



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:58 PM GMT

PDB ID : 4G3M  
Title : Complex Structure of Bacillus subtilis RibG: The Deamination Process in Riboflavin Biosynthesis  
Authors : Chen, S.C.; Shen, C.Y.; Yen, T.M.; Yu, H.C.; Chang, T.H.; Lai, W.L.; Liaw, S.H.  
Deposited on : 2012-07-15  
Resolution : 2.56 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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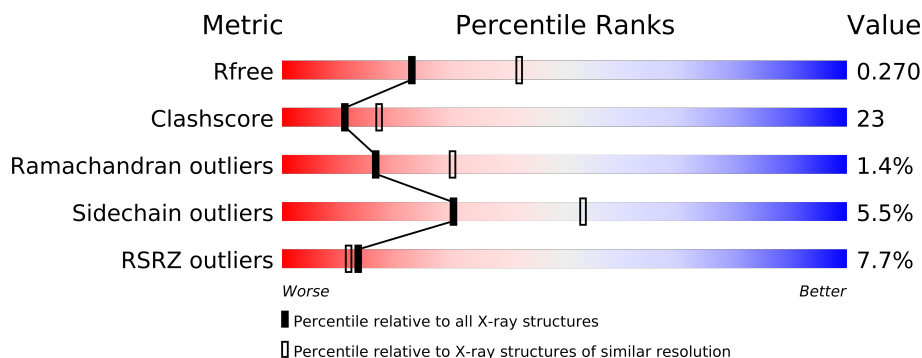
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.56 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))
$R_{free}$	66092	2347 (2.60-2.52)
Clashscore	79885	2876 (2.60-2.52)
Ramachandran outliers	78287	2826 (2.60-2.52)
Sidechain outliers	78261	2826 (2.60-2.52)
RSRZ outliers	66119	2347 (2.60-2.52)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	373	
1	B	373	
1	C	373	
1	D	373	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11519 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Riboflavin biosynthesis protein RibD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2756	1749	472	520	15			
1	B	361	Total	C	N	O	S	0	0	0
			2751	1745	471	520	15			
1	C	361	Total	C	N	O	S	0	0	0
			2751	1745	471	520	15			
1	D	361	Total	C	N	O	S	0	0	0
			2751	1745	471	520	15			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP P17618
A	-10	ARG	-	EXPRESSION TAG	UNP P17618
A	-9	GLY	-	EXPRESSION TAG	UNP P17618
A	-8	SER	-	EXPRESSION TAG	UNP P17618
A	-7	HIS	-	EXPRESSION TAG	UNP P17618
A	-6	HIS	-	EXPRESSION TAG	UNP P17618
A	-5	HIS	-	EXPRESSION TAG	UNP P17618
A	-4	HIS	-	EXPRESSION TAG	UNP P17618
A	-3	HIS	-	EXPRESSION TAG	UNP P17618
A	-2	HIS	-	EXPRESSION TAG	UNP P17618
A	-1	GLY	-	EXPRESSION TAG	UNP P17618
A	0	SER	-	EXPRESSION TAG	UNP P17618
B	-11	MET	-	EXPRESSION TAG	UNP P17618
B	-10	ARG	-	EXPRESSION TAG	UNP P17618
B	-9	GLY	-	EXPRESSION TAG	UNP P17618
B	-8	SER	-	EXPRESSION TAG	UNP P17618
B	-7	HIS	-	EXPRESSION TAG	UNP P17618
B	-6	HIS	-	EXPRESSION TAG	UNP P17618
B	-5	HIS	-	EXPRESSION TAG	UNP P17618
B	-4	HIS	-	EXPRESSION TAG	UNP P17618
B	-3	HIS	-	EXPRESSION TAG	UNP P17618

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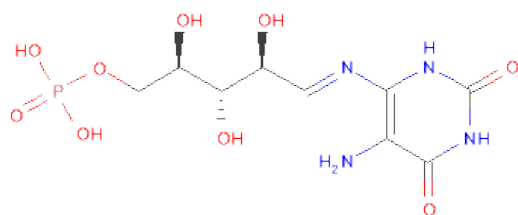
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	EXPRESSION TAG	UNP P17618
B	-1	GLY	-	EXPRESSION TAG	UNP P17618
B	0	SER	-	EXPRESSION TAG	UNP P17618
C	-11	MET	-	EXPRESSION TAG	UNP P17618
C	-10	ARG	-	EXPRESSION TAG	UNP P17618
C	-9	GLY	-	EXPRESSION TAG	UNP P17618
C	-8	SER	-	EXPRESSION TAG	UNP P17618
C	-7	HIS	-	EXPRESSION TAG	UNP P17618
C	-6	HIS	-	EXPRESSION TAG	UNP P17618
C	-5	HIS	-	EXPRESSION TAG	UNP P17618
C	-4	HIS	-	EXPRESSION TAG	UNP P17618
C	-3	HIS	-	EXPRESSION TAG	UNP P17618
C	-2	HIS	-	EXPRESSION TAG	UNP P17618
C	-1	GLY	-	EXPRESSION TAG	UNP P17618
C	0	SER	-	EXPRESSION TAG	UNP P17618
D	-11	MET	-	EXPRESSION TAG	UNP P17618
D	-10	ARG	-	EXPRESSION TAG	UNP P17618
D	-9	GLY	-	EXPRESSION TAG	UNP P17618
D	-8	SER	-	EXPRESSION TAG	UNP P17618
D	-7	HIS	-	EXPRESSION TAG	UNP P17618
D	-6	HIS	-	EXPRESSION TAG	UNP P17618
D	-5	HIS	-	EXPRESSION TAG	UNP P17618
D	-4	HIS	-	EXPRESSION TAG	UNP P17618
D	-3	HIS	-	EXPRESSION TAG	UNP P17618
D	-2	HIS	-	EXPRESSION TAG	UNP P17618
D	-1	GLY	-	EXPRESSION TAG	UNP P17618
D	0	SER	-	EXPRESSION TAG	UNP P17618

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

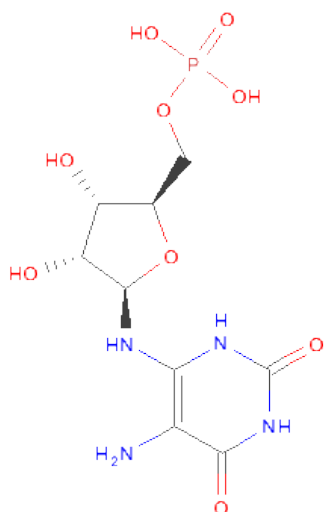
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is [(2R,3S,4S,5E)-5-[[5-AZANYL-2,4-BIS(OXIDANYLIDENE)-1H-PYRIMIDIN-6-YL]IMINO]-2,3,4-TRIS(OXIDANYL)PENTYL]DIHYDROGEN PHOSPHATE (three-letter code: AI9) (formula: C<sub>9</sub>H<sub>15</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
3	D	1	Total	C	N	O	P	0	0
			23	9	4	9	1		

- Molecule 4 is N-(5-AMINO-2,6-DIOXO-1,2,3,6-TETRAHYDROPYRIMIDIN-4-YL)-5-O-PHOSPHONO-BETA-D-RIBOFURANOSYLAMINE (three-letter code: AOF) (formula:  $C_9H_{15}N_4O_9P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
4	C	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
4	D	1	Total	C	N	O	P	0	0
			23	9	4	9	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	115	Total	O	0	0
			115	115		
5	B	70	Total	O	0	0
			70	70		
5	C	86	Total	O	0	0
			86	86		
5	D	74	Total	O	0	0
			74	74		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

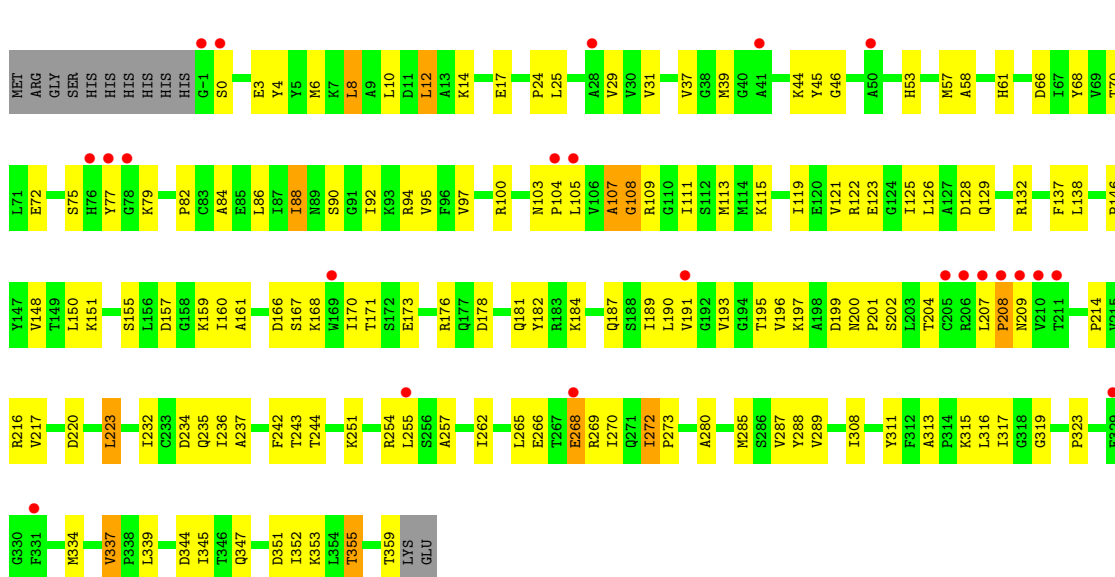
#### • Molecule 1: Riboflavin biosynthesis protein RibD

