



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:46 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 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

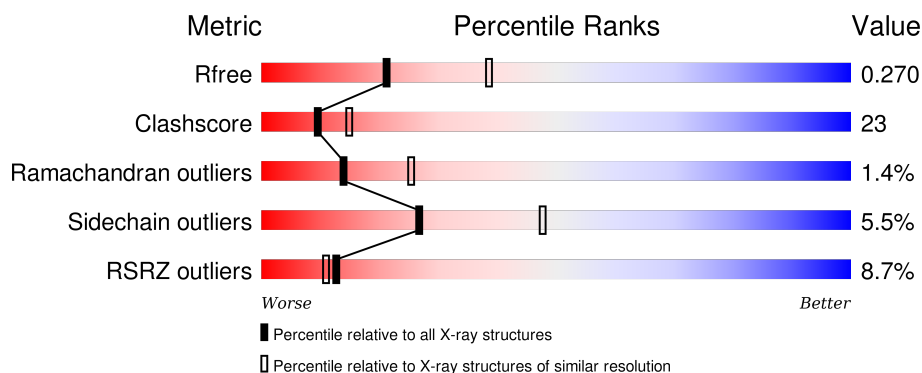
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	91344	3324 (2.60-2.52)
Clashscore	102246	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (2.60-2.52)
RSRZ outliers	91569	3333 (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 ≥ 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	373	<div> <div>4%</div> <div>71% 24% . .</div> </div>
1	B	373	<div> <div>6%</div> <div>58% 36% . .</div> </div>
1	C	373	<div> <div>11%</div> <div>60% 34% . .</div> </div>
1	D	373	<div> <div>12%</div> <div>56% 36% 5% .</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11519 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 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

Continued on next page...

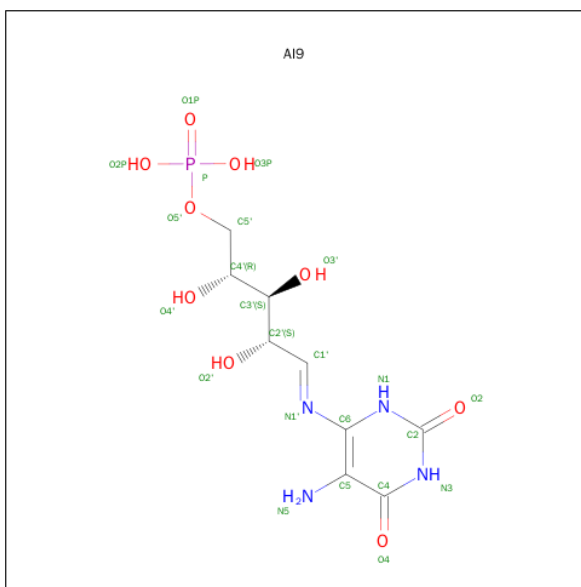
Continued from previous page...

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).

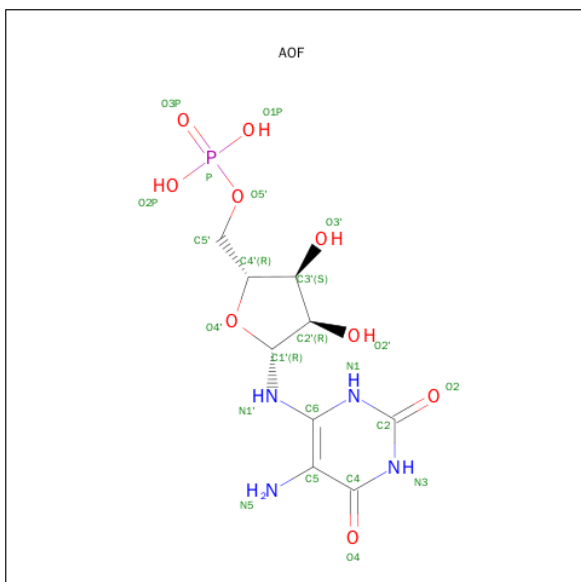
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- 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: C₉H₁₅N₄O₉P).



