Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 07:20 PM EDT

PDB ID	:	3GVD
Title	:	Crystal Structure of Serine Acetyltransferase CysE from Yersinia pestis
Authors	:	Kim, Y.; Zhou, M.; Peterson, S.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2009-03-30
Resolution	:	2.40 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:

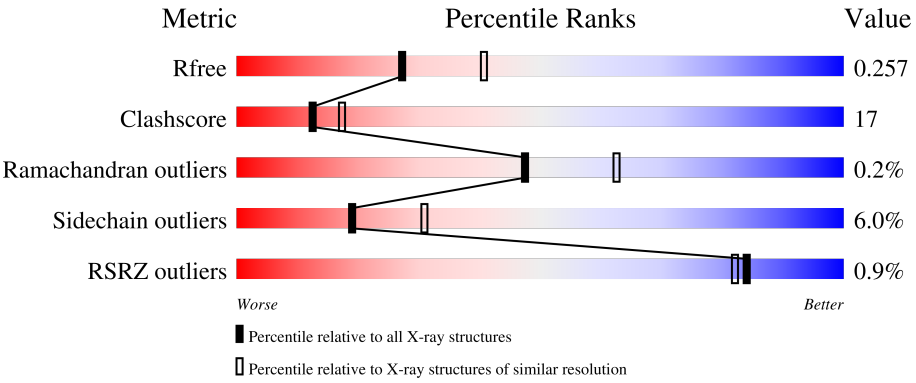
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	276	70% 26%
1	B	276	65% 28%
1	C	276	64% 29% 5%
1	D	276	65% 28% 5%
1	E	276	64% 29% 5%

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Mol	Chain	Length	Quality of chain
1	F	276	67% 25% 5%
1	G	276	58% 35% 5%
1	H	276	64% 28% 5%
1	I	276	72% 24%
1	J	276	59% 32% 5%
1	K	276	66% 26% 6%
1	L	276	66% 28% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACY	A	275	-	-	X	-
6	PG5	C	274	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 25003 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 Serine acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2039	1289	359	382	9			
1	B	265	Total	C	N	O	S	0	0	0
			1987	1254	353	371	9			
1	C	262	Total	C	N	O	S	0	0	0
			1969	1245	349	366	9			
1	D	262	Total	C	N	O	S	0	1	0
			1979	1250	353	367	9			
1	E	263	Total	C	N	O	S	0	1	0
			1984	1253	353	369	9			
1	F	261	Total	C	N	O	S	0	0	0
			1964	1242	348	365	9			
1	G	263	Total	C	N	O	S	0	1	0
			1985	1253	354	369	9			
1	H	261	Total	C	N	O	S	0	0	0
			1961	1241	347	364	9			
1	I	272	Total	C	N	O	S	0	1	0
			2054	1298	362	384	10			
1	J	261	Total	C	N	O	S	0	0	0
			1964	1242	348	365	9			
1	K	260	Total	C	N	O	S	0	0	0
			1956	1238	346	363	9			
1	L	261	Total	C	N	O	S	0	1	0
			1972	1247	349	366	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q0WKM4
A	-1	ASN	-	expression tag	UNP Q0WKM4
A	0	ALA	-	expression tag	UNP Q0WKM4
B	-2	SER	-	expression tag	UNP Q0WKM4
B	-1	ASN	-	expression tag	UNP Q0WKM4

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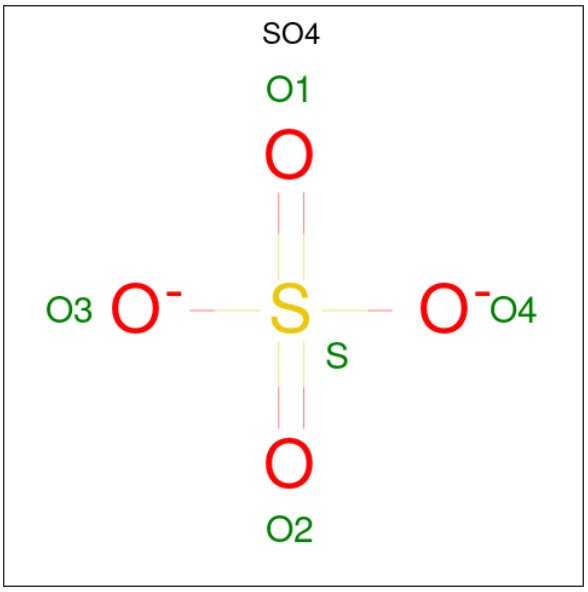
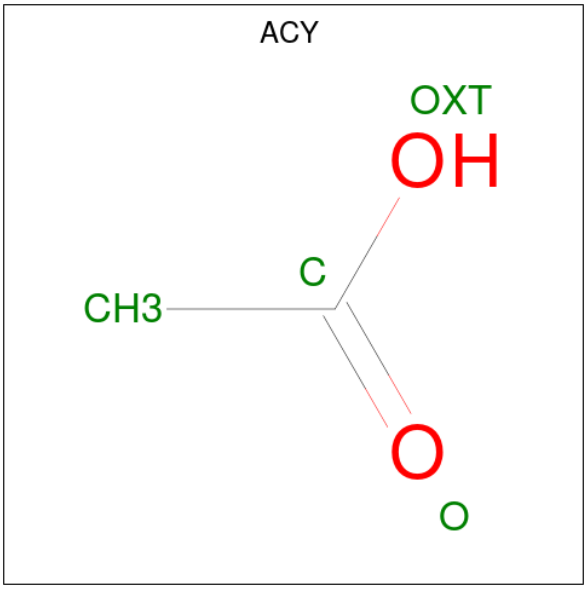
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	expression tag	UNP Q0WKM4
C	-2	SER	-	expression tag	UNP Q0WKM4
C	-1	ASN	-	expression tag	UNP Q0WKM4
C	0	ALA	-	expression tag	UNP Q0WKM4
D	-2	SER	-	expression tag	UNP Q0WKM4
D	-1	ASN	-	expression tag	UNP Q0WKM4
D	0	ALA	-	expression tag	UNP Q0WKM4
E	-2	SER	-	expression tag	UNP Q0WKM4
E	-1	ASN	-	expression tag	UNP Q0WKM4
E	0	ALA	-	expression tag	UNP Q0WKM4
F	-2	SER	-	expression tag	UNP Q0WKM4
F	-1	ASN	-	expression tag	UNP Q0WKM4
F	0	ALA	-	expression tag	UNP Q0WKM4
G	-2	SER	-	expression tag	UNP Q0WKM4
G	-1	ASN	-	expression tag	UNP Q0WKM4
G	0	ALA	-	expression tag	UNP Q0WKM4
H	-2	SER	-	expression tag	UNP Q0WKM4
H	-1	ASN	-	expression tag	UNP Q0WKM4
H	0	ALA	-	expression tag	UNP Q0WKM4
I	-2	SER	-	expression tag	UNP Q0WKM4
I	-1	ASN	-	expression tag	UNP Q0WKM4
I	0	ALA	-	expression tag	UNP Q0WKM4
J	-2	SER	-	expression tag	UNP Q0WKM4
J	-1	ASN	-	expression tag	UNP Q0WKM4
J	0	ALA	-	expression tag	UNP Q0WKM4
K	-2	SER	-	expression tag	UNP Q0WKM4
K	-1	ASN	-	expression tag	UNP Q0WKM4
K	0	ALA	-	expression tag	UNP Q0WKM4
L	-2	SER	-	expression tag	UNP Q0WKM4
L	-1	ASN	-	expression tag	UNP Q0WKM4
L	0	ALA	-	expression tag	UNP Q0WKM4

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



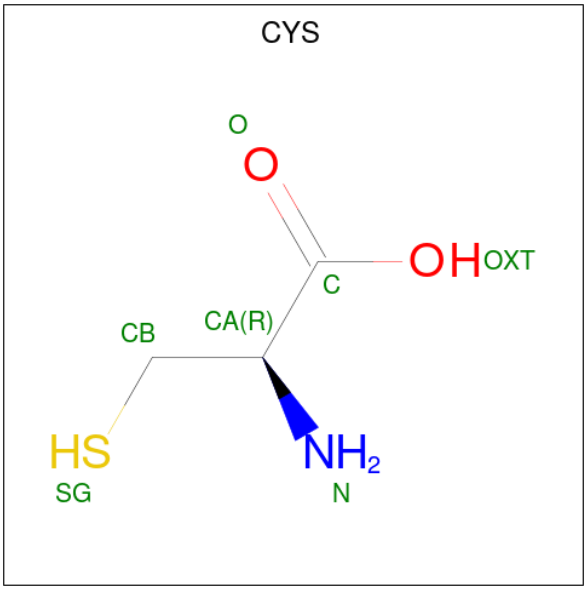
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0

- Molecule 4 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 7 3 1 2 1	0	0
4	A	1	Total C N O S 7 3 1 2 1	0	0
4	B	1	Total C N O S 7 3 1 2 1	0	0
4	D	1	Total C N O S 7 3 1 2 1	0	0
4	D	1	Total C N O S 7 3 1 2 1	0	0
4	E	1	Total C N O S 7 3 1 2 1	0	0
4	G	1	Total C N O S 7 3 1 2 1	0	0
4	H	1	Total C N O S 7 3 1 2 1	0	0

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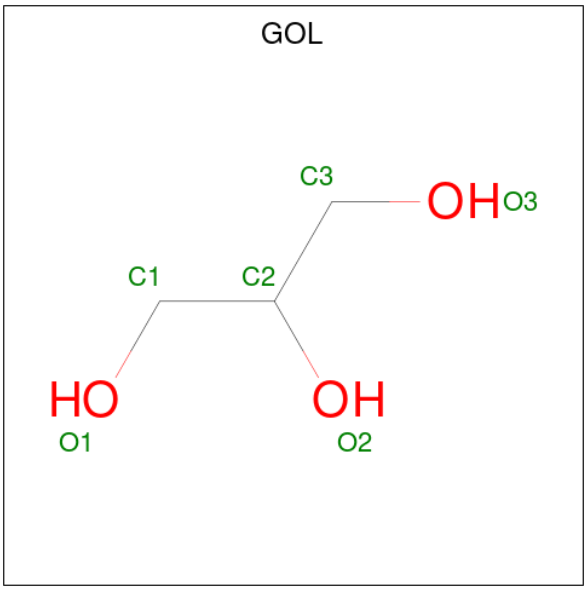
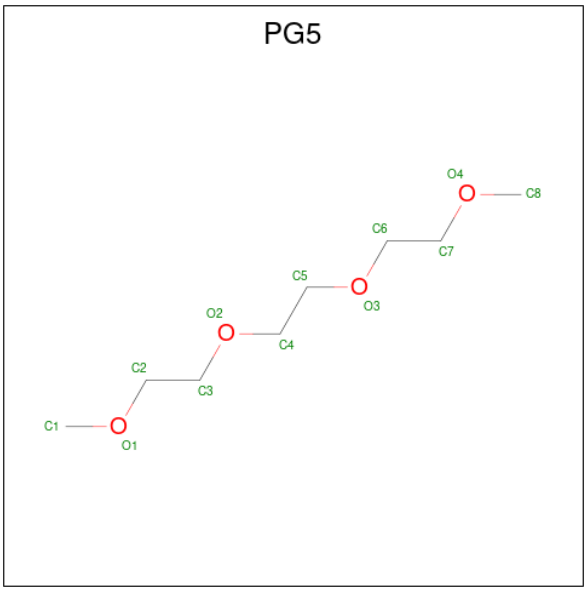
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total C N O S 7 3 1 2 1	0	0
4	J	1	Total C N O S 7 3 1 2 1	0	0
4	L	1	Total C N O S 7 3 1 2 1	0	0
4	L	1	Total C N O S 7 3 1 2 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



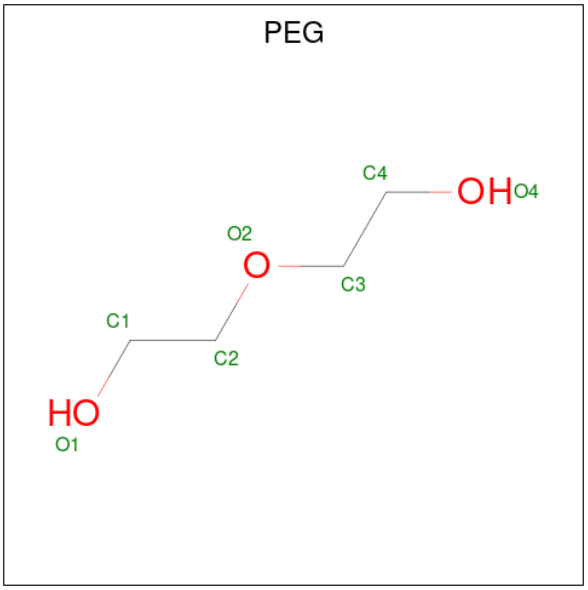
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0
5	J	1	Total C O 6 3 3	0	0

- Molecule 6 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY]-ETHANE (three-letter code: PG5) (formula: $C_8H_{18}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 12 8 4	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C O 7 4 3	0	0

- Molecule 8 is water.

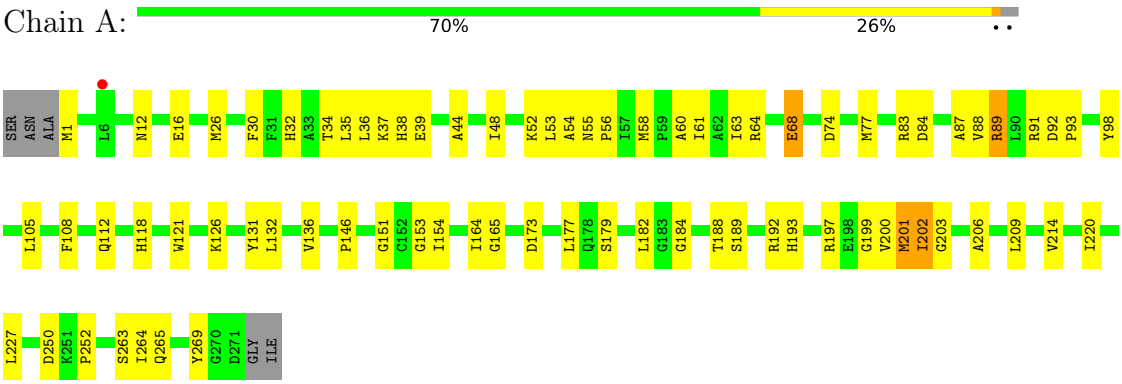
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	100	Total O 100 100	0	0
8	B	111	Total O 111 111	0	0
8	C	90	Total O 90 90	0	0
8	D	73	Total O 73 73	0	0
8	E	78	Total O 78 78	0	0
8	F	73	Total O 73 73	0	0
8	G	71	Total O 71 71	0	0
8	H	69	Total O 69 69	0	0
8	I	113	Total O 113 113	0	0
8	J	82	Total O 82 82	0	0
8	K	87	Total O 87 87	0	0
8	L	68	Total O 68 68	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.

