



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2018 – 05:18 PM EST

PDB ID : 2O1O  
Title : Cryptosporidium parvum putative polyprenyl pyrophosphate synthase (cgd4\_2550) in complex with risedronate.  
Authors : Chruszcz, M.; Artz, J.D.; Dong, A.; Dunford, J.; Lew, J.; Zhao, Y.; Kozieradski, I.; Kavanaugh, K.L.; Oppermann, U.; Sundstrom, M.; Weigelt, J.; Edwards, A.M.; Arrowsmith, C.H.; Bochkarev, A.; Hui, R.; Minor, W.; Structural Genomics Consortium (SGC)  
Deposited on : 2006-11-29  
Resolution : 2.42 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

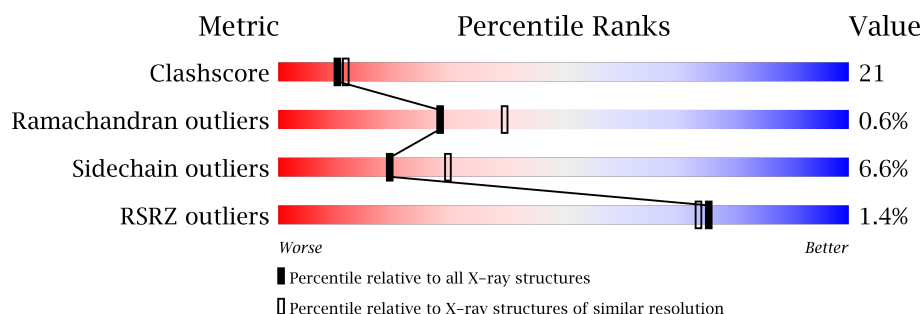
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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))
Clashscore	112137	4241 (2.44-2.40)
Ramachandran outliers	110173	4178 (2.44-2.40)
Sidechain outliers	110143	4179 (2.44-2.40)
RSRZ outliers	101464	3740 (2.44-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	368	
1	B	368	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	502	-	-	-	X
2	MG	B	501	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5378 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 Putative farnesyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2646	1725	422	488	11			
1	B	331	Total	C	N	O	S	0	0	0
			2664	1734	424	495	11			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP Q5CR09
A	2	GLY	-	CLONING ARTIFACT	UNP Q5CR09
A	3	SER	-	CLONING ARTIFACT	UNP Q5CR09
A	4	SER	-	CLONING ARTIFACT	UNP Q5CR09
A	5	HIS	-	EXPRESSION TAG	UNP Q5CR09
A	6	HIS	-	EXPRESSION TAG	UNP Q5CR09
A	7	HIS	-	EXPRESSION TAG	UNP Q5CR09
A	8	HIS	-	EXPRESSION TAG	UNP Q5CR09
A	9	HIS	-	EXPRESSION TAG	UNP Q5CR09
A	10	HIS	-	EXPRESSION TAG	UNP Q5CR09
A	11	SER	-	CLONING ARTIFACT	UNP Q5CR09
A	12	SER	-	CLONING ARTIFACT	UNP Q5CR09
A	13	GLY	-	CLONING ARTIFACT	UNP Q5CR09
A	14	ARG	-	CLONING ARTIFACT	UNP Q5CR09
A	15	GLU	-	CLONING ARTIFACT	UNP Q5CR09
A	16	ASN	-	CLONING ARTIFACT	UNP Q5CR09
A	17	LEU	-	CLONING ARTIFACT	UNP Q5CR09
A	18	TYR	-	CLONING ARTIFACT	UNP Q5CR09
A	19	PHE	-	CLONING ARTIFACT	UNP Q5CR09
A	20	GLN	-	CLONING ARTIFACT	UNP Q5CR09
A	21	GLY	-	CLONING ARTIFACT	UNP Q5CR09
B	1	MET	-	CLONING ARTIFACT	UNP Q5CR09
B	2	GLY	-	CLONING ARTIFACT	UNP Q5CR09
B	3	SER	-	CLONING ARTIFACT	UNP Q5CR09
B	4	SER	-	CLONING ARTIFACT	UNP Q5CR09