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		

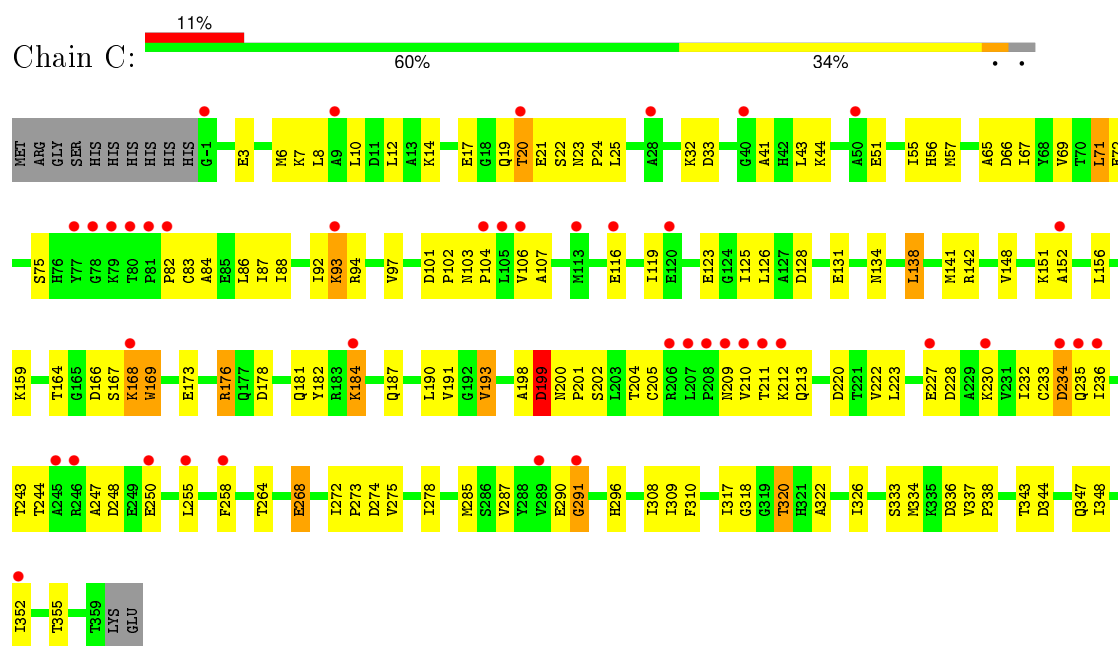
- Molecule 4 is N-(5-AMINO-2,6-DIOXO-1,2,3,6-TETRAHYDROPYRIMIDIN-4-YL)-5-O-PHOSPHONO-BETA-D-RIBOFURANOSYLAMINE (three-letter code: AOF) (formula: $C_9H_{15}N_4O_9P$).



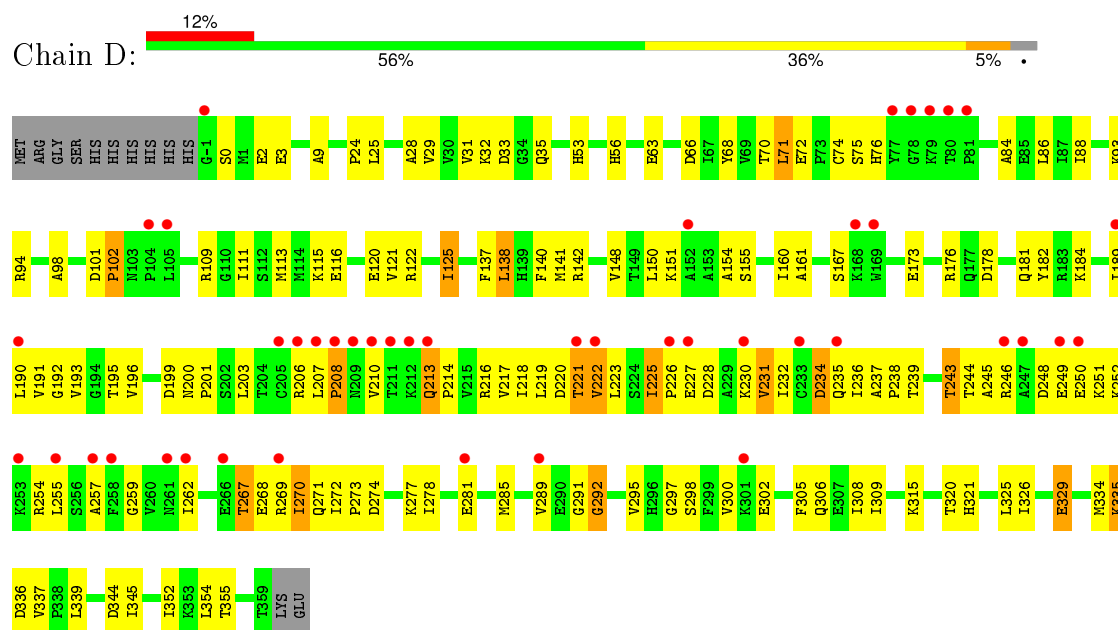
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
4	C	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
4	D	1	Total	C	N	O	P	0	0
			23	9	4	9	1		