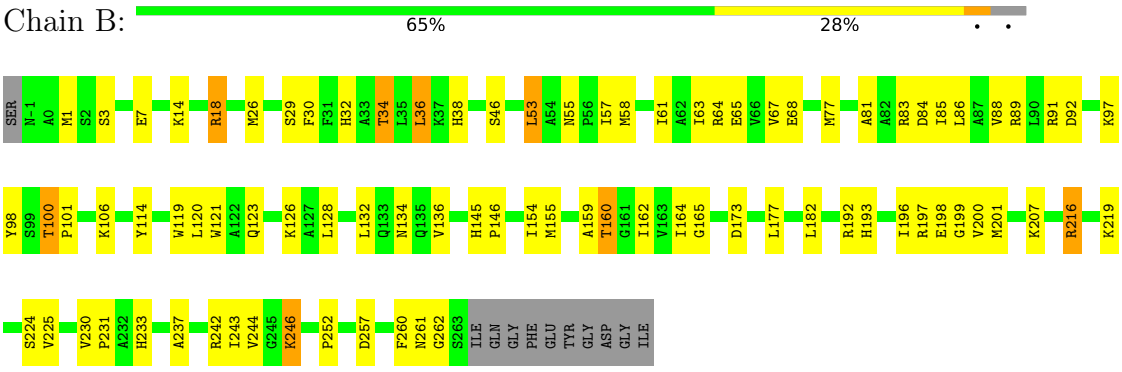
• Molecule 1: Serine acetyltransferase

Chain A:



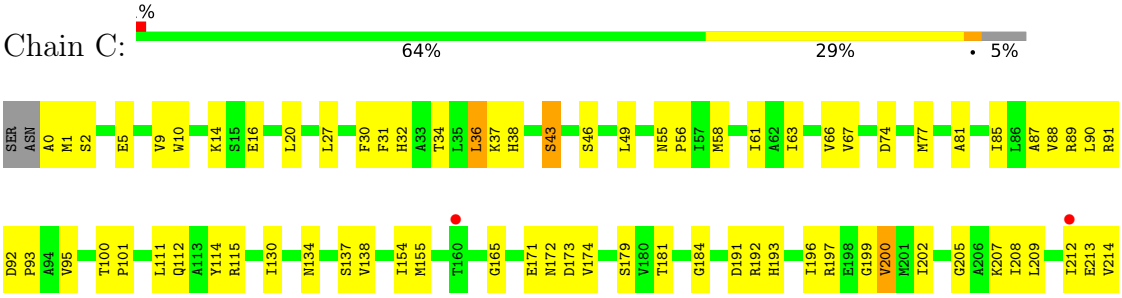
• Molecule 1: Serine acetyltransferase

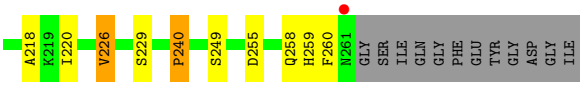
Chain B:



• Molecule 1: Serine acetyltransferase

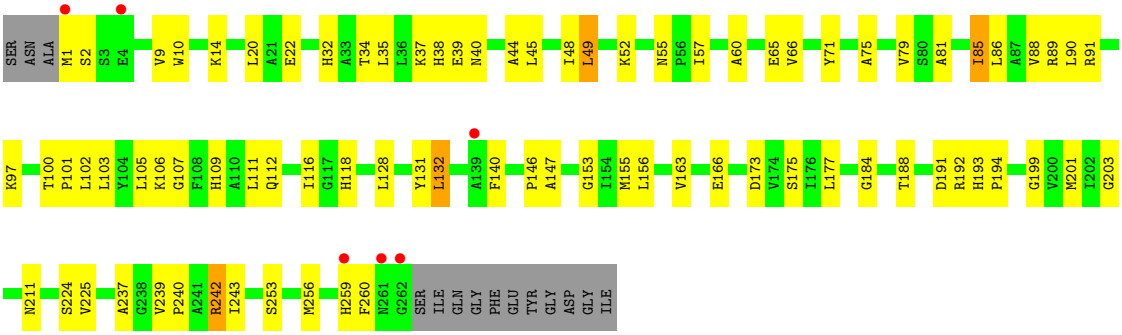
Chain C:





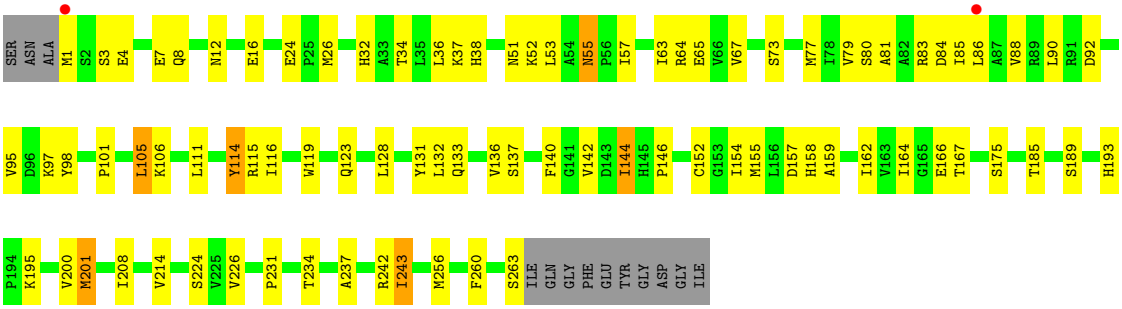
• Molecule 1: Serine acetyltransferase

Chain D:



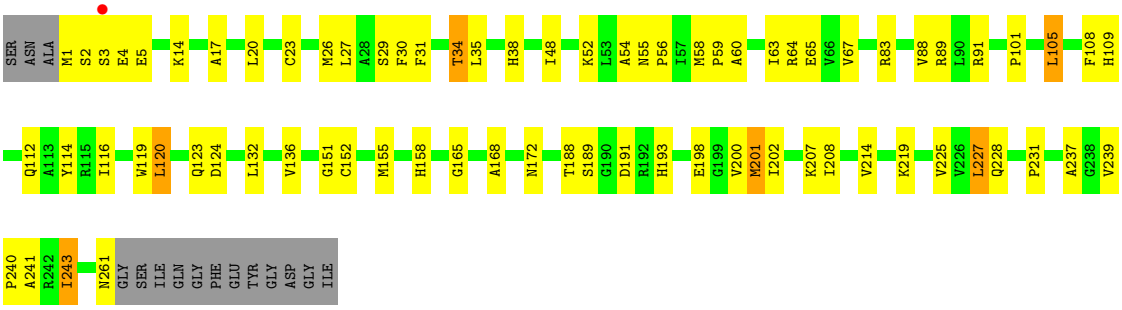
• Molecule 1: Serine acetyltransferase

Chain E:



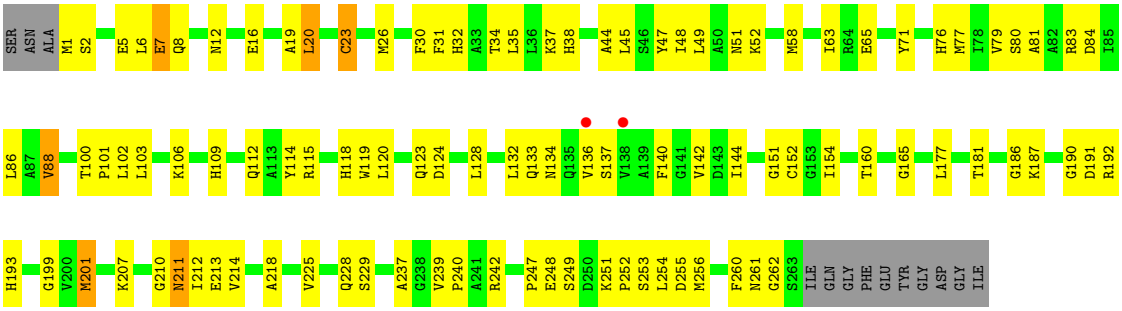
• Molecule 1: Serine acetyltransferase

Chain F:



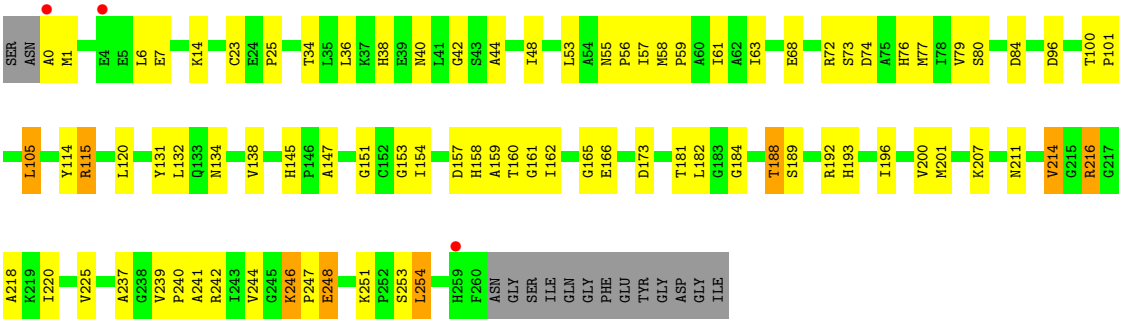
• Molecule 1: Serine acetyltransferase

Chain G:



• Molecule 1: Serine acetyltransferase

Chain H:

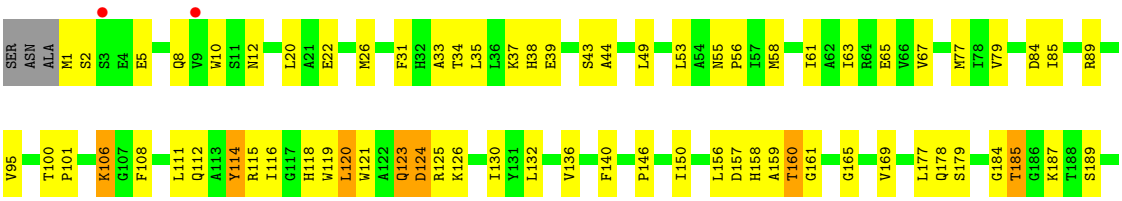


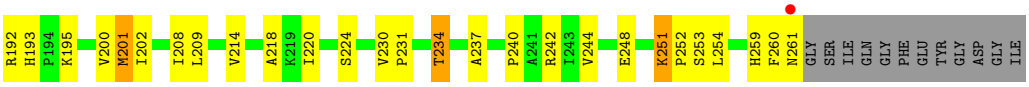
• Molecule 1: Serine acetyltransferase

Chain I:

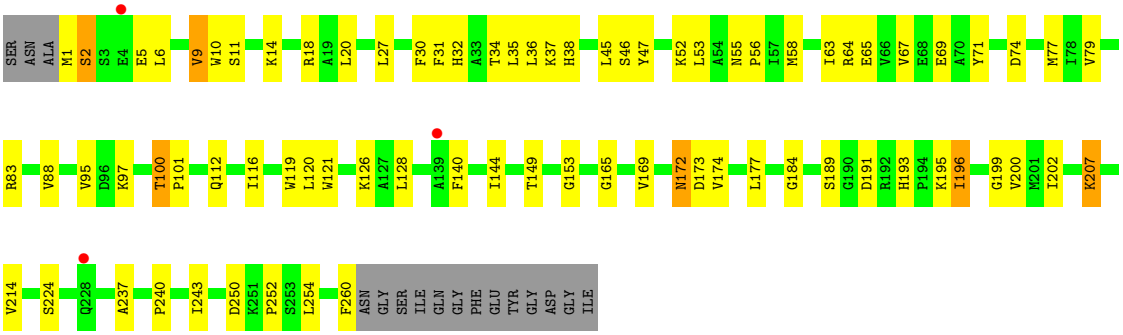
• Molecule 1: Serine acetyltransferase

Chain J:

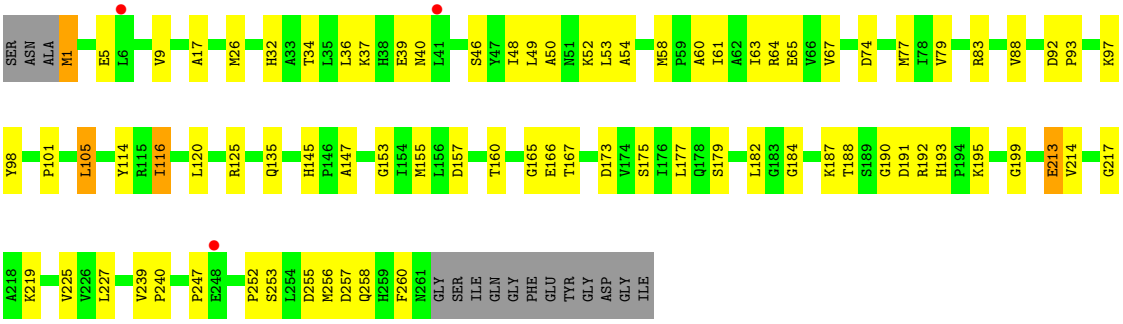




• Molecule 1: Serine acetyltransferase



• Molecule 1: Serine acetyltransferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	68.47Å 81.23Å 139.41Å 97.07° 95.32° 94.72°	Depositor
Resolution (Å)	45.99 – 2.40 45.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.0 (45.99-2.40) 97.1 (45.98-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.199 , 0.265 0.191 , 0.257	Depositor DCC
R_{free} test set	5663 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.754	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 35.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	25003	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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: PG5, ACY, GOL, PEG, SO4

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	0.42	0/2078	0.57	0/2818
1	B	0.44	0/2024	0.59	0/2746
1	C	0.43	0/2006	0.59	0/2722
1	D	0.40	0/2016	0.57	0/2734
1	E	0.41	0/2022	0.58	0/2743
1	F	0.39	0/2001	0.57	0/2715
1	G	0.39	0/2022	0.56	0/2742
1	H	0.36	0/1998	0.56	0/2711
1	I	0.42	0/2093	0.59	0/2838
1	J	0.39	0/2001	0.57	0/2715
1	K	0.38	0/1993	0.60	0/2704
1	L	0.38	0/2009	0.57	0/2725
All	All	0.40	0/24263	0.58	0/32913

