



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 11:53 am GMT

PDB ID : 1JSC  
Title : Crystal Structure of the Catalytic Subunit of Yeast Acetohydroxyacid Synthase: A target for Herbicidal Inhibitors  
Authors : Pang, S.S.; Duggleby, R.G.; Guddat, L.W.  
Deposited on : 2001-08-17  
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

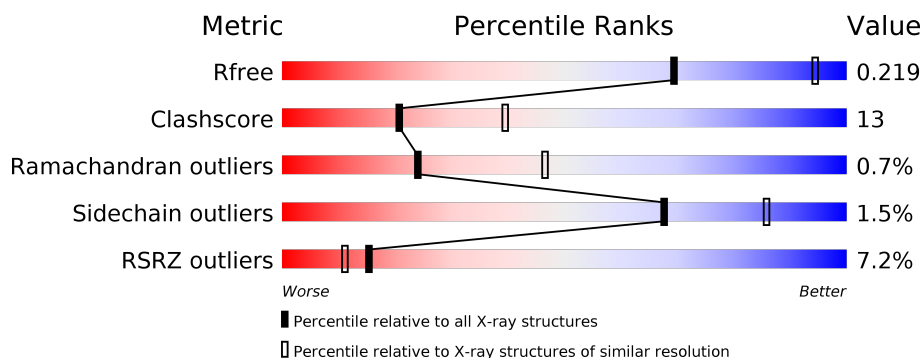
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	111664	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (2.60-2.60)

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	630	<div> <div>3%</div> <div>68%</div> <div>17%</div> <div>•</div> <div>14%</div> </div>
1	B	630	<div> <div>9%</div> <div>66%</div> <div>20%</div> <div>•</div> <div>13%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8628 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 ACETOHYDROXY-ACID SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	0	0
			4071	2577	700	775	19			
1	B	550	Total	C	N	O	S	0	0	0
			4055	2560	692	784	19			

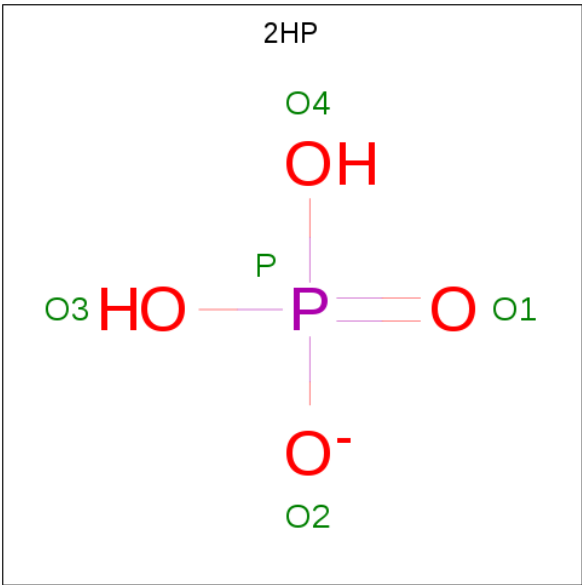
- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

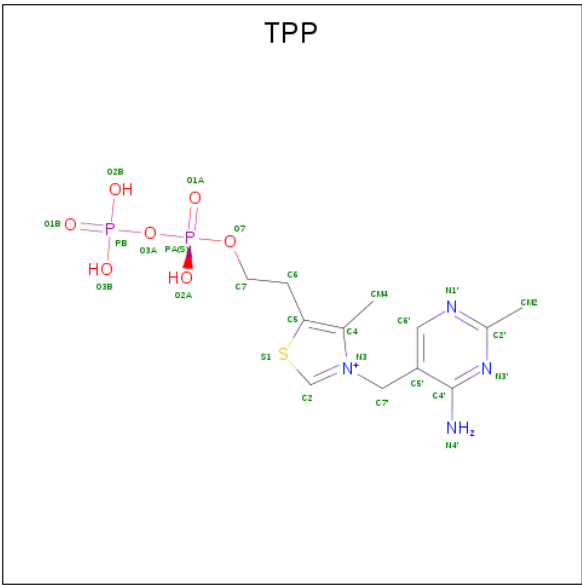
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is DIHYDROGENPHOSPHATE ION (three-letter code: 2HP) (formula: H<sub>2</sub>O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



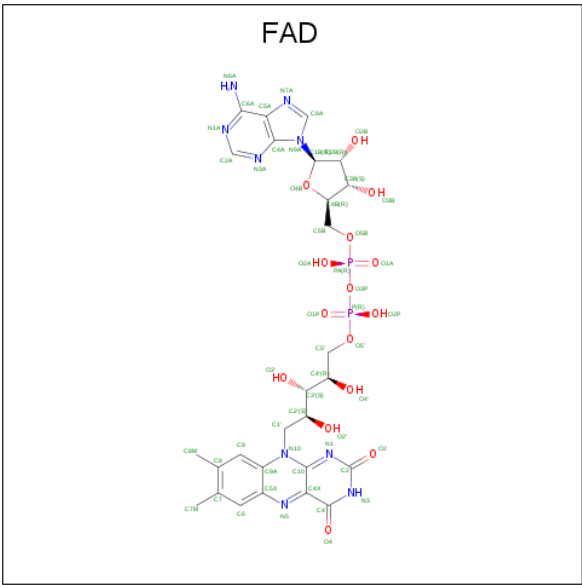
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
6	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	203	Total	O	0	0
			203	203		
7	B	122	Total	O	0	0
			122	122		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

