



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2016 – 04:09 PM EDT

PDB ID : 5SV1  
Title : Structure of the ExbB/ExbD complex from E. coli at pH 4.5  
Authors : Celia, H.; Botos, I.; Lloubes, R.; Buchanan, S.K.; Noinaj, N.  
Deposited on : 2016-08-04  
Resolution : 3.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

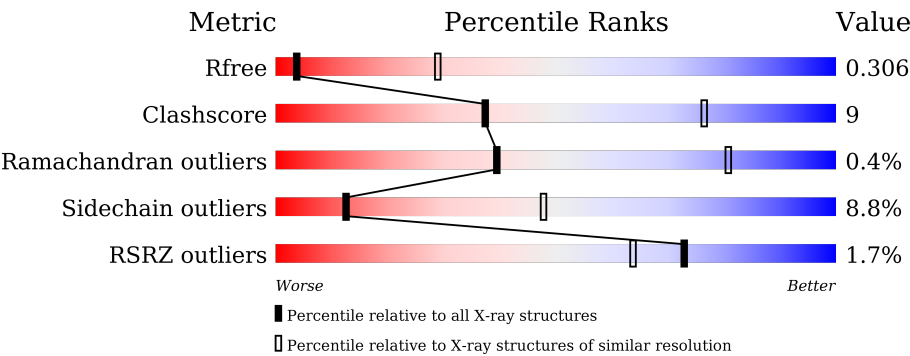
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	244	<div><div>2%</div><div><div>69%</div><div>20%</div><div>•</div><div>8%</div></div></div>
1	B	244	<div><div>68%</div><div>22%</div><div>•</div><div>8%</div></div>
1	C	244	<div><div>72%</div><div>18%</div><div>•</div><div>8%</div></div>
1	D	244	<div><div>2%</div><div><div>66%</div><div>19%</div><div>•</div><div>12%</div></div></div>
1	E	244	<div><div>%</div><div><div>73%</div><div>15%</div><div>•</div><div>9%</div></div></div>
1	F	244	<div><div>%</div><div><div>71%</div><div>18%</div><div>•</div><div>7%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	244	<div><div></div><div>67%</div><div>22%</div><div>•</div><div>8%</div></div>
1	H	244	<div><div></div><div>68%</div><div>21%</div><div>•</div><div>9%</div></div>
1	I	244	<div><div>4%</div><div></div><div>65%</div><div>21%</div><div>•</div><div>11%</div></div>
1	J	244	<div><div>%</div><div></div><div>67%</div><div>18%</div><div>5%</div><div>10%</div></div>
2	Y	58	<div><div>3%</div><div></div><div>22%</div><div>14%</div><div>•</div><div>60%</div></div>
2	Z	58	<div><div>9%</div><div></div><div>10%</div><div>21%</div><div>7%</div><div>62%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16946 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 Biopolymer transport protein ExbB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1678	1071	294	307	6			
1	B	225	Total	C	N	O	S	0	0	0
			1692	1080	295	311	6			
1	C	224	Total	C	N	O	S	0	0	0
			1665	1064	288	307	6			
1	D	215	Total	C	N	O	S	0	0	0
			1599	1018	278	298	5			
1	E	223	Total	C	N	O	S	0	0	0
			1653	1050	290	308	5			
1	F	226	Total	C	N	O	S	0	0	0
			1694	1079	297	312	6			
1	G	225	Total	C	N	O	S	0	0	0
			1694	1081	298	309	6			
1	H	222	Total	C	N	O	S	0	0	0
			1668	1062	291	309	6			
1	I	216	Total	C	N	O	S	0	0	0
			1626	1034	286	301	5			
1	J	219	Total	C	N	O	S	0	0	0
			1630	1039	286	300	5			

- Molecule 2 is a protein called Biopolymer transport protein ExbD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	23	Total	C	N	O	S	0	0	0
			171	120	23	26	2			
2	Z	22	Total	C	N	O	S	0	0	0
			166	117	22	25	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	31	GLY	-	expression tag	UNP P0ABV4

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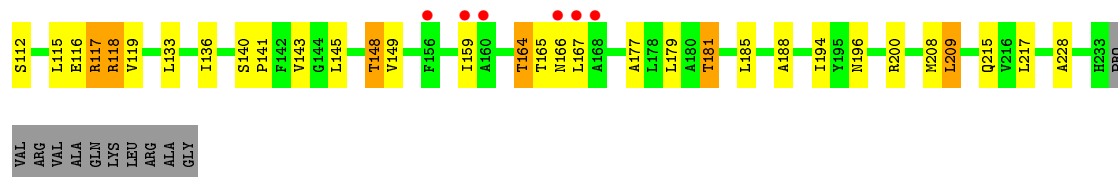
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Chain	Residue	Modelled	Actual	Comment	Reference
Y	32	GLY	-	expression tag	UNP P0ABV4
Y	33	GLY	-	expression tag	UNP P0ABV4
Y	34	GLU	-	expression tag	UNP P0ABV4
Y	35	ASN	-	expression tag	UNP P0ABV4
Y	36	LEU	-	expression tag	UNP P0ABV4
Y	37	TYR	-	expression tag	UNP P0ABV4
Y	38	PHE	-	expression tag	UNP P0ABV4
Y	39	GLN	-	expression tag	UNP P0ABV4
Z	31	GLY	-	expression tag	UNP P0ABV4
Z	32	GLY	-	expression tag	UNP P0ABV4
Z	33	GLY	-	expression tag	UNP P0ABV4
Z	34	GLU	-	expression tag	UNP P0ABV4
Z	35	ASN	-	expression tag	UNP P0ABV4
Z	36	LEU	-	expression tag	UNP P0ABV4
Z	37	TYR	-	expression tag	UNP P0ABV4
Z	38	PHE	-	expression tag	UNP P0ABV4
Z	39	GLN	-	expression tag	UNP P0ABV4

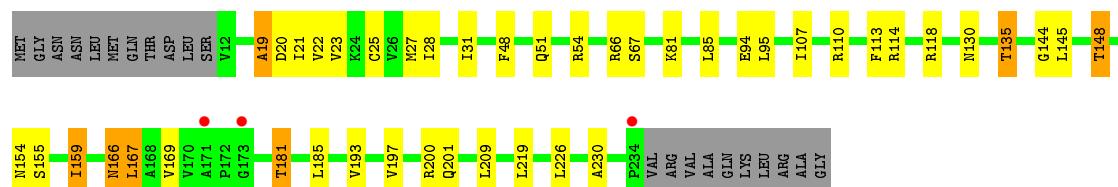
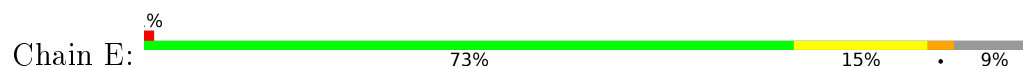
- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Hg 1 1	0	0
3	J	1	Total Hg 1 1	0	0
3	D	1	Total Hg 1 1	0	0
3	E	1	Total Hg 1 1	0	0
3	H	1	Total Hg 1 1	0	0
3	B	1	Total Hg 1 1	0	0
3	I	1	Total Hg 1 1	0	0
3	C	1	Total Hg 1 1	0	0
3	A	1	Total Hg 1 1	0	0
3	F	1	Total Hg 1 1	0	0