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2039	0	2054	57	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1987	0	2012	79	0
1	C	1969	0	1998	83	0
1	D	1979	0	2008	78	0
1	E	1984	0	2007	84	0
1	F	1964	0	1993	64	0
1	G	1985	0	2013	87	0
1	H	1961	0	1992	68	0
1	I	2054	0	2071	63	0
1	J	1964	0	1993	82	0
1	K	1956	0	1987	60	0
1	L	1972	0	2001	76	0
2	A	5	0	0	1	0
2	F	5	0	0	0	0
2	H	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	1	0
3	A	4	0	3	2	0
3	C	4	0	3	0	0
3	J	8	0	6	1	0
4	A	14	0	8	1	0
4	B	7	0	4	0	0
4	D	14	0	8	0	0
4	E	7	0	4	0	0
4	G	7	0	4	0	0
4	H	7	0	4	0	0
4	I	7	0	4	1	0
4	J	7	0	4	0	0
4	L	14	0	8	2	0
5	B	6	0	8	2	0
5	E	6	0	8	2	0
5	F	6	0	8	0	0
5	H	6	0	8	1	0
5	J	6	0	8	0	0
6	C	12	0	18	9	0
7	L	7	0	10	3	0
8	A	100	0	0	1	0
8	B	111	0	0	5	0
8	C	90	0	0	4	0
8	D	73	0	0	6	0
8	E	78	0	0	6	0
8	F	73	0	0	3	0
8	G	71	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	69	0	0	3	1
8	I	113	0	0	3	0
8	J	82	0	0	5	0
8	K	87	0	0	6	0
8	L	68	0	0	3	0
All	All	25003	0	24257	809	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (809) 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:D:57:ILE:HD11	1:F:30:PHE:HB2	1.34	1.07
1:E:114:TYR:CD1	1:E:144:ILE:HD11	1.92	1.05
1:L:120:LEU:HD22	1:L:125:ARG:HD2	1.42	1.01
1:D:91:ARG:HB2	1:D:155:MET:HE3	1.40	1.00
1:G:34:THR:HG23	1:G:35:LEU:HG	1.44	0.96
1:F:34:THR:HG22	1:F:35:LEU:HG	1.48	0.95
1:H:0:ALA:HB1	1:H:79:VAL:HG11	1.49	0.95
1:I:61:ILE:HD11	1:K:64:ARG:HD2	1.48	0.95
1:K:243:ILE:HG12	8:K:934:HOH:O	1.67	0.94
1:C:88:VAL:HA	1:C:155:MET:HE2	1.47	0.94
1:E:55:ASN:HD22	1:E:57:ILE:H	1.11	0.92
1:F:88:VAL:HA	1:F:155:MET:HE2	1.52	0.92
1:D:34:THR:HG23	1:D:35:LEU:HG	1.55	0.89
1:J:208:ILE:HD11	1:J:220:ILE:HD13	1.51	0.89
1:J:84:ASP:OD2	1:J:111:LEU:HD21	1.75	0.87
1:D:91:ARG:HB2	1:D:155:MET:CE	2.06	0.84
1:D:88:VAL:HA	1:D:155:MET:HE2	1.58	0.84
1:J:251:LYS:HG3	1:J:254:LEU:HD22	1.59	0.84
1:B:88:VAL:HA	1:B:155:MET:CE	2.09	0.83
1:F:91:ARG:HB2	1:F:155:MET:HE1	1.59	0.83
1:E:175:SER:HB3	1:E:256:MET:HE1	1.58	0.83
1:A:74:ASP:HB3	1:A:77:MET:HE2	1.60	0.82
1:F:34:THR:HG23	1:F:48:ILE:HD11	1.60	0.82
1:C:88:VAL:HA	1:C:155:MET:CE	2.08	0.82
1:C:0:ALA:H1	6:C:274:PG5:H72	1.42	0.82
1:E:114:TYR:HB2	1:E:144:ILE:HD12	1.61	0.82
1:J:202:ILE:HG12	1:J:220:ILE:HD12	1.60	0.82
1:E:77:MET:HE1	1:E:119:TRP:HB2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:TYR:HD1	1:E:144:ILE:HD11	1.46	0.80
1:I:176:ILE:HG23	1:I:180:VAL:HG21	1.60	0.80
1:D:201:MET:HG3	1:D:256:MET:HE2	1.63	0.80
1:J:214:VAL:HG21	1:J:220:ILE:HD11	1.63	0.80
1:G:151:GLY:O	1:G:154:ILE:HD11	1.83	0.79
1:C:208:ILE:HG12	1:C:226:VAL:CG1	2.13	0.79
1:E:77:MET:CE	1:E:119:TRP:HB2	2.13	0.79
1:G:2:SER:HB3	1:G:5:GLU:HG3	1.62	0.79
1:B:91:ARG:HB2	1:B:155:MET:CE	2.13	0.79
1:J:2:SER:HB2	1:J:5:GLU:HB2	1.65	0.79
1:D:57:ILE:CD1	1:F:30:PHE:HB2	2.13	0.78
1:F:88:VAL:HG22	1:F:155:MET:HG3	1.64	0.78
1:J:125:ARG:HH22	1:L:26[A]:MET:HE3	1.49	0.78
1:A:34:THR:CG2	1:A:48:ILE:HD11	2.14	0.78
1:H:101:PRO:HA	1:H:105:LEU:HB2	1.64	0.78
1:K:97:LYS:HB2	1:K:100:THR:HG22	1.66	0.77
1:E:131:TYR:HD2	1:E:132:LEU:HD12	1.48	0.77
1:A:34:THR:HG23	1:A:48:ILE:HD11	1.67	0.76
3:A:275:ACY:H1	1:B:126:LYS:HB3	1.66	0.76
1:B:197:ARG:O	1:B:200:VAL:HG23	1.86	0.76
1:E:97:LYS:HE2	8:E:889:HOH:O	1.85	0.76
1:J:208:ILE:CD1	1:J:220:ILE:HD13	2.16	0.75
1:A:214:VAL:HG11	1:A:220:ILE:HD11	1.66	0.75
1:C:81:ALA:O	1:C:85:ILE:HD12	1.86	0.75
1:K:120:LEU:HD13	1:K:128:LEU:HG	1.68	0.75
1:G:253:SER:O	1:G:256:MET:HE1	1.87	0.75
1:H:216:ARG:HG3	1:H:216:ARG:HH11	1.51	0.74
1:B:88:VAL:HA	1:B:155:MET:HE2	1.67	0.74
1:H:44:ALA:O	1:H:48:ILE:HG12	1.88	0.74
1:J:185:THR:CG2	1:L:258:GLN:H	2.00	0.74
1:H:248:GLU:H	1:H:248:GLU:CD	1.89	0.74
1:K:34:THR:O	1:K:38:HIS:HD2	1.71	0.73
1:K:172:ASN:N	1:K:172:ASN:HD22	1.84	0.73
1:C:196:ILE:HD13	1:C:202:ILE:HD11	1.69	0.73
1:J:185:THR:HG23	1:L:258:GLN:H	1.52	0.73
1:F:91:ARG:HB2	1:F:155:MET:CE	2.18	0.73
1:A:118:HIS:HD2	1:A:146:PRO:O	1.72	0.73
1:B:100:THR:HG21	8:B:295:HOH:O	1.88	0.72
1:D:177:LEU:HD12	1:D:203:GLY:HA2	1.70	0.72
1:J:240:PRO:HG3	1:L:260:PHE:CE1	2.23	0.72
1:L:120:LEU:HD22	1:L:125:ARG:CD	2.17	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:240:PRO:HG3	1:L:260:PHE:HE1	1.55	0.72
1:E:8:GLN:HE21	1:E:12:ASN:ND2	1.88	0.71
1:C:173:ASP:O	1:C:199:GLY:HA2	1.90	0.71
1:C:197:ARG:O	1:C:200:VAL:HG13	1.90	0.71
1:D:55:ASN:OD1	1:D:57:ILE:HG22	1.91	0.71
1:J:106:LYS:HD3	1:J:140:PHE:HB3	1.71	0.71
1:B:88:VAL:HG21	1:B:101:PRO:HG3	1.73	0.71
1:C:91:ARG:HB2	1:C:155:MET:CE	2.21	0.71
1:B:91:ARG:HB2	1:B:155:MET:HE3	1.73	0.71
1:G:26:MET:HG2	8:L:936:HOH:O	1.91	0.71
1:G:76:HIS:HA	1:G:79:VAL:HG22	1.71	0.71
1:I:231:PRO:HD2	1:I:234:THR:HG21	1.73	0.70
1:D:88:VAL:HA	1:D:155:MET:CE	2.20	0.70
1:C:0:ALA:N	6:C:274:PG5:H61	2.07	0.70
1:K:32:HIS:HA	1:K:36:LEU:HB2	1.72	0.70
1:H:214:VAL:HG21	1:H:220:ILE:HD11	1.72	0.70
1:G:83[B]:ARG:HA	1:G:86:LEU:HD12	1.74	0.70
1:D:201:MET:HG3	1:D:256:MET:CE	2.22	0.70
1:C:77:MET:HE3	1:C:115:ARG:HB3	1.74	0.70
1:H:74:ASP:O	1:H:77:MET:HG3	1.91	0.70
1:E:55:ASN:ND2	1:E:57:ILE:H	1.88	0.69
1:C:0:ALA:N	6:C:274:PG5:H72	2.07	0.69
1:F:67:VAL:HG22	1:F:116:ILE:HG12	1.73	0.69
1:G:12:ASN:O	1:G:16:GLU:HG3	1.92	0.69
1:H:63:ILE:HD11	8:H:633:HOH:O	1.92	0.69
1:E:97:LYS:HE3	5:E:274:GOL:O2	1.92	0.69
1:E:175:SER:HB3	1:E:256:MET:CE	2.22	0.69
1:E:114:TYR:HB2	1:E:144:ILE:CD1	2.22	0.69
1:L:5:GLU:O	1:L:9:VAL:HG23	1.92	0.69
1:A:54:ALA:HB2	1:A:60:ALA:HB2	1.75	0.68
1:I:65:GLU:OE2	1:K:38:HIS:HE1	1.77	0.68
1:F:88:VAL:HA	1:F:155:MET:CE	2.23	0.68
1:L:120:LEU:CD2	1:L:125:ARG:HD2	2.22	0.68
1:H:1:MET:HE2	1:H:79:VAL:HG13	1.76	0.68
1:G:51:ASN:HD21	1:J:61:ILE:HD11	1.59	0.68
1:C:0:ALA:H1	6:C:274:PG5:H61	1.59	0.67
1:H:242:ARG:O	1:H:244:VAL:HG23	1.95	0.67
1:A:30:PHE:CD1	1:B:57:ILE:HD12	2.29	0.67
1:D:34:THR:O	1:D:38:HIS:HD2	1.77	0.67
1:F:101:PRO:HA	1:F:105:LEU:HB2	1.76	0.67
1:L:92:ASP:HB2	1:L:155:MET:CE	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:67:VAL:HG22	1:K:116:ILE:HD13	1.76	0.66
1:G:83[A]:ARG:HA	1:G:86:LEU:HD12	1.78	0.66
1:B:77:MET:HE1	1:B:119:TRP:HB2	1.78	0.66
1:J:125:ARG:HH22	1:L:26[A]:MET:CE	2.08	0.66
1:E:101:PRO:HA	1:E:105:LEU:HD22	1.78	0.66
1:I:32:HIS:HA	1:I:36:LEU:HB2	1.78	0.66
1:L:48:ILE:O	1:L:52:LYS:HG2	1.96	0.65
1:L:88:VAL:HG13	1:L:155:MET:CE	2.26	0.65
1:I:48:ILE:O	1:I:52:LYS:HG2	1.97	0.65
1:J:100:THR:HB	1:J:101:PRO:HD3	1.78	0.65
1:H:251:LYS:HB2	1:H:254:LEU:HD22	1.78	0.65
1:C:91:ARG:HB2	1:C:155:MET:HE1	1.79	0.65
1:E:101:PRO:HA	1:E:105:LEU:HB2	1.79	0.65
1:B:38:HIS:HE1	1:D:65:GLU:OE1	1.78	0.65
1:B:26:MET:HE1	1:C:66:VAL:HG21	1.79	0.65
1:J:157:ASP:O	1:J:159:ALA:N	2.30	0.64
1:L:54:ALA:HB2	1:L:60:ALA:HB2	1.79	0.64
1:E:234:THR:HG23	1:E:243:ILE:HD12	1.80	0.64
1:I:1:MET:HG3	1:I:5:GLU:HB2	1.79	0.64
1:L:193:HIS:HE1	4:L:276:CYS:SG	2.21	0.64
1:A:209:LEU:HD13	1:C:258:GLN:HB3	1.80	0.64
1:C:0:ALA:H1	6:C:274:PG5:C7	2.09	0.64
1:G:84:ASP:O	1:G:88:VAL:HG12	1.97	0.64
1:A:32:HIS:O	1:A:37:LYS:HB2	1.97	0.64
1:D:89[B]:ARG:NH1	8:D:999:HOH:O	2.29	0.64
1:B:88:VAL:CG2	1:B:101:PRO:HG3	2.28	0.64
1:B:30:PHE:O	1:B:34:THR:HG23	1.97	0.64
1:F:165:GLY:HA3	1:F:193:HIS:CD2	2.32	0.64
1:B:3:SER:O	1:B:7:GLU:HG3	1.97	0.64
1:H:244:VAL:HG12	1:H:244:VAL:O	1.97	0.64
1:B:29:SER:HB2	1:F:29:SER:HB2	1.80	0.63
1:B:88:VAL:HA	1:B:155:MET:HE3	1.79	0.63
1:B:165:GLY:HA3	1:B:193:HIS:CD2	2.33	0.63
1:C:2:SER:OG	1:C:5:GLU:HG3	1.99	0.63
1:D:107:GLY:O	1:D:156:LEU:HD12	1.99	0.63
1:I:2:SER:OG	1:I:5:GLU:HG3	1.98	0.63
1:B:207:LYS:HB2	1:B:225:VAL:HG22	1.81	0.63
1:C:172:ASN:HD21	6:C:274:PG5:H82	1.64	0.63
1:F:101:PRO:HA	1:F:105:LEU:HD22	1.81	0.63
3:A:275:ACY:CH3	1:B:126:LYS:HB3	2.29	0.62
1:B:77:MET:CE	1:B:119:TRP:HB2	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:216:ARG:HH11	1:H:216:ARG:CG	2.12	0.62
1:C:100:THR:HB	1:C:101:PRO:HD3	1.80	0.62
1:K:254:LEU:O	1:L:187:LYS:HD3	1.99	0.62
1:A:177:LEU:HD22	1:A:203:GLY:HA2	1.81	0.62
1:A:184:GLY:HA2	1:A:192:ARG:O	2.00	0.62
1:C:165:GLY:HA3	1:C:193:HIS:CD2	2.35	0.62
1:B:106:LYS:HG2	8:B:646:HOH:O	2.00	0.62
1:H:165:GLY:HA3	1:H:193:HIS:CD2	2.35	0.62
1:K:100:THR:HG23	1:K:101:PRO:HD3	1.81	0.61
1:E:98:TYR:O	1:E:101:PRO:HD2	1.99	0.61
1:A:121:TRP:CE2	1:A:126:LYS:HE3	2.35	0.61
1:B:91:ARG:HB2	1:B:155:MET:HE1	1.82	0.61
1:E:144:ILE:HB	1:E:164:ILE:HB	1.82	0.61
1:J:260:PHE:CE1	1:K:240:PRO:HG3	2.35	0.61
1:C:184:GLY:HA2	1:C:192:ARG:O	2.01	0.61
1:G:190:GLY:O	1:G:192:ARG:HG2	2.01	0.61
1:J:58:MET:HG2	1:J:63:ILE:HG13	1.82	0.61
1:J:184:GLY:HA2	1:J:192:ARG:O	2.00	0.61
1:I:26[B]:MET:HE2	1:I:26[B]:MET:HA	1.82	0.61
1:G:20:LEU:HB3	1:G:31:PHE:CE2	2.35	0.60
1:K:55:ASN:HB3	8:K:576:HOH:O	2.01	0.60
1:H:14:LYS:HE3	1:H:36:LEU:HA	1.83	0.60
1:H:145:HIS:CE1	1:H:166:GLU:HG3	2.37	0.60
1:A:220:ILE:N	1:A:220:ILE:HD12	2.16	0.60
1:D:118:HIS:HD2	1:D:146:PRO:O	1.84	0.60
1:B:121:TRP:CZ3	1:B:126:LYS:HG2	2.37	0.59
1:C:77:MET:HE1	1:C:115:ARG:O	2.02	0.59
1:C:208:ILE:HG12	1:C:226:VAL:HG13	1.84	0.59
1:D:184:GLY:HA2	1:D:192:ARG:O	2.02	0.59
1:E:4:GLU:HA	1:E:7:GLU:HG3	1.85	0.59
1:H:58:MET:HG2	1:H:63:ILE:HG13	1.84	0.59
1:A:87:ALA:O	1:A:91:ARG:HG3	2.02	0.59
1:G:1:MET:HE3	1:G:6:LEU:HB2	1.84	0.59
1:D:177:LEU:HD13	8:D:611:HOH:O	2.02	0.59
1:G:34:THR:O	1:G:38:HIS:HD2	1.86	0.59
1:A:1:MET:HE3	1:A:83:ARG:HG2	1.83	0.59
1:D:242:ARG:HD3	1:D:243:ILE:H	1.68	0.59
1:H:38:HIS:HE1	1:L:65:GLU:OE1	1.84	0.59
1:J:200:VAL:HG21	1:J:214:VAL:HG12	1.84	0.59
1:D:100:THR:HB	1:D:101:PRO:HD3	1.84	0.59
1:L:53:LEU:HB2	1:L:63:ILE:HD13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:HIS:HA	1:A:36:LEU:HB2	1.85	0.59
1:C:212:ILE:HG22	1:C:213:GLU:N	2.17	0.59
1:K:165:GLY:HA3	1:K:193:HIS:CD2	2.38	0.59
1:E:4:GLU:CD	1:E:4:GLU:H	2.07	0.58
1:G:225:VAL:HG21	1:G:239:VAL:HG13	1.85	0.58
1:H:55:ASN:HD22	1:H:57:ILE:H	1.51	0.58
1:A:26:MET:HE2	1:D:32:HIS:HD2	1.68	0.58
1:D:34:THR:O	1:D:38:HIS:CD2	2.55	0.58
1:F:119:TRP:O	1:F:123:GLN:HG2	2.03	0.58
1:J:160:THR:HG21	8:K:825:HOH:O	2.03	0.58
1:E:34:THR:O	1:E:38:HIS:HD2	1.87	0.58
1:J:111:LEU:HD21	1:J:115:ARG:HH21	1.68	0.58
1:C:32:HIS:HA	1:C:36:LEU:HB2	1.86	0.58
1:E:224:SER:OG	1:E:237:ALA:HA	2.04	0.58
1:K:37:LYS:HD3	8:K:295:HOH:O	2.03	0.58
1:K:196:ILE:HD13	1:K:214:VAL:HG11	1.86	0.58
1:K:196:ILE:HD12	1:K:202:ILE:HD11	1.84	0.58
1:D:34:THR:CG2	1:D:35:LEU:HG	2.31	0.58
1:E:55:ASN:HD22	1:E:57:ILE:N	1.93	0.57
1:A:58:MET:HG2	1:A:63:ILE:HG12	1.86	0.57
1:J:84:ASP:OD2	1:J:111:LEU:CD2	2.51	0.57
1:C:27:LEU:O	1:C:30:PHE:HB3	2.04	0.57
1:D:52:LYS:HB3	1:D:140:PHE:HZ	1.68	0.57
1:E:131:TYR:CD2	1:E:132:LEU:HD12	2.36	0.57
1:D:109:HIS:HD2	8:D:361:HOH:O	1.88	0.57
1:L:165:GLY:HA3	1:L:193:HIS:CE1	2.40	0.57
1:G:199:GLY:C	1:G:253:SER:HB2	2.25	0.57
1:J:260:PHE:HE1	1:K:240:PRO:HG3	1.70	0.57
1:C:34:THR:O	1:C:38:HIS:HD2	1.88	0.57
1:D:253:SER:HA	1:D:256:MET:HE1	1.85	0.57
1:F:151:GLY:HA3	1:F:172:ASN:HD22	1.69	0.57
1:G:81:ALA:HB2	1:G:112:GLN:NE2	2.19	0.57
1:I:200:VAL:O	1:I:253:SER:HB3	2.05	0.57
1:A:48:ILE:O	1:A:52:LYS:HG2	2.05	0.56
1:A:131:TYR:CD2	1:A:132:LEU:HD23	2.40	0.56
1:D:260:PHE:CD1	1:D:260:PHE:O	2.59	0.56
1:G:253:SER:O	1:G:256:MET:CE	2.52	0.56
1:H:7:GLU:OE1	1:H:7:GLU:HA	2.03	0.56
1:C:0:ALA:H1	6:C:274:PG5:C6	2.17	0.56
1:I:77:MET:HE1	1:I:119:TRP:HB2	1.88	0.56
1:I:80:SER:OG	1:I:115:ARG:CZ	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:THR:O	1:H:38:HIS:HD2	1.88	0.56
1:J:201:MET:HB3	1:J:253:SER:HA	1.87	0.56
1:K:5:GLU:O	1:K:9:VAL:HG12	2.06	0.56
1:A:55:ASN:OD1	1:A:56:PRO:HD2	2.05	0.56
1:I:202:ILE:HG12	1:I:220:ILE:HD13	1.87	0.56
1:E:63:ILE:HD11	8:E:289:HOH:O	2.06	0.56
1:F:108:PHE:O	1:F:112:GLN:HG2	2.06	0.56
5:B:274:GOL:C3	1:C:130:ILE:HG13	2.36	0.56
1:B:34:THR:O	1:B:38:HIS:HD2	1.88	0.56
1:I:38:HIS:HE1	1:K:65:GLU:OE2	1.89	0.56
1:B:160:THR:HG21	8:C:277:HOH:O	2.05	0.55
1:E:260:PHE:CE2	1:F:227:LEU:HD21	2.40	0.55
1:I:77:MET:CE	1:I:119:TRP:HB2	2.36	0.55
1:J:67:VAL:HG22	1:J:116:ILE:HG12	1.87	0.55
1:L:97:LYS:NZ	7:L:275:PEG:H32	2.21	0.55
1:G:34:THR:CG2	1:G:35:LEU:HG	2.28	0.55
1:H:134:ASN:O	1:H:138:VAL:HG23	2.06	0.55
1:I:132:LEU:O	1:I:136:VAL:HG23	2.06	0.55
1:J:53:LEU:HD21	1:J:136:VAL:HG22	1.88	0.55