Chain A:



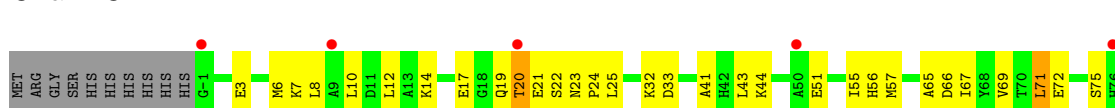
#### • Molecule 1: Riboflavin biosynthesis protein RibD

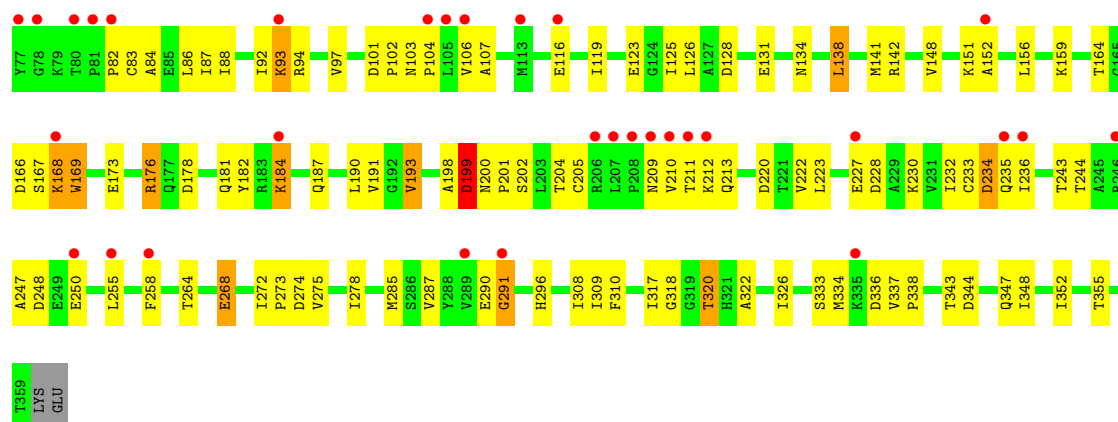
Chain B:



#### • Molecule 1: Riboflavin biosynthesis protein RibD

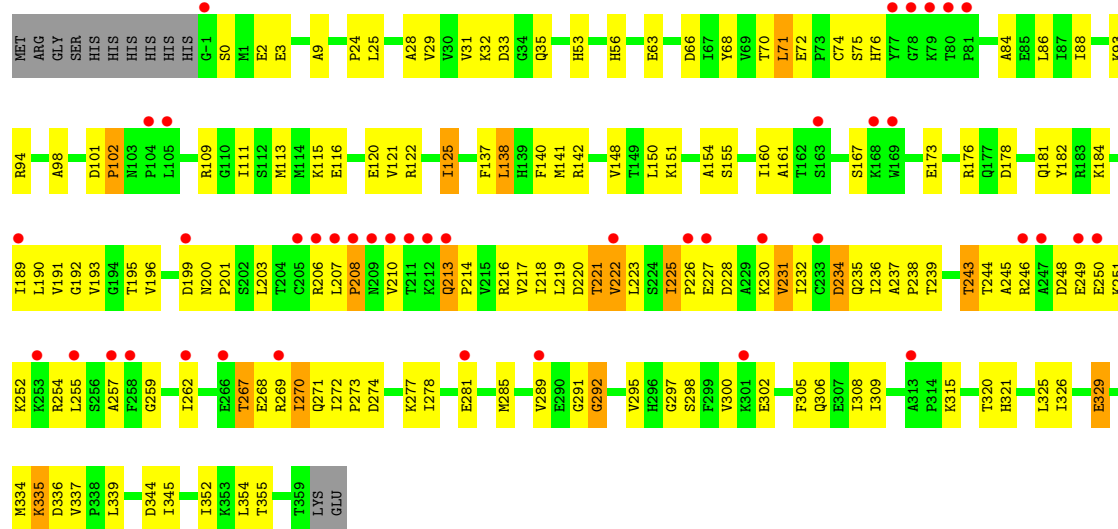
Chain C:





• Molecule 1: Riboflavin biosynthesis protein RibD

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.01Å 109.19Å 189.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.72 – 2.56 29.72 – 2.56	Depositor EDS
% Data completeness (in resolution range)	94.7 (29.72-2.56) 95.1 (29.72-2.56)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.64 (at 2.57Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.222 , 0.270 0.223 , 0.270	Depositor DCC
$R_{free}$ test set	5745 reflections (10.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.2	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 58652 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11519	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AOF, ZN, AI9

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	0.40	0/2807	0.64	0/3797
1	B	0.36	0/2802	0.60	0/3791
1	C	0.35	0/2802	0.59	0/3791
1	D	0.36	0/2802	0.59	0/3791
All	All	0.37	0/11213	0.61	0/15170