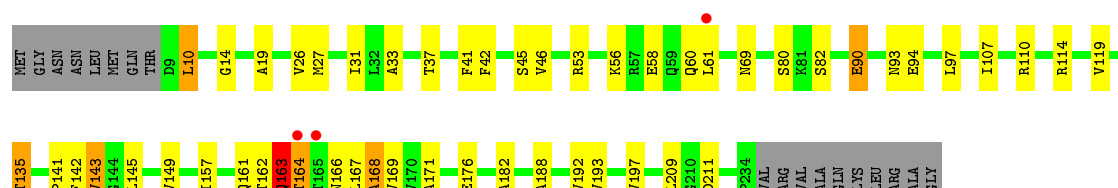




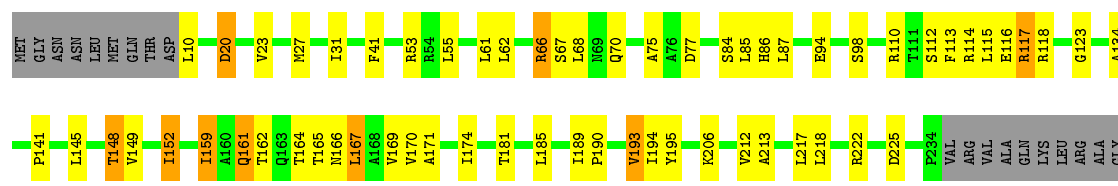
• Molecule 1: Biopolymer transport protein ExbB



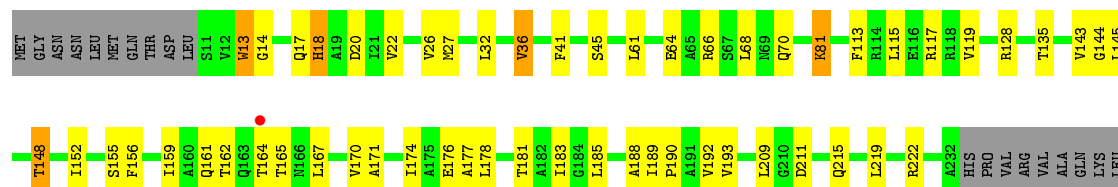
• Molecule 1: Biopolymer transport protein ExbB



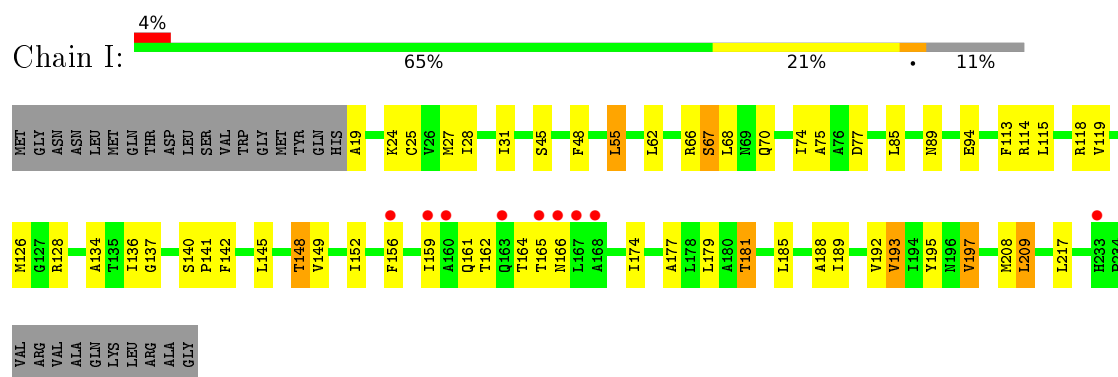
• Molecule 1: Biopolymer transport protein ExbB



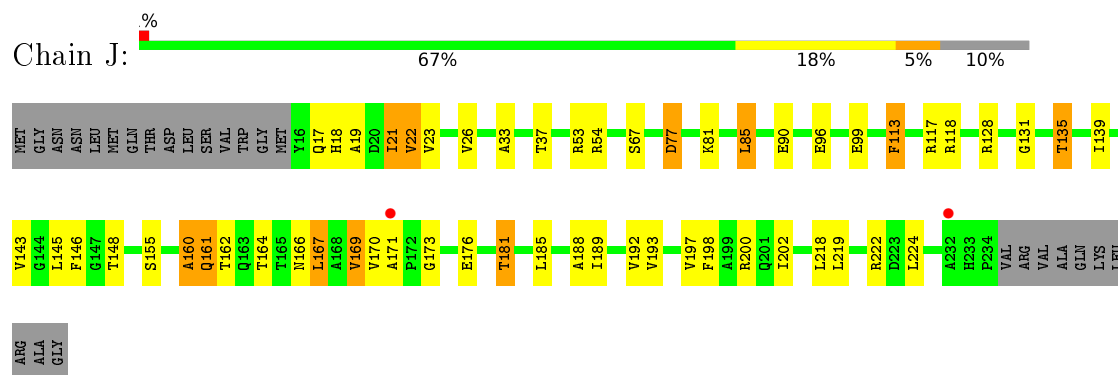
• Molecule 1: Biopolymer transport protein ExbB



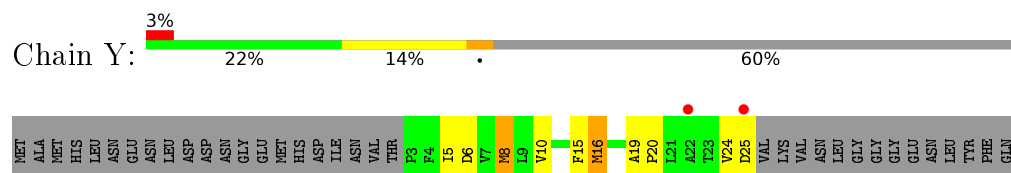
• Molecule 1: Biopolymer transport protein ExbB



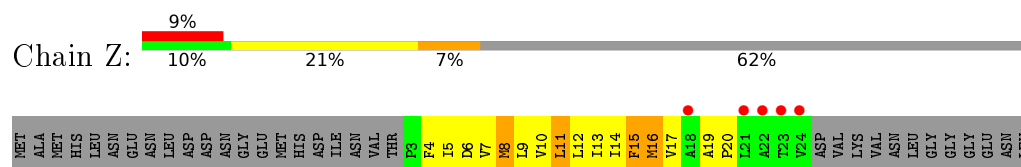
• Molecule 1: Biopolymer transport protein ExbB