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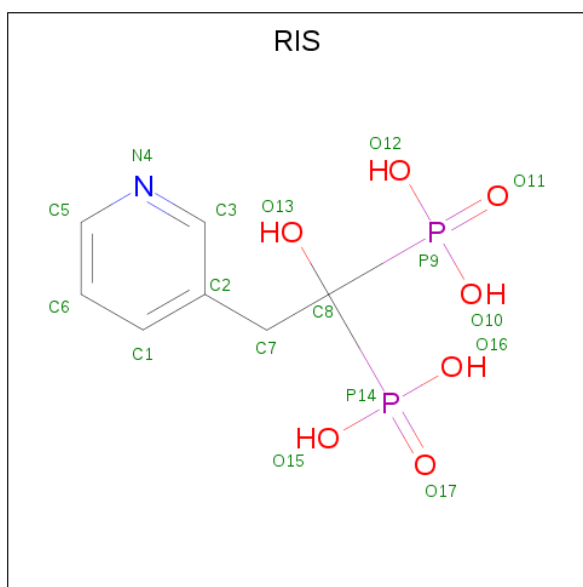
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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	HIS	-	EXPRESSION TAG	UNP Q5CR09
B	6	HIS	-	EXPRESSION TAG	UNP Q5CR09
B	7	HIS	-	EXPRESSION TAG	UNP Q5CR09
B	8	HIS	-	EXPRESSION TAG	UNP Q5CR09
B	9	HIS	-	EXPRESSION TAG	UNP Q5CR09
B	10	HIS	-	EXPRESSION TAG	UNP Q5CR09
B	11	SER	-	CLONING ARTIFACT	UNP Q5CR09
B	12	SER	-	CLONING ARTIFACT	UNP Q5CR09
B	13	GLY	-	CLONING ARTIFACT	UNP Q5CR09
B	14	ARG	-	CLONING ARTIFACT	UNP Q5CR09
B	15	GLU	-	CLONING ARTIFACT	UNP Q5CR09
B	16	ASN	-	CLONING ARTIFACT	UNP Q5CR09
B	17	LEU	-	CLONING ARTIFACT	UNP Q5CR09
B	18	TYR	-	CLONING ARTIFACT	UNP Q5CR09
B	19	PHE	-	CLONING ARTIFACT	UNP Q5CR09
B	20	GLN	-	CLONING ARTIFACT	UNP Q5CR09
B	21	GLY	-	CLONING ARTIFACT	UNP Q5CR09

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mg 3 3	0	0
2	A	3	Total Mg 3 3	0	0

- Molecule 3 is 1-HYDROXY-2-(3-PYRIDINYL)ETHYLIDENE BIS-PHOSPHONIC ACID (three-letter code: RIS) (formula: C<sub>7</sub>H<sub>11</sub>NO<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			17	7	1	7	2		
3	B	1	Total	C	N	O	P	0	0
			17	7	1	7	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	17	Total	O	0	0
			17	17		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.76 Å   101.76 Å   75.31 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	50.00 – 2.42 30.27 – 2.42	Depositor EDS
% Data completeness (in resolution range)	94.9 (50.00-2.42) 94.8 (30.27-2.42)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 2.42 Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.186 ,   0.213 0.184 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	50.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 150.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l 0.039 for h,-h-k,-l 0.016 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.69	2/2704 (0.1%)	0.65	0/3668
1	B	0.60	0/2719	0.65	0/3676
All	All	0.65	2/5423 (0.0%)	0.65	0/7344

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	SER	CB-OG	5.58	1.49	1.42
1	A	228	GLU	CD-OE2	5.45	1.31	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	PHE	Peptide
1	B	26	THR	Peptide



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2646	0	2532	109	0
1	B	2664	0	2600	113	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	17	0	7	1	0
3	B	17	0	7	0	0
4	A	11	0	0	2	0
4	B	17	0	0	1	0
All	All	5378	0	5146	218	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 21.