1:E:234:THR:CG2	1:E:243:ILE:HD12	2.35	0.55
1:G:76:HIS:HA	1:G:79:VAL:CG2	2.37	0.55
1:J:112:GLN:NE2	8:J:293:HOH:O	2.39	0.55
1:K:224:SER:OG	1:K:237:ALA:HA	2.06	0.55
1:C:88:VAL:HG12	1:C:95:VAL:HG21	1.88	0.55
1:F:188:THR:HG22	1:F:189:SER:O	2.06	0.55
1:L:17:ALA:HB3	1:L:36:LEU:HD21	1.88	0.55
1:H:25:PRO:HB2	1:K:32:HIS:CD2	2.42	0.55
1:A:34:THR:HG21	1:A:48:ILE:HD11	1.88	0.55
1:B:77:MET:HE2	8:B:896:HOH:O	2.06	0.55
1:E:67:VAL:HG22	1:E:116:ILE:HD13	1.89	0.55
1:G:32:HIS:CE1	1:G:37:LYS:HG3	2.41	0.55
1:G:151:GLY:O	1:G:154:ILE:CD1	2.55	0.55
1:L:213:GLU:HG3	1:L:214:VAL:N	2.21	0.55
1:K:172:ASN:N	1:K:172:ASN:ND2	2.54	0.55
1:A:74:ASP:HB3	1:A:77:MET:CE	2.34	0.55
1:G:112:GLN:HA	1:G:115:ARG:HG3	1.89	0.55
1:I:10:TRP:CH2	1:I:44:ALA:HB2	2.42	0.55
1:I:89:ARG:HG2	1:I:89:ARG:HH21	1.71	0.55
1:K:10:TRP:CZ2	1:K:14:LYS:HD3	2.42	0.55
1:L:116:ILE:N	1:L:116:ILE:HD13	2.22	0.55
1:D:128:LEU:O	1:D:132:LEU:HD22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASN:CG	1:A:56:PRO:HD2	2.28	0.54
1:A:118:HIS:CD2	1:A:146:PRO:O	2.57	0.54
1:D:66:VAL:CG2	1:F:26:MET:HE1	2.37	0.54
1:F:201:MET:HE2	1:F:202:ILE:N	2.22	0.54
1:L:74:ASP:HB3	1:L:77:MET:HE3	1.89	0.54
1:B:26:MET:HB3	1:C:58:MET:HE1	1.89	0.54
1:B:159:ALA:HA	1:B:162:ILE:HD12	1.89	0.54
5:B:274:GOL:H32	1:C:130:ILE:HG13	1.88	0.54
1:G:181:THR:HB	1:G:207:LYS:HD2	1.90	0.54
1:F:101:PRO:CA	1:F:105:LEU:HD22	2.37	0.54
1:G:102:LEU:O	1:G:109:HIS:HE1	1.91	0.54
1:F:30:PHE:O	1:F:34:THR:HB	2.08	0.54
1:I:167:THR:C	1:I:193:HIS:HB2	2.28	0.54
1:I:167:THR:O	1:I:193:HIS:HB2	2.07	0.54
1:L:34:THR:CG2	1:L:48:ILE:HG13	2.38	0.54
1:E:114:TYR:CD1	1:E:144:ILE:CD1	2.80	0.54
1:I:1:MET:CG	1:I:5:GLU:HB2	2.38	0.54
1:L:1:MET:HG3	1:L:83:ARG:HG2	1.90	0.54
1:E:84:ASP:O	1:E:88:VAL:HG23	2.08	0.54
1:L:88:VAL:HG13	1:L:155:MET:HE3	1.88	0.54
1:A:165:GLY:HA3	1:A:193:HIS:CD2	2.42	0.54
1:H:96:ASP:OD1	5:H:275:GOL:O2	2.26	0.54
1:L:50:ALA:HA	1:L:63:ILE:CG2	2.38	0.54
1:D:224:SER:OG	1:D:237:ALA:HA	2.09	0.54
1:B:106:LYS:HE2	1:C:137:SER:OG	2.07	0.53
1:C:58:MET:HG2	1:C:63:ILE:HG13	1.90	0.53
1:E:119:TRP:O	1:E:123:GLN:HB2	2.08	0.53
1:D:75:ALA:HB1	8:D:477:HOH:O	2.08	0.53
1:G:142:VAL:HG12	1:G:144:ILE:HG13	1.90	0.53
1:I:39:GLU:HA	1:I:39:GLU:OE2	2.08	0.53
1:C:32:HIS:O	1:C:37:LYS:HB2	2.09	0.53
1:G:114:TYR:CE1	1:G:118:HIS:HB2	2.43	0.53
1:L:97:LYS:HZ2	7:L:275:PEG:H32	1.74	0.53
1:L:145:HIS:CE1	1:L:147:ALA:HB3	2.43	0.53
1:D:57:ILE:HG23	1:D:131:TYR:OH	2.08	0.53
1:K:199:GLY:O	1:K:252:PRO:HD2	2.09	0.53
1:G:37:LYS:NZ	1:L:26[A]:MET:HE2	2.24	0.53
1:G:214:VAL:HG12	1:G:218:ALA:HB3	1.90	0.53
1:D:102:LEU:O	1:D:109:HIS:HE1	1.91	0.53
1:G:7:GLU:HG3	1:G:8:GLN:N	2.23	0.53
1:C:1:MET:HG3	1:C:5:GLU:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:201:MET:HB2	1:H:253:SER:HA	1.91	0.53
1:C:77:MET:CE	1:C:115:ARG:HB3	2.36	0.53
1:J:178:GLN:O	1:J:179:SER:HB3	2.07	0.53
1:B:32:HIS:HA	1:B:36:LEU:HB2	1.91	0.52
1:C:61:ILE:HD11	1:F:64:ARG:HD2	1.91	0.52
1:D:45:LEU:HD23	1:D:71:TYR:OH	2.08	0.52
1:D:243:ILE:N	1:D:243:ILE:HD12	2.24	0.52
1:I:176:ILE:HG23	1:I:180:VAL:CG2	2.34	0.52
1:I:176:ILE:CG2	1:I:180:VAL:HG21	2.35	0.52
1:B:260:PHE:CE1	1:C:240:PRO:HG3	2.44	0.52
1:G:151:GLY:C	1:G:154:ILE:HD11	2.28	0.52
1:G:165:GLY:HA3	1:G:193:HIS:CD2	2.45	0.52
1:E:53:LEU:HB2	1:E:63:ILE:HD13	1.91	0.52
1:H:1:MET:HE1	1:H:6:LEU:HD13	1.90	0.52
1:L:92:ASP:HB2	1:L:155:MET:HE1	1.90	0.52
1:F:152:CYS:H	1:F:172:ASN:ND2	2.08	0.52
1:G:225:VAL:CG2	1:G:239:VAL:HG13	2.40	0.52
1:J:2:SER:CB	1:J:5:GLU:HB2	2.39	0.52
1:J:161:GLY:HA2	1:L:160:THR:HG21	1.92	0.52
1:C:89:ARG:HA	1:C:95:VAL:HG23	1.92	0.52
1:F:200:VAL:HG21	1:F:214:VAL:HG12	1.92	0.52
1:H:151:GLY:O	1:H:154:ILE:HD12	2.10	0.52
1:G:35:LEU:HD11	1:G:103:LEU:HD11	1.92	0.52
1:B:121:TRP:CE3	1:B:126:LYS:HG2	2.45	0.51
1:F:1:MET:HG3	1:F:5:GLU:HG3	1.92	0.51
1:I:168:ALA:HB2	1:I:193:HIS:HB3	1.92	0.51
1:C:10:TRP:NE1	1:C:14:LYS:HD3	2.25	0.51
1:H:181:THR:HB	1:H:207:LYS:HD2	1.91	0.51
1:I:231:PRO:O	1:I:234:THR:HB	2.09	0.51
1:K:1:MET:HB3	1:K:79:VAL:HG13	1.93	0.51
1:G:212:ILE:HD11	1:G:228:GLN:C	2.31	0.51
1:H:40:ASN:ND2	1:H:42:GLY:N	2.58	0.51
1:I:20:LEU:HB3	1:I:31:PHE:CE2	2.45	0.51
1:J:34:THR:HG22	1:J:35:LEU:HG	1.93	0.51
1:L:253:SER:HA	1:L:256:MET:HE3	1.92	0.51
1:B:55:ASN:OD1	1:B:57:ILE:HG12	2.10	0.51
1:E:3:SER:O	1:E:7:GLU:HG3	2.10	0.51
1:D:34:THR:HG23	1:D:35:LEU:CG	2.36	0.51
1:F:168:ALA:HB2	1:F:193:HIS:HB3	1.92	0.51
1:F:202:ILE:HD13	1:F:208:ILE:HD11	1.90	0.51
1:I:54:ALA:HB2	1:I:60:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ASP:N	1:B:155:MET:HE1	2.25	0.51
1:F:151:GLY:HA3	1:F:172:ASN:ND2	2.26	0.51
1:G:213:GLU:O	1:G:229:SER:HA	2.11	0.51
1:A:201:MET:O	1:A:201:MET:HG3	2.11	0.51
1:B:26:MET:HE1	1:C:66:VAL:CG2	2.40	0.51
1:E:77:MET:HE3	1:E:119:TRP:HB2	1.90	0.51
1:I:34:THR:O	1:I:38:HIS:HD2	1.93	0.51
1:J:77:MET:HE2	1:J:119:TRP:HB2	1.93	0.51
1:K:45:LEU:HD23	1:K:71:TYR:OH	2.11	0.51
1:C:89:ARG:NH1	8:C:740:HOH:O	2.43	0.51
1:G:133:GLN:HG3	1:G:144:ILE:O	2.10	0.51
1:G:152:CYS:HA	1:G:154:ILE:HD12	1.93	0.51
1:G:256:MET:HG3	8:G:283:HOH:O	2.11	0.51
1:L:167:THR:H	1:L:193:HIS:CD2	2.29	0.51
1:B:260:PHE:HE1	1:C:240:PRO:HG3	1.76	0.50
1:C:34:THR:O	1:C:38:HIS:CD2	2.64	0.50
1:E:144:ILE:HD13	8:E:306:HOH:O	2.11	0.50
1:H:225:VAL:HG23	1:H:239:VAL:HG22	1.93	0.50
1:I:26[B]:MET:CE	1:J:33:ALA:HB2	2.41	0.50
1:A:214:VAL:CG1	1:A:220:ILE:HD11	2.38	0.50
1:A:227:LEU:HD11	1:C:260:PHE:CE2	2.46	0.50
1:C:46:SER:HA	1:C:67:VAL:HG11	1.93	0.50
1:H:55:ASN:ND2	1:H:56:PRO:HD2	2.27	0.50
1:C:5:GLU:O	1:C:9:VAL:HG23	2.12	0.50
1:D:118:HIS:CD2	1:D:146:PRO:O	2.64	0.50
1:F:14:LYS:O	1:F:17:ALA:HB3	2.11	0.50
1:K:149:THR:HB	1:K:169:VAL:HG22	1.92	0.50
1:L:184:GLY:HA2	1:L:192:ARG:O	2.11	0.50
1:C:208:ILE:HG12	1:C:226:VAL:HG11	1.91	0.50
1:E:97:LYS:CE	5:E:274:GOL:O2	2.59	0.50
1:E:101:PRO:CA	1:E:105:LEU:HD22	2.41	0.50
1:F:55:ASN:OD1	1:F:56:PRO:HD2	2.12	0.50
1:B:14:LYS:HG2	1:B:36:LEU:HD12	1.93	0.50
1:C:55:ASN:OD1	1:C:56:PRO:HD2	2.12	0.50
1:E:155:MET:CE	1:E:157:ASP:HB2	2.42	0.50
1:I:134:ASN:O	1:I:138:VAL:HG23	2.11	0.50
1:K:2:SER:HB3	1:K:5:GLU:OE1	2.12	0.50
1:A:153:GLY:O	1:A:173:ASP:HA	2.12	0.50
1:G:48:ILE:HG23	1:G:49:LEU:N	2.27	0.50
1:G:253:SER:C	1:G:256:MET:HE1	2.33	0.49
1:J:230:VAL:CG1	1:J:234:THR:CG2	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:26[B]:MET:HE3	1:J:33:ALA:HB2	1.94	0.49
1:I:180:VAL:HG12	1:I:206:ALA:H	1.76	0.49
1:A:197:ARG:O	1:A:200:VAL:HG23	2.13	0.49
1:D:20:LEU:HD21	1:D:97:LYS:HE2	1.94	0.49
1:H:216:ARG:CG	1:H:216:ARG:NH1	2.75	0.49
1:A:89:ARG:HG2	1:A:98:TYR:CE1	2.47	0.49
1:B:46:SER:HA	1:B:67:VAL:HG11	1.94	0.49
1:G:16:GLU:O	1:G:20:LEU:HD22	2.13	0.49
1:J:224:SER:OG	1:J:237:ALA:HA	2.12	0.49
1:L:61:ILE:HG22	8:L:937:HOH:O	2.12	0.49
1:L:145:HIS:CE1	1:L:166:GLU:HG3	2.47	0.49
1:J:156:LEU:O	1:J:159:ALA:HB2	2.12	0.49
1:K:45:LEU:HD11	1:K:112:GLN:HG3	1.95	0.49
1:A:108:PHE:O	1:A:112:GLN:HG2	2.13	0.49
1:D:57:ILE:HD11	1:F:30:PHE:CB	2.23	0.49
1:F:14:LYS:HE3	1:F:38:HIS:O	2.12	0.49
1:A:32:HIS:CE1	1:A:37:LYS:HG3	2.48	0.49
1:B:98:TYR:O	1:B:101:PRO:HD2	2.11	0.49
1:F:132:LEU:O	1:F:136:VAL:HG23	2.12	0.49
1:G:51:ASN:ND2	1:J:61:ILE:HD11	2.28	0.49
1:G:77:MET:O	1:G:80:SER:HB2	2.12	0.49
1:H:84:ASP:OD2	1:H:115:ARG:NH2	2.46	0.49
1:I:26[A]:MET:SD	1:J:37:LYS:HE3	2.53	0.49
1:J:77:MET:CE	1:J:119:TRP:HB2	2.43	0.49
1:B:233:HIS:O	1:B:246:LYS:HG3	2.12	0.49
1:E:77:MET:HE3	1:E:119:TRP:CD1	2.48	0.49
1:G:47:TYR:CZ	1:J:61:ILE:HD12	2.48	0.49
1:D:45:LEU:HG	1:D:49:LEU:HD22	1.95	0.49
1:E:260:PHE:CE1	1:F:240:PRO:HG3	2.47	0.49
1:H:115:ARG:NH1	1:H:151:GLY:O	2.46	0.49
1:J:209:LEU:HD13	1:L:258:GLN:HB3	1.95	0.49
1:L:74:ASP:HB3	1:L:77:MET:CE	2.41	0.49
1:B:224:SER:OG	1:B:237:ALA:HA	2.13	0.48
1:D:9:VAL:CG2	1:D:86:LEU:HD21	2.43	0.48
1:F:2:SER:OG	1:F:5:GLU:HG2	2.13	0.48
1:F:119:TRP:CE3	1:F:120:LEU:HD13	2.48	0.48
1:F:202:ILE:HD13	1:F:208:ILE:CD1	2.43	0.48
1:B:81:ALA:O	1:B:85:ILE:HG13	2.13	0.48
1:H:200:VAL:HG21	1:H:214:VAL:HG22	1.94	0.48
1:J:185:THR:HG23	1:L:258:GLN:HB2	1.95	0.48
1:L:32:HIS:O	1:L:37:LYS:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:MET:CB	1:G:83[B]:ARG:NH2	2.76	0.48
1:H:61:ILE:HD11	1:L:64:ARG:HD2	1.95	0.48
1:A:34:THR:HG23	1:A:48:ILE:CD1	2.42	0.48
1:E:77:MET:HE3	1:E:119:TRP:CG	2.48	0.48
1:I:34:THR:HG22	1:I:47:TYR:CD2	2.49	0.48
1:K:207:LYS:NZ	2:L:274:SO4:O3	2.47	0.48
1:A:61:ILE:HG21	1:E:51:ASN:HD21	1.79	0.48
1:F:219:LYS:NZ	8:F:834:HOH:O	2.46	0.48
1:H:188:THR:HG23	1:H:189:SER:O	2.14	0.48
1:G:213:GLU:HG3	1:G:214:VAL:N	2.28	0.48
1:J:121:TRP:CE3	1:J:126:LYS:HG2	2.49	0.48
1:B:89:ARG:HG2	1:B:89:ARG:HH11	1.79	0.48
1:B:219:LYS:HE2	1:B:257:ASP:O	2.14	0.48
1:F:58:MET:HG2	1:F:63:ILE:HG13	1.96	0.48
1:G:2:SER:HB3	1:G:5:GLU:CG	2.39	0.48
1:I:181:THR:HB	1:I:207:LYS:HD2	1.95	0.48
1:B:61:ILE:HD12	1:D:60:ALA:HB1	1.95	0.48
1:C:37:LYS:HG2	8:F:379:HOH:O	2.12	0.48
1:F:55:ASN:OD1	1:F:56:PRO:N	2.47	0.48
1:G:109:HIS:HD2	8:G:428:HOH:O	1.96	0.48
1:H:158:HIS:CD2	1:I:163:VAL:HG11	2.49	0.48
1:I:91:ARG:HD3	1:I:175:SER:OG	2.14	0.48
1:L:50:ALA:HA	1:L:63:ILE:HG21	1.95	0.48
1:L:88:VAL:HA	1:L:155:MET:HE3	1.96	0.48
1:B:196:ILE:N	1:B:196:ILE:HD12	2.29	0.47
1:H:40:ASN:ND2	1:H:42:GLY:H	2.12	0.47
1:H:182:LEU:HD22	1:H:196:ILE:HD11	1.95	0.47
1:G:1:MET:HB3	1:G:83[B]:ARG:NH2	2.29	0.47
1:I:176:ILE:CG2	1:I:180:VAL:CG2	2.92	0.47
1:L:46:SER:HA	1:L:67:VAL:HG11	1.96	0.47
1:A:34:THR:O	1:A:38:HIS:HD2	1.98	0.47
1:B:89:ARG:HD2	1:B:98:TYR:CE1	2.49	0.47
1:D:112:GLN:O	1:D:116:ILE:HD12	2.15	0.47
1:D:191:ASP:HB3	1:D:211:ASN:ND2	2.29	0.47
1:D:259:HIS:HE1	1:E:185:THR:OG1	1.97	0.47
1:G:38:HIS:HE1	1:J:65:GLU:OE2	1.96	0.47
1:E:133:GLN:HB2	1:E:146:PRO:HD3	1.95	0.47
1:I:88:VAL:HG11	1:I:101:PRO:HG3	1.96	0.47
1:K:34:THR:O	1:K:38:HIS:CD2	2.60	0.47
1:L:199:GLY:O	1:L:252:PRO:HD2	2.14	0.47
1:B:145:HIS:ND1	1:B:146:PRO:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:VAL:HG21	1:B:262:GLY:HA2	1.96	0.47
1:C:179:SER:O	1:C:205:GLY:HA2	2.15	0.47
1:F:34:THR:O	1:F:38:HIS:HD2	1.97	0.47
1:H:131:TYR:HD2	1:H:132:LEU:HD12	1.79	0.47
1:K:52:LYS:CG	1:K:140:PHE:HZ	2.27	0.47
1:A:164:ILE:HG12	1:A:182:LEU:HD12	1.97	0.47
1:B:244:VAL:HG13	1:B:261:ASN:HB2	1.96	0.47
1:E:86:LEU:O	1:E:90:LEU:HB2	2.14	0.47
1:F:27:LEU:O	1:F:30:PHE:HB3	2.15	0.47
1:E:32:HIS:O	1:E:37:LYS:HB3	2.15	0.47
1:E:80:SER:HA	1:E:152:CYS:SG	2.55	0.47
1:G:252:PRO:O	1:G:256:MET:HE2	2.14	0.47
1:E:155:MET:CE	1:E:256:MET:HE3	2.45	0.47
1:G:45:LEU:HA	1:G:48:ILE:HG22	1.96	0.47
1:H:100:THR:N	1:H:101:PRO:HD2	2.29	0.47
1:I:100:THR:HB	1:I:101:PRO:HD3	1.96	0.47
1:D:48:ILE:HD12	1:D:102:LEU:HG	1.97	0.47
1:D:259:HIS:CE1	1:E:185:THR:OG1	2.68	0.47
1:A:61:ILE:HD11	1:E:64:ARG:HD2	1.97	0.46
1:I:52:LYS:HB3	1:I:140:PHE:HZ	1.79	0.46
1:J:85:ILE:HG13	1:J:108:PHE:CE1	2.49	0.46
1:F:231:PRO:HD2	1:F:243:ILE:HD11	1.96	0.46
1:G:242:ARG:NH2	1:G:262:GLY:O	2.48	0.46
1:I:214:VAL:HG11	1:I:220:ILE:HD11	1.98	0.46
1:K:260:PHE:HZ	1:L:225:VAL:HG11	1.80	0.46
1:L:32:HIS:HB2	8:L:471:HOH:O	2.15	0.46
1:C:154:ILE:HD12	1:C:174:VAL:HB	1.97	0.46
1:F:91:ARG:CB	1:F:155:MET:HE1	2.40	0.46
1:H:159:ALA:O	1:H:160:THR:C	2.53	0.46
1:K:1:MET:HE1	1:K:6:LEU:HD13	1.98	0.46
1:L:116:ILE:N	1:L:116:ILE:CD1	2.79	0.46
1:A:12:ASN:O	1:A:16:GLU:HG3	2.16	0.46
1:E:8:GLN:HE21	1:E:12:ASN:CG	2.19	0.46
1:G:26:MET:HE2	1:H:58:MET:SD	2.55	0.46
1:I:261:ASN:ND2	1:I:267:PHE:HA	2.30	0.46
1:G:120:LEU:HD13	1:G:128:LEU:HG	1.98	0.46
1:G:186:GLY:HA3	8:G:285:HOH:O	2.15	0.46
1:H:184:GLY:HA2	1:H:192:ARG:O	2.16	0.46
1:B:77:MET:HE1	1:B:119:TRP:CB	2.43	0.46
1:E:137:SER:HA	1:E:142:VAL:O	2.16	0.46
1:G:45:LEU:HG	1:G:71:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:38:HIS:CD2	1:H:44:ALA:HA	2.51	0.46
1:L:157:ASP:HB3	1:L:177:LEU:HD13	1.98	0.46
1:A:64:ARG:O	1:A:68:GLU:HB2	2.16	0.46
1:B:38:HIS:CE1	1:D:65:GLU:OE1	2.66	0.46
1:D:131:TYR:HD2	1:D:132:LEU:HD13	1.79	0.46
1:H:68:GLU:O	1:H:72:ARG:HG3	2.16	0.46
1:I:89:ARG:HG2	1:I:89:ARG:NH2	2.31	0.46
1:G:106:LYS:HE3	1:G:140:PHE:O	2.16	0.45
1:J:119:TRP:O	1:J:123:GLN:HB2	2.16	0.45
1:L:92:ASP:HB2	1:L:155:MET:HE3	1.98	0.45
1:D:57:ILE:CG2	1:D:131:TYR:OH	2.64	0.45