• Molecule 2: Biopolymer transport protein ExbD



• Molecule 2: Biopolymer transport protein ExbD





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.94Å 196.75Å 210.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 3.50 49.29 – 3.47	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.00-3.50) 93.3 (49.29-3.47)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.24	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10 _2142: ???)	Depositor
R, $R_{free}$	0.255 , 0.300 0.252 , 0.306	Depositor DCC
$R_{free}$ test set	1877 reflections (3.56%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.7	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 20.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	16946	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.83 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4420e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.38	0/1693	0.56	0/2294
1	B	0.39	0/1707	0.59	0/2315
1	C	0.39	0/1678	0.55	0/2275
1	D	0.42	0/1609	0.58	0/2182
1	E	0.35	0/1663	0.54	0/2254
1	F	0.38	0/1709	0.54	0/2316
1	G	0.39	0/1709	0.62	1/2317 (0.0%)
1	H	0.40	0/1680	0.56	0/2275
1	I	0.44	0/1636	0.60	0/2214
1	J	0.39	0/1640	0.60	0/2221
2	Y	0.32	0/174	0.62	0/238
2	Z	0.35	0/169	0.58	0/231
All	All	0.39	0/17067	0.58	1/23132 (0.0%)

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	E	0	2
1	G	0	3
1	H	0	1
1	J	0	1
All	All	0	8

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	161	GLN	N-CA-C	-8.09	89.17	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	VAL	Peptide
1	E	166	ASN	Peptide
1	E	19	ALA	Peptide
1	G	161	GLN	Peptide
1	G	162	THR	Peptide
1	G	66	ARG	Peptide
1	H	128	ARG	Peptide
1	J	160	ALA	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1678	0	1690	40	0
1	B	1692	0	1713	35	0
1	C	1665	0	1675	29	0
1	D	1599	0	1616	33	0
1	E	1653	0	1667	25	0
1	F	1694	0	1696	36	0
1	G	1694	0	1720	40	0
1	H	1668	0	1696	36	0
1	I	1626	0	1662	41	0
1	J	1630	0	1658	34	0
2	Y	171	0	191	6	0
2	Z	166	0	189	10	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
All	All	16946	0	17173	317	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 9.