- 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		



• Molecule 1: Riboflavin biosynthesis protein RibD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.57Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.222 , 0.270 0.222 , 0.270	Depositor DCC
R_{free} test set	5745 reflections (10.18%)	DCC
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
3	A	23	0	15	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 23.

All (506) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:THR:HG22	1:C:244:THR:H	1.39	0.84
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	46	68
1	B	359/373 (96%)	320 (89%)	32 (9%)	7 (2%)	10	17
1	C	359/373 (96%)	330 (92%)	25 (7%)	4 (1%)	17	33
1	D	359/373 (96%)	322 (90%)	29 (8%)	8 (2%)	8	13
All	All	1436/1492 (96%)	1313 (91%)	103 (7%)	20 (1%)	14	25

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%)	29	51
1	B	294/305 (96%)	279 (95%)	15 (5%)	29	51
1	C	294/305 (96%)	274 (93%)	20 (7%)	20	36
1	D	294/305 (96%)	279 (95%)	15 (5%)	29	51
All	All	1177/1220 (96%)	1112 (94%)	65 (6%)	27	48

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 [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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	-	18,23,23	2.09	7 (38%)	18,33,33	2.55	7 (38%)
4	AOF	B	402	2	19,24,24	1.80	2 (10%)	19,36,36	2.76	10 (52%)
3	AI9	B	403	-	18,23,23	2.20	6 (33%)	18,33,33	2.50	5 (27%)
4	AOF	C	402	2	19,24,24	1.88	3 (15%)	19,36,36	2.65	11 (57%)
3	AI9	C	403	-	18,23,23	2.10	6 (33%)	18,33,33	2.33	4 (22%)
4	AOF	D	402	2	19,24,24	1.79	3 (15%)	19,36,36	2.73	10 (52%)
3	AI9	D	403	-	18,23,23	2.29	7 (38%)	18,33,33	2.52	5 (27%)

