



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 11:36 PM GMT

PDB ID : 2PMI  
Title : Structure of the Pho85-Pho80 CDK-cyclin Complex of the Phosphate-responsive Signal Transduction Pathway with Bound ATP-gamma-S  
Authors : Huang, K.; Ferrin-O'Connell, I.; Zhang, W.; Leonard, G.A.; O'Shea, E.K.; Quiocho, F.A.  
Deposited on : 2007-04-23  
Resolution : 2.90 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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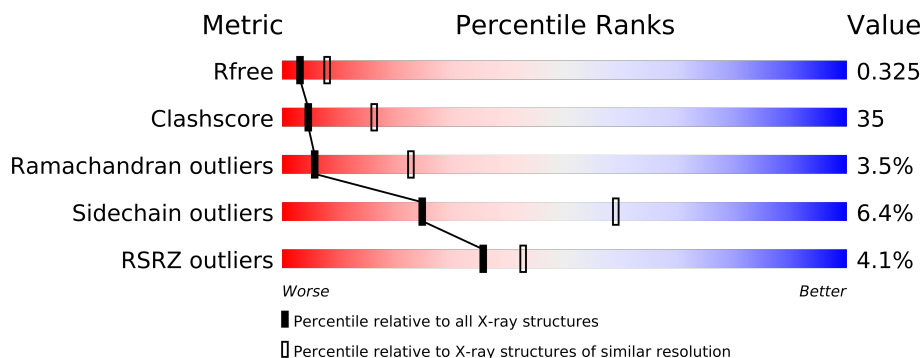
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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	317	
1	C	317	
2	B	293	
2	D	293	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8138 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 Cyclin-dependent protein kinase PHO85.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	49	0	0
			2298	1476	394	417	11			
1	C	285	Total	C	N	O	S	58	0	0
			2316	1491	397	417	11			

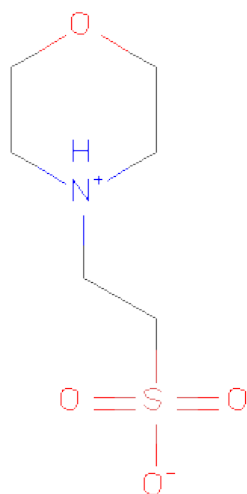
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	MET	-	EXPRESSION TAG	UNP P17157
A	307	GLY	-	EXPRESSION TAG	UNP P17157
A	308	GLY	-	EXPRESSION TAG	UNP P17157
A	309	SER	-	EXPRESSION TAG	UNP P17157
A	310	ARG	-	EXPRESSION TAG	UNP P17157
A	311	SER	-	EXPRESSION TAG	UNP P17157
A	312	HIS	-	EXPRESSION TAG	UNP P17157
A	313	HIS	-	EXPRESSION TAG	UNP P17157
A	314	HIS	-	EXPRESSION TAG	UNP P17157
A	315	HIS	-	EXPRESSION TAG	UNP P17157
A	316	HIS	-	EXPRESSION TAG	UNP P17157
A	317	HIS	-	EXPRESSION TAG	UNP P17157
C	306	MET	-	EXPRESSION TAG	UNP P17157
C	307	GLY	-	EXPRESSION TAG	UNP P17157
C	308	GLY	-	EXPRESSION TAG	UNP P17157
C	309	SER	-	EXPRESSION TAG	UNP P17157
C	310	ARG	-	EXPRESSION TAG	UNP P17157
C	311	SER	-	EXPRESSION TAG	UNP P17157
C	312	HIS	-	EXPRESSION TAG	UNP P17157
C	313	HIS	-	EXPRESSION TAG	UNP P17157
C	314	HIS	-	EXPRESSION TAG	UNP P17157
C	315	HIS	-	EXPRESSION TAG	UNP P17157
C	316	HIS	-	EXPRESSION TAG	UNP P17157
C	317	HIS	-	EXPRESSION TAG	UNP P17157

- Molecule 2 is a protein called PHO85 cyclin PHO80.

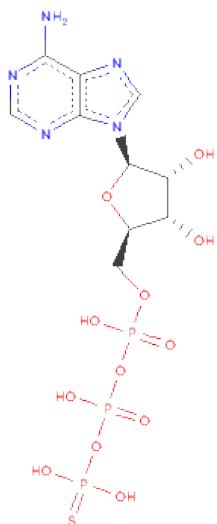
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	13	0	0
			1722	1109	298	308	7			
2	D	216	Total	C	N	O	S	14	0	0
			1747	1124	303	313	7			

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is PHOSPHOTHIOPHOSPHORICACID-ADENYLATE ESTER (three-letter code: AGS) (formula:  $C_{10}H_{16}N_5O_{12}P_3S$ ).

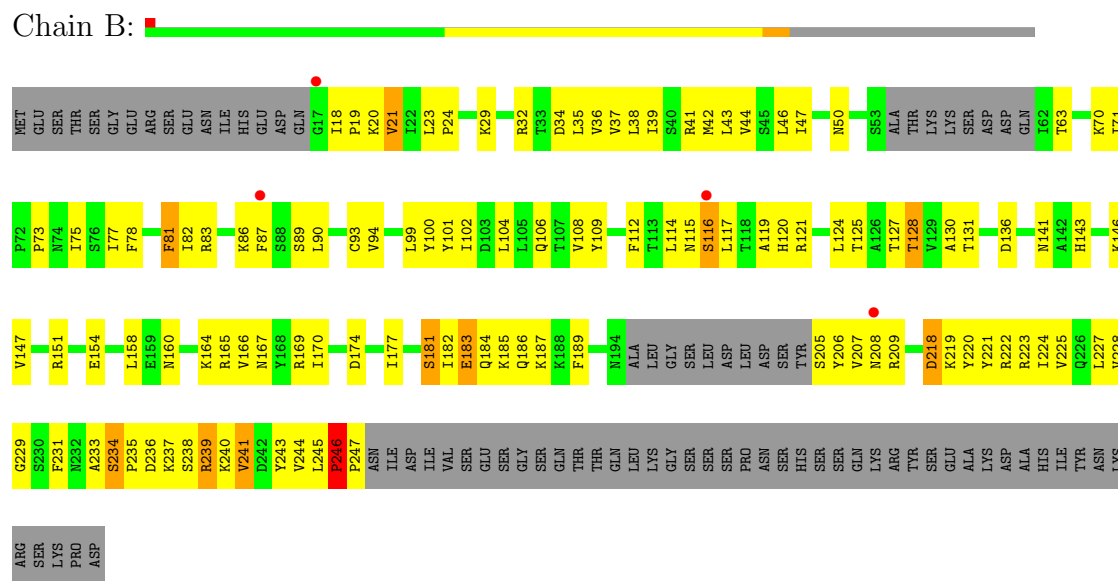


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	A	1	31	10	5	12	3	1	0	0



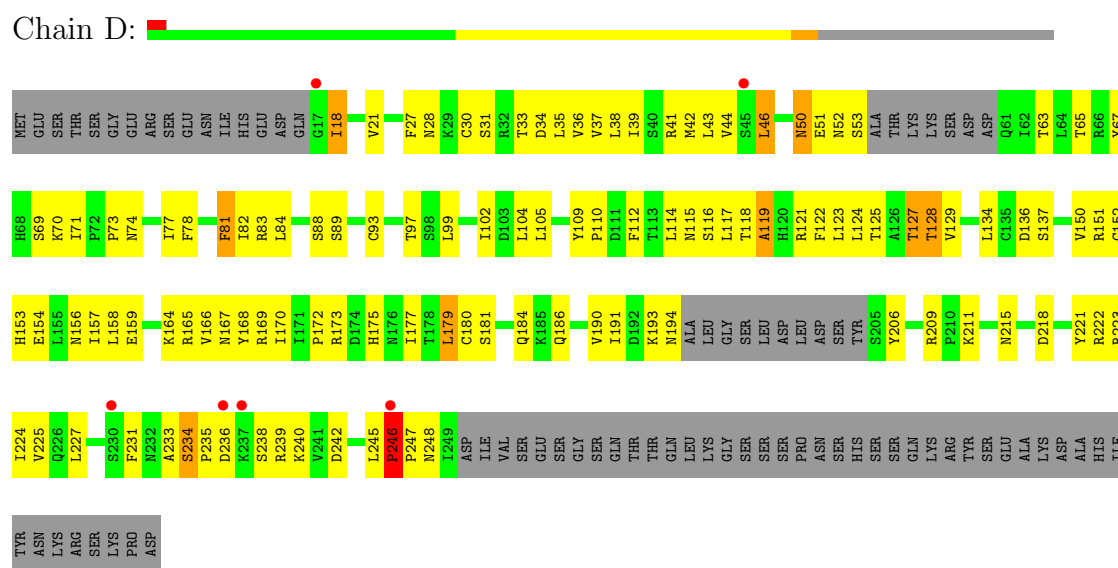
- Molecule 2: PHO85 cyclin PHO80

Chain B:



- Molecule 2: PHO85 cyclin PHO80

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.59Å 146.59Å 212.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.98 – 2.90 14.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.2 (14.98-2.90) 91.1 (14.98-2.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.289 , 0.325 0.289 , 0.325	Depositor DCC
$R_{free}$ test set	2707 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 22.2	EDS
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 53704 reflections	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	8138	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: AGS, MES

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	0.39	0/2354	0.62	1/3192 (0.0%)
1	C	0.34	0/2370	0.58	0/3207
2	B	0.43	0/1757	0.65	0/2380
2	D	0.43	0/1782	0.63	0/2414
All	All	0.40	0/8263	0.62	1/11193 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	LEU	CA-CB-CG	5.72	128.46	115.30

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	2298	0	2316	125	0
1	C	2316	0	2344	211	0
2	B	1722	0	1771	134	0
2	D	1747	0	1796	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	13	0	0
3	D	12	0	13	2	0
4	A	31	0	12	1	0
All	All	8138	0	8265	562	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 35.

All (562) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:255:ARG:HH21	1:A:259:GLN:HG2	1.14	1.09
1:A:116:GLN:NE2	1:A:147:LEU:H	1.50	1.08
1:A:39:LYS:H	1:A:39:LYS:HD3	1.17	1.05
1:A:193:TRP:HB2	1:A:285:ARG:HH11	1.23	1.03
2:D:218:ASP:HB3	2:D:222:ARG:HH22	1.28	0.98
1:C:193:TRP:HB2	1:C:285:ARG:HH21	1.30	0.92
1:A:56:LEU:HD22	1:A:129:ILE:HD13	1.52	0.91
2:B:218:ASP:HB3	2:B:222:ARG:HH12	1.36	0.91
1:A:259:GLN:HE22	1:A:266:LEU:H	1.10	0.90
1:A:116:GLN:HE22	1:A:147:LEU:H	0.93	0.89
1:C:175:ARG:HB3	1:C:180:LEU:HD21	1.53	0.89
2:D:44:VAL:HG21	2:D:235:PRO:HD3	1.54	0.89
2:D:246:PRO:HB2	2:D:247:PRO:HD3	1.54	0.88
1:C:139:LEU:HB3	1:C:147:LEU:HD11	1.57	0.87
1:C:135:LYS:HG3	1:C:137:GLN:HG2	1.53	0.87
2:D:33:THR:O	2:D:37:VAL:HG23	1.75	0.87
2:B:124:LEU:O	2:B:127:THR:HG22	1.76	0.86
1:C:101:THR:HG23	1:C:102:PRO:HD2	1.58	0.84
1:A:116:GLN:HE22	1:A:147:LEU:N	1.75	0.82
1:C:243:ASN:HB3	1:C:246:ILE:HG23	1.61	0.82
1:C:57:MET:HA	1:C:57:MET:HE2	1.62	0.82
2:B:34:ASP:O	2:B:37:VAL:HG22	1.79	0.81
1:A:193:TRP:HB2	1:A:285:ARG:NH1	1.95	0.81
2:D:109:TYR:CD2	2:D:112:PHE:HB2	2.16	0.80
1:A:87:ASN:HD22	1:A:87:ASN:H	1.27	0.80
1:C:209:PHE:CE2	1:C:221:ILE:HA	2.17	0.80
1:A:255:ARG:NH2	1:A:259:GLN:HG2	1.97	0.79
1:C:242:TYR:O	1:C:244:PRO:HD3	1.83	0.79
2:B:245:LEU:HD12	2:B:246:PRO:HD2	1.63	0.79
2:D:104:LEU:HD21	2:D:166:VAL:HG11	1.65	0.78
1:C:164:THR:HA	2:D:136:ASP:OD2	1.83	0.78
1:A:26:ASN:HB3	1:A:29:THR:O	1.84	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:74:THR:HG23	1:C:77:LYS:HB2	1.67	0.76
2:B:47:ILE:HG21	2:B:116:SER:HB3	1.68	0.76
1:A:212:THR:H	1:A:216:GLU:HG2	1.52	0.75
1:A:156:ARG:HH12	1:A:164:THR:HB	1.50	0.75
2:D:31:SER:HB3	2:D:34:ASP:OD2	1.85	0.75
2:B:73:PRO:HG2	2:B:120:HIS:HD2	1.50	0.75
2:B:41:ARG:HA	2:B:235:PRO:HG3	1.69	0.74
1:C:125:HIS:CE1	1:C:188:THR:HG23	2.21	0.74
1:C:107:LEU:HD21	1:C:266:LEU:HD23	1.68	0.74
2:B:43:LEU:HD11	2:B:102:ILE:HD11	1.69	0.73
1:C:60:LEU:HD21	1:C:129:ILE:HD12	1.69	0.73
2:B:223:ARG:NH1	2:B:227:LEU:HG	2.02	0.73
2:B:101:TYR:OH	2:B:170:ILE:HB	1.88	0.73
2:B:106:GLN:HE21	2:B:114:LEU:H	1.36	0.73
2:D:218:ASP:HB3	2:D:222:ARG:NH2	2.03	0.73
1:A:236:VAL:HG23	1:A:239:LEU:HD12	1.71	0.72
1:A:97:THR:HG21	1:A:103:ARG:HB2	1.70	0.72
2:D:123:LEU:O	2:D:127:THR:HB	1.89	0.72
2:B:233:ALA:O	2:B:234:SER:OG	2.07	0.72
2:B:218:ASP:CB	2:B:222:ARG:HH12	2.03	0.72
1:C:7:PHE:CE1	1:C:35:LEU:HD21	2.25	0.72
1:A:117:LEU:HD12	1:A:149:LEU:HD21	1.72	0.72
1:C:207:PRO:HB2	1:C:210:PRO:HG3	1.70	0.71
1:C:253:ASP:O	1:C:257:VAL:HG23	1.89	0.71
1:A:287:SER:H	1:A:290:GLN:HE21	1.39	0.70
1:C:7:PHE:HE1	1:C:35:LEU:HD21	1.57	0.70
1:C:63:GLU:O	1:C:148:LYS:HE2	1.90	0.70
1:C:181:MET:HB2	1:C:239:LEU:HD13	1.73	0.69
1:C:10:LEU:HB2	1:C:23:LYS:HB3	1.73	0.69
1:C:255:ARG:NH2	1:C:259:GLN:HE21	1.91	0.68
2:D:44:VAL:CG2	2:D:235:PRO:HD3	2.21	0.68
2:B:225:VAL:HG11	2:B:245:LEU:HB2	1.75	0.68
1:A:207:PRO:HB2	1:A:210:PRO:HG3	1.76	0.68
1:C:219:LYS:HG2	1:C:249:ARG:HH12	1.57	0.68
1:A:56:LEU:HD22	1:A:129:ILE:CD1	2.24	0.68
2:D:124:LEU:O	2:D:128:THR:HG23	1.93	0.68
1:A:106:GLU:OE2	1:A:108:ASN:HB2	1.94	0.67
1:C:279:GLN:HB2	1:C:285:ARG:HD2	1.76	0.67
1:C:237:THR:HA	1:C:242:TYR:CD1	2.30	0.67
2:D:211:LYS:HD3	2:D:215:ASN:OD1	1.94	0.67
2:D:221:TYR:O	2:D:225:VAL:HG23	1.95	0.66
1:A:209:PHE:HB3	1:A:217:GLN:NE2	2.11	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:182:GLY:HA3	1:A:240:PRO:HG2	1.78	0.66
1:C:114:GLN:NE2	1:C:199:LEU:HB2	2.11	0.66
2:B:20:LYS:HE3	2:B:244:VAL:HG21	1.77	0.65
1:A:168:GLU:OE1	2:D:152:CYS:N	2.28	0.65
1:C:181:MET:CE	1:C:242:TYR:HA	2.27	0.65
1:C:255:ARG:HA	1:C:271:MET:HE2	1.77	0.65
1:C:141:ILE:HA	1:C:146:GLN:O	1.97	0.64
1:C:193:TRP:CB	1:C:285:ARG:HH21	2.06	0.64
1:C:119:GLN:NE2	1:C:292:LEU:HD13	2.13	0.64
2:D:42:MET:CE	2:D:227:LEU:HD12	2.27	0.64
1:C:8:LYS:HB3	1:C:25:LEU:H	1.62	0.64
1:C:194:SER:O	1:C:198:ILE:HG12	1.98	0.63
1:A:212:THR:N	1:A:216:GLU:HG2	2.13	0.63
2:D:51:GLU:C	2:D:53:SER:H	2.01	0.63
1:A:161:PRO:HG2	2:B:93:CYS:SG	2.39	0.63
1:C:209:PHE:CB	1:C:217:GLN:HE22	2.12	0.63
1:C:255:ARG:HG2	1:C:271:MET:HE2	1.81	0.63
1:C:236:VAL:HG13	1:C:237:THR:N	2.14	0.63
2:D:77:ILE:HD13	2:D:119:ALA:HB1	1.80	0.63
2:B:20:LYS:CE	2:B:244:VAL:HG21	2.28	0.63
1:A:87:ASN:H	1:A:87:ASN:ND2	1.94	0.62
1:C:121:LEU:HG	1:C:125:HIS:CD2	2.34	0.62
1:C:209:PHE:HB3	1:C:217:GLN:HE22	1.64	0.62
1:C:130:LEU:HD12	1:C:158:PHE:CE2	2.34	0.62
2:B:38:LEU:HB3	2:B:224:ILE:HD12	1.82	0.62
1:A:29:THR:HB	1:A:31:VAL:HG12	1.81	0.62
2:B:234:SER:N	2:B:235:PRO:HD2	2.15	0.62
1:C:23:LYS:HG2	1:C:24:GLY:H	1.64	0.62
2:D:36:VAL:HG11	2:D:82:ILE:HG22	1.82	0.62
1:C:233:TRP:HB2	1:C:281:ASN:HB2	1.81	0.62
2:B:109:TYR:CD2	2:B:112:PHE:HB2	2.35	0.62
1:A:214:ASP:N	1:A:214:ASP:OD2	2.33	0.62
2:D:190:VAL:HG23	2:D:191:ILE:HG12	1.81	0.62
1:C:107:LEU:HD12	1:C:107:LEU:N	2.15	0.61
1:C:265:PRO:O	1:C:266:LEU:HD23	2.00	0.61
2:D:104:LEU:HD21	2:D:166:VAL:CG1	2.31	0.61
1:A:259:GLN:HE22	1:A:266:LEU:N	1.92	0.61
2:D:129:VAL:HG22	2:D:159:GLU:HG3	1.81	0.61
1:C:267:ASP:OD2	1:C:269:ASN:HB3	2.00	0.61
1:C:213:ASN:OD1	1:C:215:GLU:HB3	2.00	0.61
2:B:47:ILE:HG23	2:B:116:SER:H	1.65	0.61
2:B:231:PHE:CZ	2:B:240:LYS:HG3	2.35	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:37:VAL:HG23	2:B:38:LEU:N	2.16	0.61