All (317) 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:F:19:ALA:HB2	1:F:176:GLU:HG2	1.37	1.05
1:F:10:LEU:HG	1:F:14:GLY:HA3	1.52	0.91
1:A:21:ILE:HD11	1:I:45:SER:HB2	1.61	0.83
1:A:19:ALA:HB2	1:A:176:GLU:HG2	1.61	0.83
1:B:10:LEU:HD23	1:B:14:GLY:HA3	1.64	0.79
1:H:148:THR:HA	1:H:177:ALA:HA	1.65	0.77
1:F:141:PRO:HD3	1:F:188:ALA:HB2	1.70	0.74
1:J:21:ILE:HG23	1:J:22:VAL:H	1.53	0.73
1:F:211:ASP:OD1	1:J:117:ARG:NH1	2.23	0.72
1:G:67:SER:HB3	1:G:70:GLN:HB2	1.72	0.71
1:I:136:ILE:O	1:I:140:SER:HB2	1.91	0.70
1:D:145:LEU:HD12	1:E:185:LEU:HD11	1.73	0.70
1:A:117:ARG:NH1	1:B:211:ASP:OD1	2.25	0.70
1:A:148:THR:HA	1:A:177:ALA:HB1	1.74	0.69
1:E:20:ASP:HB3	1:E:23:VAL:HG12	1.73	0.69
1:F:27:MET:O	1:F:31:ILE:HG13	1.92	0.69
1:C:119:VAL:HG22	1:C:209:LEU:HD22	1.75	0.69
1:H:119:VAL:HG22	1:H:209:LEU:HD22	1.75	0.69
1:D:119:VAL:HG22	1:D:209:LEU:HD13	1.75	0.68
1:G:152:ILE:HG23	1:G:174:ILE:HG13	1.75	0.68
1:H:159:ILE:HA	1:H:162:THR:HG22	1.76	0.68
1:F:119:VAL:HG22	1:F:209:LEU:HD22	1.77	0.67
1:I:145:LEU:HD12	1:J:185:LEU:HD11	1.78	0.65
1:F:142:PHE:HE2	1:G:141:PRO:HG3	1.61	0.65
1:F:110:ARG:NH2	1:G:225:ASP:OD2	2.30	0.65
1:A:77:ASP:HA	1:A:78:PHE:HB2	1.79	0.64
1:E:20:ASP:OD1	1:E:21:ILE:N	2.30	0.64
1:J:160:ALA:HB3	1:J:161:GLN:HB2	1.78	0.64
1:D:141:PRO:HB3	1:D:185:LEU:HD23	1.79	0.64
1:I:119:VAL:HG22	1:I:209:LEU:HD13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:141:PRO:HB3	1:I:185:LEU:HD23	1.80	0.64
1:A:119:VAL:HG22	1:A:209:LEU:HD22	1.78	0.64
1:C:41:PHE:O	1:C:45:SER:HB3	1.97	0.64
1:B:119:VAL:HG22	1:B:209:LEU:HD22	1.79	0.63
1:G:20:ASP:N	1:G:20:ASP:OD1	2.26	0.63
1:H:178:LEU:HD11	2:Z:15:PHE:CZ	2.33	0.63
1:F:41:PHE:O	1:F:45:SER:HB2	1.99	0.62
1:I:140:SER:HB3	1:I:188:ALA:HB2	1.81	0.62
1:B:67:SER:HB3	1:B:70:GLN:HB2	1.82	0.62
1:G:94:GLU:OE2	1:H:222:ARG:NH1	2.33	0.62
1:F:90:GLU:O	1:F:114:ARG:NH2	2.33	0.61
1:F:26:VAL:HG13	1:F:143:VAL:HG13	1.80	0.61
1:A:193:VAL:HG13	1:E:135:THR:HG21	1.82	0.61
1:G:159:ILE:HD11	1:H:171:ALA:HB2	1.82	0.60
1:F:145:LEU:HD23	1:G:185:LEU:HD11	1.83	0.60
1:H:41:PHE:O	1:H:45:SER:HB3	2.00	0.60
1:F:41:PHE:O	1:F:45:SER:CB	2.49	0.60
1:G:117:ARG:NH1	1:H:211:ASP:OD1	2.35	0.60
1:A:77:ASP:HB2	1:A:79:GLY:H	1.67	0.60
1:F:193:VAL:O	1:F:197:VAL:HG23	2.01	0.60
1:B:10:LEU:HG	1:B:11:SER:H	1.66	0.59
1:I:27:MET:O	1:I:31:ILE:HG13	2.01	0.59
1:D:75:ALA:O	1:D:85:LEU:HD13	2.03	0.59
1:G:27:MET:O	1:G:31:ILE:HG13	2.03	0.59
1:C:158:GLY:O	1:C:162:THR:OG1	2.21	0.59
1:A:222:ARG:NH1	1:E:94:GLU:OE2	2.36	0.58
1:I:148:THR:HB	1:I:177:ALA:O	2.02	0.58
1:B:27:MET:O	1:B:31:ILE:HG13	2.02	0.58
1:D:104:ASN:ND2	1:D:228:ALA:HB2	2.18	0.58
1:G:110:ARG:O	1:G:114:ARG:HG3	2.02	0.58
1:G:167:LEU:O	1:G:171:ALA:N	2.33	0.58
1:H:155:SER:HB3	1:H:170:VAL:HG13	1.85	0.58
1:A:20:ASP:OD2	1:A:21:ILE:N	2.36	0.57
1:D:62:LEU:O	1:D:215:GLN:NE2	2.34	0.57
1:G:159:ILE:HD13	1:H:167:LEU:HB3	1.85	0.57
1:I:94:GLU:OE2	1:J:222:ARG:NH1	2.37	0.57
1:F:163:GLN:NE2	1:F:164:THR:O	2.38	0.56
1:C:20:ASP:OD1	1:C:21:ILE:N	2.34	0.56
1:G:98:SER:OG	1:G:110:ARG:NH1	2.39	0.56
2:Z:19:ALA:HB3	2:Z:20:PRO:HD3	1.87	0.56
1:B:145:LEU:HD12	1:C:185:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:113:PHE:CE1	1:J:117:ARG:HD2	2.40	0.56
1:I:159:ILE:HG23	1:J:167:LEU:HD11	1.87	0.56
1:A:20:ASP:O	1:A:24:LYS:HD3	2.06	0.56
1:C:22:VAL:O	1:C:26:VAL:HG23	2.06	0.56
1:I:75:ALA:O	1:I:85:LEU:HD13	2.06	0.56
1:G:123:GLY:HA3	1:G:206:LYS:HD3	1.89	0.55
1:F:33:ALA:O	1:F:37:THR:HG23	2.06	0.55
1:A:77:ASP:OD1	1:A:77:ASP:N	2.38	0.55
1:H:14:GLY:O	1:H:18:HIS:HB2	2.06	0.55
1:D:148:THR:HB	1:D:177:ALA:O	2.05	0.55
1:B:149:VAL:HG11	1:C:181:THR:HG22	1.88	0.55
1:E:23:VAL:O	1:E:27:MET:HG2	2.07	0.55
1:D:136:ILE:O	1:D:140:SER:HB2	2.08	0.54
1:B:110:ARG:O	1:B:114:ARG:HG3	2.07	0.54
1:C:14:GLY:O	1:C:18:HIS:HB2	2.06	0.54
1:G:166:ASN:O	1:G:169:VAL:HG22	2.08	0.54
1:J:173:GLY:O	1:J:176:GLU:HG2	2.07	0.54
1:A:193:VAL:O	1:A:197:VAL:HG23	2.08	0.54
1:H:66:ARG:N	1:H:70:GLN:OE1	2.40	0.54
1:A:169:VAL:HG13	1:A:170:VAL:H	1.71	0.53
2:Z:16:MET:O	2:Z:20:PRO:HD2	2.09	0.53
1:I:193:VAL:O	1:I:197:VAL:HG23	2.08	0.53
1:F:141:PRO:HD3	1:F:188:ALA:CB	2.38	0.53
1:D:149:VAL:HG21	1:E:181:THR:HG21	1.91	0.53
1:C:144:GLY:O	1:C:148:THR:HG23	2.09	0.52
1:I:165:THR:HG22	1:I:166:ASN:H	1.73	0.52
1:A:41:PHE:O	1:A:45:SER:HB2	2.10	0.52
1:G:62:LEU:HD21	1:G:75:ALA:HB2	1.91	0.52
1:A:41:PHE:O	1:A:45:SER:CB	2.57	0.52
1:F:143:VAL:HG23	1:G:189:ILE:HD13	1.90	0.52
1:B:41:PHE:HB2	1:B:194:ILE:HD13	1.92	0.52
1:J:21:ILE:HG23	1:J:22:VAL:HG12	1.91	0.52
1:D:112:SER:O	1:D:116:GLU:HG2	2.09	0.52
1:D:140:SER:HB3	1:D:188:ALA:HB2	1.91	0.51
1:E:226:LEU:O	1:E:230:ALA:HB2	2.10	0.51
1:B:115:LEU:HD12	1:B:217:LEU:HG	1.91	0.51
1:E:67:SER:O	1:E:219:LEU:HD13	2.11	0.51
1:I:25:CYS:O	1:I:28:ILE:HG13	2.10	0.51
1:G:41:PHE:HB2	1:G:194:ILE:HD13	1.92	0.51
1:H:162:THR:HG23	1:H:164:THR:H	1.75	0.51
1:J:131:GLY:O	1:J:135:THR:OG1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:84:SER:OG	1:G:212:VAL:HG11	2.11	0.51
1:A:189:ILE:O	1:A:193:VAL:HG23	2.10	0.51
1:G:145:LEU:HD12	1:H:185:LEU:HD11	1.91	0.51
1:D:82:SER:O	1:D:86:HIS:ND1	2.41	0.50
1:I:156:PHE:HA	1:I:159:ILE:HG22	1.92	0.50
1:E:19:ALA:O	1:E:20:ASP:HB2	2.11	0.50
1:J:161:GLN:O	1:J:162:THR:OG1	2.28	0.50
1:J:17:GLN:C	1:J:19:ALA:HB3	2.31	0.50
1:B:44:LYS:HB3	1:B:198:PHE:CZ	2.46	0.50
1:A:141:PRO:HD3	1:A:188:ALA:HB2	1.92	0.50
1:C:16:TYR:CE1	1:C:24:LYS:HG3	2.47	0.50
2:Y:5:ILE:O	2:Y:8:MET:N	2.45	0.50
1:I:148:THR:O	1:I:152:ILE:HG13	2.11	0.50
1:A:141:PRO:HD3	1:A:188:ALA:CB	2.42	0.50
1:G:149:VAL:HG11	1:H:181:THR:HG22	1.93	0.50
1:A:42:PHE:O	1:A:46:VAL:HG12	2.12	0.49
1:H:188:ALA:O	1:H:192:VAL:HG23	2.11	0.49
1:E:110:ARG:O	1:E:114:ARG:HG3	2.13	0.49
1:G:86:HIS:HB3	1:G:118:ARG:NH2	2.27	0.49
1:H:170:VAL:HG12	1:H:174:ILE:HG13	1.94	0.49
1:F:42:PHE:O	1:F:46:VAL:HG12	2.13	0.49
1:B:141:PRO:HD3	1:B:188:ALA:HB2	1.94	0.49
1:D:167:LEU:HD21	1:E:167:LEU:HD22	1.94	0.49
1:D:55:LEU:HD13	1:D:208:MET:HB3	1.95	0.49
1:A:135:THR:HG21	1:B:193:VAL:HG13	1.93	0.48
1:G:148:THR:O	1:G:152:ILE:HG13	2.13	0.48
1:J:167:LEU:HG	1:J:171:ALA:HB2	1.94	0.48
1:I:48:PHE:CE1	1:I:126:MET:HE3	2.48	0.48
1:F:149:VAL:HG21	1:G:181:THR:HG21	1.95	0.48
1:A:26:VAL:HG13	1:A:143:VAL:HG13	1.96	0.48
1:A:110:ARG:NH2	1:B:225:ASP:OD2	2.46	0.48
1:I:189:ILE:O	1:I:193:VAL:HG23	2.14	0.48
1:H:189:ILE:HB	1:H:190:PRO:HD3	1.95	0.48
1:I:161:GLN:HG3	1:I:162:THR:H	1.78	0.48
1:C:16:TYR:C	1:C:16:TYR:CD1	2.87	0.47
1:F:188:ALA:O	1:F:192:VAL:HG23	2.14	0.47
1:D:118:ARG:HA	1:D:118:ARG:HD3	1.46	0.47
1:I:115:LEU:HD12	1:I:217:LEU:HG	1.96	0.47
1:C:148:THR:HA	1:C:177:ALA:HA	1.95	0.47
1:I:149:VAL:HG21	1:J:181:THR:HG21	1.96	0.47
1:J:193:VAL:O	1:J:197:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:GLU:OE2	1:F:82:SER:OG	2.28	0.47
1:B:134:ALA:HB2	1:B:195:TYR:CE2	2.50	0.47
1:B:16:TYR:CE1	1:B:24:LYS:HG2	2.48	0.47
1:H:13:TRP:HZ3	1:H:17:GLN:HB2	1.80	0.47
1:F:94:GLU:OE2	1:G:222:ARG:NH1	2.48	0.47
1:J:145:LEU:HD21	2:Z:9:LEU:HD13	1.97	0.47
1:H:156:PHE:CE2	1:I:174:ILE:HG21	2.50	0.47
1:B:48:PHE:CE1	1:B:52:LYS:HD2	2.51	0.46
1:C:155:SER:HB3	1:C:170:VAL:HG13	1.96	0.46
1:D:67:SER:HG	1:D:70:GLN:H	1.58	0.46
1:J:167:LEU:O	1:J:169:VAL:N	2.48	0.46
1:J:169:VAL:HG23	1:J:170:VAL:H	1.79	0.46