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2756	0	2800	89	0
1	B	2751	0	2790	125	0
1	C	2751	0	2790	132	0
1	D	2751	0	2790	184	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	23	0	15	1	0
3	B	23	0	15	2	0
3	C	23	0	15	0	0
3	D	23	0	15	0	0
4	B	23	0	15	0	0
4	C	23	0	15	1	0
4	D	23	0	15	0	0
5	A	115	0	0	5	0
5	B	70	0	0	4	0
5	C	86	0	0	4	0
5	D	74	0	0	6	0
All	All	11519	0	11275	506	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (506) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:213:GLN:CG	1:D:237:ALA:HB2	1.52	1.39
1:C:230:LYS:O	1:C:234:ASP:HB2	1.29	1.27
1:D:213:GLN:HB3	1:D:237:ALA:CB	1.76	1.15
1:D:213:GLN:CB	1:D:237:ALA:HB2	1.76	1.15
1:D:213:GLN:HB3	1:D:237:ALA:HB1	1.31	1.12
1:D:213:GLN:HG2	1:D:237:ALA:HB2	1.17	1.10
1:C:20:THR:HG21	1:C:25:LEU:HD12	1.14	1.10
1:D:230:LYS:HG2	1:D:231:VAL:H	1.15	1.09
1:D:221:THR:O	1:D:222:VAL:HG22	1.51	1.08
1:D:270:ILE:H	1:D:270:ILE:HD13	1.14	1.06
1:D:125:ILE:HD12	1:D:125:ILE:H	1.21	1.05
1:C:20:THR:CG2	1:C:25:LEU:HD12	1.88	1.04
1:D:213:GLN:CB	1:D:237:ALA:CB	2.36	1.00
1:D:213:GLN:CG	1:D:237:ALA:CB	2.41	0.99
1:A:360:LYS:HA	1:A:360:LYS:HE3	1.44	0.99
1:C:125:ILE:HD12	1:C:125:ILE:H	1.27	0.98
1:D:221:THR:O	1:D:222:VAL:HG13	1.62	0.98
1:A:290:GLU:HG3	1:A:291:GLY:H	1.30	0.94
1:D:148:VAL:H	1:D:306:GLN:NE2	1.68	0.91
1:D:221:THR:O	1:D:222:VAL:CG2	2.22	0.88
1:D:250:GLU:O	1:D:254:ARG:HB2	1.73	0.88
1:D:270:ILE:CD1	1:D:270:ILE:H	1.87	0.86
1:A:243:THR:HG21	1:A:247:ALA:HB2	1.59	0.85
1:C:243:THR:HG22	1:C:244:THR:H	1.39	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:201:PRO:HG2	1:D:203:LEU:HD21	1.59	0.84
1:D:270:ILE:HD13	1:D:270:ILE:N	1.92	0.83
1:C:66:ASP:OD1	1:C:94:ARG:HB2	1.77	0.83
1:D:230:LYS:HG2	1:D:231:VAL:N	1.95	0.82
1:D:160:ILE:HD11	1:D:325:LEU:HD23	1.60	0.81
1:B:37:VAL:HG22	1:B:58:ALA:HA	1.63	0.81
1:C:178:ASP:O	1:C:181:GLN:HG2	1.81	0.81
1:B:220:ASP:O	1:B:243:THR:HG22	1.80	0.80
1:D:221:THR:O	1:D:222:VAL:CG1	2.29	0.80
1:D:190:LEU:HD11	1:D:219:LEU:HG	1.64	0.80
1:B:111:ILE:HG23	1:B:121:VAL:HG11	1.63	0.79
1:D:0:SER:HB3	1:D:3:GLU:HG3	1.64	0.78
1:C:205:CYS:HB3	1:C:213:GLN:HE22	1.49	0.77
1:B:187:GLN:HE22	1:B:285:MET:HG3	1.50	0.76
1:D:230:LYS:HE3	1:D:231:VAL:HG22	1.67	0.76
1:C:20:THR:HB	1:C:23:ASN:O	1.84	0.76
1:D:150:LEU:HB2	1:D:308:ILE:HD13	1.69	0.75
1:B:193:VAL:HG11	1:B:220:ASP:CG	2.07	0.75
1:C:193:VAL:HG11	1:C:220:ASP:CG	2.08	0.74
1:B:193:VAL:HG11	1:B:220:ASP:OD2	1.87	0.74
1:B:197:LYS:HD3	5:B:511:HOH:O	1.87	0.74
1:B:37:VAL:HG21	1:B:61:HIS:HB2	1.68	0.74
1:C:7:LYS:HA	1:C:10:LEU:HD12	1.69	0.74
1:B:122:ARG:HB3	1:B:122:ARG:NH1	2.03	0.74
1:B:8:LEU:HD22	1:B:12:LEU:HD22	1.70	0.73
1:D:344:ASP:HB3	1:D:355:THR:CG2	2.18	0.73
1:C:102:PRO:HG2	1:C:138:LEU:HD12	1.70	0.73
1:D:231:VAL:HG21	1:D:239:THR:HG21	1.69	0.73
1:D:201:PRO:O	1:D:230:LYS:HG3	1.88	0.72
1:D:213:GLN:HG2	1:D:237:ALA:CB	2.09	0.72
1:C:134:ASN:O	1:C:138:LEU:HD22	1.89	0.72
1:C:69:VAL:HG12	1:C:71:LEU:H	1.54	0.72
1:C:347:GLN:HG3	1:C:352:ILE:HD13	1.71	0.71
1:D:334:MET:O	1:D:337:VAL:HG12	1.90	0.71
1:D:150:LEU:HD12	1:D:308:ILE:HD11	1.73	0.71
1:D:190:LEU:HD13	1:D:217:VAL:HG12	1.73	0.70
1:A:342:PHE:CE2	1:C:352:ILE:HG12	2.26	0.70
1:A:308:ILE:HD11	1:A:310:PHE:CZ	2.26	0.70
1:A:328:GLY:O	1:C:320:THR:HG22	1.92	0.70
1:D:148:VAL:HB	1:D:305:PHE:HA	1.74	0.70
1:D:111:ILE:HG23	1:D:121:VAL:HG11	1.73	0.70
1:C:205:CYS:HB3	1:C:213:GLN:NE2	2.07	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:106:VAL:HG22	1:A:109:ARG:NH2	2.07	0.69
1:C:220:ASP:O	1:C:243:THR:HG23	1.92	0.69
1:D:262:ILE:O	1:D:262:ILE:HD12	1.92	0.68
1:D:193:VAL:HG11	1:D:220:ASP:OD2	1.94	0.68
1:B:100:ARG:NH1	1:B:108:GLY:HA2	2.08	0.68
1:A:290:GLU:HG3	1:A:291:GLY:N	2.07	0.68
1:A:223:LEU:HB2	1:A:243:THR:HG21	1.75	0.68
1:C:343:THR:HB	1:C:355:THR:HG23	1.75	0.68
1:B:105:LEU:H	1:B:105:LEU:HD23	1.58	0.68
1:A:220:ASP:O	1:A:243:THR:HG23	1.93	0.68
1:D:125:ILE:H	1:D:125:ILE:CD1	1.96	0.67
1:C:7:LYS:HE3	5:C:534:HOH:O	1.95	0.67
1:B:168:LYS:HE2	1:D:334:MET:HB3	1.75	0.67
1:A:122:ARG:HH11	1:A:122:ARG:HG2	1.58	0.67
1:B:84:ALA:O	1:B:88:ILE:HG12	1.94	0.67
1:D:221:THR:C	1:D:222:VAL:HG13	2.15	0.67
1:C:167:SER:O	1:C:169:TRP:N	2.28	0.66
1:C:125:ILE:HG22	1:C:126:LEU:HD13	1.77	0.66
1:D:178:ASP:O	1:D:181:GLN:HG2	1.95	0.66
1:D:231:VAL:HG23	1:D:232:ILE:N	2.10	0.66
1:A:360:LYS:HA	1:A:360:LYS:CE	2.24	0.66
1:A:317:ILE:HG12	1:C:337:VAL:HG21	1.77	0.66
1:B:216:ARG:HD2	1:B:237:ALA:HB3	1.79	0.65
1:A:96:PHE:CE1	1:A:122:ARG:HD2	2.32	0.65
1:C:230:LYS:O	1:C:234:ASP:CB	2.25	0.64
1:C:191:VAL:HA	1:C:291:GLY:HA2	1.78	0.64
1:C:102:PRO:CG	1:C:138:LEU:HD12	2.26	0.64
1:A:75:SER:OG	1:A:109:ARG:HD2	1.97	0.64
1:B:184:LYS:HD2	1:B:207:LEU:HD12	1.80	0.64
1:D:267:THR:HG22	1:D:268:GLU:H	1.61	0.64
1:D:221:THR:O	1:D:222:VAL:CB	2.44	0.64
1:C:24:PRO:HG3	4:C:402:AOF:H9	1.78	0.64
1:C:71:LEU:HD23	1:C:72:GLU:H	1.63	0.64
1:B:334:MET:O	1:B:337:VAL:HG13	1.98	0.64
1:D:196:VAL:HG13	1:D:230:LYS:HD3	1.80	0.64
1:D:191:VAL:CG1	1:D:195:THR:HB	2.28	0.63
1:D:125:ILE:HD12	1:D:125:ILE:N	2.06	0.63
1:C:176:ARG:HH11	1:C:176:ARG:HG2	1.62	0.63
1:D:218:ILE:HG12	1:D:230:LYS:NZ	2.15	0.62
1:D:272:ILE:HB	1:D:273:PRO:HD3	1.81	0.62
1:D:218:ILE:HG12	1:D:230:LYS:HZ1	1.63	0.62
1:C:125:ILE:CD1	1:C:125:ILE:H	2.03	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:88:ILE:HG22	1:B:119:ILE:HD13	1.80	0.62
1:C:232:ILE:HD12	1:C:255:LEU:HD22	1.82	0.62
1:C:20:THR:OG1	1:C:25:LEU:HD11	1.99	0.62
1:C:184:LYS:HB2	1:C:184:LYS:NZ	2.14	0.61
1:D:63:GLU:HB3	5:D:532:HOH:O	2.00	0.61
1:B:46:GLY:HA2	1:B:79:LYS:HE2	1.81	0.61
1:B:148:VAL:HG22	1:B:287:VAL:CG1	2.30	0.61
1:B:334:MET:HA	1:B:337:VAL:CG1	2.31	0.61
1:D:274:ASP:O	1:D:278:ILE:HG12	2.00	0.60
1:D:138:LEU:O	1:D:142:ARG:HG3	2.00	0.60
