



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:19 PM 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

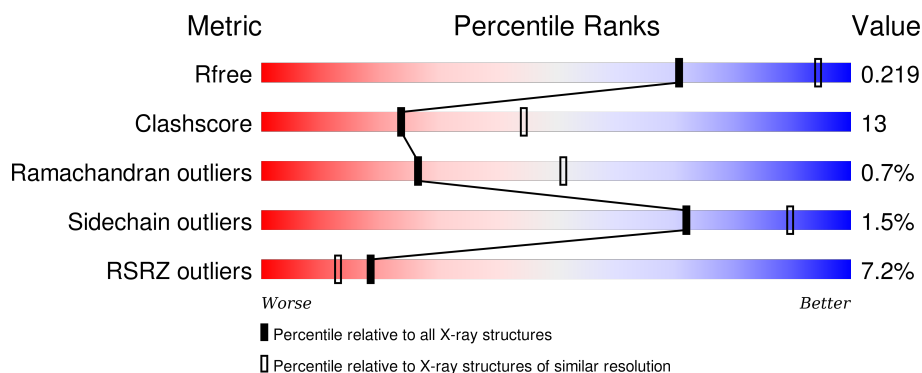
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 ≥ 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	
1	B	630	

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	K	B	1696	-	-	-	X
4	2HP	A	698	-	-	-	X
4	2HP	B	1698	-	-	-	X

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			

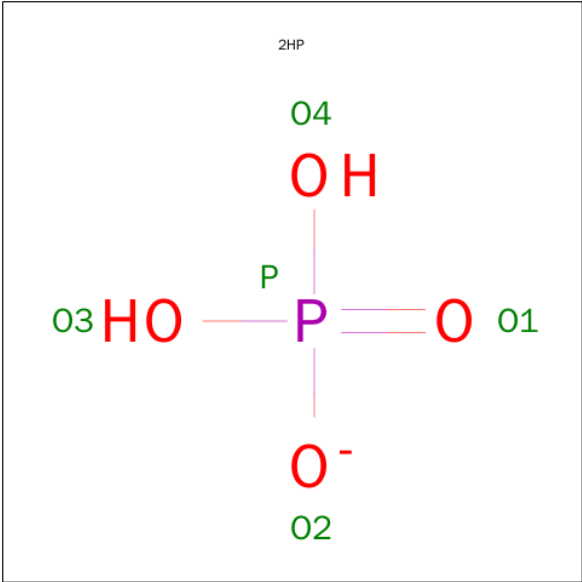
- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

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).

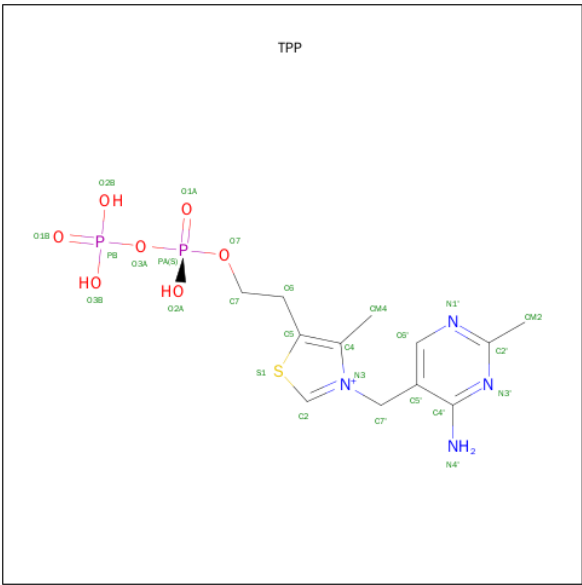
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is DIHYDROGENPHOSPHATE ION (three-letter code: 2HP) (formula: H₂O₄P).



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: C₁₂H₁₉N₄O₇P₂S).



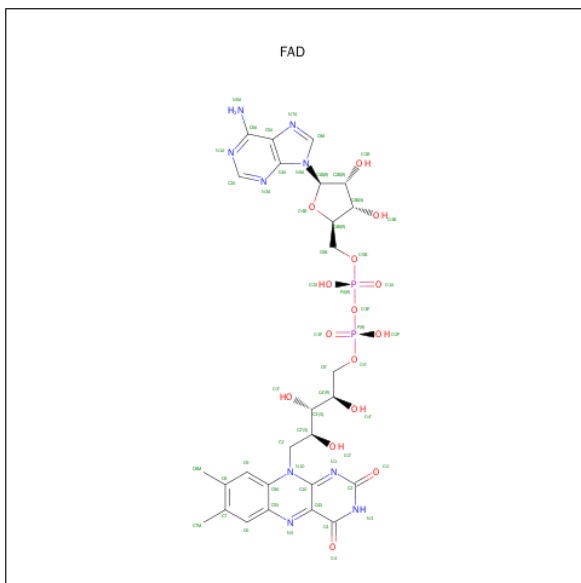
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

