS
3	X	172	PHE
3	X	209	LEU
3	X	254	ASN
3	X	347	HIS
3	X	352	ASP
3	X	390	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	363	GLN
3	I	56	HIS
3	I	363	GLN
1	J	27	ASN
1	J	255	HIS
3	L	342	ASN

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Mol	Chain	Res	Type
1	M	194	GLN
1	M	271	ASN
1	P	23	GLN
1	S	323	GLN
1	V	23	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
3	SCY	C	88	3	7,8,9	0.85	0	3,9,11	0.80	0
3	SCY	I	88	3	7,8,9	0.85	0	3,9,11	0.79	0
3	SCY	O	88	3	7,8,9	0.85	0	3,9,11	0.83	0
3	SCY	R	88	3	7,8,9	0.82	0	3,9,11	0.82	0
3	SCY	X	88	3	7,8,9	0.87	0	3,9,11	0.81	0
3	SCY	F	88	3	7,8,9	0.87	0	3,9,11	0.79	0
3	SCY	U	88	3	7,8,9	0.89	0	3,9,11	0.70	0
3	SCY	L	88	3	7,8,9	0.86	0	3,9,11	0.86	0

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	SCY	C	88	3	-	2/5/7/9	-
3	SCY	I	88	3	-	2/5/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SCY	O	88	3	-	2/5/7/9	-
3	SCY	R	88	3	-	2/5/7/9	-
3	SCY	X	88	3	-	2/5/7/9	-
3	SCY	F	88	3	-	2/5/7/9	-
3	SCY	U	88	3	-	2/5/7/9	-
3	SCY	L	88	3	-	2/5/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	88	SCY	OCD-CD-SG-CB
3	C	88	SCY	CE-CD-SG-CB
3	F	88	SCY	OCD-CD-SG-CB
3	F	88	SCY	CE-CD-SG-CB
3	I	88	SCY	OCD-CD-SG-CB
3	I	88	SCY	CE-CD-SG-CB
3	L	88	SCY	OCD-CD-SG-CB
3	L	88	SCY	CE-CD-SG-CB
3	O	88	SCY	OCD-CD-SG-CB
3	O	88	SCY	CE-CD-SG-CB
3	R	88	SCY	OCD-CD-SG-CB
3	R	88	SCY	CE-CD-SG-CB
3	U	88	SCY	OCD-CD-SG-CB
3	U	88	SCY	CE-CD-SG-CB
3	X	88	SCY	OCD-CD-SG-CB
3	X	88	SCY	CE-CD-SG-CB

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	88	SCY	2	0
3	O	88	SCY	1	0
3	L	88	SCY	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
5	13X	L	500	-	9,9,9	0.87	0	12,12,12	0.41	0
5	13X	O	500	-	9,9,9	0.88	0	12,12,12	0.39	0
5	13X	C	500	-	9,9,9	0.88	0	12,12,12	0.41	0
5	13X	R	500	-	9,9,9	0.89	0	12,12,12	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	13X	L	500	-	-	-	0/1/1/1
5	13X	O	500	-	-	-	0/1/1/1
5	13X	C	500	-	-	-	0/1/1/1
5	13X	R	500	-	-	-	0/1/1/1