All (218) 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:B:24:ASP:CA	1:B:25:TYR:HB2	1.70	1.20
1:B:24:ASP:HA	1:B:25:TYR:CB	1.64	1.20
1:B:319:GLU:HG3	1:B:322:ARG:NH2	1.67	1.07
1:A:238:LEU:HD11	1:A:331:LEU:CD1	1.92	0.99
1:B:318:LEU:O	1:B:322:ARG:HG3	1.66	0.95
1:A:279:GLN:OE1	1:A:280:LYS:HG2	1.68	0.92
1:B:300:ASN:OD1	1:B:302:SER:HB2	1.70	0.92
1:A:227:SER:O	1:A:228:GLU:HG2	1.71	0.91
1:B:239:ILE:HA	1:B:242:ILE:HD12	1.55	0.89
1:A:332:VAL:HG11	1:A:345:ILE:HG12	1.55	0.89
1:A:255:ASP:HB3	1:A:275:THR:HG22	1.56	0.88
1:A:213:ARG:O	1:A:217:TYR:HB3	1.74	0.87
1:A:238:LEU:CD1	1:A:331:LEU:HD11	2.05	0.85
1:B:328:LEU:HB3	1:B:348:ILE:HD12	1.58	0.84
1:B:327:TYR:HA	1:B:330:LYS:HD2	1.58	0.83
1:B:280:LYS:HE3	1:B:284:ILE:HD11	1.60	0.83
1:A:33:ASP:O	1:A:37:VAL:HG23	1.81	0.79
1:A:238:LEU:CD1	1:A:331:LEU:CD1	2.61	0.78
1:B:172:ILE:HD13	1:B:221:PHE:HB3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:GLU:CG	1:B:322:ARG:NH2	2.48	0.75
1:B:97:ILE:HG12	1:B:226:LEU:HD13	1.68	0.75
1:A:74:ILE:HD11	1:A:354:LEU:HD11	1.69	0.74
1:B:161:PHE:HB3	1:B:165:ILE:HG12	1.72	0.71
1:A:252:VAL:HG12	1:A:317:TYR:HE1	1.54	0.71
1:A:118:MET:HE3	1:A:188:LEU:HD11	1.74	0.69
1:A:279:GLN:OE1	1:A:280:LYS:CG	2.39	0.69
1:B:260:LEU:HD23	1:B:261:PHE:CE2	2.28	0.69
1:B:191:PHE:CB	1:B:199:ILE:HD11	2.22	0.69
1:A:312:LYS:O	1:A:315:GLU:HB3	1.92	0.68
1:A:155:PHE:CE2	1:B:171:LYS:HG3	2.30	0.67
1:A:238:LEU:HD11	1:A:331:LEU:HD12	1.75	0.66
1:B:24:ASP:HA	1:B:25:TYR:HB2	0.78	0.65
1:A:276:TRP:HB3	1:A:277:PRO:HD3	1.79	0.65
1:B:199:ILE:HG13	1:B:274:LEU:HD11	1.79	0.64
1:A:83:SER:OG	1:A:223:GLY:HA2	1.97	0.64
1:A:177:ILE:O	1:A:181:VAL:HG23	1.97	0.64
1:A:153:LEU:HA	1:A:156:GLU:HG3	1.81	0.63
1:A:252:VAL:HG12	1:A:317:TYR:CE1	2.34	0.63
1:A:279:GLN:CD	1:A:280:LYS:HG2	2.18	0.63
1:A:316:HIS:CD2	1:A:316:HIS:H	2.18	0.62
1:A:224:LEU:C	1:A:224:LEU:HD12	2.21	0.61
1:A:283:GLU:HG3	1:A:284:ILE:HG23	1.81	0.61
1:A:81:LEU:O	1:A:85:LEU:HB2	2.01	0.61