1:D:231:VAL:HB	1:D:239:THR:OG1	2.01	0.60
1:B:232:ILE:HD13	1:B:255:LEU:HD22	1.84	0.60
1:C:347:GLN:O	1:C:348:ILE:HD13	2.01	0.60
1:A:152:ALA:HB3	1:A:310:PHE:CE1	2.36	0.60
1:A:243:THR:CG2	1:A:247:ALA:HB2	2.30	0.60
1:A:159:LYS:HE2	5:C:508:HOH:O	2.01	0.59
1:D:193:VAL:HG11	1:D:220:ASP:CG	2.23	0.59
1:B:187:GLN:HE22	1:B:285:MET:CG	2.14	0.59
1:D:268:GLU:HG3	1:D:269:ARG:HG2	1.85	0.59
1:A:184:LYS:HE3	1:A:207:LEU:HD12	1.83	0.59
1:C:274:ASP:O	1:C:278:ILE:HG12	2.03	0.59
1:C:102:PRO:O	1:C:104:PRO:HD3	2.03	0.58
1:D:111:ILE:HG22	1:D:115:LYS:HE2	1.85	0.58
1:C:93:LYS:HD2	1:C:94:ARG:H	1.69	0.58
1:C:166:ASP:OD1	1:C:168:LYS:HG3	2.02	0.58
1:B:190:LEU:HD13	1:B:191:VAL:N	2.16	0.58
1:D:221:THR:C	1:D:222:VAL:HG22	2.22	0.58
1:B:344:ASP:HB3	1:B:355:THR:HG23	1.84	0.58
1:B:269:ARG:HD3	5:B:546:HOH:O	2.03	0.58
1:C:84:ALA:O	1:C:88:ILE:HG13	2.03	0.58
1:D:32:LYS:HE2	1:D:33:ASP:OD2	2.04	0.58
1:D:76:HIS:HB3	1:D:109:ARG:HH12	1.68	0.58
1:D:250:GLU:CB	1:D:254:ARG:HH21	2.17	0.58
1:B:122:ARG:HB3	1:B:122:ARG:CZ	2.33	0.58
1:B:168:LYS:CE	1:D:334:MET:HB3	2.32	0.58
1:C:32:LYS:HE3	1:C:33:ASP:OD2	2.04	0.58
1:C:199:ASP:HB3	1:C:201:PRO:HD3	1.86	0.57
1:A:193:VAL:HG22	1:A:219:LEU:O	2.05	0.57
1:D:210:VAL:O	1:D:210:VAL:HG23	2.04	0.57
1:D:216:ARG:CZ	1:D:231:VAL:HG12	2.34	0.57
1:A:246:ARG:HH11	1:A:246:ARG:HB3	1.69	0.57
1:A:355:THR:HG23	5:A:559:HOH:O	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:3:GLU:HB2	1:C:126:LEU:HD11	1.87	0.57
1:D:232:ILE:HD12	1:D:255:LEU:HD22	1.85	0.57
1:B:184:LYS:CD	1:B:207:LEU:HD12	2.35	0.57
1:B:12:LEU:HD21	1:B:39:MET:HB3	1.86	0.57
1:D:154:ALA:HB2	1:D:160:ILE:HD13	1.87	0.56
1:D:320:THR:O	1:D:321:HIS:HB2	2.05	0.56
1:B:75:SER:HB2	1:B:113:MET:CE	2.35	0.56
1:B:146:PRO:HD3	1:B:280:ALA:HB2	1.87	0.56
1:C:20:THR:CG2	1:C:25:LEU:CD1	2.75	0.56
1:C:193:VAL:HG11	1:C:220:ASP:OD2	2.06	0.56
1:C:93:LYS:HD2	1:C:94:ARG:N	2.20	0.56
1:B:97:VAL:O	1:B:123:GLU:HA	2.06	0.56
1:B:24:PRO:HD3	1:B:137:PHE:CE2	2.41	0.56
1:D:217:VAL:C	1:D:218:ILE:HD12	2.26	0.56
1:C:44:LYS:HE2	5:C:546:HOH:O	2.06	0.56
1:C:308:ILE:HD11	1:C:310:PHE:CZ	2.41	0.56
1:B:207:LEU:HB3	1:B:208:PRO:CD	2.35	0.56
1:B:344:ASP:HB3	1:B:355:THR:CG2	2.35	0.56
1:A:246:ARG:NH1	1:A:246:ARG:HB3	2.19	0.56
1:D:191:VAL:HA	1:D:291:GLY:HA3	1.88	0.56
1:D:148:VAL:H	1:D:306:GLN:HE21	1.51	0.56
1:B:223:LEU:HD23	1:B:243:THR:CG2	2.36	0.56
1:D:234:ASP:OD1	1:D:236:ILE:HD13	2.06	0.56
1:B:345:ILE:O	1:B:345:ILE:HG13	2.05	0.56
1:D:148:VAL:H	1:D:306:GLN:HE22	1.51	0.56
1:D:344:ASP:HB3	1:D:355:THR:HG21	1.87	0.56
1:D:230:LYS:HE3	1:D:231:VAL:CG2	2.36	0.56
1:C:125:ILE:HD12	1:C:125:ILE:N	2.09	0.56
1:A:122:ARG:NH1	1:A:122:ARG:HG2	2.20	0.56
1:D:102:PRO:HG3	1:D:138:LEU:HD12	1.89	0.55
1:B:265:LEU:HD23	5:B:537:HOH:O	2.06	0.55
1:C:234:ASP:O	1:C:235:GLN:HB3	2.07	0.55
1:A:272:ILE:HB	1:A:273:PRO:HD3	1.88	0.55
1:C:20:THR:OG1	1:C:25:LEU:CD1	2.54	0.55
1:C:347:GLN:HG3	1:C:352:ILE:CD1	2.36	0.55
1:C:6:MET:HB3	1:C:126:LEU:HD22	1.89	0.55
1:B:196:VAL:HA	1:B:201:PRO:HD2	1.88	0.55
1:B:315:LYS:HE2	1:D:339:LEU:HD13	1.89	0.55
1:C:83:CYS:O	1:C:87:ILE:HG12	2.07	0.55
1:D:150:LEU:HD23	1:D:289:VAL:HB	1.89	0.55
1:C:65:ALA:O	1:C:92:ILE:HG23	2.06	0.55
1:B:150:LEU:HD23	1:B:289:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:298:SER:O	1:D:302:GLU:HG2	2.08	0.54
1:C:234:ASP:HB3	1:C:236:ILE:HG12	1.88	0.54
1:D:190:LEU:HD13	1:D:217:VAL:CG1	2.37	0.54
1:A:106:VAL:HG22	1:A:109:ARG:HH21	1.72	0.54
1:A:222:VAL:O	1:A:222:VAL:HG12	2.06	0.54
1:D:291:GLY:O	1:D:292:GLY:O	2.24	0.54
1:B:242:PHE:HD2	1:B:265:LEU:HD11	1.72	0.54
1:B:167:SER:HA	1:D:334:MET:HE3	1.90	0.54
1:A:2:GLU:HB3	1:A:125:ILE:HD13	1.90	0.54
1:A:345:ILE:HG23	1:A:354:LEU:CD2	2.38	0.54
1:C:344:ASP:H	1:C:355:THR:HG22	1.73	0.54
1:D:102:PRO:CG	1:D:138:LEU:HD12	2.38	0.54
1:B:159:LYS:HE2	5:D:533:HOH:O	2.07	0.54
1:A:326:ILE:HG22	5:A:572:HOH:O	2.08	0.54
1:C:184:LYS:HB2	1:C:184:LYS:HZ3	1.73	0.53
1:D:71:LEU:HD23	1:D:72:GLU:H	1.72	0.53
1:D:231:VAL:CG2	1:D:232:ILE:N	2.71	0.53
1:A:278:ILE:O	1:A:282:GLU:HG2	2.08	0.53
1:A:35:GLN:OE1	1:B:44:LYS:NZ	2.40	0.53
1:B:0:SER:HB3	1:B:3:GLU:HB3	1.89	0.53
1:A:310:PHE:CD2	1:C:156:LEU:HG	2.43	0.53
1:D:71:LEU:HD23	1:D:72:GLU:N	2.24	0.53
1:C:232:ILE:HG22	1:C:233:CYS:SG	2.48	0.53
1:C:210:VAL:O	1:C:211:THR:OG1	2.20	0.53
1:B:311:TYR:CE1	1:B:353:LYS:HD2	2.44	0.53
1:A:243:THR:HG22	1:A:244:THR:H	1.74	0.53
1:D:189:ILE:HG13	1:D:214:PRO:HB2	1.90	0.53
1:D:151:LYS:HD3	1:D:151:LYS:C	2.29	0.53
1:A:201:PRO:HB3	3:A:402:AI9:H8	1.91	0.53
1:A:169:TRP:N	1:A:169:TRP:CE3	2.77	0.53
1:C:169:TRP:HA	1:C:169:TRP:HE3	1.73	0.52
1:D:203:LEU:N	1:D:203:LEU:HD22	2.24	0.52
1:D:335:LYS:HG3	1:D:336:ASP:OD1	2.09	0.52
1:A:272:ILE:O	1:A:275:VAL:HG22	2.10	0.52
1:C:148:VAL:HG22	1:C:287:VAL:CG1	2.39	0.52
1:D:230:LYS:HE3	1:D:231:VAL:HG13	1.91	0.52
1:A:310:PHE:HD2	1:C:156:LEU:HG	1.75	0.52
1:C:41:ALA:O	1:C:43:LEU:HD22	2.09	0.52
1:D:72:GLU:OE1	1:D:111:ILE:HG12	2.10	0.52
1:C:169:TRP:HA	1:C:169:TRP:CE3	2.45	0.52
1:C:222:VAL:HG12	1:C:222:VAL:O	2.09	0.52
1:C:202:SER:HB2	1:C:204:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:243:THR:HG22	1:C:244:THR:N	2.17	0.52
1:C:181:GLN:HG3	1:C:182:TYR:N	2.24	0.52
1:D:221:THR:OG1	1:D:270:ILE:HD12	2.10	0.52
1:C:55:ILE:HD11	1:C:67:ILE:HD12	1.92	0.52
1:B:347:GLN:HG3	1:B:351:ASP:O	2.09	0.52
1:D:235:GLN:HG2	1:D:235:GLN:O	2.10	0.52
1:B:187:GLN:NE2	1:B:285:MET:HB2	2.24	0.51
1:A:331:PHE:HB2	1:A:337:VAL:HG12	1.92	0.51
1:D:102:PRO:HG2	1:D:137:PHE:HE1	1.75	0.51
1:D:277:LYS:O	1:D:281:GLU:HG3	2.11	0.51
1:B:129:GLN:HG2	1:B:132:ARG:HH21	1.75	0.51
1:D:235:GLN:OE1	1:D:235:GLN:N	2.42	0.51
1:A:51:GLU:OE1	1:A:51:GLU:N	2.35	0.51
1:C:159:LYS:HD2	1:C:322:ALA:HB3	1.92	0.51
1:D:267:THR:HG22	1:D:268:GLU:N	2.26	0.51