1:E:32:HIS:HA	1:E:36:LEU:HB2	1.98	0.45
1:G:134:ASN:HA	1:G:137:SER:HB3	1.97	0.45
1:K:55:ASN:OD1	1:K:56:PRO:HD2	2.16	0.45
1:H:77:MET:HE1	1:H:115:ARG:HB3	1.99	0.45
1:L:1:MET:HB3	1:L:79:VAL:HG13	1.98	0.45
1:D:1:MET:HE2	1:D:86:LEU:HD11	1.98	0.45
1:D:153:GLY:O	1:D:173:ASP:HA	2.16	0.45
1:E:4:GLU:CD	1:E:4:GLU:N	2.69	0.45
1:E:34:THR:O	1:E:38:HIS:CD2	2.66	0.45
1:H:214:VAL:HG23	1:H:218:ALA:HB3	1.98	0.45
1:J:244:VAL:HG11	1:J:261:ASN:C	2.37	0.45
1:K:121:TRP:CE3	1:K:126:LYS:HG2	2.51	0.45
1:I:159:ALA:O	1:I:160:THR:C	2.55	0.45
1:K:34:THR:HG22	1:K:35:LEU:HG	1.97	0.45
1:C:49:LEU:HD21	1:C:112:GLN:HB2	1.98	0.45
1:E:260:PHE:HE1	1:F:240:PRO:HG3	1.81	0.45
1:J:242:ARG:O	1:J:244:VAL:HG23	2.17	0.45
1:J:244:VAL:O	1:J:244:VAL:HG12	2.17	0.45
1:L:105:LEU:HD12	1:L:105:LEU:HA	1.84	0.45
1:L:145:HIS:CE1	1:L:147:ALA:CB	2.99	0.45
1:E:92:ASP:OD2	1:E:95:VAL:HG23	2.17	0.45
1:G:132:LEU:O	1:G:136:VAL:HG23	2.16	0.45
1:I:37:LYS:HG3	1:I:37:LYS:O	2.17	0.45
1:I:156:LEU:HA	1:I:176:ILE:O	2.16	0.45
1:D:57:ILE:HD12	8:D:982:HOH:O	2.16	0.45
1:G:100:THR:HB	1:G:101:PRO:HD3	1.97	0.45
1:H:0:ALA:HA	8:H:276:HOH:O	2.16	0.45
1:H:192:ARG:HA	1:H:211:ASN:HB2	1.99	0.45
1:B:216:ARG:HG3	8:B:609:HOH:O	2.16	0.45
1:B:230:VAL:HA	1:B:231:PRO:HD3	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:97:LYS:HD2	7:L:275:PEG:H21	1.98	0.45
1:A:26:MET:HE2	1:A:26:MET:HA	1.99	0.45
1:C:92:ASP:HA	1:C:93:PRO:HD3	1.81	0.45
1:C:181:THR:HB	1:C:207:LYS:HD2	1.98	0.45
1:D:147:ALA:HB3	1:D:166:GLU:HG3	1.99	0.45
1:H:1:MET:HE3	1:H:6:LEU:HB2	1.98	0.45
1:K:83:ARG:HD2	8:K:835:HOH:O	2.16	0.45
1:G:19:ALA:O	1:G:23:CYS:HB2	2.17	0.44
1:G:58:MET:HG2	1:G:63:ILE:HG13	2.00	0.44
1:H:220:ILE:N	1:H:220:ILE:HD12	2.31	0.44
1:C:212:ILE:CG2	1:C:213:GLU:N	2.81	0.44
1:E:159:ALA:HA	1:E:162:ILE:HD12	1.98	0.44
1:E:231:PRO:O	1:E:234:THR:HB	2.17	0.44
1:H:237:ALA:O	1:H:241:ALA:HA	2.17	0.44
1:K:69:GLU:HG2	1:K:119:TRP:CH2	2.52	0.44
1:L:145:HIS:NE2	1:L:166:GLU:HG3	2.32	0.44
1:A:151:GLY:O	1:A:154:ILE:HD12	2.18	0.44
1:B:91:ARG:HH22	1:B:173:ASP:HA	1.82	0.44
1:E:52:LYS:HB3	1:E:140:PHE:HZ	1.82	0.44
1:B:198:GLU:O	1:B:216:ARG:HB2	2.18	0.44
1:C:20:LEU:HB3	1:C:31:PHE:CE2	2.53	0.44
1:C:74:ASP:O	1:C:77:MET:HG3	2.17	0.44
1:D:81:ALA:O	1:D:85:ILE:HD12	2.18	0.44
1:F:55:ASN:OD1	1:F:56:PRO:CD	2.66	0.44
1:I:61:ILE:HD12	1:K:47:TYR:CE1	2.53	0.44
1:J:26:MET:HE3	8:K:924:HOH:O	2.17	0.44
1:B:100:THR:HG23	1:B:101:PRO:HD3	1.99	0.44
1:C:16:GLU:O	1:C:20:LEU:HG	2.18	0.44
1:C:154:ILE:HD11	1:C:171:GLU:O	2.16	0.44
1:F:225:VAL:HG23	1:F:239:VAL:HG22	1.99	0.44
1:J:119:TRP:HE3	1:J:120:LEU:HD13	1.83	0.44
1:L:239:VAL:HA	1:L:240:PRO:HA	1.86	0.44
6:C:274:PG5:H22	8:C:520:HOH:O	2.17	0.44
1:H:59:PRO:HG3	8:H:417:HOH:O	2.17	0.44
1:I:199:GLY:O	1:I:252:PRO:HD2	2.18	0.44
1:K:58:MET:HG2	1:K:63:ILE:HG13	1.99	0.44
1:K:88:VAL:HG11	1:K:101:PRO:HG3	1.99	0.44
8:A:894:HOH:O	1:C:259:HIS:HE1	2.01	0.44
1:F:2:SER:H	1:F:5:GLU:CD	2.21	0.44
1:H:153:GLY:O	1:H:173:ASP:HA	2.18	0.44
1:I:114:TYR:HA	8:I:543:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ILE:HG22	1:A:206:ALA:HB3	1.99	0.44
1:B:53:LEU:HD12	1:B:53:LEU:HA	1.82	0.44
1:B:84:ASP:HB3	8:B:302:HOH:O	2.17	0.44
1:E:12:ASN:O	1:E:16:GLU:HG3	2.18	0.44
1:B:14:LYS:HE3	1:B:38:HIS:O	2.17	0.44
1:B:38:HIS:CE1	1:B:64:ARG:HH22	2.36	0.44
1:D:91:ARG:HD3	1:D:253:SER:O	2.18	0.44
1:G:48:ILE:HG23	1:G:49:LEU:H	1.83	0.44
1:I:61:ILE:HD12	1:K:47:TYR:CD1	2.52	0.44
1:I:80:SER:HB2	1:I:152:CYS:HB3	2.00	0.44
1:J:118:HIS:HD2	1:J:146:PRO:O	2.01	0.44
1:K:184:GLY:N	1:K:193:HIS:CD2	2.86	0.44
1:B:18:ARG:HH21	1:L:195:LYS:HE3	1.82	0.43
1:C:214:VAL:HG13	1:C:220:ILE:HD11	1.99	0.43
1:D:163:VAL:HG11	1:F:158:HIS:CD2	2.53	0.43
1:E:81:ALA:O	1:E:85:ILE:HG13	2.18	0.43
1:E:166:GLU:HG2	1:E:167:THR:HG23	2.00	0.43
1:H:157:ASP:O	1:H:159:ALA:N	2.45	0.43
1:L:98:TYR:O	1:L:101:PRO:HD2	2.18	0.43
1:I:114:TYR:CE2	1:I:150:ILE:HB	2.52	0.43
1:J:124:ASP:HA	8:J:732:HOH:O	2.18	0.43
1:C:38:HIS:HE1	1:F:65:GLU:OE2	2.02	0.43
1:J:8:GLN:O	1:J:12:ASN:OD1	2.36	0.43
1:J:185:THR:HG22	1:L:257:ASP:HA	2.00	0.43
1:K:46:SER:HA	1:K:67:VAL:HG11	2.00	0.43
1:G:201:MET:HE1	1:G:256:MET:HA	1.99	0.43
1:I:-1:ASN:HB2	1:I:83:ARG:NE	2.33	0.43
1:J:251:LYS:HA	1:J:252:PRO:HD2	1.95	0.43
1:B:199:GLY:O	1:B:252:PRO:HD2	2.19	0.43
1:E:88:VAL:HG11	1:E:105:LEU:HD23	2.00	0.43
1:E:157:ASP:O	1:E:158:HIS:HB2	2.19	0.43
1:E:193:HIS:O	1:E:195:LYS:HE3	2.19	0.43
1:J:10:TRP:CH2	1:J:44:ALA:HB2	2.53	0.43
1:K:6:LEU:O	1:K:9:VAL:HG13	2.18	0.43
1:D:1:MET:HB3	1:D:79:VAL:CG1	2.48	0.43
1:D:37:LYS:HB3	1:D:37:LYS:HE2	1.79	0.43
1:F:237:ALA:O	1:F:241:ALA:HA	2.19	0.43
1:G:191:ASP:HB3	1:G:211:ASN:ND2	2.34	0.43
1:G:248:GLU:CD	1:G:248:GLU:H	2.21	0.43
1:J:55:ASN:OD1	1:J:56:PRO:HD2	2.18	0.43
1:J:106:LYS:HE2	8:J:697:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:THR:O	1:A:38:HIS:CD2	2.71	0.43
1:A:38:HIS:CD2	1:A:44:ALA:HA	2.54	0.43
1:B:65:GLU:OE2	1:D:38:HIS:HE1	2.02	0.43
1:C:212:ILE:CG2	1:C:229:SER:HA	2.49	0.43
1:D:260:PHE:O	1:D:260:PHE:HD1	2.01	0.43
1:E:260:PHE:HZ	1:F:225:VAL:HG11	1.83	0.43
1:I:59:PRO:HB2	8:I:426:HOH:O	2.18	0.43
1:K:128:LEU:HD12	1:K:128:LEU:O	2.18	0.43
1:K:196:ILE:CD1	1:K:202:ILE:HD11	2.47	0.43
1:F:52:LYS:HE2	1:F:109:HIS:ND1	2.34	0.43
3:J:276:ACY:OXT	8:J:286:HOH:O	2.21	0.43
1:C:130:ILE:HD13	1:C:130:ILE:HA	1.84	0.43
1:K:27:LEU:O	1:K:30:PHE:HB3	2.19	0.43
1:K:83:ARG:HE	1:K:83:ARG:HB3	1.62	0.43
1:L:153:GLY:O	1:L:173:ASP:HA	2.18	0.43
1:A:39:GLU:OE2	1:A:39:GLU:HA	2.18	0.43
1:C:77:MET:HE1	1:C:115:ARG:C	2.39	0.43
1:D:199:GLY:O	1:D:253:SER:HB3	2.18	0.43
1:I:91:ARG:HD3	1:I:253:SER:O	2.18	0.43
1:J:165:GLY:HA3	1:J:193:HIS:CD2	2.54	0.43
1:D:44:ALA:O	1:D:48:ILE:HG13	2.19	0.42
1:J:20:LEU:HB3	1:J:31:PHE:CE2	2.54	0.42
1:J:231:PRO:HD2	1:J:234:THR:HG21	2.01	0.42
1:K:27:LEU:HB2	1:K:31:PHE:CE2	2.55	0.42
1:E:208:ILE:HG23	1:E:226:VAL:HB	2.01	0.42
1:F:20:LEU:HB3	1:F:31:PHE:CE2	2.54	0.42
1:H:76:HIS:ND1	1:H:79:VAL:HB	2.34	0.42
1:J:108:PHE:O	1:J:112:GLN:HG2	2.19	0.42
1:J:248:GLU:HG3	8:J:304:HOH:O	2.19	0.42
1:A:92:ASP:HA	1:A:93:PRO:HD2	1.85	0.42
1:B:164:ILE:HG12	1:B:182:LEU:HD12	2.01	0.42
1:B:165:GLY:HA3	1:B:193:HIS:NE2	2.34	0.42
1:E:24:GLU:OE1	1:E:26:MET:HB2	2.19	0.42
1:G:239:VAL:HA	1:G:240:PRO:HA	1.80	0.42
1:J:132:LEU:O	1:J:136:VAL:HG23	2.19	0.42
1:A:121:TRP:CZ2	1:A:126:LYS:HE3	2.54	0.42
1:B:97:LYS:HB2	1:B:100:THR:HG22	2.01	0.42
1:D:106:LYS:HG2	8:E:292:HOH:O	2.19	0.42
1:D:177:LEU:CD1	8:D:611:HOH:O	2.63	0.42
1:E:1:MET:HG2	1:E:79:VAL:HG13	2.01	0.42
1:H:246:LYS:HD3	1:H:247:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:174:VAL:HG13	1:K:200:VAL:O	2.18	0.42
1:A:44:ALA:O	1:A:48:ILE:HG12	2.18	0.42
1:C:87:ALA:HB1	1:C:91:ARG:CZ	2.50	0.42
1:C:91:ARG:HB2	1:C:155:MET:HE3	1.99	0.42
1:D:1:MET:HB3	1:D:79:VAL:HG13	2.01	0.42
1:E:115:ARG:HD2	8:E:593:HOH:O	2.20	0.42
1:G:1:MET:HB2	1:G:83[B]:ARG:NH2	2.35	0.42
1:J:1:MET:HB3	1:J:79:VAL:CG1	2.49	0.42
1:K:1:MET:CE	1:K:6:LEU:HD13	2.50	0.42
1:B:88:VAL:CA	1:B:155:MET:HE2	2.46	0.42
1:E:111:LEU:HD21	1:E:154:ILE:HB	2.00	0.42
1:I:80:SER:OG	1:I:115:ARG:NE	2.53	0.42
1:L:157:ASP:OD2	4:L:501:CYS:N	2.53	0.42
1:D:225:VAL:HG23	1:D:239:VAL:HG22	2.01	0.42
1:J:114:TYR:CE2	1:J:150:ILE:HB	2.54	0.42
1:A:84:ASP:O	1:A:88:VAL:HG23	2.19	0.42
1:C:134:ASN:O	1:C:138:VAL:HG23	2.20	0.42
1:D:256:MET:CE	1:D:256:MET:H	2.33	0.42
1:H:80:SER:HB3	1:H:115:ARG:CZ	2.50	0.42
1:I:157:ASP:OD2	4:I:501:CYS:N	2.53	0.42
1:J:38:HIS:HB3	1:J:43:SER:HB2	2.01	0.42
1:L:34:THR:CG2	1:L:48:ILE:CG1	2.98	0.42
1:F:231:PRO:HD2	1:F:243:ILE:CD1	2.50	0.42
1:H:207:LYS:O	1:H:225:VAL:HA	2.20	0.42
1:L:49:LEU:HD23	1:L:49:LEU:HA	1.89	0.42
1:G:201:MET:O	1:G:201:MET:HG3	2.19	0.42
1:E:260:PHE:CZ	1:F:227:LEU:HD21	2.54	0.41
1:G:119:TRP:O	1:G:123:GLN:HG2	2.20	0.41
1:G:249:SER:HB3	1:G:255:ASP:OD2	2.19	0.41
1:K:18:ARG:HG2	1:K:36:LEU:HD21	2.02	0.41
1:L:92:ASP:HA	1:L:93:PRO:HD2	1.90	0.41
1:L:217:GLY:O	1:L:247:PRO:HG2	2.20	0.41
1:I:55:ASN:HB3	8:I:275:HOH:O	2.20	0.41
1:K:153:GLY:O	1:K:173:ASP:HA	2.20	0.41
1:L:175:SER:HB2	1:L:256:MET:HE3	2.02	0.41
1:A:34:THR:HG22	1:A:35:LEU:HG	2.02	0.41
1:D:39:GLU:O	1:D:40:ASN:HB3	2.19	0.41
1:E:1:MET:HB2	1:E:83:ARG:NH1	2.35	0.41
1:G:1:MET:HE2	1:G:6:LEU:HD13	2.02	0.41
1:J:169:VAL:CG2	1:J:195:LYS:HD3	2.49	0.41
1:C:173:ASP:OD1	6:C:274:PG5:H32	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:MET:HE2	1:D:256:MET:HA	2.03	0.41
1:F:54:ALA:HB2	1:F:60:ALA:HB2	2.01	0.41
1:I:167:THR:HG21	1:I:190:GLY:O	2.20	0.41
1:K:95:VAL:O	1:K:95:VAL:HG12	2.19	0.41
1:A:105:LEU:HD23	1:B:134:ASN:OD1	2.20	0.41
1:B:1:MET:HE2	1:B:83:ARG:NH1	2.35	0.41
1:C:88:VAL:HG23	8:C:899:HOH:O	2.21	0.41
1:E:132:LEU:O	1:E:136:VAL:HG23	2.21	0.41
1:H:40:ASN:HD22	1:H:42:GLY:H	1.68	0.41
1:J:20:LEU:HD23	1:J:20:LEU:HA	1.91	0.41
1:J:244:VAL:O	1:J:244:VAL:CG1	2.67	0.41
1:A:53:LEU:HD21	1:A:136:VAL:HG22	2.02	0.41
1:B:18:ARG:NE	1:L:191:ASP:OD2	2.45	0.41
1:B:132:LEU:O	1:B:136:VAL:HG23	2.21	0.41
1:D:256:MET:H	1:D:256:MET:HE3	1.86	0.41
1:E:97:LYS:HG3	8:E:889:HOH:O	2.20	0.41
1:E:195:LYS:HA	1:E:195:LYS:HD3	1.81	0.41
1:F:201:MET:O	1:F:201:MET:HG3	2.20	0.41
1:J:130:ILE:HD13	1:J:130:ILE:HA	1.85	0.41
1:J:185:THR:HG23	1:L:258:GLN:N	2.29	0.41
1:L:167:THR:HG21	1:L:190:GLY:O	2.21	0.41
1:A:38:HIS:HE1	1:E:65:GLU:OE2	2.02	0.41
2:A:274:SO4:O3	1:C:207:LYS:NZ	2.47	0.41
1:D:66:VAL:HG22	1:F:26:MET:HE1	2.02	0.41
1:F:1:MET:HB2	1:F:83:ARG:NH2	2.35	0.41
1:K:74:ASP:O	1:K:77:MET:HE2	2.21	0.41
1:K:260:PHE:CE2	1:L:227:LEU:HD11	2.56	0.41
1:B:120:LEU:HD13	1:B:128:LEU:HG	2.03	0.41
1:D:57:ILE:HD12	1:D:57:ILE:O	2.20	0.41
1:G:247:PRO:HB3	1:G:252:PRO:HG3	2.03	0.41
1:H:1:MET:CE	1:H:6:LEU:HD13	2.50	0.41
1:A:92:ASP:OD1	4:A:276:CYS:N	2.53	0.41
1:A:199:GLY:O	1:A:252:PRO:HD2	2.21	0.41
1:B:18:ARG:NH2	1:L:195:LYS:HE3	2.36	0.41
1:C:89:ARG:HA	1:C:95:VAL:CG2	2.51	0.41
1:C:111:LEU:HD12	1:C:111:LEU:HA	1.87	0.41
1:C:249:SER:HB3	1:C:255:ASP:OD2	2.20	0.41
1:D:175:SER:HB2	1:D:256:MET:HE1	2.02	0.41
1:E:175:SER:CB	1:E:256:MET:CE	2.96	0.41
1:E:200:VAL:HG21	1:E:214:VAL:HG12	2.03	0.41
1:E:200:VAL:CG1	1:E:201:MET:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:251:LYS:HD2	1:G:254:LEU:HD11	2.02	0.41
1:H:159:ALA:O	1:H:162:ILE:HG13	2.21	0.41
1:I:230:VAL:HA	1:I:231:PRO:HD3	1.95	0.41
1:K:20:LEU:HD23	1:K:20:LEU:HA	1.94	0.41
1:D:243:ILE:N	1:D:243:ILE:CD1	2.83	0.41
1:G:34:THR:O	1:G:38:HIS:CD2	2.69	0.41
1:G:44:ALA:O	1:G:48:ILE:HG22	2.21	0.41
1:G:76:HIS:O	1:G:79:VAL:HG23	2.21	0.41
1:G:160:THR:HG21	1:H:161:GLY:HA2	2.03	0.41
1:H:100:THR:H	1:H:101:PRO:HD2	1.85	0.41
1:H:145:HIS:CE1	1:H:147:ALA:HB3	2.56	0.41
1:B:88:VAL:CG2	1:B:101:PRO:CG	2.98	0.40
1:B:88:VAL:HG12	1:B:155:MET:HG3	2.01	0.40
1:D:10:TRP:NE1	1:D:14:LYS:HD2	2.36	0.40
1:E:128:LEU:O	1:E:132:LEU:HD13	2.20	0.40
1:J:187:LYS:HD3	1:L:255:ASP:HA	2.03	0.40
1:J:230:VAL:HG13	1:J:234:THR:CG2	2.52	0.40
1:B:58:MET:HG2	1:B:63:ILE:HG13	2.03	0.40
1:B:243:ILE:H	1:B:243:ILE:HD12	1.86	0.40
1:G:30:PHE:O	1:G:34:THR:HG22	2.22	0.40
1:G:152:CYS:HA	1:G:154:ILE:CD1	2.51	0.40
1:G:237:ALA:HB1	1:G:260:PHE:CE1	2.56	0.40
1:J:209:LEU:CD1	1:L:258:GLN:HB3	2.51	0.40
1:C:88:VAL:HG11	1:C:101:PRO:HG3	2.02	0.40
1:C:196:ILE:CD1	1:C:202:ILE:HD11	2.46	0.40
1:C:209:LEU:O	1:C:212:ILE:CD1	2.69	0.40
1:D:193:HIS:HA	1:D:194:PRO:HD3	1.89	0.40
1:E:133:GLN:HG3	1:E:144:ILE:O	2.21	0.40
1:F:58:MET:HA	1:F:59:PRO:HD3	1.80	0.40
1:F:124:ASP:HA	8:F:501:HOH:O	2.21	0.40
1:J:200:VAL:HA	1:J:218:ALA:O	2.21	0.40
1:L:101:PRO:HA	1:L:105:LEU:HD22	2.03	0.40
1:C:58:MET:HB2	1:C:58:MET:HE3	1.78	0.40
1:D:10:TRP:CE3	1:D:10:TRP:HA	2.57	0.40
1:G:123:GLN:O	1:G:124:ASP:HB3	2.22	0.40
1:G:210:GLY:O	1:G:212:ILE:HG22	2.20	0.40
1:J:231:PRO:O	1:J:234:THR:HG22	2.21	0.40
1:C:38:HIS:HB3	1:C:43:SER:HB2	2.02	0.40
1:C:200:VAL:HB	1:C:218:ALA:O	2.21	0.40
1:G:2:SER:O	1:G:5:GLU:N	2.55	0.40
1:H:157:ASP:C	1:H:159:ALA:H	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:188:THR:HG22	1:I:189:SER:O	2.21	0.40
1:J:1:MET:HB3	1:J:79:VAL:HG13	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:TYR:OH	8:H:729:HOH:O[1_444]	2.19	0.01