1:B:235:GLN:HG3	1:B:235:GLN:O	1.99	0.61
1:B:292:LYS:HE2	1:B:303:LEU:HD13	1.83	0.60
1:B:319:GLU:HG3	1:B:322:ARG:HH22	1.63	0.60
1:B:100:LEU:HD23	1:B:226:LEU:HD11	1.83	0.59
1:A:74:ILE:HD11	1:A:354:LEU:CD1	2.31	0.59
1:A:179:PHE:CB	1:A:213:ARG:HG3	2.32	0.59
1:B:72:LYS:NZ	4:B:513:HOH:O	2.36	0.59
1:A:193:LEU:HD21	1:A:196:ALA:HB2	1.83	0.59
1:B:180:THR:HG23	1:B:210:LYS:O	2.03	0.59
1:B:24:ASP:HB2	1:B:26:THR:N	2.17	0.59
1:A:166:VAL:O	1:A:170:GLN:HG3	2.03	0.58
1:B:92:ILE:O	1:B:92:ILE:HG23	2.03	0.58
1:A:255:ASP:HB3	1:A:275:THR:CG2	2.32	0.58
1:A:73:HIS:O	1:A:77:LYS:HG3	2.02	0.58
1:B:172:ILE:CD1	1:B:221:PHE:HB3	2.32	0.58
1:A:155:PHE:HE2	1:B:171:LYS:HG3	1.67	0.58
1:A:74:ILE:HD12	1:A:354:LEU:HD13	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:HD11	1:A:331:LEU:CG	2.35	0.57
1:A:268:ASP:O	1:A:271:ARG:O	2.23	0.57
1:A:269:ILE:O	1:A:298:GLY:HA2	2.04	0.57
1:B:276:TRP:HB3	1:B:277:PRO:HD3	1.85	0.57
1:B:277:PRO:HA	1:B:313:ILE:HD12	1.87	0.57
1:A:130:TRP:HA	1:A:133:VAL:HG22	1.87	0.57
1:A:32:TYR:CE2	1:A:69:LYS:HD2	2.39	0.56
1:A:136:GLN:OE1	1:B:136:GLN:NE2	2.38	0.56
1:A:193:LEU:CD2	1:A:196:ALA:HB2	2.36	0.56
1:A:54:LYS:HD2	1:A:57:ILE:HD11	1.87	0.56
1:A:74:ILE:CD1	1:A:354:LEU:CD1	2.83	0.56
1:B:208:GLU:HB2	1:B:244:TYR:HE1	1.71	0.56
1:A:249:PHE:CE1	1:A:321:GLN:HG2	2.42	0.55
1:A:271:ARG:O	1:A:273:LYS:N	2.39	0.55
1:A:249:PHE:HE1	1:A:321:GLN:HG2	1.71	0.55
1:B:260:LEU:HB3	1:B:261:PHE:CD2	2.42	0.55
1:A:270:CYS:HA	1:A:298:GLY:HA2	1.89	0.55
1:A:83:SER:HA	1:A:227:SER:HB3	1.89	0.55
1:B:24:ASP:HB2	1:B:26:THR:H	1.71	0.55
1:A:202:ARG:O	1:A:206:MET:HB2	2.06	0.54
1:B:103:VAL:O	1:B:107:ILE:HG13	2.07	0.54
1:B:280:LYS:O	1:B:283:GLU:HB3	2.07	0.54
1:A:328:LEU:O	1:A:332:VAL:HG23	2.07	0.54
1:B:70:LYS:HB3	1:B:125:ARG:HD2	1.89	0.54
1:A:306:ASP:O	1:A:309:ASN:HB3	2.08	0.54
1:B:165:ILE:CD1	1:B:165:ILE:N	2.71	0.54
1:A:221:PHE:CZ	1:A:239:ILE:HD11	2.42	0.53
1:A:262:ASN:N	1:A:262:ASN:ND2	2.55	0.53
1:A:269:ILE:O	1:A:298:GLY:N	2.41	0.53