[illegible]

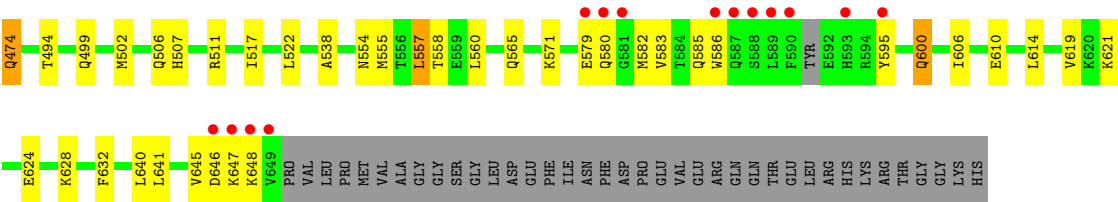
Chain B:

9% 66% 20% 13%

ALA PRO SER PHE ASN VAL ASP PRO LEU GLU GLN PRO ALA GLU PRO SER LYS LEU ALA LYS LYS LEU ARG ALA E82 E83 F89 E100 R101 M102 V107 F111 G115 L119 P120 M127 S128 D129 L135 P136 K137 G141 A142 M145 R151 A152 S153 V159

V159 P302 V303 L304 V305 V306 H313 R318 L319 L323 S324 D325 R326 A327 Q328 I329 P330 V331 T332 T333 Q336 D342 Q343 E344 L352 G353 M354 H355 A360 N361 V364 Q365 L366 A367 D368 L369 T370 I371 D378 R380 V381 N384 A389 P390 G391 A392 R393 A394 A395

A396 ALA GLU GLY ARG GLY T403 T404 H405 F406 E407 M414 Q418 T419 Q420 L421 T428 G432 K433 K434 M435 S436 K437 I438 F439 P440 V441 LYS R444 S445 E446 W447 F448 A449 Q450 Q451 M452 E457 Y458 PRD TYR ALA TYR MET E464 E465 T466 P467 G468 A469 K470 T472



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.55Å 109.40Å 178.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.60 41.93 – 2.59	Depositor EDS
% Data completeness (in resolution range)	94.1 (100.00-2.60) 93.2 (41.93-2.59)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.93 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.188 , 0.219 0.188 , 0.219	Depositor DCC
$R_{free}$ test set	5807 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.2	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8628	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 3.29% 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: 2HP, MG, K, FAD, TPP

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	0.33	0/4152	0.60	1/5639 (0.0%)
1	B	0.32	0/4131	0.57	0/5619
All	All	0.32	0/8283	0.58	1/11258 (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	614	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	4071	0	4066	113	0
1	B	4055	0	3938	111	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	26	0	16	0	0
5	B	26	0	16	1	0
6	A	53	0	31	0	0
6	B	53	0	31	0	0
7	A	203	0	0	6	0
7	B	122	0	0	2	0
All	All	8628	0	8098	216	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 13.