1:D:84:ALA:O	1:D:88:ILE:HG13	2.10	0.51
1:A:57:MET:HG3	1:B:53:HIS:CD2	2.45	0.51
1:D:230:LYS:HG2	1:D:231:VAL:HG13	1.92	0.51
1:D:320:THR:O	1:D:321:HIS:CB	2.58	0.51
1:B:262:ILE:N	1:B:262:ILE:HD12	2.26	0.51
1:C:187:GLN:HE22	1:C:285:MET:HG3	1.75	0.51
1:C:152:ALA:HB3	1:C:310:PHE:CD1	2.46	0.51
1:C:202:SER:CB	1:C:204:THR:HG23	2.41	0.51
1:A:51:GLU:CD	1:A:51:GLU:H	2.14	0.51
1:B:31:VAL:CG2	1:B:66:ASP:HB2	2.41	0.51
1:D:246:ARG:HD2	1:D:246:ARG:O	2.11	0.51
1:D:193:VAL:HG13	1:D:219:LEU:O	2.11	0.51
1:B:223:LEU:HD23	1:B:243:THR:HG21	1.91	0.51
1:B:254:ARG:O	1:B:257:ALA:HB3	2.11	0.51
1:D:74:CYS:HB2	1:D:76:HIS:CE1	2.46	0.50
1:D:243:THR:HG22	1:D:244:THR:H	1.76	0.50
1:B:168:LYS:NZ	1:D:335:LYS:HB3	2.26	0.50
1:B:150:LEU:CD2	1:B:289:VAL:HB	2.41	0.50
1:B:189:ILE:HD11	1:B:214:PRO:HG3	1.92	0.50
1:A:152:ALA:HB3	1:A:310:PHE:CD1	2.47	0.50
1:C:234:ASP:OD1	1:C:236:ILE:CG1	2.60	0.50
1:D:271:GLN:HB2	1:D:274:ASP:OD2	2.12	0.50
1:A:353:LYS:HG2	5:A:559:HOH:O	2.11	0.50
1:B:207:LEU:HB3	1:B:208:PRO:HD2	1.94	0.50
1:C:176:ARG:NH1	1:C:176:ARG:HG2	2.27	0.50
1:D:155:SER:HB2	1:D:315:LYS:O	2.12	0.50
1:A:8:LEU:HD11	1:A:39:MET:HE3	1.92	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:111:ILE:HD12	1:D:121:VAL:HG11	1.95	0.49
1:C:10:LEU:CD1	1:C:126:LEU:HD23	2.43	0.49
1:A:193:VAL:HG22	1:A:220:ASP:HA	1.95	0.49
1:C:71:LEU:HD23	1:C:72:GLU:N	2.26	0.49
1:C:344:ASP:HB3	1:C:355:THR:CG2	2.43	0.49
1:B:88:ILE:HG22	1:B:119:ILE:CD1	2.42	0.49
1:B:190:LEU:HD12	1:B:289:VAL:HG13	1.94	0.49
1:D:252:LYS:HB2	1:D:252:LYS:NZ	2.26	0.49
1:D:150:LEU:HD12	1:D:308:ILE:CD1	2.41	0.49
1:B:178:ASP:O	1:B:181:GLN:HG2	2.13	0.49
1:A:271:GLN:HG3	5:A:575:HOH:O	2.11	0.49
1:B:202:SER:O	1:B:204:THR:HG23	2.12	0.49
1:D:291:GLY:O	1:D:295:VAL:HB	2.13	0.49
1:A:82:PRO:HG2	1:A:85:GLU:HB2	1.95	0.49
1:D:201:PRO:CG	1:D:203:LEU:HD21	2.35	0.49
1:D:227:GLU:HA	1:D:232:ILE:HG13	1.95	0.49
1:C:151:LYS:HA	1:C:309:ILE:O	2.13	0.49
1:D:223:LEU:O	1:D:251:LYS:NZ	2.46	0.48
1:C:102:PRO:HB2	1:C:141:MET:CB	2.42	0.48
1:C:290:GLU:O	1:C:291:GLY:O	2.30	0.48
1:A:169:TRP:HA	1:A:169:TRP:HE3	1.78	0.48
1:B:173:GLU:OE2	1:B:176:ARG:HD2	2.13	0.48
1:D:140:PHE:CD1	1:D:285:MET:HA	2.48	0.48
1:C:347:GLN:C	1:C:348:ILE:HD13	2.33	0.48
1:B:103:ASN:OD1	1:B:104:PRO:HD2	2.13	0.48
1:D:102:PRO:HG2	1:D:137:PHE:CE1	2.48	0.48
1:D:235:GLN:CD	1:D:235:GLN:H	2.16	0.48
1:A:169:TRP:CA	1:A:169:TRP:CE3	2.96	0.48
1:D:227:GLU:CD	1:D:251:LYS:HE3	2.34	0.48
1:A:345:ILE:HG12	1:A:354:LEU:HD22	1.96	0.48
1:D:231:VAL:CG2	1:D:239:THR:HG21	2.39	0.48
1:B:223:LEU:HB2	1:B:243:THR:HG21	1.94	0.48
1:D:161:ALA:HB2	1:D:167:SER:HB3	1.96	0.48
1:A:67:ILE:HB	1:A:92:ILE:HD13	1.95	0.48
1:C:103:ASN:O	1:C:107:ALA:N	2.45	0.48
1:A:9:ALA:O	1:A:27:GLY:HA3	2.13	0.48
1:B:90:SER:OG	1:B:92:ILE:HG12	2.14	0.48
1:C:131:GLU:OE1	1:C:142:ARG:NH1	2.44	0.48
1:A:169:TRP:HA	1:A:169:TRP:CE3	2.49	0.48
1:A:337:VAL:O	1:A:337:VAL:HG23	2.13	0.48
1:C:184:LYS:NZ	1:C:205:CYS:SG	2.86	0.48
1:B:193:VAL:HG11	1:B:220:ASP:CB	2.44	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:66:ASP:OD1	1:D:94:ARG:HB3	2.13	0.48
1:C:333:SER:HB2	1:C:336:ASP:OD2	2.13	0.47
1:D:70:THR:O	1:D:98:ALA:HB3	2.13	0.47
1:D:207:LEU:HD23	1:D:208:PRO:HD2	1.94	0.47
1:A:223:LEU:HD13	1:A:251:LYS:HD3	1.96	0.47
1:C:92:ILE:O	1:C:119:ILE:HD12	2.14	0.47
1:D:160:ILE:O	1:D:160:ILE:HG22	2.15	0.47
1:A:308:ILE:HG22	1:A:356:ALA:O	2.13	0.47
1:B:75:SER:HB2	1:B:113:MET:HE3	1.97	0.47
1:C:8:LEU:HG	1:C:12:LEU:CD2	2.43	0.47
1:D:267:THR:HG22	1:D:269:ARG:H	1.80	0.47
1:B:6:MET:HB3	1:B:126:LEU:HD12	1.97	0.47
1:B:111:ILE:HG22	1:B:115:LYS:HE3	1.97	0.47
1:D:31:VAL:HA	1:D:35:GLN:O	2.15	0.47
1:D:230:LYS:O	1:D:232:ILE:N	2.48	0.47
1:A:221:THR:O	1:A:243:THR:HG22	2.14	0.47
1:B:223:LEU:HD11	1:B:255:LEU:CD1	2.44	0.47
1:B:223:LEU:CD1	1:B:251:LYS:HE2	2.45	0.47
1:B:160:ILE:O	1:B:161:ALA:HB2	2.15	0.47
1:A:69:VAL:HG12	1:A:71:LEU:H	1.79	0.47
1:C:164:THR:O	1:C:164:THR:HG22	2.13	0.47
1:D:75:SER:OG	1:D:109:ARG:HD2	2.15	0.47
1:D:120:GLU:HG3	5:D:569:HOH:O	2.14	0.47
1:B:66:ASP:OD1	1:B:94:ARG:HG3	2.15	0.47
1:B:199:ASP:O	1:B:200:ASN:C	2.53	0.46
1:D:191:VAL:HG12	1:D:192:GLY:N	2.30	0.46
1:C:187:GLN:NE2	1:C:285:MET:HB2	2.30	0.46
1:C:227:GLU:HB2	5:C:575:HOH:O	2.15	0.46
1:D:337:VAL:HG13	1:D:337:VAL:O	2.16	0.46
1:C:243:THR:HG21	1:C:247:ALA:HB2	1.97	0.46
1:D:216:ARG:NE	1:D:231:VAL:HG12	2.29	0.46
1:D:308:ILE:O	1:D:355:THR:HA	2.15	0.46
1:B:4:TYR:C	1:B:4:TYR:CD1	2.89	0.46
1:B:182:TYR:C	1:B:184:LYS:H	2.19	0.46
1:B:339:LEU:O	1:B:359:THR:HG22	2.16	0.46
1:D:225:ILE:HD13	1:D:226:PRO:N	2.31	0.46
1:D:222:VAL:H	1:D:243:THR:HG22	1.80	0.46
1:C:344:ASP:HB3	1:C:355:THR:HG21	1.97	0.45
1:D:196:VAL:HA	1:D:201:PRO:HD2	1.98	0.45
1:A:76:HIS:O	1:A:82:PRO:HB3	2.16	0.45
1:A:167:SER:O	1:A:169:TRP:N	2.48	0.45
1:A:47:GLU:OE2	1:B:61:HIS:HE1	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:191:VAL:HA	1:C:291:GLY:CA	2.45	0.45
1:D:101:ASP:OD1	1:D:102:PRO:HD2	2.16	0.45
1:B:10:LEU:HD23	1:B:70:THR:CG2	2.46	0.45
1:B:268:GLU:CD	1:B:268:GLU:H	2.20	0.45
1:C:56:HIS:NE2	1:D:56:HIS:CE1	2.84	0.45
1:C:258:PHE:N	1:C:258:PHE:CD1	2.84	0.45
1:C:230:LYS:HB3	1:C:234:ASP:OD2	2.17	0.45
1:B:223:LEU:HD11	1:B:255:LEU:HD11	1.97	0.45
1:D:138:LEU:HB3	1:D:142:ARG:NH1	2.32	0.45
1:D:24:PRO:HD3	1:D:137:PHE:CE2	2.52	0.45
1:C:209:ASN:O	1:C:211:THR:HG23	2.16	0.45
1:C:19:GLN:HB2	1:C:43:LEU:O	2.17	0.45
1:B:160:ILE:HG12	1:B:323:PRO:O	2.17	0.45
1:D:248:ASP:OD1	1:D:249:GLU:N	2.50	0.45
1:D:250:GLU:HB3	1:D:254:ARG:HH21	1.82	0.44
1:D:102:PRO:HB3	1:D:141:MET:HB2	1.99	0.44
1:C:17:GLU:HA	1:C:25:LEU:HD21	1.99	0.44
1:D:230:LYS:O	1:D:231:VAL:C	2.56	0.44
1:D:0:SER:OG	1:D:2:GLU:HG2	2.17	0.44
1:B:100:ARG:HH11	1:B:108:GLY:HA2	1.78	0.44
1:C:151:LYS:C	1:C:151:LYS:HD3	2.38	0.44