1:C:298:ALA:C	1:C:300:TYR:H	2.03	0.61
2:D:42:MET:HE1	2:D:227:LEU:HB2	1.83	0.61
1:A:144:ARG:HD3	1:A:144:ARG:N	2.15	0.61
1:A:39:LYS:CD	1:A:39:LYS:H	1.99	0.60
2:B:77:ILE:HD12	2:B:120:HIS:CE1	2.36	0.60
1:C:72:ILE:HB	1:C:79:THR:OG1	2.00	0.60
1:A:116:GLN:NE2	1:A:147:LEU:N	2.35	0.60
1:A:57:MET:HA	1:A:57:MET:HE2	1.82	0.60
1:C:243:ASN:CB	1:C:246:ILE:HG23	2.32	0.60
1:C:107:LEU:HD21	1:C:266:LEU:CD2	2.30	0.60
1:C:39:LYS:C	1:C:39:LYS:HD3	2.21	0.60
1:A:287:SER:H	1:A:290:GLN:NE2	2.00	0.59
1:C:181:MET:HE2	1:C:242:TYR:HA	1.84	0.59
2:D:165:ARG:HG2	2:D:165:ARG:HH11	1.67	0.59
1:C:26:ASN:HB3	1:C:29:THR:O	2.01	0.59
1:C:73:HIS:CG	2:D:164:LYS:HE2	2.37	0.59
2:B:234:SER:H	2:B:235:PRO:HD2	1.67	0.59
1:C:193:TRP:HB2	1:C:285:ARG:NH2	2.12	0.59
2:D:43:LEU:HD11	2:D:102:ILE:CD1	2.32	0.59
1:C:132:ARG:HD3	1:C:154:LEU:O	2.02	0.59
2:D:181:SER:O	2:D:184:GLN:HB2	2.02	0.58
1:A:107:LEU:HB2	1:A:264:GLU:OE1	2.03	0.58
1:A:39:LYS:HD3	1:A:39:LYS:N	2.01	0.58
1:C:161:PRO:HG2	2:D:93:CYS:SG	2.42	0.58
1:A:233:TRP:N	1:A:234:PRO:HD3	2.19	0.58
1:C:209:PHE:HB3	1:C:217:GLN:NE2	2.18	0.58
2:B:82:ILE:HG13	2:B:83:ARG:N	2.18	0.58
1:C:247:GLN:O	1:C:249:ARG:HG3	2.04	0.58
1:C:125:HIS:ND1	1:C:188:THR:HG23	2.18	0.58
2:B:73:PRO:CG	2:B:120:HIS:HD2	2.17	0.58
1:C:199:LEU:HD13	1:C:274:LEU:HD13	1.85	0.58
2:B:42:MET:HE3	2:B:227:LEU:HD12	1.86	0.58
2:B:70:LYS:O	2:B:71:ILE:HG23	2.04	0.58
1:C:61:LYS:HE2	1:C:61:LYS:HA	1.86	0.58
2:D:233:ALA:O	2:D:234:SER:OG	2.19	0.57
1:C:223:ASP:O	1:C:252:ARG:HD3	2.04	0.57
1:C:221:ILE:HG13	1:C:222:PHE:HD2	1.69	0.57
1:A:107:LEU:HD13	1:A:264:GLU:CD	2.24	0.57
2:D:127:THR:HG22	2:D:128:THR:HG22	1.86	0.57
1:C:161:PRO:CG	2:D:28:ASN:HD21	2.17	0.57
2:B:125:THR:OG1	2:B:158:LEU:HG	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:194:SER:O	1:A:198:ILE:HG12	2.04	0.57
2:D:46:LEU:O	2:D:50:ASN:HB2	2.05	0.57
1:C:172:LEU:O	1:C:175:ARG:HB2	2.05	0.57
2:B:160:ASN:ND2	2:B:164:LYS:NZ	2.53	0.57
1:A:101:THR:HB	1:A:102:PRO:CD	2.35	0.57
1:C:255:ARG:HG2	1:C:271:MET:CE	2.35	0.57
1:A:87:ASN:HD22	1:A:87:ASN:N	1.92	0.56
1:A:66:VAL:HG21	1:A:140:LEU:HD22	1.86	0.56
2:B:233:ALA:HB3	2:B:235:PRO:HD2	1.87	0.56
2:B:43:LEU:HD11	2:B:102:ILE:CD1	2.35	0.56
1:A:222:PHE:CE2	1:A:228:PRO:HD3	2.40	0.56
1:C:117:LEU:HD13	1:C:139:LEU:HD21	1.86	0.56
1:A:25:LEU:HD12	1:A:25:LEU:O	2.06	0.56
1:A:125:HIS:ND1	1:A:188:THR:HB	2.21	0.56
1:C:297:PHE:O	1:C:299:GLU:N	2.39	0.56
2:B:205:SER:OG	2:B:207:VAL:HG23	2.06	0.56
1:C:85:MET:HB2	1:C:140:LEU:HD23	1.87	0.55
2:D:127:THR:HG22	2:D:128:THR:N	2.21	0.55
1:C:87:ASN:O	1:C:140:LEU:HA	2.06	0.55
1:C:38:VAL:CG1	1:C:47:PRO:HG2	2.37	0.55
2:D:206:TYR:O	2:D:209:ARG:HB3	2.07	0.55
1:A:21:VAL:HG23	1:A:35:LEU:C	2.27	0.55
1:A:33:VAL:C	1:A:84:PHE:HB2	2.27	0.55
2:D:165:ARG:HG2	2:D:165:ARG:NH1	2.22	0.55
2:B:104:LEU:HD21	2:B:166:VAL:HG13	1.89	0.55
1:C:175:ARG:NE	1:C:179:VAL:HG11	2.22	0.55
1:A:40:LEU:HB2	1:A:76:ASN:HA	1.89	0.55
1:C:10:LEU:CB	1:C:23:LYS:HB3	2.37	0.55
1:A:97:THR:HG23	1:A:97:THR:O	2.07	0.54
2:B:234:SER:C	2:B:236:ASP:H	2.11	0.54
2:B:223:ARG:HH12	2:B:227:LEU:HG	1.69	0.54
2:D:166:VAL:O	2:D:166:VAL:HG12	2.08	0.54
2:B:47:ILE:CG2	2:B:116:SER:HB3	2.37	0.54
1:C:62:HIS:HB2	1:C:123:PHE:CD2	2.43	0.54
1:C:117:LEU:HD12	1:C:149:LEU:HD21	1.89	0.54
1:A:111:LYS:HG3	1:A:297:PHE:CE1	2.43	0.54
1:C:177:PRO:HB3	1:C:221:ILE:HD11	1.89	0.54
1:A:164:THR:HA	2:B:136:ASP:OD2	2.07	0.54
2:B:231:PHE:CE2	2:B:236:ASP:HA	2.43	0.54
1:C:6:GLN:OE1	1:C:72:ILE:HD13	2.07	0.54
2:D:37:VAL:O	2:D:41:ARG:HG3	2.07	0.53
2:B:82:ILE:O	2:B:86:LYS:HG2	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:66:VAL:HG23	1:C:149:LEU:O	2.08	0.53
1:A:125:HIS:CE1	1:A:188:THR:HB	2.43	0.53
2:D:168:TYR:O	2:D:170:ILE:N	2.41	0.53
1:C:7:PHE:HB2	1:C:25:LEU:O	2.08	0.53
1:A:63:GLU:O	1:A:148:LYS:HE2	2.08	0.53
1:C:107:LEU:CD1	1:C:107:LEU:H	2.21	0.53
2:D:231:PHE:CE2	2:D:236:ASP:HA	2.44	0.53
1:C:57:MET:HA	1:C:57:MET:CE	2.36	0.53
1:C:227:THR:HG21	1:C:248:GLN:HA	1.91	0.53
1:C:142:ASN:HD21	1:C:146:GLN:HB2	1.74	0.53
2:B:221:TYR:O	2:B:224:ILE:HG12	2.09	0.53
1:C:114:GLN:HE22	1:C:199:LEU:HB2	1.73	0.53
1:C:127:ASN:O	1:C:129:ILE:HG13	2.08	0.53
2:B:104:LEU:HD12	2:B:177:ILE:HG12	1.91	0.53
1:C:282:PRO:C	1:C:284:MET:H	2.12	0.52
2:B:77:ILE:CG2	2:B:78:PHE:N	2.72	0.52
2:D:167:ASN:N	2:D:167:ASN:HD22	2.06	0.52
2:D:246:PRO:O	2:D:248:ASN:N	2.36	0.52
2:D:102:ILE:HD13	2:D:114:LEU:HD22	1.91	0.52
2:B:104:LEU:HD21	2:B:166:VAL:CG1	2.39	0.52
2:D:99:LEU:HD12	2:D:102:ILE:HD12	1.91	0.52
2:D:84:LEU:O	2:D:88:SER:HB2	2.09	0.52
2:D:246:PRO:HB2	2:D:247:PRO:CD	2.35	0.52
2:B:104:LEU:O	2:B:108:VAL:HG22	2.10	0.52
2:B:225:VAL:O	2:B:229:GLY:HA3	2.09	0.52
1:C:121:LEU:HD13	1:C:134:LEU:HD11	1.92	0.52
1:A:138:ASN:O	1:A:139:LEU:HD23	2.08	0.52
1:A:73:HIS:O	1:A:74:THR:HB	2.09	0.52
1:C:175:ARG:CB	1:C:180:LEU:HD21	2.34	0.52
2:B:41:ARG:HG2	2:B:235:PRO:HG2	1.91	0.52
1:A:97:THR:CG2	1:A:103:ARG:HB2	2.40	0.52
1:C:126:GLU:OE2	1:C:126:GLU:HA	2.09	0.52
1:C:282:PRO:O	1:C:284:MET:N	2.42	0.52
2:B:160:ASN:ND2	2:B:164:LYS:HE3	2.24	0.52
2:B:46:LEU:O	2:B:50:ASN:HB2	2.10	0.52
1:A:229:ASN:O	1:A:231:SER:N	2.41	0.52
1:C:222:PHE:CE1	1:C:228:PRO:HD3	2.45	0.52
1:C:253:ASP:OD1	1:C:256:GLN:HG2	2.09	0.52
1:C:161:PRO:HG2	2:D:28:ASN:HD21	1.75	0.52
1:C:258:LEU:CD1	1:C:274:LEU:HD21	2.39	0.51
1:C:270:LEU:HD13	1:C:296:TRP:CE2	2.45	0.51
1:C:279:GLN:HG3	1:C:284:MET:HB3	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:236:VAL:CG1	1:C:237:THR:N	2.73	0.51
2:D:81:PHE:CG	2:D:123:LEU:HD21	2.46	0.51
2:B:166:VAL:O	2:B:166:VAL:HG12	2.10	0.51
1:C:208:LEU:HG	1:C:209:PHE:CZ	2.45	0.51
1:C:26:ASN:OD1	1:C:27:LYS:N	2.43	0.51
2:D:246:PRO:CB	2:D:247:PRO:HD3	2.35	0.51
1:C:93:MET:CE	1:C:202:MET:HA	2.40	0.51
1:C:142:ASN:ND2	1:C:146:GLN:HB2	2.25	0.51
1:A:101:THR:HB	1:A:102:PRO:HD2	1.92	0.51
2:B:34:ASP:O	2:B:37:VAL:CG2	2.56	0.51
2:D:46:LEU:HD23	2:D:46:LEU:N	2.25	0.51
1:C:106:GLU:HA	1:C:264:GLU:OE2	2.11	0.51
1:A:209:PHE:CB	1:A:217:GLN:NE2	2.73	0.51
1:A:21:VAL:HG22	1:A:22:TYR:N	2.26	0.51
1:A:96:ARG:HG3	1:A:96:ARG:HH11	1.76	0.51
1:C:243:ASN:HB3	1:C:246:ILE:CG2	2.38	0.51
2:D:65:THR:HG22	2:D:109:TYR:OH	2.11	0.51
1:A:135:LYS:HA	1:A:198:ILE:HD11	1.93	0.51
1:A:26:ASN:O	1:A:29:THR:O	2.29	0.50
2:D:77:ILE:CD1	2:D:119:ALA:HB1	2.41	0.50
2:B:185:LYS:C	2:B:186:GLN:HE21	2.14	0.50
2:D:150:VAL:HG23	2:D:151:ARG:O	2.11	0.50
1:A:94:ASP:O	1:A:98:VAL:N	2.43	0.50
1:C:90:LYS:HD2	1:C:137:GLN:NE2	2.26	0.50
2:D:42:MET:HE1	2:D:227:LEU:HD12	1.93	0.50
1:A:227:THR:HG21	1:A:248:GLN:HA	1.94	0.50