All (216) 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:A:474:GLN:HE21	1:A:474:GLN:H	1.09	1.01
1:A:403:ILE:H	1:A:420:GLN:HE21	1.07	0.94
1:A:151:ARG:HH22	1:A:336:GLN:HE22	1.20	0.87
1:B:365:GLN:HA	1:B:390:PRO:HD2	1.56	0.84
1:B:499:GLN:HE22	1:B:580:GLN:NE2	1.77	0.83
1:B:306:VAL:HG13	1:B:333:THR:HG22	1.61	0.82
1:A:474:GLN:NE2	1:A:474:GLN:H	1.76	0.82
1:B:474:GLN:H	1:B:474:GLN:NE2	1.81	0.79
1:A:151:ARG:NH2	1:A:336:GLN:HE22	1.82	0.77
1:A:385:ILE:HD11	1:A:417:VAL:CG1	2.15	0.77
1:A:338:LEU:HD11	1:A:351:MET:CE	2.16	0.75
1:A:462:TYR:HE2	1:A:478:LYS:HD2	1.51	0.75
1:A:313:HIS:HD2	1:A:315:ASP:H	1.36	0.74
1:B:368:ASP:O	1:B:392:ALA:HA	1.88	0.73
1:B:352:LEU:HD12	1:B:360:ALA:HB1	1.72	0.71
1:A:403:ILE:N	1:A:420:GLN:HE21	1.87	0.69
1:A:474:GLN:N	1:A:474:GLN:HE21	1.86	0.69
1:B:414:ASN:OD1	1:B:419:THR:HG22	1.92	0.68
1:B:499:GLN:HE22	1:B:580:GLN:HE22	1.41	0.66
1:A:462:TYR:CE2	1:A:478:LYS:HD2	2.31	0.66
1:A:450:GLN:HE21	1:A:450:GLN:HA	1.61	0.65
1:A:403:ILE:H	1:A:420:GLN:NE2	1.88	0.65
1:B:313:HIS:CD2	1:B:428:THR:HG21	2.31	0.65
1:B:390:PRO:HG2	1:B:391:GLU:H	1.60	0.65
1:A:554:ASN:HA	1:A:557:LEU:HD13	1.79	0.65
1:A:338:LEU:HD11	1:A:351:MET:HE3	1.77	0.64
1:A:386:SER:HA	1:A:393:ARG:HH22	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:HD12	1:A:421:ILE:HD12	1.79	0.63
1:B:621:LYS:O	1:B:624:GLU:HG2	1.99	0.63
1:A:335:LEU:HD12	1:A:351:MET:HE1	1.81	0.62
1:A:458:TYR:N	1:A:459:PRO:HD3	2.15	0.62
1:B:226:LEU:HB3	1:B:227:PRO:HD3	1.82	0.62
1:B:302:PRO:O	1:B:330:PRO:HD2	2.00	0.62
1:B:473:PRO:HG3	1:B:645:VAL:HG11	1.81	0.62
1:B:299:ALA:HB1	1:B:368:ASP:OD2	2.00	0.61
1:B:342:ASP:OD2	1:B:344:GLU:HB2	2.00	0.61
1:A:621:LYS:O	1:A:624:GLU:HG2	1.99	0.61
1:B:355:HIS:ND1	1:B:502:MET:HG3	2.16	0.61
1:A:151:ARG:HD2	1:A:182:ILE:CD1	2.31	0.61
1:A:520:GLY:HA3	7:A:1003:HOH:O	2.00	0.61
1:B:228:LEU:O	1:B:232:GLU:HG3	2.02	0.59
1:B:302:PRO:HG2	1:B:329:ILE:HG23	1.84	0.59
1:B:648:LYS:N	1:B:648:LYS:HD2	2.18	0.59
1:B:151:ARG:NH2	7:B:804:HOH:O	2.34	0.59
1:A:226:LEU:HB3	1:A:227:PRO:HD3	1.84	0.59
1:B:554:ASN:HA	1:B:557:LEU:HD13	1.84	0.59
1:B:474:GLN:HE21	1:B:474:GLN:H	1.49	0.58
1:B:353:GLY:HA2	1:B:381:VAL:HA	1.84	0.58
1:A:102:MET:HE3	1:A:107:VAL:HG11	1.84	0.58
1:A:385:ILE:HD11	1:A:417:VAL:HG12	1.84	0.58
1:A:151:ARG:NH2	1:A:336:GLN:NE2	2.51	0.58
1:B:151:ARG:HD2	1:B:182:ILE:CD1	2.34	0.57
1:A:228:LEU:O	1:A:232:GLU:HG3	2.04	0.57
1:B:434:MET:O	1:B:434:MET:HG2	2.04	0.57
1:A:141:GLY:O	1:A:145:MET:HG3	2.04	0.57
1:A:606:ILE:O	1:A:610:GLU:HG3	2.04	0.57
1:B:141:GLY:O	1:B:145:MET:HG3	2.05	0.57
1:A:87:THR:HG22	1:A:261:PRO:HG3	1.86	0.56
1:B:389:ALA:O	1:B:393:ARG:HB2	2.05	0.56
1:B:292:ALA:HB2	1:B:421:ILE:HG21	1.88	0.56
1:B:389:ALA:HB1	1:B:392:ALA:HB3	1.88	0.56
1:B:606:ILE:O	1:B:610:GLU:HG3	2.05	0.56
1:A:450:GLN:HA	1:A:450:GLN:NE2	2.19	0.55
1:A:619:VAL:HG22	1:A:628:LYS:HG3	1.86	0.55
1:A:555:MET:CE	7:A:761:HOH:O	2.54	0.55
1:B:102:MET:HE3	1:B:107:VAL:HG11	1.89	0.55
1:B:619:VAL:HG22	1:B:628:LYS:HG3	1.88	0.55
1:B:439:PHE:N	1:B:439:PHE:CD1	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ARG:HH21	1:B:319:LEU:HD21	1.71	0.54
1:A:600:GLN:NE2	7:A:759:HOH:O	2.40	0.54
1:A:465:GLU:CD	1:A:472:LYS:H	2.11	0.54
1:B:304:LEU:HD12	1:B:331:VAL:HG22	1.90	0.54
1:B:361:ASN:O	1:B:365:GLN:HG2	2.08	0.54
1:B:405:HIS:CE1	1:B:407:GLU:HB2	2.43	0.54