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	-	-	0/16/19/19	0/1/1/1
4	AOF	B	402	2	-	0/10/26/26	0/2/2/2
3	AI9	B	403	-	-	0/16/19/19	0/1/1/1
4	AOF	C	402	2	-	0/10/26/26	0/2/2/2
3	AI9	C	403	-	-	0/16/19/19	0/1/1/1
4	AOF	D	402	2	-	0/10/26/26	0/2/2/2
3	AI9	D	403	-	-	0/16/19/19	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	AI9	C5-C6	2.02	1.43	1.40
4	C	402	AOF	P-O1P	2.23	1.62	1.54
4	D	402	AOF	P-O1P	2.25	1.62	1.54
3	C	403	AI9	C4-N3	2.55	1.37	1.33
3	D	403	AI9	C5-C6	2.60	1.44	1.40
3	A	402	AI9	C4-N3	3.02	1.38	1.33
3	D	403	AI9	C4-N3	3.03	1.38	1.33
3	C	403	AI9	P-O3P	3.05	1.65	1.54
3	A	402	AI9	P-O3P	3.12	1.65	1.54
3	C	403	AI9	O4-C4	3.13	1.32	1.24
3	A	402	AI9	P-O2P	3.18	1.66	1.54
3	B	403	AI9	C5'-C4'	3.21	1.56	1.51
3	A	402	AI9	C5'-C4'	3.33	1.56	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	AI9	P-O3P	3.34	1.66	1.54
3	B	403	AI9	C4-N3	3.34	1.39	1.33
3	D	403	AI9	C5'-C4'	3.40	1.56	1.51
3	B	403	AI9	P-O2P	3.41	1.67	1.54
3	B	403	AI9	O4-C4	3.46	1.33	1.24
3	D	403	AI9	P-O2P	3.47	1.67	1.54
3	D	403	AI9	P-O3P	3.47	1.67	1.54
3	A	402	AI9	O4-C4	3.52	1.33	1.24
3	C	403	AI9	P-O2P	3.55	1.67	1.54
3	C	403	AI9	P-O1P	3.75	1.63	1.51
3	A	402	AI9	P-O1P	3.86	1.63	1.51
3	D	403	AI9	O4-C4	3.88	1.34	1.24
3	D	403	AI9	P-O1P	4.05	1.64	1.51
3	C	403	AI9	C5'-C4'	4.06	1.57	1.51
3	B	403	AI9	P-O1P	4.19	1.64	1.51
4	D	402	AOF	C6-N1	4.35	1.42	1.34
4	B	402	AOF	C6-N1	4.68	1.43	1.34
4	C	402	AOF	C6-N1	4.84	1.43	1.34
4	B	402	AOF	C4-N3	5.57	1.43	1.33
4	D	402	AOF	C4-N3	5.72	1.43	1.33
4	C	402	AOF	C4-N3	5.82	1.43	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	AOF	O3'-C3'-C4'	-5.54	94.44	111.05
4	D	402	AOF	O3'-C3'-C4'	-5.31	95.12	111.05
4	C	402	AOF	O3'-C3'-C4'	-4.59	97.30	111.05
4	D	402	AOF	O4'-C4'-C5'	-3.86	95.51	109.32
4	C	402	AOF	O1P-P-O5'	-3.77	95.72	106.56
4	C	402	AOF	O4'-C4'-C5'	-3.73	95.99	109.32
4	B	402	AOF	O1P-P-O5'	-3.72	95.84	106.56
4	D	402	AOF	O1P-P-O5'	-3.66	96.02	106.56
4	B	402	AOF	O4'-C4'-C5'	-3.61	96.42	109.32
3	A	402	AI9	O4'-C4'-C5'	-2.50	104.75	110.19
3	A	402	AI9	O3'-C3'-C2'	-2.27	104.92	108.93
3	A	402	AI9	C6-C5-N5	-2.22	118.43	121.63
3	D	403	AI9	O4'-C4'-C5'	-2.06	105.71	110.19
3	B	403	AI9	C6-C5-N5	-2.01	118.73	121.63
4	C	402	AOF	O2P-P-O1P	2.00	115.00	107.38
3	C	403	AI9	C6-N1'-C1'	2.10	124.60	120.40
4	C	402	AOF	C5'-C4'-C3'	2.16	123.78	115.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	AOF	C5'-C4'-C3'	2.25	124.12	115.21
4	C	402	AOF	O2'-C2'-C1'	2.25	117.78	109.94