1:C:148:THR:HG21	1:C:181:THR:OG1	2.15	0.46
1:E:48:PHE:CZ	1:E:201:GLN:HB3	2.51	0.46
1:I:141:PRO:HB3	1:I:185:LEU:CD2	2.45	0.46
1:B:141:PRO:HD3	1:B:188:ALA:CB	2.45	0.46
1:C:135:THR:HG1	1:D:196:ASN:HD22	1.56	0.46
1:H:20:ASP:HB2	1:H:176:GLU:OE2	2.16	0.46
1:H:32:LEU:O	1:H:36:VAL:HG12	2.16	0.46
1:E:193:VAL:O	1:E:197:VAL:HG23	2.16	0.46
1:E:145:LEU:HD21	2:Y:10:VAL:HG21	1.96	0.46
1:A:58:GLU:CD	1:A:82:SER:HG	2.19	0.46
1:F:163:GLN:HE21	1:F:163:GLN:HB3	1.53	0.46
1:A:80:SER:O	1:A:82:SER:N	2.49	0.45
1:H:215:GLN:O	1:H:219:LEU:HG	2.16	0.45
1:I:55:LEU:CD1	1:I:208:MET:HB3	2.47	0.45
1:B:30:LEU:HD13	1:B:184:GLY:HA2	1.98	0.45
1:J:18:HIS:HA	1:J:19:ALA:C	2.36	0.45
1:H:113:PHE:O	1:H:117:ARG:HB3	2.16	0.45
1:H:148:THR:HG21	1:H:181:THR:OG1	2.15	0.45
1:I:185:LEU:O	1:I:189:ILE:HG12	2.16	0.45
1:C:188:ALA:O	1:C:192:VAL:HG23	2.17	0.45
1:I:85:LEU:HG	1:I:89:ASN:ND2	2.32	0.45
1:A:155:SER:O	1:A:159:ILE:HG13	2.17	0.45
1:D:30:LEU:HD21	1:D:143:VAL:HG13	1.98	0.45
1:H:144:GLY:O	1:H:148:THR:HG23	2.16	0.45
1:B:53:ARG:HH12	1:H:161:GLN:HG3	1.82	0.45
1:B:84:SER:OG	1:B:212:VAL:HG11	2.16	0.45
1:G:170:VAL:HG13	1:G:174:ILE:HD13	1.99	0.45
1:I:114:ARG:HG2	1:J:218:LEU:HD11	1.99	0.45
1:B:148:THR:O	1:B:152:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:GLN:O	1:B:219:LEU:HG	2.17	0.45
1:D:117:ARG:HA	1:D:117:ARG:HD2	1.70	0.45
1:J:54:ARG:HH12	1:J:81:LYS:HG3	1.82	0.45
1:E:144:GLY:O	1:E:148:THR:HG23	2.17	0.45
1:F:167:LEU:O	1:F:169:VAL:N	2.50	0.45
1:H:81:LYS:HD2	1:H:81:LYS:N	2.32	0.45
1:A:67:SER:O	1:A:219:LEU:HD13	2.18	0.44
1:F:166:ASN:O	1:F:168:ALA:N	2.50	0.44
1:H:61:LEU:HA	1:H:61:LEU:HD23	1.79	0.44
1:G:167:LEU:H	1:G:167:LEU:HD13	1.81	0.44
1:H:22:VAL:O	1:H:26:VAL:HG23	2.17	0.44
1:I:48:PHE:CD1	1:I:126:MET:HE3	2.53	0.44
1:I:55:LEU:HA	1:I:55:LEU:HD23	1.75	0.44
1:J:77:ASP:N	1:J:77:ASP:OD1	2.44	0.44
1:J:85:LEU:HD23	1:J:85:LEU:HA	1.76	0.44
1:B:162:THR:N	1:B:163:GLN:HA	2.32	0.44
1:G:115:LEU:HD12	1:G:217:LEU:HG	1.98	0.44
1:G:23:VAL:HG12	1:G:27:MET:HE2	2.00	0.44
1:I:134:ALA:HB2	1:I:195:TYR:CE1	2.53	0.44
1:J:67:SER:O	1:J:219:LEU:HD13	2.17	0.44
1:E:25:CYS:O	1:E:28:ILE:HG13	2.18	0.44
1:E:28:ILE:O	1:E:31:ILE:HG13	2.17	0.44
1:I:70:GLN:O	1:I:74:ILE:HG13	2.18	0.44
1:D:145:LEU:HA	1:D:181:THR:HG23	1.99	0.44
1:E:148:THR:HG21	1:E:181:THR:OG1	2.18	0.44
1:I:137:GLY:HA3	1:I:192:VAL:HG23	1.99	0.44
1:A:159:ILE:HG13	1:A:159:ILE:H	1.66	0.43
1:J:224:LEU:HD23	1:J:224:LEU:HA	1.84	0.43
1:C:70:GLN:O	1:C:74:ILE:HG13	2.19	0.43
1:B:48:PHE:CE2	1:B:205:PHE:HB2	2.54	0.43
1:D:55:LEU:HA	1:D:55:LEU:HD23	1.74	0.43
1:H:27:MET:HG2	1:H:183:ILE:HD12	1.99	0.43
1:I:159:ILE:CG2	1:J:167:LEU:HD11	2.48	0.43
1:A:161:GLN:HG2	1:A:161:GLN:H	1.70	0.43
1:C:217:LEU:HD23	1:C:217:LEU:HA	1.82	0.43
1:H:14:GLY:O	1:H:18:HIS:N	2.47	0.43
2:Y:5:ILE:HA	2:Y:8:MET:SD	2.58	0.43
1:C:16:TYR:C	1:C:16:TYR:HD1	2.21	0.43
1:I:145:LEU:HA	1:I:181:THR:HG23	1.99	0.43
2:Z:9:LEU:O	2:Z:13:ILE:HB	2.19	0.43
1:E:209:LEU:HD12	1:E:209:LEU:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:GLY:HA3	1:B:206:LYS:HE2	2.01	0.43
1:C:151:GLY:HA3	1:C:177:ALA:HB2	2.00	0.43
1:F:135:THR:HG21	1:G:193:VAL:HG13	1.99	0.43
1:G:61:LEU:HA	1:G:61:LEU:HD23	1.78	0.43
1:D:25:CYS:O	1:D:28:ILE:HG13	2.18	0.43
1:I:19:ALA:N	1:I:24:LYS:HE2	2.34	0.43
1:J:23:VAL:O	1:J:26:VAL:HG22	2.18	0.43
1:C:189:ILE:HB	1:C:190:PRO:HD3	2.00	0.43
1:C:28:ILE:O	1:C:32:LEU:HG	2.19	0.43
1:A:143:VAL:HG23	1:B:189:ILE:HD13	2.00	0.42
1:B:159:ILE:HD13	1:C:167:LEU:HB3	2.01	0.42
1:E:20:ASP:OD2	1:E:154:ASN:ND2	2.52	0.42
1:F:157:ILE:O	1:F:161:GLN:HG2	2.19	0.42
2:Z:11:LEU:HD22	2:Z:11:LEU:HA	1.82	0.42
1:C:20:ASP:O	1:C:24:LYS:HB2	2.20	0.42
1:D:179:LEU:HD23	1:D:179:LEU:HA	1.73	0.42
1:E:107:ILE:HA	1:E:110:ARG:NH1	2.34	0.42
1:F:93:ASN:O	1:F:97:LEU:HG	2.19	0.42
1:G:185:LEU:HA	1:G:185:LEU:HD23	1.88	0.42
2:Y:19:ALA:HB3	2:Y:20:PRO:HD3	2.00	0.42
1:A:93:ASN:HB3	1:A:114:ARG:HH22	1.83	0.42
1:I:142:PHE:HB3	1:J:189:ILE:HD11	2.02	0.42
2:Y:24:VAL:HB	2:Y:25:ASP:CA	2.48	0.42
1:D:209:LEU:HD23	1:D:209:LEU:HA	1.91	0.42
1:F:168:ALA:HA	1:F:171:ALA:HB2	2.01	0.42
1:F:61:LEU:HA	1:F:61:LEU:HD23	1.86	0.42
1:B:30:LEU:HA	1:B:30:LEU:HD23	1.88	0.42
1:D:165:THR:HG22	1:D:166:ASN:H	1.84	0.42
1:I:118:ARG:HD3	1:I:118:ARG:HA	1.90	0.42
1:A:48:PHE:CZ	1:A:201:GLN:HB3	2.55	0.42
1:A:149:VAL:HG21	1:B:181:THR:HG21	2.00	0.42
1:D:85:LEU:HG	1:D:89:ASN:ND2	2.35	0.42
1:F:107:ILE:HA	1:F:110:ARG:NH1	2.35	0.42
1:F:168:ALA:HA	1:F:171:ALA:CB	2.50	0.42
1:A:81:LYS:HB2	1:A:81:LYS:HE3	1.56	0.42
1:C:93:ASN:O	1:C:97:LEU:HG	2.20	0.42
1:J:188:ALA:O	1:J:192:VAL:HG13	2.19	0.42
1:B:94:GLU:OE2	1:C:222:ARG:NH1	2.52	0.42
1:B:112:SER:O	1:B:116:GLU:HG2	2.20	0.41
1:G:87:LEU:HD13	1:G:213:ALA:HB2	2.02	0.41
1:C:232:ALA:HB3	1:C:233:HIS:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:62:LEU:HD23	1:I:62:LEU:HA	1.81	0.41
1:J:17:GLN:O	1:J:19:ALA:HB3	2.20	0.41
1:B:14:GLY:O	1:B:18:HIS:N	2.53	0.41
1:B:42:PHE:CZ	1:I:31:ILE:HD13	2.55	0.41
1:J:33:ALA:O	1:J:37:THR:HG23	2.21	0.41
1:C:215:GLN:O	1:C:219:LEU:HG	2.21	0.41
1:H:115:LEU:HD23	1:H:115:LEU:HA	1.81	0.41
1:E:54:ARG:HH12	1:E:81:LYS:HE2	1.85	0.41
1:G:194:ILE:HD13	1:G:194:ILE:HG21	1.90	0.41
1:H:145:LEU:HD21	2:Z:7:VAL:HG13	2.02	0.41
2:Z:5:ILE:HB	2:Z:8:MET:CE	2.50	0.41
1:A:188:ALA:O	1:A:192:VAL:HG23	2.21	0.41
1:D:115:LEU:HD12	1:D:217:LEU:HG	2.03	0.41
1:G:134:ALA:HB2	1:G:195:TYR:CE2	2.55	0.41
1:G:189:ILE:N	1:G:190:PRO:HD2	2.36	0.41
1:H:13:TRP:O	1:H:13:TRP:HE3	2.04	0.41
1:D:44:LYS:HD2	1:D:44:LYS:HA	1.91	0.41
1:A:171:ALA:HB2	1:E:159:ILE:HD11	2.02	0.41
1:E:95:LEU:HD23	1:E:95:LEU:HA	1.88	0.41
1:F:93:ASN:HB3	1:F:114:ARG:HH22	1.85	0.41
1:G:218:LEU:HD23	1:G:218:LEU:HA	1.83	0.41
1:I:179:LEU:HD23	1:I:179:LEU:HA	1.79	0.41
1:I:142:PHE:HZ	2:Z:4:PHE:HE1	1.67	0.41
1:D:78:PHE:HA	1:D:78:PHE:HD1	1.74	0.41
1:F:56:LYS:O	1:F:60:GLN:HG3	2.21	0.41
1:A:123:GLY:HA3	1:A:206:LYS:HE2	2.03	0.40
1:D:164:THR:HG22	1:D:165:THR:H	1.85	0.40
1:J:135:THR:O	1:J:139:ILE:HG12	2.21	0.40
1:G:189:ILE:O	1:G:193:VAL:HG23	2.20	0.40
1:H:189:ILE:O	1:H:193:VAL:HG22	2.22	0.40
1:A:16:TYR:CE1	1:A:24:LYS:HE3	2.57	0.40
2:Z:10:VAL:O	2:Z:14:ILE:HB	2.21	0.40
1:A:77:ASP:CA	1:A:78:PHE:HB2	2.49	0.40
1:F:182:ALA:HB1	1:J:146:PHE:HE1	1.86	0.40
1:G:112:SER:O	1:G:116:GLU:HG2	2.20	0.40
1:A:171:ALA:HB3	1:A:172:PRO:HD3	2.03	0.40
1:C:128:ARG:O	1:D:200:ARG:NH1	2.31	0.40
1:D:133:LEU:HD13	1:D:194:ILE:HG22	2.03	0.40
1:D:87:LEU:HD22	1:D:115:LEU:HD22	2.02	0.40
1:J:198:PHE:O	1:J:202:ILE:HB	2.21	0.40
2:Y:16:MET:O	2:Y:20:PRO:HD2	2.20	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	221/244 (91%)	209 (95%)	11 (5%)	1 (0%)	34	78
1	B	222/244 (91%)	213 (96%)	8 (4%)	1 (0%)	34	78
1	C	221/244 (91%)	212 (96%)	9 (4%)	0	100	100
1	D	212/244 (87%)	202 (95%)	10 (5%)	0	100	100
1	E	220/244 (90%)	214 (97%)	6 (3%)	0	100	100
1	F	223/244 (91%)	211 (95%)	8 (4%)	4 (2%)	11	53
1	G	222/244 (91%)	214 (96%)	8 (4%)	0	100	100
1	H	219/244 (90%)	210 (96%)	9 (4%)	0	100	100
1	I	213/244 (87%)	203 (95%)	9 (4%)	1 (0%)	34	78
1	J	216/244 (88%)	208 (96%)	6 (3%)	2 (1%)	21	68
2	Y	21/58 (36%)	19 (90%)	2 (10%)	0	100	100
2	Z	20/58 (34%)	17 (85%)	3 (15%)	0	100	100
All	All	2230/2556 (87%)	2132 (96%)	89 (4%)	9 (0%)	39	81