1:B:502:MET:O	1:B:506:GLN:HG3	2.08	0.54
1:B:354:MET:SD	1:B:380:ARG:CZ	2.96	0.53
1:A:499:GLN:HE22	1:A:648:LYS:CB	2.21	0.53
1:B:355:HIS:HB3	1:B:502:MET:HE2	1.90	0.53
1:B:582:MET:HE1	1:B:600:GLN:HG2	1.89	0.53
1:B:119:LEU:HB3	1:B:120:PRO:HD3	1.90	0.53
1:B:172:THR:HB	1:B:173:PRO:HD3	1.91	0.53
1:B:447:TRP:HA	1:B:447:TRP:CE3	2.43	0.53
1:B:378:ASP:HB3	1:B:381:VAL:HG23	1.92	0.52
1:A:165:PRO:HD3	1:B:522:LEU:HG	1.91	0.52
1:B:555:MET:CE	7:B:760:HOH:O	2.57	0.52
1:A:471:ILE:HG12	1:A:622:GLN:HG2	1.93	0.51
1:A:136:PRO:HB3	1:A:145:MET:HE2	1.92	0.51
1:A:289:ILE:HG23	1:A:434:MET:HB2	1.92	0.51
1:A:571:LYS:HB3	1:A:632:PHE:CZ	2.45	0.51
1:A:169:ASN:ND2	1:B:172:THR:OG1	2.43	0.51
1:A:335:LEU:CD1	1:A:351:MET:HE1	2.40	0.51
1:A:172:THR:HB	1:A:173:PRO:HD3	1.92	0.51
1:A:465:GLU:OE1	1:A:471:ILE:HA	2.11	0.51
1:B:323:LEU:HA	1:B:435:MET:HE1	1.93	0.50
1:B:571:LYS:HB3	1:B:632:PHE:CZ	2.46	0.50
1:A:502:MET:O	1:A:506:GLN:HG3	2.11	0.50
1:A:170:VAL:C	1:A:173:PRO:HD2	2.32	0.50
1:A:600:GLN:HG3	1:B:137:LYS:HE3	1.92	0.49
1:B:470:LYS:HB3	1:B:646:ASP:HB2	1.94	0.49
1:A:469:SER:H	1:A:622:GLN:NE2	2.09	0.49
1:A:172:THR:OG1	1:B:169:ASN:ND2	2.45	0.49
1:A:281:GLN:HG3	1:A:284:PHE:HB3	1.94	0.49
1:A:469:SER:H	1:A:622:GLN:HE21	1.59	0.49
1:A:473:PRO:HD3	1:A:645:VAL:HG13	1.95	0.49
1:A:640:LEU:C	1:A:640:LEU:HD23	2.32	0.49
1:B:170:VAL:C	1:B:173:PRO:HD2	2.33	0.49
1:B:414:ASN:CG	1:B:419:THR:HG22	2.32	0.49
1:B:448:PHE:HB3	1:B:452:ASN:HD21	1.78	0.48
1:A:115:GLY:HA3	1:A:162:THR:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LEU:HG	1:B:165:PRO:HD3	1.95	0.48
1:B:640:LEU:C	1:B:640:LEU:HD23	2.33	0.48
1:B:102:MET:CE	1:B:107:VAL:HG11	2.43	0.48
1:A:151:ARG:HD2	1:A:182:ILE:HD11	1.94	0.48
1:B:447:TRP:HA	1:B:447:TRP:HE3	1.79	0.48
1:A:119:LEU:HB3	1:A:120:PRO:HD3	1.96	0.48
1:B:557:LEU:HD23	1:B:558:THR:N	2.29	0.47
1:A:384:ASN:ND2	1:A:386:SER:OG	2.46	0.47
1:B:439:PHE:HD1	1:B:439:PHE:H	1.62	0.47
1:A:151:ARG:HD2	1:A:182:ILE:HD13	1.97	0.47
1:A:349:LEU:O	1:A:350:ASP:HB2	2.14	0.47
1:B:115:GLY:HA3	1:B:162:THR:HB	1.97	0.47
1:A:102:MET:CE	1:A:107:VAL:HG11	2.45	0.47
1:A:102:MET:HE2	1:A:158:VAL:HG11	1.97	0.47
1:B:585:GLN:HG3	1:B:586:TRP:HD1	1.80	0.47
1:A:136:PRO:HG3	1:A:142:ALA:HB2	1.96	0.47
1:A:434:MET:O	1:A:434:MET:HG2	2.14	0.46
1:B:494:THR:HA	1:B:517:ILE:O	2.15	0.46
1:A:269:PRO:O	1:A:270:SER:HB2	2.15	0.46
1:B:136:PRO:HG3	1:B:142:ALA:HB2	1.97	0.46
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.80	0.46
1:B:218:VAL:HG22	1:B:219:MET:N	2.30	0.46
1:B:439:PHE:N	1:B:439:PHE:HD1	2.14	0.46
1:A:145:MET:HE3	1:A:145:MET:HB2	1.82	0.46
1:A:281:GLN:O	1:A:281:GLN:HG2	2.16	0.46
1:A:494:THR:HA	1:A:517:ILE:O	2.16	0.45
1:B:211:ARG:HH11	1:B:211:ARG:HG3	1.81	0.45
1:A:218:VAL:HG22	1:A:219:MET:N	2.30	0.45
1:B:136:PRO:HB3	1:B:145:MET:HE2	1.98	0.45
1:B:153:SER:HB3	1:B:538:ALA:HB1	1.99	0.45
1:A:335:LEU:HA	1:A:351:MET:CE	2.45	0.45
1:A:474:GLN:O	1:A:478:LYS:HG3	2.16	0.45
1:A:102:MET:CE	1:A:158:VAL:HG11	2.47	0.45
1:A:246:LEU:HD23	1:A:246:LEU:C	2.37	0.45
1:B:246:LEU:C	1:B:246:LEU:HD23	2.37	0.45
1:A:119:LEU:HD11	1:B:583:VAL:HG13	1.98	0.45
1:A:281:GLN:C	1:A:283:GLU:N	2.71	0.44
1:A:555:MET:HE2	7:A:761:HOH:O	2.17	0.44
1:A:286:MET:O	1:A:286:MET:HE3	2.16	0.44
1:B:289:ILE:HG21	1:B:433:LYS:O	2.17	0.44