3	C	403	AI9	O5'-P-O1P	2.40	113.25	107.14
4	B	402	AOF	C5'-C4'-C3'	2.47	125.01	115.21
4	B	402	AOF	O2'-C2'-C1'	2.53	118.77	109.94
4	B	402	AOF	O3'-C3'-C2'	2.63	120.39	111.83
4	D	402	AOF	O2'-C2'-C1'	2.63	119.13	109.94
4	C	402	AOF	O2P-P-O5'	2.73	114.43	106.56
4	D	402	AOF	O2P-P-O5'	2.75	114.48	106.56
4	C	402	AOF	O3'-C3'-C2'	2.76	120.82	111.83
3	A	402	AI9	C6-N1'-C1'	2.77	125.94	120.40
4	D	402	AOF	C3'-C2'-C1'	2.79	106.99	101.40
3	B	403	AI9	C6-N1'-C1'	2.88	126.16	120.40
4	B	402	AOF	O2P-P-O5'	2.92	114.96	106.56
3	D	403	AI9	O5'-P-O1P	2.93	114.60	107.14
4	D	402	AOF	O3'-C3'-C2'	2.94	121.38	111.83
4	C	402	AOF	C3'-C2'-C1'	2.96	107.33	101.40
4	B	402	AOF	C3'-C2'-C1'	2.97	107.35	101.40
3	D	403	AI9	C6-N1'-C1'	3.02	126.43	120.40
3	B	403	AI9	O5'-P-O1P	3.22	115.35	107.14
4	D	402	AOF	C4-C5-C6	3.32	117.07	114.43
3	A	402	AI9	O5'-P-O1P	3.52	116.10	107.14
3	B	403	AI9	C2-N1-C6	3.80	121.02	114.85
4	C	402	AOF	C4-C5-C6	3.81	117.47	114.43
3	D	403	AI9	C2-N1-C6	3.97	121.29	114.85
3	C	403	AI9	C2-N1-C6	3.98	121.31	114.85
4	B	402	AOF	C4-C5-C6	3.98	117.60	114.43
3	A	402	AI9	C2-N1-C6	4.08	121.47	114.85
4	B	402	AOF	C4-N3-C2	4.39	119.04	115.25
4	C	402	AOF	C4-N3-C2	4.52	119.16	115.25
4	D	402	AOF	C4-N3-C2	4.90	119.48	115.25
3	C	403	AI9	C4-N3-C2	6.93	121.24	115.25
3	A	402	AI9	C4-N3-C2	7.27	121.53	115.25
3	D	403	AI9	C4-N3-C2	7.42	121.66	115.25
3	B	403	AI9	C4-N3-C2	7.50	121.73	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	AI9	1	0
3	B	403	AI9	2	0
4	C	402	AOF	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, 95th 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	361/373 (96%)	0.10	16 (4%)	38 35	33, 49, 64, 78	0
1	B	361/373 (96%)	0.34	23 (6%)	23 20	40, 58, 73, 85	0
1	C	361/373 (96%)	0.56	42 (11%)	6 5	42, 60, 77, 84	0
1	D	361/373 (96%)	0.57	44 (12%)	5 5	37, 61, 82, 87	0
All	All	1444/1492 (96%)	0.39	125 (8%)	13 11	33, 56, 77, 87	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-1	GLY	7.5
1	D	169	TRP	7.2
1	C	105	LEU	6.9
1	B	169	TRP	6.2
1	B	208	PRO	6.1
1	D	80	THR	5.9
1	D	209	ASN	5.8
1	D	207	LEU	5.7
1	D	208	PRO	5.7
1	D	79	LYS	5.6
1	D	77	TYR	5.5
1	C	210	VAL	5.5
1	D	211	THR	5.4
1	C	209	ASN	5.2
1	D	78	GLY	5.0
1	B	209	ASN	5.0
1	B	0	SER	5.0
1	B	105	LEU	4.8
1	C	208	PRO	4.6
1	B	77	TYR	4.6
1	A	208	PRO	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	211	THR	4.4
1	C	-1	GLY	4.3
1	C	78	GLY	4.1
1	D	81	PRO	4.0
1	C	104	PRO	4.0
1	C	235	GLN	3.9
1	C	77	TYR	3.9