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	162	THR
1	I	67	SER
1	J	21	ILE
1	F	163	GLN
1	F	168	ALA
1	A	20	ASP
1	B	68	LEU
1	F	164	THR
1	J	166	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/189 (88%)	155 (93%)	12 (7%)	18	57
1	B	171/189 (90%)	157 (92%)	14 (8%)	14	51
1	C	165/189 (87%)	152 (92%)	13 (8%)	15	53
1	D	160/189 (85%)	146 (91%)	14 (9%)	12	48
1	E	164/189 (87%)	148 (90%)	16 (10%)	10	42
1	F	168/189 (89%)	160 (95%)	8 (5%)	31	71
1	G	171/189 (90%)	154 (90%)	17 (10%)	10	41
1	H	169/189 (89%)	158 (94%)	11 (6%)	21	62
1	I	165/189 (87%)	152 (92%)	13 (8%)	15	53
1	J	162/189 (86%)	142 (88%)	20 (12%)	6	29
2	Y	19/50 (38%)	15 (79%)	4 (21%)	1	8
2	Z	19/50 (38%)	12 (63%)	7 (37%)	0	1
All	All	1700/1990 (85%)	1551 (91%)	149 (9%)	12	48

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	24	LYS
1	A	68	LEU
1	A	77	ASP
1	A	90	GLU
1	A	118	ARG
1	A	130	ASN
1	A	143	VAL
1	A	161	GLN
1	A	170	VAL
1	A	179	LEU
1	A	186	VAL
1	B	17	GLN
1	B	55	LEU