1:A:292:ALA:HB3	1:A:434:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:MET:HE3	1:B:107:VAL:HG21	1.99	0.44
1:B:325:ASP:O	1:B:328:GLN:NE2	2.51	0.44
1:B:494:THR:HG22	1:B:517:ILE:HB	1.99	0.44
1:A:457:GLU:C	1:A:459:PRO:HD3	2.38	0.44
1:A:557:LEU:HD23	1:A:558:THR:N	2.32	0.44
1:B:151:ARG:HD2	1:B:182:ILE:HD13	1.99	0.44
1:A:416:VAL:HG12	1:A:417:VAL:HG13	2.00	0.44
1:B:145:MET:HB2	1:B:145:MET:HE3	1.82	0.44
1:B:329:ILE:HA	1:B:330:PRO:HD3	1.88	0.44
1:B:336:GLN:HA	1:B:336:GLN:OE1	2.18	0.43
1:B:365:GLN:CA	1:B:390:PRO:HD2	2.39	0.43
1:B:151:ARG:HD2	1:B:182:ILE:HD11	1.98	0.43
1:B:304:LEU:HD23	1:B:371:ILE:HB	2.00	0.43
1:A:224:GLU:HG3	1:A:258:LEU:HD11	2.01	0.43
1:B:473:PRO:HG3	1:B:645:VAL:CG1	2.48	0.43
1:B:432:GLY:C	1:B:434:MET:H	2.21	0.43
1:B:619:VAL:HG23	1:B:641:LEU:HD11	2.00	0.43
1:A:458:TYR:N	1:A:459:PRO:CD	2.81	0.43
1:B:167:ALA:O	1:B:170:VAL:HG22	2.19	0.43
1:B:344:GLU:HG3	1:B:511:ARG:CZ	2.49	0.43
1:B:435:MET:CE	1:B:435:MET:HA	2.48	0.43
1:B:645:VAL:HG13	1:B:646:ASP:N	2.33	0.43
1:B:619:VAL:HG13	1:B:624:GLU:HG3	2.00	0.43
1:A:139:GLU:OE2	5:B:1700:TPP:N1'	2.52	0.42
1:A:299:ALA:HB2	7:A:812:HOH:O	2.18	0.42
1:A:384:ASN:ND2	1:A:387:LYS:HG3	2.34	0.42
1:B:89:PHE:HE2	1:B:100:GLU:HG2	1.83	0.42
1:A:161:VAL:CG2	1:A:188:THR:HG22	2.49	0.42
1:B:102:MET:CE	1:B:158:VAL:HG11	2.49	0.42
1:B:579:GLU:HB2	1:B:647:LYS:CB	2.49	0.42
1:A:291:LYS:HB3	1:A:421:ILE:CD1	2.49	0.42
1:A:350:ASP:HB3	7:A:860:HOH:O	2.18	0.42
1:B:369:LEU:HD12	1:B:403:ILE:N	2.35	0.42
1:B:557:LEU:HD23	1:B:557:LEU:C	2.40	0.42
1:A:619:VAL:HG13	1:A:624:GLU:HG3	2.01	0.42
1:A:384:ASN:HD22	1:A:387:LYS:HG3	1.85	0.41
1:B:111:PHE:O	1:B:159:VAL:HA	2.20	0.41
1:B:582:MET:HE1	1:B:600:GLN:CG	2.50	0.41
1:B:224:GLU:HG3	1:B:258:LEU:HD11	2.02	0.41
1:A:118:ILE:HG13	1:A:118:ILE:O	2.20	0.41
1:A:555:MET:HB3	1:A:555:MET:HE3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LYS:HB3	1:A:421:ILE:HD13	2.03	0.41
1:A:453:LYS:O	1:A:457:GLU:HB2	2.20	0.41
1:A:494:THR:HG22	1:A:517:ILE:HB	2.01	0.41
1:B:394:ARG:C	1:B:396:ALA:H	2.23	0.41
1:A:111:PHE:O	1:A:159:VAL:HA	2.20	0.41
1:B:228:LEU:HB2	1:B:266:THR:HB	2.03	0.41
1:A:450:GLN:HE21	1:A:450:GLN:CA	2.28	0.41
1:A:201:PHE:CE2	1:A:202:GLN:HG3	2.56	0.41
1:A:385:ILE:HD12	1:A:385:ILE:HA	1.86	0.41
1:B:304:LEU:O	1:B:332:THR:HG22	2.21	0.41
1:A:291:LYS:HA	1:A:291:LYS:HD3	1.90	0.41
1:A:409:SER:HA	1:A:410:PRO:HD3	1.93	0.41
1:B:115:GLY:HA3	1:B:162:THR:CB	2.51	0.41
1:A:119:LEU:HG	1:A:123:ASP:OD2	2.21	0.40
1:A:600:GLN:NE2	1:B:565:GLN:OE1	2.55	0.40
1:A:115:GLY:HA3	1:A:162:THR:CB	2.51	0.40
1:A:385:ILE:HD11	1:A:417:VAL:HG11	2.01	0.40
1:B:201:PHE:CE2	1:B:202:GLN:HG3	2.57	0.40
1:B:474:GLN:HG3	1:B:507:HIS:CD2	2.56	0.40
1:A:598:THR:HG23	1:B:135:LEU:HD11	2.03	0.40
1:B:365:GLN:O	1:B:390:PRO:HG2	2.22	0.40
1:B:595:TYR:CD1	1:B:595:TYR:N	2.89	0.40
1:A:201:PHE:CZ	1:A:202:GLN:HG3	2.57	0.40
1:A:335:LEU:HA	1:A:351:MET:HE2	2.02	0.40
1:A:313:HIS:CD2	1:A:315:ASP:H	2.26	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	535/630 (85%)	517 (97%)	15 (3%)	3 (1%)	27 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	536/630 (85%)	502 (94%)	29 (5%)	5 (1%)	19	38
All	All	1071/1260 (85%)	1019 (95%)	44 (4%)	8 (1%)	24	46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	464	GLU
1	B	394	ARG
1	A	597	HIS
1	B	390	PRO
1	B	437	LYS
1	A	459	PRO
1	B	433	LYS
1	B	440	PRO