1:A:179:PHE:HB3	1:A:213:ARG:HG3	1.90	0.53
1:A:206:MET:HE3	1:A:207:VAL:HG23	1.90	0.53
1:A:74:ILE:CD1	1:A:354:LEU:HD13	2.39	0.53
1:B:57:ILE:O	1:B:61:LEU:HG	2.08	0.53
1:A:256:VAL:HG21	1:A:317:TYR:CD1	2.44	0.52
1:A:216:PHE:HZ	1:A:250:TYR:CD2	2.28	0.52
1:B:108:GLN:OE1	1:B:109:ALA:N	2.42	0.52
1:B:144:PHE:O	1:B:148:MET:HG2	2.10	0.52
1:B:161:PHE:CZ	1:B:226:LEU:HD22	2.45	0.52
1:A:246:LEU:HD21	1:A:348:ILE:HG12	1.92	0.51
1:B:140:ILE:HA	1:B:143:ILE:HD12	1.92	0.51
1:B:93:LYS:O	1:B:97:ILE:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TRP:O	1:A:133:VAL:HG22	2.10	0.51
1:A:238:LEU:HD11	1:A:331:LEU:HG	1.93	0.51
1:A:322:ARG:O	1:A:326:ASP:HB2	2.10	0.51
1:B:271:ARG:NH1	1:B:273:LYS:HD3	2.25	0.51
1:B:178:PHE:CE2	1:B:182:LEU:HD11	2.46	0.51
1:B:218:MET:HB3	1:B:219:PRO:HD3	1.92	0.51
1:B:64:ILE:HG23	1:B:68:VAL:HG21	1.92	0.51
1:B:165:ILE:HD12	1:B:165:ILE:N	2.26	0.50
1:A:227:SER:C	1:A:228:GLU:HG2	2.31	0.50
1:A:258:ASP:O	1:A:262:ASN:ND2	2.44	0.50
1:B:113:ILE:CD1	1:B:143:ILE:HG13	2.42	0.50
1:B:208:GLU:HB2	1:B:244:TYR:CE1	2.47	0.50
1:A:71:GLY:HA2	1:A:125:ARG:HG2	1.93	0.50
1:A:237:ASN:ND2	4:A:509:HOH:O	2.44	0.49
1:A:332:VAL:CG1	1:A:345:ILE:HG12	2.36	0.49
1:A:252:VAL:HG22	1:A:276:TRP:CD1	2.46	0.49
1:B:216:PHE:CE2	1:B:247:GLY:HA2	2.48	0.49
1:B:81:LEU:O	1:B:84:SER:CB	2.60	0.49
1:A:140:ILE:HA	1:A:143:ILE:HD12	1.94	0.49
1:A:153:LEU:HA	1:A:156:GLU:CG	2.41	0.49
1:A:256:VAL:HG21	1:A:317:TYR:CG	2.48	0.49
1:B:266:ALA:C	1:B:271:ARG:HE	2.14	0.49
1:B:93:LYS:HG2	1:B:160:VAL:HG12	1.94	0.49
1:B:337:ASP:C	1:B:339:SER:H	2.16	0.48
1:A:153:LEU:O	1:A:156:GLU:HB2	2.13	0.48
1:B:124:ARG:O	1:B:125:ARG:HB2	2.12	0.48
1:B:267:ASP:OD1	1:B:270:CYS:HB2	2.12	0.48
1:A:269:ILE:O	1:A:298:GLY:CA	2.61	0.48
1:A:220:VAL:O	1:A:224:LEU:HG	2.13	0.48
1:B:110:LEU:HA	1:B:113:ILE:HG12	1.96	0.48
1:A:353:GLU:O	1:A:356:THR:N	2.47	0.48
1:B:176:SER:HA	1:B:213:ARG:HG2	1.95	0.47
1:A:315:GLU:HG2	1:A:316:HIS:N	2.30	0.47