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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	500	13X	2	0
5	O	500	13X	1	0
5	C	500	13X	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	358/362 (98%)	-0.42	0 100 100	25, 37, 57, 169	0
1	D	359/362 (99%)	-0.44	0 100 100	27, 38, 55, 213	0
1	G	359/362 (99%)	-0.06	3 (0%) 86 83	36, 53, 71, 93	0
1	J	359/362 (99%)	-0.32	1 (0%) 94 92	27, 39, 59, 153	0
1	M	359/362 (99%)	-0.34	0 100 100	30, 39, 57, 87	0
1	P	358/362 (98%)	0.09	11 (3%) 49 48	34, 49, 65, 84	0
1	S	358/362 (98%)	-0.30	1 (0%) 94 92	29, 41, 58, 85	0
1	V	359/362 (99%)	-0.29	0 100 100	34, 46, 64, 116	0
2	B	145/146 (99%)	-0.11	4 (2%) 53 51	30, 44, 67, 87	0
2	E	145/146 (99%)	0.04	2 (1%) 75 72	32, 45, 69, 79	0
2	H	145/146 (99%)	-0.30	1 (0%) 87 85	32, 48, 70, 96	0
2	K	145/146 (99%)	-0.20	1 (0%) 87 85	30, 45, 65, 74	0
2	N	145/146 (99%)	0.02	6 (4%) 37 36	33, 46, 72, 92	0
2	Q	145/146 (99%)	-0.05	3 (2%) 63 62	35, 48, 78, 90	0
2	T	145/146 (99%)	0.01	8 (5%) 25 26	33, 47, 72, 85	0
2	W	145/146 (99%)	0.18	6 (4%) 37 36	38, 55, 88, 95	0
3	C	394/398 (98%)	-0.02	4 (1%) 82 79	32, 47, 59, 75	0
3	F	394/398 (98%)	-0.17	3 (0%) 86 83	37, 49, 65, 88	0
3	I	395/398 (99%)	0.00	5 (1%) 77 74	40, 56, 71, 155	0
3	L	395/398 (99%)	-0.16	1 (0%) 94 92	36, 51, 69, 88	0
3	O	395/398 (99%)	0.08	9 (2%) 60 58	37, 50, 64, 81	0
3	R	394/398 (98%)	0.00	6 (1%) 73 71	38, 52, 66, 94	0
3	U	395/398 (99%)	-0.05	6 (1%) 73 71	33, 48, 63, 88	0
3	X	395/398 (99%)	-0.01	7 (1%) 68 66	42, 57, 76, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	7186/7248 (99%)	-0.13	88 (1%)	79	76	25, 48, 68, 213	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	35	GLU	3.7
3	R	265	ASP	3.7
3	X	265	ASP	3.6
2	T	38	ASN	3.6
2	T	55	SER	3.5
3	R	398	ASP	3.4
2	T	34	CYS	3.0
2	T	54	LEU	2.9
2	T	36	GLU	2.9
3	U	3	ALA	2.8
3	X	192	PRO	2.8
3	O	398	ASP	2.8
2	H	2	SER	2.7
3	X	196	LEU	2.7
2	Q	38	ASN	2.7
3	L	227	HIS	2.7
2	W	36	GLU	2.6
2	T	53	SER	2.6
3	F	265	ASP	2.6
3	C	196	LEU	2.6
2	Q	36	GLU	2.5
2	W	114	GLN	2.5
3	U	373	LYS	2.5
3	O	3	ALA	2.5
2	W	146	ILE	2.5
3	O	325	GLU	2.4
2	B	146	ILE	2.4
3	U	227	HIS	2.4
2	W	55	SER	2.4
2	N	36	GLU	2.4
3	R	366	GLY	2.4
1	S	293	PRO	2.4
3	I	324	LEU	2.4
3	O	294	VAL	2.4
3	R	396	SER	2.4
2	N	52	ASN	2.3
3	I	321	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	2	SER	2.3
2	N	146	ILE	2.3
3	O	324	LEU	2.3
2	B	113	GLN	2.3
2	N	2	SER	2.3
3	X	157	GLN	2.3
2	Q	2	SER	2.3
3	C	330	LEU	2.3
2	E	40	ILE	2.3
3	C	227	HIS	2.3
1	P	233	PRO	2.3
3	U	326	GLY	2.2
2	W	34	CYS	2.2
3	X	195	SER	2.2
3	R	264	LYS	2.2
3	O	227	HIS	2.2
1	P	235	ASP	2.2
1	P	260	PRO	2.2
3	C	192	PRO	2.2
1	G	259	ASN	2.2
3	O	9	VAL	2.2
1	G	261	LYS	2.2
3	R	376	ARG	2.2
1	P	230	HIS	2.2
3	X	189	TYR	2.1
1	P	227	ALA	2.1
3	O	331	ASP	2.1
1	P	314	THR	2.1
3	I	322	PHE	2.1
3	F	193	ILE	2.1
3	I	163	GLY	2.1
1	P	232	SER	2.1
2	B	111	ASP	2.1
2	W	52	ASN	2.1
3	X	197	GLU	2.1
2	K	33	GLN	2.1
3	U	330	LEU	2.1
2	N	38	ASN	2.1
2	T	52	ASN	2.1
3	O	329	ALA	2.1
1	G	256	LEU	2.1
2	N	50	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	264	LYS	2.1
1	J	325	HIS	2.1
1	P	42	GLY	2.0
1	P	234	ALA	2.0
3	U	369	ASP	2.0
1	P	229	LEU	2.0
1	P	236	TYR	2.0
2	E	64	SER	2.0
3	I	323	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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	SCY	U	88	9/10	0.92	0.23	37,48,62,64	0
3	SCY	O	88	9/10	0.93	0.20	37,44,52,53	0
3	SCY	I	88	9/10	0.93	0.30	51,53,69,75	0
3	SCY	X	88	9/10	0.93	0.27	48,51,59,63	0
3	SCY	L	88	9/10	0.94	0.26	40,44,54,57	0
3	SCY	C	88	9/10	0.94	0.21	44,45,56,57	0
3	SCY	F	88	9/10	0.95	0.29	41,44,70,77	0
3	SCY	R	88	9/10	0.95	0.17	48,52,58,58	0

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
5	13X	O	500	9/9	0.85	0.29	50,56,60,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	13X	R	500	9/9	0.85	0.26	52,56,61,63	0
5	13X	C	500	9/9	0.90	0.23	42,56,59,61	0
5	13X	L	500	9/9	0.91	0.23	50,56,58,60	0
4	ZN	B	200	1/1	0.94	0.04	116,116,116,116	0
4	ZN	T	200	1/1	0.94	0.14	132,132,132,132	0
4	ZN	H	200	1/1	0.95	0.04	81,81,81,81	0
4	ZN	W	200	1/1	0.95	0.16	135,135,135,135	0
4	ZN	Q	200	1/1	0.97	0.07	162,162,162,162	0
4	ZN	K	200	1/1	0.99	0.09	104,104,104,104	0
4	ZN	N	200	1/1	0.99	0.14	97,97,97,97	0
4	ZN	E	200	1/1	0.99	0.08	96,96,96,96	0

6.5 Other polymers (i)

There are no such residues in this entry.