### 5.3.2 Protein sidechains [i](#)

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	434/518 (84%)	428 (99%)	6 (1%)	69	87
1	B	422/518 (82%)	415 (98%)	7 (2%)	63	83
All	All	856/1036 (83%)	843 (98%)	13 (2%)	67	86

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	PRO
1	A	357	CYS
1	A	474	GLN
1	A	557	LEU
1	A	560	LEU
1	A	614	LEU
1	B	439	PHE
1	B	447	TRP

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Mol	Chain	Res	Type
1	B	474	GLN
1	B	557	LEU
1	B	560	LEU
1	B	600	GLN
1	B	614	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	169	ASN
1	A	313	HIS
1	A	336	GLN
1	A	384	ASN
1	A	420	GLN
1	A	450	GLN
1	A	474	GLN
1	A	499	GLN
1	A	512	ASN
1	A	554	ASN
1	A	600	GLN
1	A	622	GLN
1	B	169	ASN
1	B	313	HIS
1	B	412	ASN
1	B	418	GLN
1	B	452	ASN
1	B	474	GLN
1	B	499	GLN
1	B	512	ASN
1	B	554	ASN
1	B	600	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [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
4	2HP	A	698	-	4,4,4	1.32	0	6,6,6	0.39	0
5	TPP	A	700	3	21,27,27	1.59	4 (19%)	26,40,40	1.67	7 (26%)
6	FAD	A	701	-	51,58,58	2.58	24 (47%)	57,89,89	1.84	6 (10%)
4	2HP	B	1697	-	4,4,4	1.34	0	6,6,6	0.39	0
4	2HP	B	1698	-	4,4,4	1.33	0	6,6,6	0.38	0
5	TPP	B	1700	3	21,27,27	1.55	4 (19%)	26,40,40	1.73	7 (26%)
6	FAD	B	1701	-	51,58,58	2.55	23 (45%)	57,89,89	1.75	5 (8%)

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	2HP	A	698	-	-	0/0/0/0	0/0/0/0
5	TPP	A	700	3	-	0/16/17/17	0/2/2/2
6	FAD	A	701	-	-	0/28/50/50	0/6/6/6
4	2HP	B	1697	-	-	0/0/0/0	0/0/0/0
4	2HP	B	1698	-	-	0/0/0/0	0/0/0/0
5	TPP	B	1700	3	-	0/16/17/17	0/2/2/2
6	FAD	B	1701	-	-	0/28/50/50	0/6/6/6