1:B:276:TRP:CH2	1:B:317:TYR:HA	2.49	0.47
1:B:64:ILE:HG23	1:B:68:VAL:CG2	2.44	0.47
1:B:337:ASP:HB2	1:B:340:LEU:HB3	1.97	0.47
1:B:113:ILE:CD1	1:B:143:ILE:CG1	2.93	0.47
1:B:70:LYS:HB2	1:B:125:ARG:HH21	1.80	0.47
1:A:130:TRP:HA	1:A:133:VAL:CG2	2.45	0.46
1:B:275:THR:OG1	1:B:277:PRO:HD2	2.15	0.46
1:B:319:GLU:CG	1:B:322:ARG:HH21	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:THR:HG22	1:A:216:PHE:CD2	2.51	0.46
1:A:258:ASP:HB2	4:A:514:HOH:O	2.14	0.46
1:A:180:THR:HA	1:A:210:LYS:HA	1.98	0.46
1:A:217:TYR:HA	1:A:243:LEU:HD13	1.98	0.46
1:B:265:ASN:HA	1:B:270:CYS:SG	2.56	0.46
1:B:91:ASN:HB3	1:B:93:LYS:CD	2.46	0.46
1:A:262:ASN:N	1:A:262:ASN:HD22	2.13	0.46
1:B:319:GLU:HA	1:B:322:ARG:NE	2.30	0.46
1:A:301:SER:O	1:A:305:LYS:N	2.47	0.45
1:A:136:GLN:NE2	1:B:136:GLN:OE1	2.48	0.45
1:B:79:LEU:HD11	1:B:100:LEU:HG	1.97	0.45
1:B:91:ASN:ND2	1:B:92:ILE:H	2.14	0.45
1:A:71:GLY:CA	1:A:125:ARG:HG2	2.47	0.45
1:A:270:CYS:CA	1:A:298:GLY:HA2	2.46	0.45
1:A:316:HIS:HA	1:A:319:GLU:HG3	1.98	0.45
1:B:55:PRO:O	1:B:58:GLU:HG3	2.15	0.45
1:A:277:PRO:HB3	1:A:313:ILE:HG21	1.97	0.45
1:A:289:MET:C	1:A:291:LEU:H	2.20	0.45
1:B:292:LYS:CE	1:B:303:LEU:HD13	2.46	0.45
1:A:253:HIS:HA	1:A:317:TYR:OH	2.16	0.44
1:B:91:ASN:HB3	1:B:93:LYS:HD2	1.98	0.44
1:B:27:ASP:N	1:B:27:ASP:OD1	2.50	0.44
1:B:326:ASP:HA	1:B:329:ILE:HD12	1.99	0.44
1:B:252:VAL:HG22	1:B:276:TRP:CD1	2.52	0.44
1:B:104:VAL:HA	1:B:107:ILE:HD12	1.98	0.44
1:B:113:ILE:HD11	1:B:143:ILE:HA	1.99	0.44
1:B:158:SER:O	1:B:162:GLY:HA2	2.17	0.44
1:B:281:SER:OG	1:B:282:PHE:N	2.50	0.44
1:B:99:LEU:O	1:B:103:VAL:HG23	2.18	0.44
1:A:289:MET:HE1	1:A:310:LEU:HD23	1.99	0.44
1:B:113:ILE:HD11	1:B:143:ILE:CG1	2.47	0.44
1:A:286:ASP:O	1:A:290:LYS:HB2	2.18	0.43
1:B:186:LEU:HB2	1:B:206:MET:HG3	1.99	0.43
1:B:267:ASP:O	1:B:271:ARG:N	2.51	0.43
1:A:220:VAL:HG21	1:A:243:LEU:HD21	1.99	0.43
1:B:297:TYR:HA	1:B:298:GLY:HA2	1.61	0.43
1:B:293:ILE:O	1:B:297:TYR:HB2	2.18	0.43
1:A:100:LEU:HD23	1:A:226:LEU:HD11	2.00	0.43