1:D:225:ILE:O	1:D:225:ILE:HG23	2.17	0.44
1:D:300:VAL:HG21	1:D:326:ILE:HD13	1.98	0.44
1:C:234:ASP:OD1	1:C:236:ILE:HD11	2.17	0.44
1:C:101:ASP:HA	1:C:102:PRO:HD3	1.81	0.44
1:C:272:ILE:HB	1:C:273:PRO:HD3	1.99	0.44
1:D:297:GLY:HA2	1:D:326:ILE:HG23	1.98	0.44
1:A:28:ALA:HA	1:A:68:TYR:O	2.17	0.44
1:C:125:ILE:CG2	1:C:126:LEU:HD13	2.45	0.44
1:D:250:GLU:HB2	1:D:254:ARG:HH21	1.82	0.44
1:B:166:ASP:OD1	1:D:334:MET:HB2	2.17	0.44
1:B:190:LEU:CD2	1:B:217:VAL:HB	2.47	0.44
1:B:345:ILE:HG21	1:D:352:ILE:HD12	2.00	0.44
1:B:170:ILE:HB	3:B:403:AI9:O4	2.18	0.44
1:B:14:LYS:HG3	5:B:514:HOH:O	2.17	0.44
1:A:7:LYS:NZ	1:A:129:GLN:NE2	2.66	0.44
1:D:190:LEU:HD12	1:D:191:VAL:N	2.32	0.44
1:A:32:LYS:HG3	1:A:61:HIS:O	2.18	0.44
1:B:191:VAL:HG21	1:B:195:THR:HG21	2.00	0.44
1:C:344:ASP:H	1:C:355:THR:CG2	2.30	0.44
1:B:6:MET:CE	1:B:70:THR:HG22	2.48	0.44
1:D:182:TYR:CZ	1:D:309:ILE:HD13	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:150:LEU:HB2	1:D:308:ILE:CD1	2.44	0.43
1:C:51:GLU:O	1:C:55:ILE:HD13	2.18	0.43
1:C:258:PHE:N	1:C:258:PHE:HD1	2.16	0.43
1:D:176:ARG:NH2	5:D:531:HOH:O	2.51	0.43
1:D:244:THR:O	1:D:245:ALA:C	2.57	0.43
1:A:96:PHE:HE1	1:A:122:ARG:HD2	1.80	0.43
1:A:169:TRP:N	1:A:169:TRP:CD2	2.85	0.43
1:B:243:THR:HB	1:B:244:THR:H	1.60	0.43
1:A:106:VAL:O	1:A:109:ARG:HB2	2.18	0.43
1:B:181:GLN:HG3	1:B:182:TYR:N	2.33	0.43
1:B:266:GLU:CD	1:B:266:GLU:H	2.21	0.43
1:A:178:ASP:O	1:A:181:GLN:HB2	2.18	0.43
1:D:228:ASP:O	1:D:228:ASP:OD1	2.37	0.43
1:D:182:TYR:C	1:D:184:LYS:H	2.22	0.43
1:B:17:GLU:HA	1:B:25:LEU:HD11	1.99	0.43
1:D:199:ASP:O	1:D:200:ASN:HB3	2.19	0.43
1:B:319:GLY:HA2	1:D:329:GLU:O	2.18	0.43
1:C:223:LEU:HB2	1:C:243:THR:HG21	2.01	0.43
1:B:166:ASP:OD1	1:B:168:LYS:HG2	2.18	0.43
1:B:45:TYR:CZ	1:B:79:LYS:HE3	2.53	0.43
1:A:193:VAL:CG2	1:A:220:ASP:HA	2.48	0.43
1:D:113:MET:O	1:D:116:GLU:HB3	2.19	0.43
1:B:316:LEU:O	1:D:337:VAL:HG23	2.19	0.43
1:B:189:ILE:HD11	1:B:214:PRO:CG	2.49	0.43
1:A:180:GLN:OE1	1:A:205:CYS:HA	2.18	0.43
1:B:352:ILE:HD13	1:D:345:ILE:HD12	2.01	0.43
1:D:220:ASP:OD1	1:D:221:THR:N	2.52	0.42
1:A:340:LEU:HD12	1:A:340:LEU:N	2.34	0.42
1:D:28:ALA:HA	1:D:68:TYR:O	2.19	0.42
1:D:236:ILE:HG12	5:D:515:HOH:O	2.20	0.42
1:A:275:VAL:HG23	1:A:276:LEU:N	2.34	0.42
1:A:12:LEU:HD11	1:A:39:MET:CE	2.49	0.42
1:B:151:LYS:HD2	1:B:288:TYR:OH	2.19	0.42
1:D:230:LYS:HE2	1:D:230:LYS:HB3	1.92	0.42
1:D:230:LYS:CE	1:D:231:VAL:HG22	2.43	0.42
1:C:57:MET:HG3	1:D:53:HIS:CD2	2.54	0.42
1:B:107:ALA:C	1:B:109:ARG:H	2.22	0.42
1:D:71:LEU:HB2	5:D:554:HOH:O	2.19	0.42
1:A:302:GLU:HA	1:A:302:GLU:OE1	2.20	0.42
1:A:53:HIS:CD2	1:B:57:MET:HG3	2.55	0.42
1:C:200:ASN:HD21	1:C:230:LYS:HG3	1.84	0.42
1:A:222:VAL:CG1	1:A:222:VAL:O	2.67	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:297:GLY:HA2	1:A:326:ILE:CG2	2.49	0.42
1:A:210:VAL:HG23	1:A:210:VAL:O	2.20	0.42
1:B:201:PRO:HB3	3:B:403:AI9:H8	2.01	0.42
1:B:173:GLU:OE2	1:B:176:ARG:NH1	2.53	0.42
1:B:171:THR:HG22	1:B:313:ALA:HB2	2.01	0.42
1:D:345:ILE:HD12	1:D:354:LEU:HD22	2.02	0.42
1:B:272:ILE:N	1:B:273:PRO:CD	2.83	0.42
1:C:268:GLU:H	1:C:268:GLU:CD	2.23	0.42
1:D:201:PRO:HG2	1:D:203:LEU:CD2	2.40	0.42
1:C:173:GLU:HG2	1:C:176:ARG:HH21	1.84	0.42
1:D:237:ALA:HB1	1:D:238:PRO:CD	2.50	0.42
1:C:21:GLU:OE2	1:C:212:LYS:NZ	2.53	0.42
1:B:190:LEU:HD13	1:B:190:LEU:C	2.40	0.41
1:A:311:TYR:CE1	1:A:353:LYS:HD2	2.55	0.41
1:D:254:ARG:O	1:D:257:ALA:HB3	2.19	0.41
1:B:234:ASP:OD2	1:B:236:ILE:HB	2.21	0.41
1:B:79:LYS:NZ	1:B:79:LYS:CB	2.83	0.41
1:B:190:LEU:HD22	1:B:217:VAL:HB	2.01	0.41
1:C:296:HIS:HB3	1:C:326:ILE:HD12	2.02	0.41
1:D:191:VAL:CG1	1:D:192:GLY:N	2.83	0.41
1:B:216:ARG:HD2	1:B:237:ALA:CB	2.49	0.41
1:D:226:PRO:C	1:D:228:ASP:N	2.74	0.41
1:A:177:GLN:O	1:A:180:GLN:HB3	2.21	0.41
1:C:248:ASP:OD2	1:C:250:GLU:HB2	2.20	0.41
1:A:132:ARG:HA	1:A:132:ARG:NE	2.35	0.41
1:D:225:ILE:HA	1:D:226:PRO:HD3	1.91	0.41
1:D:206:ARG:HH11	1:D:206:ARG:HG3	1.86	0.41
1:C:97:VAL:O	1:C:123:GLU:HA	2.21	0.41
1:C:337:VAL:HA	1:C:338:PRO:HD3	1.90	0.41
1:A:7:LYS:NZ	1:A:129:GLN:HE22	2.19	0.41
1:C:317:ILE:HG22	1:C:318:GLY:O	2.21	0.41
1:C:182:TYR:C	1:C:184:LYS:H	2.23	0.41
1:B:157:ASP:OD1	1:B:316:LEU:HA	2.20	0.41
1:B:66:ASP:OD1	1:B:94:ARG:CG	2.69	0.41
1:A:161:ALA:HB2	1:A:167:SER:HB3	2.03	0.41
1:C:103:ASN:HB2	1:C:106:VAL:HB	2.03	0.41
1:C:212:LYS:NZ	1:C:212:LYS:HB2	2.35	0.41
1:D:191:VAL:HG11	1:D:195:THR:HB	2.00	0.41
1:C:220:ASP:CG	1:C:223:LEU:HA	2.41	0.41
1:A:93:LYS:HA	1:A:93:LYS:HD3	1.83	0.41
1:A:345:ILE:CD1	1:C:352:ILE:HD12	2.51	0.41
1:B:148:VAL:HG22	1:B:287:VAL:HG13	1.99	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:206:ARG:NH1	1:D:206:ARG:HG3	2.36	0.41
1:B:77:TYR:CD1	1:B:82:PRO:HD3	2.56	0.41
1:A:329:GLU:N	5:A:585:HOH:O	2.54	0.41
1:C:190:LEU:HD23	1:C:191:VAL:N	2.36	0.40
1:B:79:LYS:HB3	1:B:79:LYS:HZ3	1.85	0.40
1:D:161:ALA:CB	1:D:167:SER:HB3	2.51	0.40
1:A:170:ILE:HG12	1:C:334:MET:CE	2.50	0.40
1:B:68:TYR:N	1:B:68:TYR:CD1	2.89	0.40
1:C:200:ASN:ND2	1:C:230:LYS:HG3	2.36	0.40
1:D:227:GLU:HG2	1:D:255:LEU:HD21	2.02	0.40
1:B:88:ILE:HG12	1:B:88:ILE:H	1.58	0.40
1:B:31:VAL:HG22	1:B:66:ASP:HB2	2.03	0.40
1:B:103:ASN:OD1	1:B:105:LEU:HD23	2.22	0.40
1:D:252:LYS:HB2	1:D:252:LYS:HZ3	1.87	0.40
1:B:155:SER:HB3	1:B:317:ILE:HG12	2.03	0.40
1:D:9:ALA:HB2	1:D:29:VAL:HG13	2.03	0.40
1:C:243:THR:CG2	1:C:244:THR:H	2.20	0.40
1:D:2:GLU:H	1:D:2:GLU:HG2	1.57	0.40
1:A:345:ILE:HD11	1:C:352:ILE:CD1	2.51	0.40
1:C:75:SER:HA	1:C:82:PRO:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	359/373 (96%)	341 (95%)	17 (5%)	1 (0%)	50	74
1	B	359/373 (96%)	320 (89%)	32 (9%)	7 (2%)	12	21
1	C	359/373 (96%)	330 (92%)	25 (7%)	4 (1%)	21	39
1	D	359/373 (96%)	322 (90%)	29 (8%)	8 (2%)	10	17
All	All	1436/1492 (96%)	1313 (91%)	103 (7%)	20 (1%)	16	30