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1700	TPP	C4-N3	-3.45	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	700	TPP	C4-N3	-2.70	1.37	1.39
5	A	700	TPP	PB-O2B	-2.11	1.46	1.54
5	B	1700	TPP	PB-O2B	-2.10	1.46	1.54
6	B	1701	FAD	C2-N3	2.10	1.42	1.38
5	B	1700	TPP	C6'-C5'	2.13	1.42	1.37
6	A	701	FAD	C4'-C3'	2.18	1.57	1.53
5	B	1700	TPP	C7'-C5'	2.23	1.55	1.51
6	A	701	FAD	C2-N3	2.23	1.42	1.38
6	A	701	FAD	C1'-N10	2.30	1.50	1.48
6	A	701	FAD	O4B-C1B	2.31	1.44	1.41
5	A	700	TPP	C6'-C5'	2.34	1.42	1.37
6	B	1701	FAD	O4'-C4'	2.35	1.48	1.43
6	B	1701	FAD	C6-C5X	2.43	1.45	1.41
6	A	701	FAD	C5A-C4A	2.44	1.46	1.40
6	B	1701	FAD	C5A-C4A	2.62	1.46	1.40
6	B	1701	FAD	O4B-C1B	2.70	1.45	1.41
6	B	1701	FAD	C2A-N1A	2.75	1.39	1.33
6	A	701	FAD	C2A-N1A	2.81	1.39	1.33
6	B	1701	FAD	C5X-N5	2.83	1.39	1.35
6	A	701	FAD	C6-C5X	2.85	1.46	1.41
6	A	701	FAD	O4'-C4'	2.85	1.49	1.43
6	A	701	FAD	C4A-N3A	2.91	1.39	1.35
6	B	1701	FAD	C4-C4X	2.91	1.46	1.41
5	A	700	TPP	C7'-C5'	2.98	1.57	1.51
6	A	701	FAD	C4-C4X	3.01	1.46	1.41
6	B	1701	FAD	C4X-N5	3.03	1.37	1.33
6	A	701	FAD	C5X-N5	3.07	1.40	1.35
6	B	1701	FAD	C1'-N10	3.11	1.51	1.48
6	B	1701	FAD	C4A-N3A	3.14	1.40	1.35
6	A	701	FAD	C9-C9A	3.25	1.47	1.40
6	B	1701	FAD	C9-C9A	3.31	1.47	1.40
6	A	701	FAD	C4X-N5	3.46	1.38	1.33
6	B	1701	FAD	C6-C7	3.46	1.46	1.37
6	A	701	FAD	C2A-N3A	3.50	1.37	1.32
6	A	701	FAD	C6-C7	3.58	1.47	1.37
6	A	701	FAD	C4X-C10	3.66	1.47	1.41
6	A	701	FAD	C7M-C7	3.66	1.58	1.51
6	A	701	FAD	C9-C8	3.75	1.47	1.37
6	B	1701	FAD	C9-C8	3.76	1.47	1.37
6	B	1701	FAD	C7M-C7	3.76	1.58	1.51
6	B	1701	FAD	C2A-N3A	3.77	1.38	1.32
6	B	1701	FAD	C8A-N9A	3.86	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1701	FAD	C4X-C10	3.90	1.47	1.41
6	B	1701	FAD	C9A-C5X	4.00	1.50	1.42
6	A	701	FAD	C9A-C5X	4.02	1.50	1.42
6	A	701	FAD	C8A-N9A	4.17	1.42	1.36
6	B	1701	FAD	C8-C7	4.46	1.52	1.40
6	B	1701	FAD	C10-N1	4.60	1.39	1.33
6	A	701	FAD	C10-N1	4.63	1.39	1.33
6	A	701	FAD	C8-C7	4.63	1.52	1.40
6	A	701	FAD	C4-N3	5.34	1.42	1.33
6	B	1701	FAD	C4-N3	5.51	1.42	1.33
6	B	1701	FAD	C9A-N10	6.31	1.46	1.38
6	A	701	FAD	C9A-N10	6.62	1.46	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	701	FAD	C4X-C4-N3	-5.19	116.09	123.47
6	B	1701	FAD	C4X-C4-N3	-5.14	116.16	123.47
5	B	1700	TPP	N1'-C2'-N3'	-2.89	120.45	125.55
5	A	700	TPP	N1'-C2'-N3'	-2.72	120.76	125.55
5	B	1700	TPP	CM4-C4-C5	-2.60	121.92	127.60
5	A	700	TPP	CM4-C4-C5	-2.53	122.07	127.60
5	B	1700	TPP	C5'-C6'-N1'	-2.52	119.57	123.83
5	A	700	TPP	C5'-C6'-N1'	-2.34	119.86	123.83
6	A	701	FAD	C1'-N10-C10	-2.14	116.32	118.46
6	B	1701	FAD	C6-C5X-C9A	2.01	121.71	119.01
5	B	1700	TPP	C2'-N3'-C4'	2.01	121.55	118.14
6	A	701	FAD	C6-C5X-C9A	2.02	121.72	119.01
5	A	700	TPP	C2'-N3'-C4'	2.03	121.59	118.14
5	A	700	TPP	CM2-C2'-N1'	2.92	120.31	117.07
5	A	700	TPP	C5-C4-N3	3.13	113.83	107.57
5	B	1700	TPP	C5-C4-N3	3.17	113.91	107.57
5	B	1700	TPP	CM2-C2'-N1'	3.24	120.67	117.07
5	B	1700	TPP	C6'-N1'-C2'	3.43	121.92	115.95
5	A	700	TPP	C6'-N1'-C2'	3.43	121.93	115.95
6	B	1701	FAD	C1'-N10-C9A	4.18	122.03	118.31
6	B	1701	FAD	C4X-N5-C5X	4.22	121.18	116.76
6	A	701	FAD	C4X-N5-C5X	4.23	121.19	116.76
6	A	701	FAD	C1'-N10-C9A	5.00	122.75	118.31
6	B	1701	FAD	C4-N3-C2	8.35	122.25	115.14
6	A	701	FAD	C4-N3-C2	8.59	122.45	115.14