1:A:276:TRP:N	1:A:277:PRO:CD	2.81	0.42
1:B:113:ILE:HD12	1:B:143:ILE:HG13	2.00	0.42
1:B:55:PRO:CA	1:B:58:GLU:HG2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ARG:O	1:A:125:ARG:HB2	2.18	0.42
1:A:199:ILE:HG13	1:A:274:LEU:HD11	2.00	0.42
1:B:31:TYR:CE1	1:B:34:LYS:HD2	2.54	0.42
1:B:45:LYS:HE2	1:B:45:LYS:HA	2.00	0.42
1:A:118:MET:CE	1:A:188:LEU:HD11	2.48	0.42
1:B:267:ASP:O	1:B:271:ARG:HB2	2.20	0.42
1:A:23:TYR:HD2	1:A:81:LEU:HD13	1.84	0.42
1:A:208:GLU:HB2	1:A:244:TYR:HE1	1.83	0.42
1:B:260:LEU:HB3	1:B:261:PHE:CE2	2.54	0.42
1:B:284:ILE:HB	1:B:311:LEU:HD21	2.02	0.42
1:B:141:ASN:O	1:B:144:PHE:HB2	2.20	0.42
1:B:208:GLU:HG2	1:B:209:MET:HE3	2.02	0.42
1:B:296:ASN:O	1:B:298:GLY:HA2	2.20	0.42
1:B:337:ASP:O	1:B:338:ASP:HB2	2.19	0.42
1:A:229:ILE:HA	1:A:230:GLN:HA	1.63	0.41
1:A:148:MET:HE1	1:B:173:TYR:CE2	2.55	0.41
1:B:45:LYS:HB2	1:B:46:LEU:HA	2.02	0.41
1:B:328:LEU:HB3	1:B:348:ILE:CD1	2.41	0.41
1:A:100:LEU:CD2	1:A:226:LEU:HD11	2.51	0.41
1:B:266:ALA:O	1:B:271:ARG:NE	2.36	0.41
1:B:45:LYS:N	1:B:46:LEU:HA	2.36	0.41
1:A:208:GLU:HB2	1:A:244:TYR:CE1	2.55	0.41
1:A:107:ILE:O	1:A:110:LEU:HG	2.21	0.41
1:B:210:LYS:HG3	1:B:211:THR:OG1	2.20	0.41
1:B:285:ALA:HB3	1:B:290:LYS:HG3	2.02	0.41
3:A:400:RIS:C2	3:A:400:RIS:O17	2.69	0.41
1:A:250:TYR:CE2	1:A:351:ILE:HD12	2.56	0.41
1:B:24:ASP:CA	1:B:25:TYR:CB	2.50	0.41
1:B:113:ILE:O	1:B:117:ILE:HG13	2.21	0.40
1:B:216:PHE:HE2	1:B:247:GLY:HA2	1.85	0.40
1:B:208:GLU:HA	1:B:212:SER:HB2	2.02	0.40
1:A:224:LEU:C	1:A:224:LEU:CD1	2.90	0.40
1:A:42:VAL:O	1:A:44:LYS:N	2.46	0.40
1:B:311:LEU:HD23	1:B:311:LEU:O	2.22	0.40
1:B:292:LYS:NZ	1:B:303:LEU:HD22	2.36	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	333/368 (90%)	295 (89%)	36 (11%)	2 (1%)	28	40
1	B	327/368 (89%)	301 (92%)	24 (7%)	2 (1%)	28	40
All	All	660/736 (90%)	596 (90%)	60 (9%)	4 (1%)	28	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	231	VAL
1	B	92	ILE
1	A	47	PRO
1	A	272	PHE