2:B:124:LEU:O	2:B:128:THR:HG23	2.12	0.50
2:B:234:SER:N	2:B:235:PRO:CD	2.74	0.50
1:C:87:ASN:HD22	1:C:87:ASN:N	2.10	0.50
1:A:73:HIS:HA	1:A:78:LEU:HD12	1.93	0.50
1:C:89:LEU:HD12	1:C:139:LEU:HD12	1.93	0.50
1:C:107:LEU:CD1	1:C:107:LEU:N	2.74	0.50
1:C:233:TRP:HZ3	1:C:280:LEU:HB3	1.75	0.50
1:C:62:HIS:HB3	1:C:65:ILE:HD12	1.94	0.50
2:B:42:MET:HE1	2:B:227:LEU:CB	2.42	0.50
1:C:224:ILE:HG22	1:C:224:ILE:O	2.12	0.50
2:B:82:ILE:HG13	2:B:83:ARG:H	1.77	0.50
2:B:184:GLN:HA	2:B:184:GLN:OE1	2.12	0.50
2:D:73:PRO:HG3	3:D:2001:MES:H22	1.94	0.50
2:B:219:LYS:HA	2:B:222:ARG:NH2	2.26	0.49
1:C:116:GLN:HE22	1:C:146:GLN:HA	1.76	0.49
1:C:299:GLU:HG3	1:C:300:TYR:CD2	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:66:VAL:HG13	1:A:83:GLU:HG2	1.94	0.49
1:C:59:GLU:HG3	2:D:173:ARG:NH1	2.26	0.49
1:C:83:GLU:OE2	1:C:148:LYS:HD2	2.12	0.49
2:D:35:LEU:O	2:D:39:ILE:HG13	2.11	0.49
1:C:119:GLN:HE22	1:C:292:LEU:HD13	1.78	0.49
2:B:42:MET:CE	2:B:227:LEU:HD12	2.42	0.49
1:A:130:LEU:HD12	1:A:130:LEU:N	2.28	0.49
2:D:44:VAL:HG21	2:D:235:PRO:CD	2.35	0.49
2:D:109:TYR:CD2	2:D:112:PHE:CB	2.93	0.49
2:D:109:TYR:CE2	2:D:112:PHE:HB2	2.47	0.49
1:A:211:GLY:HA2	1:A:216:GLU:HG2	1.93	0.49
1:C:217:GLN:O	1:C:221:ILE:HG23	2.13	0.49
1:A:65:ILE:O	1:A:66:VAL:C	2.51	0.49
1:C:106:GLU:HG3	1:C:109:LEU:H	1.78	0.49
1:C:73:HIS:CD2	2:D:164:LYS:HG2	2.47	0.49
2:B:37:VAL:HG21	2:B:243:TYR:OH	2.13	0.49
1:C:177:PRO:HB3	1:C:221:ILE:CD1	2.43	0.49
1:A:236:VAL:CG2	1:A:239:LEU:HD12	2.40	0.49
1:C:255:ARG:HH21	1:C:259:GLN:HE21	1.56	0.49
1:A:209:PHE:CE2	1:A:221:ILE:HA	2.47	0.49
1:C:237:THR:HA	1:C:242:TYR:CE1	2.47	0.49
1:C:33:VAL:HG22	1:C:82:PHE:O	2.13	0.49
2:B:44:VAL:HG21	2:B:235:PRO:HD3	1.94	0.48
1:C:270:LEU:HD13	1:C:296:TRP:CZ2	2.47	0.48
1:C:279:GLN:HG3	1:C:284:MET:CB	2.43	0.48
1:A:138:ASN:ND2	1:A:151:ASP:HB3	2.28	0.48
1:C:31:VAL:HG13	1:C:31:VAL:O	2.14	0.48
2:D:184:GLN:O	2:D:186:GLN:NE2	2.47	0.48
1:C:140:LEU:N	1:C:140:LEU:HD12	2.28	0.48
2:B:115:ASN:O	2:B:117:LEU:N	2.39	0.48
1:C:198:ILE:O	1:C:199:LEU:C	2.50	0.48
2:D:104:LEU:HD13	2:D:177:ILE:HG12	1.94	0.48
1:C:137:GLN:H	1:C:137:GLN:CD	2.13	0.48
1:A:119:GLN:HE22	1:A:292:LEU:HD13	1.77	0.48
2:B:36:VAL:HG13	2:B:81:PHE:CD2	2.49	0.48
1:C:198:ILE:O	1:C:201:GLU:N	2.45	0.48
1:C:156:ARG:CZ	1:C:162:VAL:HG23	2.44	0.48
2:B:41:ARG:HG2	2:B:235:PRO:CG	2.44	0.48
1:C:33:VAL:HG21	1:C:81:VAL:CG1	2.44	0.48
2:B:127:THR:HG23	2:B:128:THR:N	2.29	0.47
2:B:82:ILE:O	2:B:86:LYS:N	2.41	0.47
2:B:160:ASN:HD21	2:B:164:LYS:NZ	2.11	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:82:ILE:HG13	2:D:83:ARG:N	2.27	0.47
1:A:80:LEU:N	1:A:80:LEU:HD23	2.30	0.47
1:C:166:SER:HB3	1:C:175:ARG:HH21	1.79	0.47
2:B:23:LEU:HD11	2:B:243:TYR:HB3	1.97	0.47
1:C:201:GLU:HG3	1:C:206:LYS:C	2.35	0.47
1:C:216:GLU:O	1:C:219:LYS:N	2.46	0.47
1:A:96:ARG:HG3	1:A:96:ARG:NH1	2.30	0.47
2:D:97:THR:HG21	2:D:134:LEU:HD11	1.96	0.47
1:C:104:GLY:O	1:C:105:LEU:HD23	2.14	0.47
1:C:101:THR:HG23	1:C:102:PRO:CD	2.36	0.47
2:D:18:ILE:HD12	2:D:242:ASP:OD2	2.14	0.47
2:D:121:ARG:HG2	2:D:121:ARG:NH1	2.29	0.47
2:B:47:ILE:HG23	2:B:116:SER:N	2.28	0.47
2:B:99:LEU:HD12	2:B:102:ILE:HD12	1.96	0.47
1:C:181:MET:HE1	1:C:242:TYR:HA	1.96	0.47
2:D:51:GLU:C	2:D:53:SER:N	2.68	0.47
2:D:36:VAL:HG12	2:D:78:PHE:CE2	2.49	0.47
1:C:299:GLU:HG3	1:C:300:TYR:HD2	1.78	0.47
1:C:298:ALA:C	1:C:300:TYR:N	2.68	0.47
2:D:67:TYR:O	2:D:118:THR:HA	2.15	0.47
1:A:170:VAL:HG23	1:A:171:THR:HG23	1.97	0.47
1:C:88:ASP:HA	1:C:139:LEU:O	2.14	0.47
2:D:166:VAL:HG13	2:D:180:CYS:SG	2.55	0.47
2:B:77:ILE:HA	2:B:120:HIS:HE1	1.80	0.47
2:B:101:TYR:HH	2:B:170:ILE:HB	1.80	0.47
2:B:151:ARG:O	2:B:154:GLU:HB2	2.14	0.47
2:D:231:PHE:CE2	2:D:240:LYS:HA	2.50	0.47
2:B:47:ILE:HD11	2:B:119:ALA:HB2	1.96	0.46
1:C:106:GLU:O	1:C:110:VAL:HG23	2.15	0.46
1:A:131:HIS:O	1:A:132:ARG:HB2	2.15	0.46
1:A:87:ASN:HB2	1:A:91:LYS:HB3	1.97	0.46
2:B:143:HIS:HE1	2:D:137:SER:OG	1.99	0.46
2:D:99:LEU:O	2:D:102:ILE:HB	2.15	0.46
1:C:203:ILE:HG22	1:C:204:THR:N	2.30	0.46
1:C:201:GLU:HG3	1:C:206:LYS:O	2.15	0.46
1:C:93:MET:HE3	1:C:202:MET:HA	1.96	0.46
1:C:8:LYS:HB3	1:C:25:LEU:HB2	1.98	0.46
1:C:269:ASN:ND2	1:C:296:TRP:HA	2.30	0.46
2:B:207:VAL:O	2:B:208:ASN:HB2	2.15	0.46
1:C:175:ARG:HE	1:C:179:VAL:HG11	1.81	0.46
2:B:18:ILE:HG21	2:B:240:LYS:HG2	1.97	0.46
1:C:62:HIS:CE1	1:C:64:ASN:HB2	2.51	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:271:MET:HE3	1:A:271:MET:HA	1.97	0.46
1:A:112:TYR:O	1:A:115:TRP:HB3	2.16	0.46
2:B:37:VAL:CG2	2:B:38:LEU:N	2.79	0.46
1:A:211:GLY:HA2	1:A:216:GLU:CG	2.45	0.46
2:B:239:ARG:HE	2:B:239:ARG:CA	2.28	0.46
1:A:39:LYS:HA	1:A:77:LYS:HA	1.98	0.46
2:D:18:ILE:HG22	2:D:240:LYS:CG	2.46	0.46
1:A:254:LEU:HD12	1:A:275:HIS:NE2	2.31	0.46
1:C:273:PHE:CE2	1:C:291:ALA:HB1	2.51	0.46
1:C:248:GLN:C	1:C:249:ARG:HG3	2.36	0.45
2:B:239:ARG:HB3	2:B:241:VAL:HG23	1.97	0.45
2:D:38:LEU:HB3	2:D:224:ILE:HD12	1.97	0.45
1:A:44:GLU:HA	2:B:141:ASN:H	1.81	0.45
1:C:36:LYS:HD3	1:C:80:LEU:HD12	1.98	0.45
1:C:254:LEU:HD23	1:C:254:LEU:O	2.17	0.45
2:B:94:VAL:HG13	2:B:130:ALA:HB3	1.98	0.45
2:D:234:SER:H	2:D:235:PRO:HD2	1.82	0.45
1:C:23:LYS:CG	1:C:24:GLY:H	2.27	0.45
2:B:154:GLU:O	2:B:158:LEU:HB2	2.16	0.45
2:B:89:SER:CB	2:D:89:SER:OG	2.64	0.45
2:D:109:TYR:HA	2:D:110:PRO:HD2	1.72	0.45
2:B:246:PRO:HA	2:B:247:PRO:HD3	1.84	0.45
2:B:160:ASN:CG	2:B:164:LYS:HE3	2.36	0.45
1:C:181:MET:HG2	1:C:218:LEU:HD11	1.97	0.45
2:D:43:LEU:HD11	2:D:102:ILE:HD11	1.98	0.45
2:B:160:ASN:ND2	2:B:164:LYS:CE	2.79	0.45
2:B:37:VAL:HG23	2:B:38:LEU:H	1.81	0.45
1:C:201:GLU:OE1	1:C:207:PRO:HA	2.16	0.45
1:C:23:LYS:HG2	1:C:24:GLY:N	2.30	0.45
1:C:269:ASN:OD1	1:C:295:PRO:HB2	2.17	0.45
1:C:298:ALA:O	1:C:300:TYR:N	2.48	0.45
2:B:35:LEU:O	2:B:36:VAL:C	2.54	0.45
1:C:135:LYS:HG3	1:C:137:GLN:CG	2.37	0.45
1:A:209:PHE:N	1:A:210:PRO:HD3	2.32	0.45
1:C:294:HIS:CE1	1:C:296:TRP:H	2.33	0.45
2:B:70:LYS:O	2:B:71:ILE:CG2	2.64	0.45
1:A:237:THR:O	2:D:74:ASN:ND2	2.43	0.45
1:C:259:GLN:N	1:C:260:PRO:HD2	2.32	0.44
2:D:153:HIS:O	2:D:156:ASN:HB2	2.17	0.44
2:B:127:THR:CG2	2:B:128:THR:N	2.80	0.44
2:B:90:LEU:HD13	2:B:127:THR:OG1	2.18	0.44
1:C:187:SER:OG	1:C:188:THR:N	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:233:TRP:CD1	1:C:235:SER:HB2	2.52	0.44
2:D:167:ASN:ND2	2:D:167:ASN:N	2.65	0.44
1:A:140:LEU:N	1:A:140:LEU:HD12	2.32	0.44
1:A:64:ASN:HA	1:A:148:LYS:HG2	1.98	0.44
2:D:115:ASN:O	2:D:117:LEU:N	2.45	0.44
2:D:109:TYR:CZ	2:D:165:ARG:NE	2.86	0.44
1:C:10:LEU:HB3	1:C:11:GLU:H	1.60	0.44
1:C:115:TRP:O	1:C:119:GLN:HB2	2.17	0.44
2:B:23:LEU:HA	2:B:24:PRO:HD3	1.79	0.44