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
5	B	1700	TPP	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, 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	541/630 (85%)	-0.17	21 (3%) 39 31	33, 48, 90, 140	0
1	B	550/630 (87%)	0.31	58 (10%) 6 3	33, 56, 136, 147	0
All	All	1091/1260 (86%)	0.07	79 (7%) 15 11	33, 50, 125, 147	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	649	VAL	8.0
1	B	590	PHE	6.6
1	B	82	GLU	6.3
1	B	396	ALA	6.2
1	B	593	HIS	5.5
1	B	595	TYR	5.3
1	B	83	PRO	5.1
1	A	463	MET	5.1
1	A	596	SER	4.8
1	B	298	LEU	4.8
1	A	461	ALA	4.6
1	B	466	THR	4.5
1	B	458	TYR	4.5
1	B	280	ALA	4.4
1	B	648	LYS	4.4
1	B	467	PRO	4.3
1	B	366	ASN	4.2
1	A	467	PRO	4.2
1	B	384	ASN	4.2
1	A	599	HIS	4.2
1	B	586	TRP	3.9
1	B	392	ALA	3.9
1	A	83	PRO	3.8
1	B	589	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	468	GLY	3.7
1	A	460	TYR	3.7
1	B	127	ASN	3.6
1	A	597	HIS	3.5
1	B	389	ALA	3.4
1	B	435	MET	3.4
1	B	587	GLN	3.3
1	B	441	VAL	3.3
1	B	283	GLU	3.2
1	A	456	LYS	3.2
1	B	369	LEU	3.2
1	A	462	TYR	3.2
1	A	281	GLN	3.2
1	B	391	GLU	3.1
1	B	364	VAL	3.1
1	B	447	TRP	3.1
1	B	464	GLU	3.0
1	B	588	SER	3.0
1	B	439	PHE	2.8
1	A	468	GLY	2.8
1	B	457	GLU	2.8
1	B	445	SER	2.7
1	B	278	SER	2.7
1	A	466	THR	2.6
1	B	448	PHE	2.6
1	B	647	LYS	2.6
1	B	418	GLN	2.6
1	B	326	ARG	2.6
1	A	598	THR	2.5
1	B	450	GLN	2.5
1	B	129	ASP	2.5
1	B	286	MET	2.5
1	B	579	GLU	2.5
1	B	451	ILE	2.5
1	A	458	TYR	2.5
1	B	328	GLN	2.4
1	B	436	SER	2.4
1	B	277	THR	2.4
1	B	361	ASN	2.4
1	A	270	SER	2.4
1	B	393	ARG	2.4
1	B	449	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	465	GLU	2.3
1	B	367	ALA	2.2
1	A	84	ASP	2.2
1	B	581	GLY	2.2
1	A	268	LEU	2.1
1	B	302	PRO	2.1
1	A	464	GLU	2.1
1	A	283	GLU	2.1
1	B	420	GLN	2.1
1	B	276	LEU	2.1
1	A	96	GLN	2.1
1	B	646	ASP	2.0
1	B	580	GLN	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	2HP	B	1698	5/5	0.83	0.26	133,133,133,133	0
4	2HP	A	698	5/5	0.85	0.24	120,120,121,121	0
4	2HP	B	1697	5/5	0.92	0.12	115,115,115,115	0
6	FAD	B	1701	53/53	0.95	0.19	54,60,86,87	0
5	TPP	A	700	26/26	0.98	0.13	36,46,49,50	0
6	FAD	A	701	53/53	0.98	0.16	40,49,73,74	0
3	MG	A	699	1/1	0.98	0.06	47,47,47,47	0
2	K	B	1696	1/1	0.98	0.20	43,43,43,43	0
2	K	A	696	1/1	0.99	0.19	32,32,32,32	0
3	MG	B	1699	1/1	0.99	0.06	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	TPP	B	1700	26/26	0.99	0.13	35,42,45,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.