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	269/276 (98%)	256 (95%)	13 (5%)	0	100	100
1	B	263/276 (95%)	253 (96%)	9 (3%)	1 (0%)	34	48
1	C	260/276 (94%)	249 (96%)	11 (4%)	0	100	100
1	D	261/276 (95%)	249 (95%)	11 (4%)	1 (0%)	34	48
1	E	262/276 (95%)	253 (97%)	9 (3%)	0	100	100
1	F	259/276 (94%)	246 (95%)	12 (5%)	1 (0%)	34	48
1	G	262/276 (95%)	250 (95%)	11 (4%)	1 (0%)	34	48
1	H	259/276 (94%)	246 (95%)	13 (5%)	0	100	100
1	I	271/276 (98%)	256 (94%)	14 (5%)	1 (0%)	34	48
1	J	259/276 (94%)	246 (95%)	11 (4%)	2 (1%)	19	29
1	K	258/276 (94%)	248 (96%)	10 (4%)	0	100	100
1	L	260/276 (94%)	247 (95%)	13 (5%)	0	100	100
All	All	3143/3312 (95%)	2999 (95%)	137 (4%)	7 (0%)	47	62

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	192	ARG
1	D	2	SER
1	F	198	GLU
1	G	211	ASN
1	J	158	HIS
1	J	124	ASP
1	B	192	ARG