2:B:20:LYS:HE2	2:B:244:VAL:HG21	2.00	0.44
2:D:42:MET:HE3	2:D:227:LEU:HD12	1.96	0.44
1:C:54:ILE:HD11	1:C:80:LEU:HD21	2.00	0.44
1:A:58:LYS:HE3	2:B:167:ASN:O	2.18	0.44
1:C:193:TRP:NE1	1:C:197:CYS:SG	2.91	0.44
2:B:222:ARG:HG3	2:B:222:ARG:HH11	1.82	0.44
1:C:107:LEU:HD12	1:C:107:LEU:H	1.80	0.44
1:C:253:ASP:CG	1:C:256:GLN:HG2	2.37	0.44
2:B:24:PRO:HG2	2:B:29:LYS:O	2.18	0.44
2:D:168:TYR:O	2:D:170:ILE:HG13	2.18	0.44
2:B:44:VAL:CG2	2:B:235:PRO:HD3	2.47	0.43
2:D:73:PRO:CG	3:D:2001:MES:H22	2.48	0.43
2:D:51:GLU:O	2:D:53:SER:N	2.51	0.43
2:B:151:ARG:HB3	1:C:168:GLU:OE2	2.18	0.43
2:B:182:ILE:O	2:B:184:GLN:N	2.51	0.43
2:B:143:HIS:O	2:B:147:VAL:HG23	2.17	0.43
1:C:209:PHE:N	1:C:210:PRO:HD3	2.33	0.43
1:C:209:PHE:HB2	1:C:217:GLN:HE22	1.82	0.43
2:D:127:THR:CG2	2:D:128:THR:N	2.79	0.43
1:C:214:ASP:N	1:C:214:ASP:OD2	2.48	0.43
1:A:25:LEU:HD23	1:A:32:TYR:CE2	2.53	0.43
1:A:229:ASN:C	1:A:231:SER:H	2.22	0.43
2:B:18:ILE:CG2	2:B:240:LYS:HE2	2.49	0.43
2:B:42:MET:HE1	2:B:227:LEU:HB2	1.99	0.43
2:B:42:MET:HA	2:B:228:VAL:HG11	1.99	0.43
2:D:102:ILE:HG13	2:D:122:PHE:CE2	2.53	0.43
1:C:57:MET:HE1	1:C:152:PHE:CD1	2.54	0.43
1:C:219:LYS:O	1:C:222:PHE:N	2.51	0.43
1:C:213:ASN:O	1:C:215:GLU:N	2.52	0.43
2:D:105:LEU:O	2:D:109:TYR:HB3	2.18	0.43
1:C:38:VAL:HB	1:C:78:LEU:HB3	2.00	0.43
2:B:109:TYR:CD2	2:B:165:ARG:HD3	2.54	0.43
2:B:207:VAL:C	2:B:209:ARG:H	2.22	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:106:GLU:O	1:C:106:GLU:HG3	2.18	0.43
2:B:39:ILE:HG23	2:B:99:LEU:HD13	2.00	0.43
2:B:151:ARG:HH22	1:C:214:ASP:H	1.66	0.43
2:B:169:ARG:HD2	2:B:183:GLU:OE1	2.18	0.43
2:D:121:ARG:HH22	2:D:154:GLU:HG2	1.83	0.43
1:A:258:LEU:O	1:A:259:GLN:C	2.57	0.43
2:B:75:ILE:O	2:B:75:ILE:HG23	2.19	0.43
2:B:235:PRO:O	2:B:236:ASP:C	2.57	0.43
2:B:109:TYR:CZ	2:B:165:ARG:CZ	3.02	0.42
1:C:132:ARG:NH1	1:C:156:ARG:HB2	2.34	0.42
1:A:52:ARG:HD3	1:A:155:ALA:O	2.19	0.42
2:B:73:PRO:HG2	2:B:120:HIS:CD2	2.41	0.42
1:A:140:LEU:CD1	1:A:140:LEU:N	2.82	0.42
1:A:64:ASN:O	1:A:65:ILE:HG12	2.18	0.42
2:B:174:ASP:HB3	2:B:209:ARG:HH11	1.84	0.42
1:A:40:LEU:O	1:A:76:ASN:HB3	2.19	0.42
2:B:89:SER:HB3	2:D:89:SER:OG	2.19	0.42
2:B:166:VAL:HG12	2:B:169:ARG:H	1.83	0.42
1:A:271:MET:HE3	1:A:271:MET:CA	2.49	0.42
1:C:23:LYS:O	1:C:35:LEU:HD12	2.19	0.42
2:D:69:SER:O	2:D:70:LYS:C	2.58	0.42
1:C:169:VAL:HG23	1:C:172:LEU:HD23	2.02	0.42
1:C:175:ARG:HE	1:C:179:VAL:CG1	2.32	0.42
2:B:109:TYR:CG	2:B:165:ARG:HD3	2.55	0.42
1:C:109:LEU:O	1:C:112:TYR:HB3	2.19	0.42
1:C:59:GLU:CG	2:D:173:ARG:HH11	2.33	0.42
2:B:181:SER:O	2:B:184:GLN:HB2	2.20	0.42
1:C:200:ALA:O	1:C:203:ILE:HB	2.19	0.42
2:B:94:VAL:HG11	2:B:131:THR:OG1	2.19	0.42
2:D:27:PHE:O	2:D:30:CYS:HB3	2.20	0.42
1:C:221:ILE:HG13	1:C:222:PHE:CD2	2.53	0.42
1:C:130:LEU:HD12	1:C:158:PHE:CZ	2.55	0.42
1:C:269:ASN:O	1:C:296:TRP:HB2	2.20	0.42
2:B:77:ILE:HG23	2:B:78:PHE:N	2.34	0.42
1:A:138:ASN:HD21	1:A:151:ASP:HB3	1.85	0.42
1:A:139:LEU:CD2	1:A:149:LEU:HD23	2.50	0.42
1:A:130:LEU:HD22	1:A:158:PHE:CZ	2.54	0.42
2:B:187:LYS:O	2:B:189:PHE:CD1	2.73	0.42
2:B:87:PHE:N	2:B:87:PHE:CD1	2.88	0.42
1:A:100:ASN:N	1:A:100:ASN:OD1	2.53	0.42
1:A:21:VAL:HG11	4:A:3001:AGS:O4'	2.20	0.41
2:D:121:ARG:HG2	2:D:121:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:125:THR:OG1	2:D:158:LEU:HG	2.19	0.41
1:C:25:LEU:HD11	1:C:32:TYR:CE2	2.55	0.41
1:A:89:LEU:HD12	1:A:139:LEU:HD12	2.02	0.41
1:C:67:ARG:H	1:C:83:GLU:HG2	1.84	0.41
1:A:268:GLY:O	1:A:271:MET:HB2	2.20	0.41
2:B:237:LYS:HD2	2:B:237:LYS:O	2.20	0.41
1:A:141:ILE:HA	1:A:146:GLN:O	2.20	0.41
1:C:83:GLU:HG3	1:C:83:GLU:O	2.19	0.41
2:D:154:GLU:O	2:D:157:ILE:HG12	2.20	0.41
1:A:58:LYS:O	1:A:61:LYS:HE3	2.19	0.41
1:A:27:LYS:HA	1:A:27:LYS:HD3	1.86	0.41
1:A:118:LEU:HA	1:A:118:LEU:HD23	1.86	0.41
2:D:97:THR:O	2:D:97:THR:HG22	2.20	0.41
1:A:51:ILE:O	1:A:55:SER:HB2	2.21	0.41
1:A:230:GLU:OE2	1:A:242:TYR:OH	2.38	0.41
1:C:175:ARG:HH11	1:C:175:ARG:HG2	1.85	0.41
1:A:26:ASN:CG	1:A:29:THR:H	2.22	0.41
2:D:190:VAL:HG23	2:D:191:ILE:N	2.35	0.41
2:D:109:TYR:HD2	2:D:112:PHE:HB2	1.78	0.41
1:A:208:LEU:O	1:A:209:PHE:CD2	2.72	0.41
1:A:223:ASP:HB3	1:A:252:ARG:NH2	2.35	0.41
1:C:211:GLY:HA3	1:C:217:GLN:OE1	2.21	0.41
1:C:223:ASP:OD1	1:C:249:ARG:NH1	2.54	0.41
1:C:236:VAL:C	1:C:238:LYS:H	2.23	0.41
1:A:93:MET:O	1:A:96:ARG:HB3	2.20	0.41
2:D:115:ASN:C	2:D:117:LEU:H	2.23	0.41
2:B:100:TYR:HD1	2:B:220:TYR:CZ	2.39	0.41
1:C:208:LEU:HG	1:C:209:PHE:CE1	2.55	0.41
1:C:74:THR:O	1:C:75:GLU:C	2.60	0.41
2:D:77:ILE:O	2:D:81:PHE:HB2	2.21	0.41
1:A:101:THR:CB	1:A:102:PRO:CD	2.99	0.41
2:D:18:ILE:HG22	2:D:240:LYS:HG3	2.02	0.41
2:B:117:LEU:HA	2:B:117:LEU:HD12	1.95	0.41
2:D:97:THR:HG21	2:D:134:LEU:CD1	2.51	0.41
2:B:100:TYR:HA	2:B:220:TYR:CE1	2.56	0.41
1:A:62:HIS:HB2	1:A:123:PHE:CD2	2.56	0.41
2:B:146:LYS:HE3	2:B:146:LYS:HB2	1.95	0.41
1:A:243:ASN:ND2	2:D:71:ILE:HD13	2.36	0.41
1:C:160:ILE:HD12	2:D:172:PRO:HG2	2.03	0.41
2:B:218:ASP:N	2:B:218:ASP:OD1	2.54	0.41
1:A:87:ASN:N	1:A:87:ASN:ND2	2.56	0.41
1:C:255:ARG:HA	1:C:271:MET:CE	2.49	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:233:TRP:N	1:C:234:PRO:HD3	2.35	0.41
1:A:57:MET:HA	1:A:57:MET:CE	2.51	0.41
2:B:206:TYR:O	2:B:209:ARG:HB3	2.21	0.41
1:A:33:VAL:HG12	1:A:69:TYR:HE2	1.86	0.41
2:B:187:LYS:O	2:B:189:PHE:HD1	2.04	0.41
1:C:233:TRP:CZ3	1:C:280:LEU:HB3	2.54	0.40
2:B:124:LEU:O	2:B:128:THR:CG2	2.70	0.40
1:A:211:GLY:HA2	1:A:220:LEU:HD11	2.03	0.40
1:C:255:ARG:HB3	1:C:255:ARG:HE	1.58	0.40
1:C:277:LEU:HD12	1:C:277:LEU:N	2.36	0.40
2:D:175:HIS:O	2:D:179:LEU:HD12	2.22	0.40
1:C:243:ASN:ND2	1:C:246:ILE:HG22	2.36	0.40
1:C:199:LEU:O	1:C:202:MET:HB2	2.21	0.40
1:C:239:LEU:HB2	1:C:242:TYR:HB2	2.04	0.40
1:C:132:ARG:HH11	1:C:156:ARG:HB2	1.85	0.40
2:B:35:LEU:HD23	2:B:35:LEU:HA	1.86	0.40
2:B:21:VAL:H	2:B:21:VAL:HG12	1.67	0.40
2:D:222:ARG:HG3	2:D:222:ARG:HH21	1.86	0.40
2:D:235:PRO:O	2:D:238:SER:HB2	2.22	0.40
1:A:130:LEU:CD1	1:A:130:LEU:N	2.85	0.40
2:D:223:ARG:HE	2:D:227:LEU:HD21	1.87	0.40
1:C:29:THR:C	1:C:31:VAL:H	2.25	0.40
1:A:51:ILE:O	1:A:55:SER:CB	2.70	0.40
1:C:160:ILE:CD1	2:D:172:PRO:HG2	2.51	0.40
1:C:278:LEU:HD23	1:C:278:LEU:HA	1.89	0.40
2:D:193:LYS:O	2:D:194:ASN:HB3	2.21	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	282/317 (89%)	232 (82%)	39 (14%)	11 (4%)	5	18
1	C	279/317 (88%)	218 (78%)	49 (18%)	12 (4%)	4	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	207/293 (71%)	169 (82%)	32 (16%)	6 (3%)	7	28
2	D	210/293 (72%)	177 (84%)	28 (13%)	5 (2%)	9	35
All	All	978/1220 (80%)	796 (81%)	148 (15%)	34 (4%)	6	23