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Mol	Chain	Res	Type
1	B	57	ARG
1	B	66	ARG
1	B	68	LEU
1	B	113	PHE
1	B	117	ARG
1	B	118	ARG
1	B	148	THR
1	B	152	ILE
1	B	159	ILE
1	B	162	THR
1	B	181	THR
1	B	193	VAL
1	C	11	SER
1	C	12	VAL
1	C	13	TRP
1	C	16	TYR
1	C	18	HIS
1	C	25	CYS
1	C	36	VAL
1	C	64	GLU
1	C	90	GLU
1	C	118	ARG
1	C	135	THR
1	C	162	THR
1	C	181	THR
1	D	22	VAL
1	D	32	LEU
1	D	46	VAL
1	D	55	LEU
1	D	68	LEU
1	D	77	ASP
1	D	80	SER
1	D	117	ARG
1	D	118	ARG
1	D	148	THR
1	D	159	ILE
1	D	164	THR
1	D	181	THR
1	D	209	LEU
1	E	22	VAL
1	E	51	GLN
1	E	66	ARG

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Mol	Chain	Res	Type
1	E	85	LEU
1	E	113	PHE
1	E	118	ARG
1	E	130	ASN
1	E	135	THR
1	E	148	THR
1	E	155	SER
1	E	159	ILE
1	E	166	ASN
1	E	167	LEU
1	E	169	VAL
1	E	181	THR
1	E	200	ARG
1	F	10	LEU
1	F	53	ARG
1	F	69	ASN
1	F	80	SER
1	F	90	GLU
1	F	135	THR
1	F	143	VAL
1	F	163	GLN
1	G	10	LEU
1	G	20	ASP
1	G	53	ARG
1	G	55	LEU
1	G	66	ARG
1	G	68	LEU
1	G	77	ASP
1	G	85	LEU
1	G	113	PHE
1	G	117	ARG
1	G	148	THR
1	G	152	ILE
1	G	159	ILE
1	G	164	THR
1	G	165	THR
1	G	167	LEU
1	G	193	VAL
1	H	13	TRP
1	H	18	HIS
1	H	36	VAL
1	H	64	GLU

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Mol	Chain	Res	Type
1	H	68	LEU
1	H	81	LYS
1	H	135	THR
1	H	143	VAL
1	H	148	THR
1	H	152	ILE
1	H	165	THR
1	I	55	LEU
1	I	66	ARG
1	I	67	SER
1	I	68	LEU
1	I	77	ASP
1	I	113	PHE
1	I	128	ARG
1	I	148	THR
1	I	164	THR
1	I	181	THR
1	I	193	VAL
1	I	197	VAL
1	I	209	LEU
1	J	22	VAL
1	J	53	ARG
1	J	77	ASP
1	J	85	LEU
1	J	90	GLU
1	J	96	GLU
1	J	99	GLU
1	J	113	PHE
1	J	118	ARG
1	J	128	ARG
1	J	135	THR
1	J	143	VAL
1	J	148	THR
1	J	155	SER
1	J	161	GLN
1	J	164	THR
1	J	167	LEU
1	J	169	VAL
1	J	181	THR
1	J	200	ARG
2	Y	6	ASP
2	Y	8	MET