1	D	247	ALA	3.8
1	C	207	LEU	3.8
1	C	106	VAL	3.7
1	C	236	ILE	3.7
1	D	246	ARG	3.7
1	D	205	CYS	3.7
1	C	211	THR	3.6
1	D	213	GLN	3.5
1	D	250	GLU	3.4
1	D	212	LYS	3.4
1	D	227	GLU	3.4
1	C	246	ARG	3.3
1	C	81	PRO	3.3
1	D	255	LEU	3.3
1	B	210	VAL	3.3
1	A	360	LYS	3.3
1	B	104	PRO	3.3
1	D	222	VAL	3.2
1	D	249	GLU	3.2
1	D	258	PHE	3.2
1	C	79	LYS	3.2
1	D	269	ARG	3.2
1	C	82	PRO	3.1
1	D	210	VAL	3.1
1	C	20	THR	3.0
1	C	50	ALA	3.0
1	C	152	ALA	3.0
1	B	207	LEU	3.0
1	D	105	LEU	3.0
1	D	-1	GLY	2.9
1	A	266	GLU	2.8
1	B	50	ALA	2.8
1	D	281	GLU	2.8
1	C	80	THR	2.8
1	C	230	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	257	ALA	2.8
1	B	41	ALA	2.8
1	B	211	THR	2.7
1	C	291	GLY	2.7
1	B	78	GLY	2.7
1	D	189	ILE	2.6
1	B	206	ARG	2.6
1	C	234	ASP	2.6
1	D	235	GLN	2.6
1	B	76	HIS	2.6
1	D	104	PRO	2.5
1	C	206	ARG	2.5
1	A	291	GLY	2.5
1	C	116	GLU	2.5
1	A	40	GLY	2.5
1	D	262	ILE	2.5
1	D	301	LYS	2.5
1	B	28	ALA	2.5
1	D	261	ASN	2.5
1	C	28	ALA	2.5
1	B	205	CYS	2.4
1	D	206	ARG	2.4
1	C	93	LYS	2.4
1	C	245	ALA	2.4
1	A	105	LEU	2.4
1	D	226	PRO	2.4
1	A	132	ARG	2.4
1	C	184	LYS	2.4
1	B	255	LEU	2.4
1	C	289	VAL	2.3
1	D	233	CYS	2.3
1	D	266	GLU	2.3
1	D	289	VAL	2.3
1	A	28	ALA	2.3
1	C	258	PHE	2.3
1	C	255	LEU	2.3
1	C	9	ALA	2.3
1	D	168	LYS	2.3
1	A	289	VAL	2.3
1	C	40	GLY	2.2
1	B	191	VAL	2.2
1	C	212	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	209	ASN	2.2
1	A	310	PHE	2.2
1	C	227	GLU	2.2
1	D	253	LYS	2.2
1	A	41	ALA	2.2
1	A	309	ILE	2.2
1	D	190	LEU	2.2
1	A	39	MET	2.2
1	D	152	ALA	2.1
1	D	230	LYS	2.1
1	A	45	TYR	2.1
1	B	329	GLU	2.1
1	C	168	LYS	2.1
1	C	250	GLU	2.1
1	C	113	MET	2.1
1	B	3	GLU	2.1
1	C	120	GLU	2.0
1	C	352	ILE	2.0
1	D	221	THR	2.0
1	B	291	GLY	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 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, 95th 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 ²)	Q<0.9
2	ZN	A	401	1/1	0.98	0.16	0.89	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	AI9	C	403	23/23	0.89	0.20	0.21	62,73,80,81	0
4	AOF	D	402	23/23	0.86	0.24	0.15	71,73,76,77	0
3	AI9	B	403	23/23	0.84	0.20	0.05	70,78,81,83	0
3	AI9	A	402	23/23	0.95	0.14	-0.26	52,60,62,63	0
3	AI9	D	403	23/23	0.87	0.18	-0.27	75,77,81,81	0
4	AOF	C	402	23/23	0.92	0.18	-0.44	67,72,74,74	0
4	AOF	B	402	23/23	0.90	0.17	-0.51	63,66,69,72	0
2	ZN	B	401	1/1	0.98	0.12	-1.22	63,63,63,63	0
2	ZN	D	401	1/1	0.99	0.04	-1.27	53,53,53,53	0
2	ZN	C	401	1/1	1.00	0.07	-1.62	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.