All (20) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	C	168	LYS
1	C	291	GLY
1	D	222	VAL
1	D	231	VAL
1	D	267	THR
1	D	292	GLY
1	B	270	ILE
1	C	198	ALA
1	D	329	GLU
1	A	168	LYS
1	C	199	ASP
1	D	234	ASP
1	D	259	GLY
1	B	107	ALA
1	B	209	ASN
1	B	208	PRO
1	B	235	GLN
1	B	108	GLY
1	B	125	ILE
1	D	102	PRO

### 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	295/305 (97%)	280 (95%)	15 (5%)	33	57
1	B	294/305 (96%)	279 (95%)	15 (5%)	33	57
1	C	294/305 (96%)	274 (93%)	20 (7%)	22	40
1	D	294/305 (96%)	279 (95%)	15 (5%)	33	57
All	All	1177/1220 (96%)	1112 (94%)	65 (6%)	30	53

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	71	LEU
1	A	86	LEU

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Mol	Chain	Res	Type
1	A	128	ASP
1	A	135	GLU
1	A	138	LEU
1	A	181	GLN
1	A	193	VAL
1	A	223	LEU
1	A	243	THR
1	A	246	ARG
1	A	261	ASN
1	A	343	THR
1	A	350	ARG
1	A	360	LYS
1	B	8	LEU
1	B	12	LEU
1	B	29	VAL
1	B	72	GLU
1	B	86	LEU
1	B	88	ILE
1	B	95	VAL
1	B	128	ASP
1	B	138	LEU
1	B	223	LEU
1	B	268	GLU
1	B	272	ILE
1	B	308	ILE
1	B	337	VAL
1	B	355	THR
1	C	14	LYS
1	C	20	THR
1	C	22	SER
1	C	71	LEU
1	C	86	LEU
1	C	93	LYS
1	C	116	GLU
1	C	128	ASP
1	C	138	LEU
1	C	169	TRP
1	C	176	ARG
1	C	184	LYS
1	C	193	VAL
1	C	199	ASP
1	C	228	ASP

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Mol	Chain	Res	Type
1	C	234	ASP
1	C	264	THR
1	C	268	GLU
1	C	275	VAL
1	C	320	THR
1	D	25	LEU
1	D	71	LEU
1	D	86	LEU
1	D	93	LYS
1	D	122	ARG
1	D	125	ILE
1	D	138	LEU
1	D	173	GLU
1	D	208	PRO
1	D	213	GLN
1	D	221	THR
1	D	225	ILE
1	D	243	THR
1	D	270	ILE
1	D	335	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	53	HIS
1	A	129	GLN
1	A	181	GLN
1	A	341	GLN
1	B	23	ASN
1	B	53	HIS
1	B	61	HIS
1	B	180	GLN
1	B	187	GLN
1	B	235	GLN
1	B	271	GLN
1	B	341	GLN
1	C	23	ASN
1	C	187	GLN
1	C	341	GLN
1	D	23	ASN
1	D	53	HIS

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Mol	Chain	Res	Type
1	D	129	GLN
1	D	180	GLN
1	D	186	HIS
1	D	261	ASN
1	D	306	GLN
1	D	347	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	AI9	A	402	-	23,23,23	2.08	7 (30%)	28,33,33	1.62	5 (17%)
4	AOF	B	402	2	24,24,24	1.65	4 (16%)	32,36,36	2.89	16 (50%)
3	AI9	B	403	-	23,23,23	2.25	7 (30%)	28,33,33	1.58	5 (17%)
4	AOF	C	402	2	24,24,24	1.69	5 (20%)	32,36,36	2.78	15 (46%)
3	AI9	C	403	-	23,23,23	2.12	7 (30%)	28,33,33	1.50	5 (17%)
4	AOF	D	402	2	24,24,24	1.55	5 (20%)	32,36,36	3.04	17 (53%)
3	AI9	D	403	-	23,23,23	2.25	6 (26%)	28,33,33	1.58	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AI9	A	402	-	-	0/18/19/19	0/1/1/1
4	AOF	B	402	2	-	0/10/26/26	0/2/2/2
3	AI9	B	403	-	-	0/18/19/19	0/1/1/1
4	AOF	C	402	2	-	0/10/26/26	0/2/2/2
3	AI9	C	403	-	-	0/18/19/19	0/1/1/1
4	AOF	D	402	2	-	0/10/26/26	0/2/2/2
3	AI9	D	403	-	-	0/18/19/19	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	AI9	O2-C2	5.43	1.34	1.23
3	D	403	AI9	O2-C2	4.98	1.33	1.23
3	D	403	AI9	O4-C4	4.84	1.34	1.24
3	C	403	AI9	O2-C2	4.75	1.33	1.23
3	A	402	AI9	O2-C2	4.69	1.33	1.23
3	A	402	AI9	O4-C4	4.40	1.33	1.24
3	B	403	AI9	O4-C4	4.33	1.33	1.24
3	B	403	AI9	P-O1P	4.09	1.64	1.51
4	C	402	AOF	C4-N3	3.99	1.43	1.37
3	D	403	AI9	P-O1P	3.96	1.64	1.51
3	C	403	AI9	O4-C4	3.93	1.32	1.24
3	C	403	AI9	C5'-C4'	3.91	1.57	1.51
4	C	402	AOF	C2-N3	3.89	1.44	1.37
4	D	402	AOF	C4-N3	3.88	1.43	1.37
3	A	402	AI9	P-O1P	3.77	1.63	1.51
4	B	402	AOF	C4-N3	3.72	1.43	1.37
3	C	403	AI9	P-O1P	3.66	1.63	1.51
4	D	402	AOF	C2-N3	3.62	1.44	1.37
4	B	402	AOF	C2-N3	3.55	1.44	1.37
3	C	403	AI9	P-O2P	3.48	1.67	1.54
4	B	402	AOF	C2-N1	3.46	1.44	1.37
3	D	403	AI9	P-O3P	3.41	1.67	1.54
3	D	403	AI9	P-O2P	3.40	1.67	1.54
3	B	403	AI9	P-O2P	3.35	1.67	1.54
4	C	402	AOF	C6-N1	3.34	1.43	1.35
3	B	403	AI9	P-O3P	3.28	1.66	1.54
3	D	403	AI9	C5'-C4'	3.27	1.56	1.51
4	C	402	AOF	C2-N1	3.22	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	AOF	C6-N1	3.21	1.43	1.35
3	A	402	AI9	C5'-C4'	3.20	1.56	1.51
3	A	402	AI9	P-O2P	3.12	1.66	1.54
3	B	403	AI9	C5'-C4'	3.09	1.56	1.51
3	A	402	AI9	P-O3P	3.06	1.65	1.54
3	C	403	AI9	P-O3P	3.00	1.65	1.54
4	D	402	AOF	C6-N1	2.94	1.42	1.35
4	D	402	AOF	C2-N1	2.68	1.42	1.37
3	C	403	AI9	C6-N1'	-2.34	1.33	1.38
4	D	402	AOF	P-O1P	2.21	1.62	1.54
4	C	402	AOF	P-O1P	2.19	1.62	1.54
3	B	403	AI9	C6-N1'	-2.18	1.33	1.38
3	A	402	AI9	C6-N1'	-2.06	1.33	1.38