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	212/215 (99%)	201 (95%)	11 (5%)	23	38
1	B	207/215 (96%)	191 (92%)	16 (8%)	13	20
1	C	205/215 (95%)	197 (96%)	8 (4%)	32	50
1	D	206/215 (96%)	195 (95%)	11 (5%)	22	37
1	E	207/215 (96%)	196 (95%)	11 (5%)	22	37
1	F	205/215 (95%)	190 (93%)	15 (7%)	14	22
1	G	207/215 (96%)	197 (95%)	10 (5%)	25	41
1	H	204/215 (95%)	190 (93%)	14 (7%)	15	25
1	I	214/215 (100%)	204 (95%)	10 (5%)	26	42
1	J	205/215 (95%)	188 (92%)	17 (8%)	11	17
1	K	204/215 (95%)	190 (93%)	14 (7%)	15	25
1	L	206/215 (96%)	193 (94%)	13 (6%)	18	28
All	All	2482/2580 (96%)	2332 (94%)	150 (6%)	19	31

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	GLU
1	A	89	ARG
1	A	179	SER
1	A	188	THR

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Mol	Chain	Res	Type
1	A	189	SER
1	A	201	MET
1	A	202	ILE
1	A	250	ASP
1	A	263	SER
1	A	264	ILE
1	A	265	GLN
1	B	18	ARG
1	B	34	THR
1	B	36	LEU
1	B	53	LEU
1	B	68	GLU
1	B	86	LEU
1	B	100	THR
1	B	114	TYR
1	B	123	GLN
1	B	154	ILE
1	B	160	THR
1	B	177	LEU
1	B	201	MET
1	B	216	ARG
1	B	242	ARG
1	B	246	LYS
1	C	36	LEU
1	C	43	SER
1	C	90	LEU
1	C	114	TYR
1	C	191	ASP
1	C	200	VAL
1	C	226	VAL
1	C	240	PRO
1	D	22	GLU
1	D	49	LEU
1	D	85	ILE
1	D	90	LEU
1	D	103	LEU
1	D	105	LEU
1	D	111	LEU
1	D	132	LEU
1	D	188	THR
1	D	240	PRO
1	D	242	ARG

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Mol	Chain	Res	Type
1	E	55	ASN
1	E	73	SER
1	E	105	LEU
1	E	106	LYS
1	E	114	TYR
1	E	144	ILE
1	E	189	SER
1	E	201	MET
1	E	242	ARG
1	E	243	ILE
1	E	263	SER
1	F	3	SER
1	F	4	GLU
1	F	23	CYS
1	F	34	THR
1	F	89	ARG
1	F	105	LEU
1	F	114	TYR
1	F	120	LEU
1	F	191	ASP
1	F	201	MET
1	F	207	LYS
1	F	227	LEU
1	F	228	GLN
1	F	243	ILE
1	F	261	ASN
1	G	7	GLU
1	G	20	LEU
1	G	23	CYS
1	G	52	LYS
1	G	65	GLU
1	G	88	VAL
1	G	177	LEU
1	G	187	LYS
1	G	201	MET
1	G	261	ASN
1	H	23	CYS
1	H	53	LEU
1	H	73	SER
1	H	105	LEU
1	H	114	TYR
1	H	115	ARG