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Mol	Chain	Res	Type
2	Y	15	PHE
2	Y	16	MET
2	Z	6	ASP
2	Z	8	MET
2	Z	11	LEU
2	Z	12	LEU
2	Z	15	PHE
2	Z	16	MET
2	Z	17	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	E	125	GLN
1	F	17	GLN
1	F	163	GLN
1	I	215	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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	$\# Z  > 2$
1	MLY	A	108	1	8,10,11	0.45	0	9,11,13	1.03	1 (11%)
1	MLY	B	108	1	8,10,11	0.49	0	9,11,13	1.18	1 (11%)
1	MLY	C	108	1	8,10,11	0.49	0	9,11,13	0.97	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	D	108	1	8,10,11	0.55	0	9,11,13	1.06	1 (11%)
1	MLY	E	108	1	8,10,11	0.46	0	9,11,13	1.05	1 (11%)
1	MLY	F	108	1	8,10,11	0.44	0	9,11,13	1.00	1 (11%)
1	MLY	G	108	1	8,10,11	0.60	0	9,11,13	1.27	2 (22%)
1	MLY	H	108	1	8,10,11	0.42	0	9,11,13	1.06	1 (11%)
1	MLY	I	108	1	8,10,11	0.49	0	9,11,13	1.01	1 (11%)
1	MLY	J	108	1	8,10,11	0.54	0	9,11,13	1.18	1 (11%)

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
1	MLY	A	108	1	-	0/7/9/11	0/0/0/0
1	MLY	B	108	1	-	0/7/9/11	0/0/0/0
1	MLY	C	108	1	-	0/7/9/11	0/0/0/0
1	MLY	D	108	1	-	0/7/9/11	0/0/0/0
1	MLY	E	108	1	-	0/7/9/11	0/0/0/0
1	MLY	F	108	1	-	0/7/9/11	0/0/0/0
1	MLY	G	108	1	-	0/7/9/11	0/0/0/0
1	MLY	H	108	1	-	0/7/9/11	0/0/0/0
1	MLY	I	108	1	-	0/7/9/11	0/0/0/0
1	MLY	J	108	1	-	0/7/9/11	0/0/0/0

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	108	MLY	O-C-CA	-2.39	119.31	125.72
1	A	108	MLY	O-C-CA	-2.34	119.44	125.72
1	B	108	MLY	O-C-CA	-2.33	119.46	125.72
1	G	108	MLY	O-C-CA	-2.29	119.57	125.72
1	D	108	MLY	O-C-CA	-2.25	119.68	125.72
1	F	108	MLY	O-C-CA	-2.21	119.81	125.72
1	C	108	MLY	O-C-CA	-2.20	119.83	125.72
1	E	108	MLY	O-C-CA	-2.19	119.84	125.72
1	I	108	MLY	O-C-CA	-2.15	119.96	125.72
1	H	108	MLY	O-C-CA	-2.09	120.11	125.72
1	G	108	MLY	CH2-NZ-CH1	-2.02	104.39	109.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	223/244 (91%)	-0.27	6 (2%) 58 47	61, 84, 137, 199	0
1	B	224/244 (91%)	-0.50	0 100 100	53, 78, 133, 169	0
1	C	223/244 (91%)	-0.33	1 (0%) 93 90	50, 89, 136, 180	0
1	D	214/244 (87%)	-0.30	6 (2%) 56 46	48, 74, 166, 244	0
1	E	222/244 (90%)	-0.29	3 (1%) 78 68	57, 94, 157, 209	0
1	F	225/244 (92%)	-0.30	3 (1%) 79 70	52, 89, 151, 183	0
1	G	224/244 (91%)	-0.38	0 100 100	62, 81, 129, 154	0
1	H	221/244 (90%)	-0.43	1 (0%) 91 88	40, 77, 136, 181	0
1	I	215/244 (88%)	-0.20	9 (4%) 40 31	44, 74, 162, 243	0
1	J	218/244 (89%)	-0.14	2 (0%) 85 78	56, 87, 141, 168	0
2	Y	23/58 (39%)	0.67	2 (8%) 13 12	119, 141, 167, 170	0
2	Z	22/58 (37%)	0.73	5 (22%) 1 1	98, 151, 168, 180	0
All	All	2254/2556 (88%)	-0.29	38 (1%) 73 64	40, 84, 151, 244	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	THR	7.2
1	D	166	ASN	6.9
1	I	166	ASN	5.7
1	A	165	THR	4.5
1	D	159	ILE	4.5
1	I	159	ILE	4.1
1	C	233	HIS	4.0
2	Y	22	ALA	3.9
1	I	168	ALA	3.3
2	Z	24	VAL	3.2
1	J	232	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	I	165	THR	3.2
2	Z	21	LEU	3.1
1	I	233	HIS	3.1
1	D	167	LEU	3.1
1	F	164	THR	2.9
1	D	160	ALA	2.8
1	A	163	GLN	2.8
2	Y	25	ASP	2.7
1	H	164	THR	2.7
1	E	173	GLY	2.6
1	E	171	ALA	2.5
2	Z	23	THR	2.5
2	Z	18	ALA	2.5
1	D	168	ALA	2.4
1	F	165	THR	2.4
1	F	61	LEU	2.4
1	D	156	PHE	2.4
1	A	166	ASN	2.3
1	I	156	PHE	2.3
2	Z	22	ALA	2.3
1	A	169	VAL	2.3
1	A	168	ALA	2.2
1	I	160	ALA	2.2
1	I	163	GLN	2.2
1	J	171	ALA	2.2
1	I	167	LEU	2.2
1	E	234	PRO	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	MLY	F	108	11/12	0.96	0.16	-	46,51,62,70	0
1	MLY	I	108	11/12	0.95	0.22	-	57,63,79,97	0
1	MLY	G	108	11/12	0.94	0.18	-	61,62,66,75	0
1	MLY	E	108	11/12	0.93	0.25	-	57,60,67,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	J	108	11/12	0.96	0.19	-	59,59,63,94	0
1	MLY	C	108	11/12	0.93	0.19	-	46,49,69,84	0
1	MLY	A	108	11/12	0.94	0.20	-	70,72,94,108	0
1	MLY	B	108	11/12	0.96	0.18	-	48,49,71,80	0
1	MLY	H	108	11/12	0.96	0.15	-	40,41,48,49	0
1	MLY	D	108	11/12	0.96	0.17	-	47,48,52,109	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HG	F	301	1/1	0.97	0.43	-	487,487,487,487	0
3	HG	D	301	1/1	0.60	0.18	-	598,598,598,598	0
3	HG	J	301	1/1	0.65	0.11	-	593,593,593,593	0
3	HG	H	301	1/1	0.47	0.50	-	563,563,563,563	0
3	HG	A	301	1/1	0.92	0.28	-	370,370,370,370	0
3	HG	E	301	1/1	0.74	0.13	-	582,582,582,582	0
3	HG	C	301	1/1	0.71	0.26	-	467,467,467,467	0
3	HG	I	301	1/1	0.85	0.26	-	683,683,683,683	0
3	HG	G	301	1/1	0.49	0.14	-	502,502,502,502	0
3	HG	B	301	1/1	0.28	0.27	-	514,514,514,514	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.