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	AOF	O4'-C1'-N1'	-8.69	101.44	109.91
4	C	402	AOF	O4'-C1'-N1'	-7.64	102.46	109.91
4	D	402	AOF	C6-N1'-C1'	6.97	131.30	123.15
4	B	402	AOF	C6-N1'-C1'	6.90	131.22	123.15
4	B	402	AOF	O4'-C1'-N1'	-6.44	103.63	109.91
4	B	402	AOF	O3'-C3'-C4'	-5.64	94.44	111.08
4	C	402	AOF	C6-N1'-C1'	5.55	129.64	123.15
4	D	402	AOF	O3'-C3'-C4'	-5.42	95.12	111.08
4	C	402	AOF	O3'-C3'-C4'	-4.68	97.30	111.08
4	C	402	AOF	O1P-P-O5'	-3.96	95.72	106.65
4	B	402	AOF	O1P-P-O5'	-3.91	95.84	106.65
4	D	402	AOF	O4'-C4'-C5'	-3.88	95.51	109.36
4	D	402	AOF	O1P-P-O5'	-3.85	96.02	106.65
4	B	402	AOF	C4-C5-C6	3.83	117.60	114.43
4	C	402	AOF	O4'-C4'-C5'	-3.74	95.99	109.36
4	C	402	AOF	C4-C5-C6	3.67	117.47	114.43
4	B	402	AOF	O4'-C4'-C5'	-3.62	96.42	109.36
3	A	402	AI9	C6-C5-N5	-3.52	118.43	123.83
3	B	403	AI9	C6-C5-N5	-3.32	118.73	123.83
4	B	402	AOF	O4'-C1'-C2'	-3.27	102.39	105.99
3	D	403	AI9	C6-C5-N5	-3.24	118.86	123.83
3	A	402	AI9	O5'-P-O1P	3.20	116.10	106.71
4	D	402	AOF	C4-C5-C6	3.19	117.07	114.43
4	D	402	AOF	O4'-C1'-C2'	-3.15	102.52	105.99
3	C	403	AI9	C6-C5-N5	-3.13	119.03	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	AOF	C4-N3-C2	-3.12	119.04	125.36
4	C	402	AOF	C4-N3-C2	-3.06	119.16	125.36
4	B	402	AOF	C3'-C2'-C1'	3.03	107.35	101.35
4	C	402	AOF	C3'-C2'-C1'	3.02	107.33	101.35
4	B	402	AOF	O2P-P-O5'	3.01	114.96	106.65
3	A	402	AI9	C2-N1-C6	2.96	121.47	117.78
4	D	402	AOF	C5-C6-N1	2.96	123.93	115.37
3	B	403	AI9	O5'-P-O1P	2.95	115.35	106.71
4	D	402	AOF	O3'-C3'-C2'	2.93	121.38	111.83
4	D	402	AOF	C4-N3-C2	-2.90	119.48	125.36
4	B	402	AOF	C5-C4-N3	2.87	121.32	113.95
4	D	402	AOF	C3'-C2'-C1'	2.85	106.99	101.35
4	D	402	AOF	O2P-P-O5'	2.84	114.48	106.65
4	C	402	AOF	C5-C4-N3	2.83	121.22	113.95
3	C	403	AI9	C2-N1-C6	2.83	121.31	117.78
3	D	403	AI9	C2-N1-C6	2.82	121.29	117.78
4	C	402	AOF	O2P-P-O5'	2.82	114.43	106.65
4	C	402	AOF	C5-C6-N1	2.81	123.52	115.37
4	C	402	AOF	O3'-C3'-C2'	2.76	120.82	111.83
4	D	402	AOF	C5-C4-N3	2.73	120.96	113.95
4	B	402	AOF	C5-C6-N1	2.70	123.19	115.37
3	D	403	AI9	O5'-P-O1P	2.69	114.60	106.71
4	D	402	AOF	O2'-C2'-C1'	2.67	119.13	110.04
4	B	402	AOF	O3'-C3'-C2'	2.63	120.39	111.83
3	A	402	AI9	O4'-C4'-C5'	-2.61	104.75	110.12
3	B	403	AI9	C2-N1-C6	2.60	121.02	117.78
4	B	402	AOF	O2'-C2'-C1'	2.57	118.77	110.04
4	C	402	AOF	C4'-O4'-C1'	2.47	114.38	108.62
4	B	402	AOF	C5'-C4'-C3'	2.44	125.01	115.21
4	D	402	AOF	C4'-O4'-C1'	2.39	114.19	108.62
4	B	402	AOF	C4'-O4'-C1'	2.38	114.17	108.62
4	C	402	AOF	O2'-C2'-C1'	2.28	117.78	110.04
3	B	403	AI9	C5'-C4'-C3'	-2.27	107.77	112.06
3	C	403	AI9	O5'-P-O1P	2.23	113.25	106.71
4	D	402	AOF	C5'-C4'-C3'	2.22	124.12	115.21
3	A	402	AI9	O3'-C3'-C2'	-2.21	104.92	108.86
4	D	402	AOF	N1'-C6-N1	-2.15	115.28	120.09
3	D	403	AI9	O4'-C4'-C5'	-2.15	105.71	110.12
4	C	402	AOF	C5'-C4'-C3'	2.14	123.78	115.21
3	D	403	AI9	O2'-C2'-C3'	2.08	114.00	109.70
3	C	403	AI9	C5-C4-N3	2.06	119.24	113.95
3	C	403	AI9	C4-N3-C2	-2.03	121.24	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	AI9	C5-C4-N3	2.01	119.12	113.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	361/373 (96%)	0.09	11 (3%)	48 48	33, 49, 64, 78	0
1	B	361/373 (96%)	0.34	23 (6%)	19 17	40, 58, 73, 85	0
1	C	361/373 (96%)	0.52	36 (9%)	8 6	42, 60, 77, 84	0
1	D	361/373 (96%)	0.55	42 (11%)	5 4	37, 61, 82, 87	0
All	All	1444/1492 (96%)	0.37	112 (7%)	13 11	33, 56, 77, 87	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	169	TRP	8.0
1	B	-1	GLY	6.5
1	C	105	LEU	6.5
1	B	208	PRO	6.4
1	B	169	TRP	6.0
1	B	209	ASN	6.0
1	D	207	LEU	5.8
1	D	80	THR	5.8
1	D	77	TYR	5.5
1	D	209	ASN	5.2
1	C	209	ASN	5.2
1	D	211	THR	5.1
1	C	210	VAL	5.1
1	C	77	TYR	5.0
1	D	208	PRO	4.9
1	D	79	LYS	4.8
1	B	77	TYR	4.8
1	D	78	GLY	4.5
1	B	105	LEU	4.2
1	C	207	LEU	4.2
1	C	-1	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	81	PRO	4.1
1	C	208	PRO	4.1
1	A	211	THR	3.9
1	B	207	LEU	3.9
1	B	0	SER	3.9
1	A	208	PRO	3.7
1	D	258	PHE	3.7
1	C	104	PRO	3.7
1	D	255	LEU	3.6
1	C	106	VAL	3.6
1	D	247	ALA	3.6
1	C	211	THR	3.6
1	C	50	ALA	3.5
1	D	213	GLN	3.4
1	D	212	LYS	3.4
1	B	210	VAL	3.4
1	C	246	ARG	3.3
1	A	360	LYS	3.3
1	D	205	CYS	3.3
1	C	78	GLY	3.2
1	D	246	ARG	3.2
1	D	269	ARG	3.2
1	C	81	PRO	3.1
1	D	227	GLU	3.0
1	B	50	ALA	3.0
1	B	211	THR	2.9
1	C	235	GLN	2.9
1	B	104	PRO	2.9
1	C	236	ILE	2.9
1	D	168	LYS	2.9
1	D	105	LEU	2.8
1	C	20	THR	2.8
1	C	9	ALA	2.7
1	A	266	GLU	2.7
1	D	-1	GLY	2.7
1	C	82	PRO	2.7
1	B	78	GLY	2.7
1	D	257	ALA	2.7
1	D	222	VAL	2.6
1	D	189	ILE	2.6
1	D	250	GLU	2.6
1	B	255	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	105	LEU	2.6
1	B	41	ALA	2.5
1	C	206	ARG	2.5
1	B	76	HIS	2.5
1	D	253	LYS	2.5
1	C	258	PHE	2.5
1	D	249	GLU	2.5
1	B	206	ARG	2.5
1	B	205	CYS	2.4
1	D	210	VAL	2.4
1	D	281	GLU	2.4
1	A	291	GLY	2.4
1	C	227	GLU	2.4
1	D	233	CYS	2.4
1	C	93	LYS	2.4
1	C	116	GLU	2.3
1	C	113	MET	2.3
1	A	132	ARG	2.3
1	C	152	ALA	2.3
1	C	80	THR	2.3
1	C	291	GLY	2.3
1	A	40	GLY	2.3
1	D	289	VAL	2.3
1	D	230	LYS	2.3
1	A	310	PHE	2.2
1	C	255	LEU	2.2
1	B	28	ALA	2.2
1	C	168	LYS	2.2
1	A	209	ASN	2.2
1	A	289	VAL	2.2
1	B	191	VAL	2.2
1	D	262	ILE	2.2
1	B	329	GLU	2.2
1	C	76	HIS	2.1
1	D	206	ARG	2.1
1	D	313	ALA	2.1
1	C	335	LYS	2.1
1	D	301	LYS	2.1
1	D	266	GLU	2.1
1	B	331	PHE	2.1
1	B	268	GLU	2.1
1	C	184	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	250	GLU	2.1
1	D	163	SER	2.0
1	D	226	PRO	2.0
1	C	289	VAL	2.0
1	D	199	ASP	2.0
1	C	212	LYS	2.0
1	D	104	PRO	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	A	401	1/1	0.16	0.92	39,39,39,39	0
3	AI9	C	403	23/23	0.20	0.31	62,73,80,81	0
4	AOF	D	402	23/23	0.23	0.07	71,73,76,77	0
3	AI9	B	403	23/23	0.20	0.06	70,78,81,83	0
3	AI9	D	403	23/23	0.19	-0.13	75,77,81,81	0
3	AI9	A	402	23/23	0.14	-0.26	52,60,62,63	0
4	AOF	B	402	23/23	0.17	-0.55	63,66,69,72	0
4	AOF	C	402	23/23	0.16	-0.72	67,72,74,74	0
2	ZN	D	401	1/1	0.05	-1.14	53,53,53,53	0
2	ZN	B	401	1/1	0.14	-1.42	63,63,63,63	0
2	ZN	C	401	1/1	0.08	-1.67	69,69,69,69	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.