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Mol	Chain	Res	Type
1	H	120	LEU
1	H	188	THR
1	H	214	VAL
1	H	216	ARG
1	H	240	PRO
1	H	246	LYS
1	H	248	GLU
1	H	254	LEU
1	I	-1	ASN
1	I	3	SER
1	I	37	LYS
1	I	39	GLU
1	I	61	ILE
1	I	80	SER
1	I	114	TYR
1	I	132	LEU
1	I	216	ARG
1	I	234	THR
1	J	22	GLU
1	J	39	GLU
1	J	49	LEU
1	J	89	ARG
1	J	95	VAL
1	J	106	LYS
1	J	114	TYR
1	J	120	LEU
1	J	123	GLN
1	J	160	THR
1	J	177	LEU
1	J	185	THR
1	J	189	SER
1	J	201	MET
1	J	234	THR
1	J	251	LYS
1	J	259	HIS
1	K	2	SER
1	K	9	VAL
1	K	11	SER
1	K	53	LEU
1	K	100	THR
1	K	144	ILE
1	K	172	ASN

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Mol	Chain	Res	Type
1	K	177	LEU
1	K	189	SER
1	K	191	ASP
1	K	195	LYS
1	K	196	ILE
1	K	207	LYS
1	K	250	ASP
1	L	1	MET
1	L	39	GLU
1	L	40	ASN
1	L	58	MET
1	L	105	LEU
1	L	114	TYR
1	L	116	ILE
1	L	135	GLN
1	L	179	SER
1	L	182	LEU
1	L	188	THR
1	L	213	GLU
1	L	219	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	38	HIS
1	A	76	HIS
1	A	118	HIS
1	A	258	GLN
1	B	38	HIS
1	B	172	ASN
1	C	38	HIS
1	C	76	HIS
1	C	123	GLN
1	C	259	HIS
1	D	32	HIS
1	D	38	HIS
1	D	51	ASN
1	D	109	HIS
1	D	118	HIS
1	E	8	GLN
1	E	38	HIS

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Mol	Chain	Res	Type
1	E	51	ASN
1	E	55	ASN
1	E	118	HIS
1	E	258	GLN
1	F	38	HIS
1	F	51	ASN
1	F	172	ASN
1	F	259	HIS
1	F	261	ASN
1	G	32	HIS
1	G	38	HIS
1	G	51	ASN
1	G	55	ASN
1	G	109	HIS
1	G	112	GLN
1	G	258	GLN
1	H	38	HIS
1	H	40	ASN
1	H	55	ASN
1	H	259	HIS
1	I	-1	ASN
1	I	8	GLN
1	I	38	HIS
1	I	55	ASN
1	I	261	ASN
1	J	32	HIS
1	J	112	GLN
1	J	118	HIS
1	J	123	GLN
1	J	259	HIS
1	K	38	HIS
1	K	172	ASN
1	K	258	GLN
1	L	12	ASN
1	L	40	ASN
1	L	51	ASN
1	L	193	HIS
1	L	228	GLN
1	L	258	GLN

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)

28 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	L	274	-	4,4,4	0.17	0	6,6,6	0.29	0
5	GOL	B	274	-	5,5,5	0.31	0	5,5,5	0.48	0
2	SO4	H	274	-	4,4,4	0.15	0	6,6,6	0.28	0
4	CYS	D	501	-	5,6,6	0.94	0	5,7,7	1.83	2 (40%)
4	CYS	A	501	-	5,6,6	1.31	1 (20%)	5,7,7	1.41	2 (40%)
4	CYS	L	276	-	5,6,6	1.09	1 (20%)	5,7,7	1.78	2 (40%)
3	ACY	A	275	-	3,3,3	0.63	0	3,3,3	1.41	0
4	CYS	J	501	-	5,6,6	1.11	1 (20%)	5,7,7	1.77	2 (40%)
6	PG5	C	274	-	11,11,11	0.47	0	10,10,10	1.48	1 (10%)
5	GOL	H	275	-	5,5,5	0.41	0	5,5,5	0.14	0
4	CYS	A	276	-	5,6,6	1.01	0	5,7,7	1.58	2 (40%)
4	CYS	L	501	-	5,6,6	1.04	0	5,7,7	1.45	1 (20%)
2	SO4	F	274	-	4,4,4	0.18	0	6,6,6	0.22	0
3	ACY	J	276	-	3,3,3	0.77	0	3,3,3	0.82	0
5	GOL	F	275	-	5,5,5	0.37	0	5,5,5	0.24	0
2	SO4	K	274	-	4,4,4	0.13	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ACY	J	275	-	3,3,3	0.70	0	3,3,3	1.15	0
5	GOL	J	274	-	5,5,5	0.40	0	5,5,5	0.35	0
7	PEG	L	275	-	6,6,6	0.50	0	5,5,5	1.54	0
4	CYS	G	501	-	5,6,6	1.07	1 (20%)	5,7,7	1.80	1 (20%)
4	CYS	H	501	-	5,6,6	0.99	1 (20%)	5,7,7	1.74	2 (40%)
5	GOL	E	274	-	5,5,5	0.43	0	5,5,5	0.44	0
4	CYS	D	274	-	5,6,6	1.14	0	5,7,7	1.53	2 (40%)
2	SO4	A	274	-	4,4,4	0.17	0	6,6,6	0.46	0
4	CYS	E	501	-	5,6,6	0.93	0	5,7,7	1.31	1 (20%)
3	ACY	C	275	-	3,3,3	0.89	0	3,3,3	0.58	0
4	CYS	B	501	-	5,6,6	1.08	1 (20%)	5,7,7	1.23	0
4	CYS	I	501	-	5,6,6	1.16	1 (20%)	5,7,7	1.93	2 (40%)

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	GOL	B	274	-	-	2/4/4/4	-
4	CYS	D	501	-	-	0/6/6/6	-
4	CYS	A	501	-	-	0/6/6/6	-
4	CYS	L	276	-	-	0/6/6/6	-
4	CYS	J	501	-	-	1/6/6/6	-
6	PG5	C	274	-	-	5/9/9/9	-
5	GOL	H	275	-	-	4/4/4/4	-
4	CYS	A	276	-	-	0/6/6/6	-
4	CYS	L	501	-	-	0/6/6/6	-
5	GOL	F	275	-	-	4/4/4/4	-
5	GOL	J	274	-	-	4/4/4/4	-
7	PEG	L	275	-	-	2/4/4/4	-
4	CYS	G	501	-	-	0/6/6/6	-
4	CYS	H	501	-	-	0/6/6/6	-
5	GOL	E	274	-	-	0/4/4/4	-
4	CYS	D	274	-	-	0/6/6/6	-
4	CYS	E	501	-	-	0/6/6/6	-
4	CYS	B	501	-	-	0/6/6/6	-
4	CYS	I	501	-	-	0/6/6/6	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	501	CYS	OXT-C	-2.34	1.22	1.30
4	A	501	CYS	OXT-C	-2.26	1.23	1.30
4	I	501	CYS	OXT-C	-2.22	1.23	1.30
4	B	501	CYS	OXT-C	-2.14	1.23	1.30
4	G	501	CYS	OXT-C	-2.09	1.23	1.30
4	L	276	CYS	OXT-C	-2.08	1.23	1.30
4	H	501	CYS	OXT-C	-2.05	1.23	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	501	CYS	OXT-C-O	-3.46	116.22	124.09
4	J	501	CYS	OXT-C-O	-3.22	116.79	124.09
4	G	501	CYS	CB-CA-C	-2.90	107.00	109.89
4	H	501	CYS	OXT-C-O	-2.79	117.75	124.09
4	D	501	CYS	OXT-C-O	-2.74	117.87	124.09
4	L	276	CYS	OXT-C-O	-2.73	117.89	124.09
4	D	501	CYS	OXT-C-CA	2.63	122.33	113.38
4	A	276	CYS	OXT-C-O	-2.57	118.25	124.09
4	L	276	CYS	OXT-C-CA	2.53	122.00	113.38
4	H	501	CYS	OXT-C-CA	2.47	121.80	113.38
4	I	501	CYS	OXT-C-CA	2.46	121.76	113.38
4	A	276	CYS	OXT-C-CA	2.37	121.46	113.38
4	L	501	CYS	OXT-C-O	-2.34	118.78	124.09
4	D	274	CYS	OXT-C-CA	2.32	121.29	113.38
4	A	501	CYS	OXT-C-O	-2.30	118.87	124.09
4	J	501	CYS	OXT-C-CA	2.29	121.19	113.38
6	C	274	PG5	O2-C3-C2	2.20	120.34	110.39
4	E	501	CYS	OXT-C-O	-2.04	119.46	124.09
4	D	274	CYS	OXT-C-O	-2.04	119.47	124.09
4	A	501	CYS	OXT-C-CA	2.03	120.29	113.38

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	274	GOL	O1-C1-C2-C3
5	F	275	GOL	O1-C1-C2-C3
5	H	275	GOL	O1-C1-C2-C3
5	J	274	GOL	O1-C1-C2-C3
6	C	274	PG5	O1-C2-C3-O2
6	C	274	PG5	O3-C6-C7-O4

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Mol	Chain	Res	Type	Atoms
5	H	275	GOL	C1-C2-C3-O3
5	B	274	GOL	O1-C1-C2-O2
5	H	275	GOL	O1-C1-C2-O2
5	J	274	GOL	O1-C1-C2-O2
7	L	275	PEG	O2-C3-C4-O4
5	H	275	GOL	O2-C2-C3-O3
7	L	275	PEG	C1-C2-O2-C3
5	F	275	GOL	O1-C1-C2-O2
6	C	274	PG5	C5-C4-O2-C3
5	F	275	GOL	C1-C2-C3-O3
5	J	274	GOL	C1-C2-C3-O3
6	C	274	PG5	C3-C2-O1-C1
5	F	275	GOL	O2-C2-C3-O3
5	J	274	GOL	O2-C2-C3-O3
6	C	274	PG5	C6-C7-O4-C8
4	J	501	CYS	O-C-CA-N

There are no ring outliers.

13 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	274	SO4	1	0
5	B	274	GOL	2	0
4	L	276	CYS	1	0
3	A	275	ACY	2	0
6	C	274	PG5	9	0
5	H	275	GOL	1	0
4	A	276	CYS	1	0
4	L	501	CYS	1	0
3	J	276	ACY	1	0
7	L	275	PEG	3	0
5	E	274	GOL	2	0
2	A	274	SO4	1	0
4	I	501	CYS	1	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	271/276 (98%)	-0.30	1 (0%) 92 91	29, 41, 65, 89	0
1	B	265/276 (96%)	-0.39	0 100 100	29, 40, 55, 84	0
1	C	262/276 (94%)	-0.34	3 (1%) 80 79	26, 39, 59, 97	0
1	D	262/276 (94%)	-0.23	6 (2%) 60 58	33, 43, 68, 104	0
1	E	263/276 (95%)	-0.14	2 (0%) 86 84	31, 43, 68, 102	0
1	F	261/276 (94%)	-0.24	1 (0%) 92 91	31, 42, 71, 97	0
1	G	263/276 (95%)	-0.24	2 (0%) 86 84	33, 47, 67, 93	0
1	H	261/276 (94%)	-0.16	3 (1%) 80 79	33, 48, 72, 120	0
1	I	272/276 (98%)	-0.27	0 100 100	31, 43, 59, 83	0
1	J	261/276 (94%)	-0.20	3 (1%) 80 79	32, 45, 68, 88	0
1	K	260/276 (94%)	-0.03	3 (1%) 79 77	36, 49, 72, 97	0
1	L	261/276 (94%)	-0.17	3 (1%) 80 79	32, 47, 72, 90	0
All	All	3162/3312 (95%)	-0.23	27 (0%) 84 82	26, 44, 68, 120	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	9	VAL	3.2
1	D	261	ASN	3.1
1	E	1	MET	3.0
1	H	0	ALA	3.0
1	D	4	GLU	2.9
1	A	6	LEU	2.8
1	K	139	ALA	2.7
1	D	139	ALA	2.5
1	K	228	GLN	2.5
1	D	1	MET	2.4
1	D	262	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	212	ILE	2.4
1	C	160	THR	2.3
1	J	261	ASN	2.3
1	F	3	SER	2.2
1	L	248	GLU	2.2
1	G	136	VAL	2.1
1	K	4	GLU	2.1
1	E	86	LEU	2.1
1	L	41	LEU	2.1
1	G	138	VAL	2.1
1	C	261	ASN	2.1
1	H	259	HIS	2.0
1	H	4	GLU	2.0
1	D	259	HIS	2.0
1	J	3	SER	2.0
1	L	6	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
6	PG5	C	274	12/12	0.71	0.25	63,65,68,68	0
5	GOL	J	274	6/6	0.74	0.13	66,66,66,66	0
3	ACY	C	275	4/4	0.75	0.21	47,50,50,50	0
7	PEG	L	275	7/7	0.83	0.21	40,42,43,43	0
2	SO4	K	274	5/5	0.84	0.40	200,200,200,200	0
3	ACY	J	276	4/4	0.87	0.15	55,55,56,57	0
5	GOL	B	274	6/6	0.90	0.20	43,44,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACY	J	275	4/4	0.92	0.16	51,51,52,53	0
4	CYS	E	501	7/7	0.92	0.14	32,34,35,37	0
4	CYS	L	501	7/7	0.93	0.12	39,40,41,43	0
5	GOL	F	275	6/6	0.93	0.13	55,55,56,57	0
5	GOL	H	275	6/6	0.93	0.17	54,55,55,55	0
4	CYS	J	501	7/7	0.94	0.16	35,36,39,47	0
4	CYS	L	276	7/7	0.94	0.11	40,42,43,45	0
2	SO4	L	274	5/5	0.95	0.18	53,55,55,56	0
4	CYS	A	276	7/7	0.95	0.14	35,35,37,38	0
5	GOL	E	274	6/6	0.95	0.12	49,49,49,49	0
4	CYS	D	274	7/7	0.95	0.12	27,30,31,32	0
3	ACY	A	275	4/4	0.96	0.17	43,45,45,45	0
4	CYS	B	501	7/7	0.97	0.14	37,39,39,39	0
4	CYS	D	501	7/7	0.97	0.11	37,38,39,40	0
4	CYS	A	501	7/7	0.97	0.08	28,29,31,43	0
2	SO4	A	274	5/5	0.97	0.22	50,52,53,53	0
4	CYS	H	501	7/7	0.97	0.10	42,48,50,50	0
4	CYS	G	501	7/7	0.98	0.09	35,37,38,39	0
2	SO4	F	274	5/5	0.98	0.16	47,48,49,50	0
2	SO4	H	274	5/5	0.99	0.14	49,50,51,52	0
4	CYS	I	501	7/7	0.99	0.08	31,33,34,39	0

6.5 Other polymers (i)

There are no such residues in this entry.