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ASP
2	B	234	SER
2	B	238	SER
1	C	8	LYS
1	C	98	VAL
1	C	100	ASN
1	C	198	ILE
1	C	298	ALA
2	D	234	SER
2	D	246	PRO
1	A	65	ILE
1	A	74	THR
1	A	151	ASP
1	A	230	GLU
2	B	19	PRO
1	C	214	ASP
1	C	283	ASP
1	C	299	GLU
1	A	101	THR
1	A	247	GLN
2	B	116	SER
1	C	75	GLU
1	C	199	LEU
2	D	52	ASN
2	D	116	SER
2	D	119	ALA
1	A	66	VAL
2	B	183	GLU
1	C	203	ILE
1	A	259	GLN
2	B	246	PRO
1	C	30	GLY
1	A	211	GLY
1	A	161	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	256/284 (90%)	239 (93%)	17 (7%)	24	57
1	C	258/284 (91%)	240 (93%)	18 (7%)	21	53
2	B	199/271 (73%)	188 (94%)	11 (6%)	30	68
2	D	202/271 (74%)	189 (94%)	13 (6%)	25	59
All	All	915/1110 (82%)	856 (94%)	59 (6%)	25	59

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	39	LYS
1	A	49	THR
1	A	80	LEU
1	A	87	ASN
1	A	88	ASP
1	A	89	LEU
1	A	98	VAL
1	A	100	ASN
1	A	144	ARG
1	A	164	THR
1	A	212	THR
1	A	214	ASP
1	A	245	ASN
1	A	253	ASP
1	A	262	THR
1	A	277	LEU
2	B	21	VAL
2	B	32	ARG
2	B	63	THR
2	B	81	PHE
2	B	121	ARG
2	B	128	THR
2	B	181	SER
2	B	218	ASP
2	B	239	ARG