### 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	276/341 (81%)	255 (92%)	21 (8%)	15	23
1	B	287/341 (84%)	271 (94%)	16 (6%)	25	38
All	All	563/682 (83%)	526 (93%)	37 (7%)	19	30

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	TYR
1	A	25	TYR

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Mol	Chain	Res	Type
1	A	27	ASP
1	A	53	ARG
1	A	148	MET
1	A	155	PHE
1	A	202	ARG
1	A	233	SER
1	A	239	ILE
1	A	259	TYR
1	A	262	ASN
1	A	263	ASP
1	A	268	ASP
1	A	275	THR
1	A	279	GLN
1	A	286	ASP
1	A	289	MET
1	A	312	LYS
1	A	314	ASN
1	A	350	GLN
1	A	355	ILE
1	B	27	ASP
1	B	36	LYS
1	B	92	ILE
1	B	133	VAL
1	B	147	LYS
1	B	164	ASP
1	B	165	ILE
1	B	213	ARG
1	B	232	SER
1	B	235	GLN
1	B	259	TYR
1	B	264	SER
1	B	279	GLN
1	B	314	ASN
1	B	334	ASP
1	B	354	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	170	GLN
1	A	262	ASN



### 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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	RIS	A	400	2	17,17,17	2.94	5 (29%)	27,27,27	1.95	7 (25%)
3	RIS	B	400	2	17,17,17	2.81	5 (29%)	27,27,27	1.75	8 (29%)

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	RIS	A	400	2	-	0/23/23/23	0/1/1/1
3	RIS	B	400	2	-	0/23/23/23	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	RIS	P14-C8	-9.03	1.78	1.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	RIS	P14-C8	-7.31	1.79	1.85
3	B	400	RIS	P9-C8	-5.42	1.81	1.85
3	A	400	RIS	P9-C8	-4.58	1.81	1.85
3	B	400	RIS	P14-O15	-3.90	1.47	1.54
3	A	400	RIS	P14-O16	-3.84	1.47	1.54
3	A	400	RIS	P14-O15	-3.62	1.48	1.54
3	B	400	RIS	P14-O16	-3.57	1.48	1.54
3	A	400	RIS	O13-C8	-2.32	1.41	1.44
3	B	400	RIS	C1-C2	2.33	1.43	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	RIS	O17-P14-C8	-5.39	95.60	109.92
3	B	400	RIS	O17-P14-C8	-4.32	98.43	109.92
3	A	400	RIS	O10-P9-O11	-3.16	105.97	113.05
3	B	400	RIS	O10-P9-O11	-3.09	106.13	113.05
3	B	400	RIS	C7-C2-C1	-2.95	116.95	121.07
3	A	400	RIS	C7-C2-C1	-2.59	117.46	121.07
3	B	400	RIS	O11-P9-C8	-2.51	103.24	109.92
3	A	400	RIS	O11-P9-C8	-2.33	103.73	109.92
3	B	400	RIS	P14-C8-C7	2.06	114.79	109.23
3	B	400	RIS	C7-C2-C3	2.11	124.89	121.55
3	A	400	RIS	O12-P9-O11	2.17	117.91	113.05
3	A	400	RIS	C5-N4-C3	2.21	120.71	116.83
3	B	400	RIS	O10-P9-O12	2.26	114.44	108.09
3	B	400	RIS	C5-N4-C3	2.61	121.40	116.83
3	A	400	RIS	O10-P9-O12	3.21	117.10	108.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	RIS	1	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	335/368 (91%)	-0.31	8 (2%) 59 56	29, 60, 103, 131	0
1	B	331/368 (89%)	-0.39	1 (0%) 93 93	29, 56, 96, 125	0
All	All	666/736 (90%)	-0.35	9 (1%) 75 73	29, 58, 100, 131	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	ALA	3.7
1	A	356	THR	3.6
1	A	86	SER	3.5
1	A	57	ILE	2.7
1	A	227	SER	2.7
1	A	226	LEU	2.3
1	B	361	ASN	2.2
1	A	74	ILE	2.2
1	A	214	TYR	2.1

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	502	1/1	0.96	0.32	4.03	58,58,58,58	0
2	MG	B	501	1/1	0.97	0.20	2.92	60,60,60,60	0
2	MG	B	503	1/1	0.84	0.15	0.88	48,48,48,48	0
3	RIS	B	400	17/17	0.98	0.16	0.35	33,46,56,59	0
3	RIS	A	400	17/17	0.98	0.14	-0.41	31,42,47,62	0
2	MG	B	502	1/1	0.94	0.18	-	44,44,44,44	0
2	MG	A	503	1/1	0.97	0.18	-	56,56,56,56	0
2	MG	A	501	1/1	0.90	0.19	-	65,65,65,65	0

## 6.5 Other polymers

There are no such residues in this entry.