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Mol	Chain	Res	Type
2	B	241	VAL
2	B	246	PRO
1	C	7	PHE
1	C	11	GLU
1	C	44	GLU
1	C	59	GLU
1	C	61	LYS
1	C	87	ASN
1	C	89	LEU
1	C	108	ASN
1	C	137	GLN
1	C	164	THR
1	C	175	ARG
1	C	199	LEU
1	C	218	LEU
1	C	221	ILE
1	C	245	ASN
1	C	272	ASP
1	C	285	ARG
1	C	286	LEU
2	D	18	ILE
2	D	21	VAL
2	D	46	LEU
2	D	50	ASN
2	D	63	THR
2	D	81	PHE
2	D	127	THR
2	D	128	THR
2	D	169	ARG
2	D	179	LEU
2	D	239	ARG
2	D	245	LEU
2	D	246	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	116	GLN
1	A	119	GLN
1	A	138	ASN
1	A	245	ASN

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Mol	Chain	Res	Type
1	A	259	GLN
1	A	279	GLN
1	A	290	GLN
2	B	50	ASN
2	B	79	ASN
2	B	92	HIS
2	B	106	GLN
2	B	120	HIS
2	B	141	ASN
2	B	143	HIS
2	B	153	HIS
2	B	156	ASN
2	B	160	ASN
2	B	167	ASN
2	B	186	GLN
1	C	87	ASN
1	C	116	GLN
1	C	119	GLN
1	C	217	GLN
1	C	245	ASN
1	C	259	GLN
1	C	279	GLN
1	C	290	GLN
2	D	28	ASN
2	D	50	ASN
2	D	61	GLN
2	D	79	ASN
2	D	92	HIS
2	D	141	ASN
2	D	156	ASN
2	D	167	ASN
2	D	194	ASN
2	D	226	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

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	AGS	A	3001	-	33,33,33	1.35	4 (12%)	52,52,52	2.53	16 (30%)
3	MES	B	1001	-	12,12,12	0.93	1 (8%)	16,16,16	0.93	0
3	MES	D	2001	-	12,12,12	0.94	0	16,16,16	0.89	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	A	3001	-	1/1/7/7	0/21/38/38	0/1/3/3
3	MES	B	1001	-	-	0/6/14/14	1/1/1/1
3	MES	D	2001	-	-	0/6/14/14	1/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3001	AGS	O4'-C1'	3.33	1.46	1.41
4	A	3001	AGS	PG-O3G	2.28	1.61	1.56
3	B	1001	MES	C8-S	2.23	1.82	1.78
4	A	3001	AGS	C8-N7	-2.23	1.30	1.34
4	A	3001	AGS	PG-O2G	2.21	1.61	1.56

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3001	AGS	N3-C2-N1	-10.72	119.75	128.71
4	A	3001	AGS	O3A-PB-O3B	6.49	114.86	101.66
4	A	3001	AGS	O2G-PG-S1G	-5.08	107.38	112.73
4	A	3001	AGS	N3-C4-N9	4.36	133.31	125.43
4	A	3001	AGS	O4'-C1'-N9	3.57	111.76	108.44
4	A	3001	AGS	PB-O3B-PG	-3.32	120.46	131.81
4	A	3001	AGS	O3G-PG-S1G	-3.10	109.47	112.73
4	A	3001	AGS	C4-C5-N7	-3.09	106.88	109.52
4	A	3001	AGS	C2-N3-C4	3.04	122.66	114.01
4	A	3001	AGS	O4'-C4'-C5'	2.97	119.95	109.36
4	A	3001	AGS	C5-C4-N3	-2.96	119.26	125.70
4	A	3001	AGS	C8-N9-C4	-2.89	104.69	106.90
4	A	3001	AGS	O5'-C5'-C4'	2.40	117.74	108.94
4	A	3001	AGS	PA-O3A-PB	-2.31	124.91	131.68
4	A	3001	AGS	O2A-PA-O3A	2.28	115.94	105.14
4	A	3001	AGS	C2-N1-C6	2.01	122.40	118.77

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	3001	AGS	C3'

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2001	MES	C2-C3-C5-C6-N4-O1
3	B	1001	MES	C2-C3-C5-C6-N4-O1

## 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	284/317 (89%)	0.35	10 (3%)	42 50	14, 39, 79, 107	13 (4%)
1	C	285/317 (89%)	0.63	21 (7%)	14 17	27, 64, 108, 131	17 (5%)
2	B	213/293 (72%)	0.32	4 (1%)	64 72	16, 37, 62, 78	6 (2%)
2	D	216/293 (73%)	0.36	6 (2%)	50 59	16, 38, 67, 107	4 (1%)
All	All	998/1220 (81%)	0.43	41 (4%)	35 43	14, 44, 92, 131	40 (4%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	102	PRO	7.9
1	C	30	GLY	5.3
1	C	21	VAL	4.4
1	C	26	ASN	4.2
1	C	27	LYS	4.1
1	A	102	PRO	3.5
1	C	29	THR	3.4
1	A	232	LEU	3.3
1	C	77	LYS	3.2
2	B	17	GLY	3.1
1	C	223	ASP	3.0
2	D	45	SER	3.0
1	A	40	LEU	2.9
2	D	17	GLY	2.9
1	C	257	VAL	2.8
1	A	20	THR	2.8
1	C	38	VAL	2.8
1	C	74	THR	2.8
1	A	41	ASP	2.7
2	D	236	ASP	2.7
2	B	208	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	30	GLY	2.6
2	B	116	SER	2.6
2	B	87	PHE	2.5
1	A	137	GLN	2.5
1	C	207	PRO	2.4
1	C	44	GLU	2.3
1	A	272	ASP	2.3
1	C	101	THR	2.3
1	C	107	LEU	2.3
2	D	237	LYS	2.3
1	C	96	ARG	2.3
1	C	284	MET	2.3
1	C	262	THR	2.2
1	C	28	THR	2.1
1	C	206	LYS	2.1
1	A	251	PRO	2.1
2	D	246	PRO	2.1
1	C	103	ARG	2.1
2	D	230	SER	2.1
1	A	22	TYR	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
3	MES	D	2001	12/12	0.23	1.55	43,47,49,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MES	B	1001	12/12	0.25	0.83	56,61,68,70	0
4	AGS	A	3001	31/31	0.24	0.19	71,97,115,118	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.