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

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

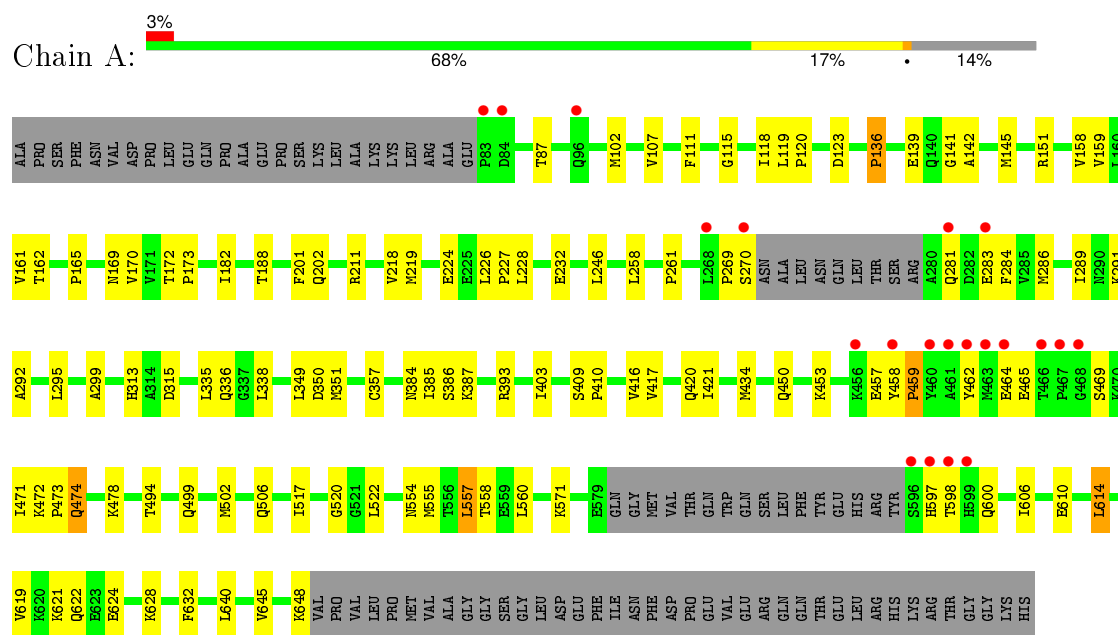
- Molecule 7 is water.

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

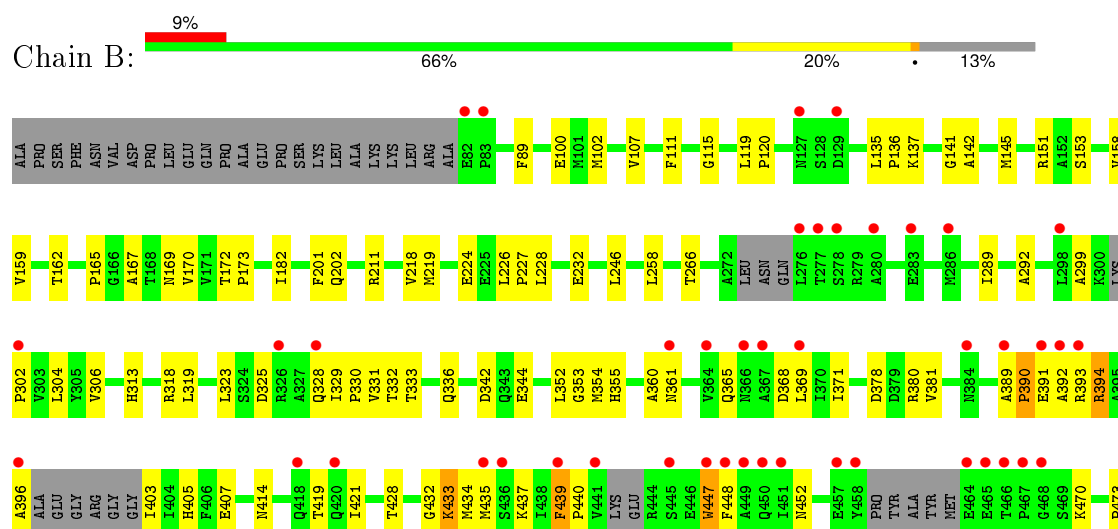
3 Residue-property plots [i](#)

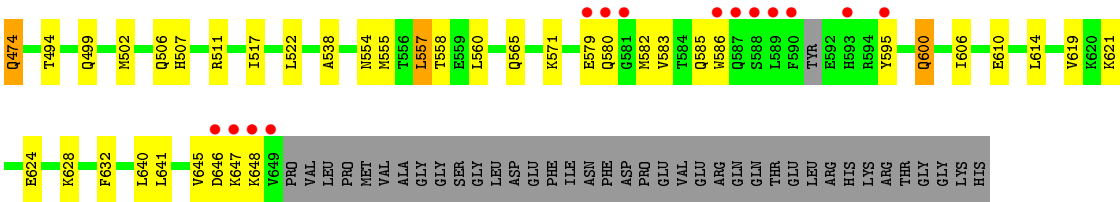
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: ACETOHYDROXY-ACID SYNTHASE



• Molecule 1: ACETOHYDROXY-ACID SYNTHASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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	5574 reflections (10.15%)	DCC
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 57455 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8628	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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:385:ILE:HD11	1:A:417:VAL:HG12	1.84	0.58
1:A:102:MET:HE3	1:A:107:VAL:HG11	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:389:ALA:HB1	1:B:392:ALA:HB3	1.88	0.56
1:B:292:ALA:HB2	1:B:421:ILE:HG21	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:619:VAL:HG22	1:B:628:LYS:HG3	1.88	0.55
1:B:102:MET:HE3	1:B:107:VAL:HG11	1.89	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:361:ASN:O	1:B:365:GLN:HG2	2.08	0.54
1:B:304:LEU:HD12	1:B:331:VAL:HG22	1.90	0.54
1:B:502:MET:O	1:B:506:GLN:HG3	2.08	0.54
1:B:405:HIS:CE1	1:B:407:GLU:HB2	2.43	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:465:GLU:OE1	1:A:471:ILE:HA	2.11	0.51
1:A:172:THR:HB	1:A:173:PRO:HD3	1.92	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:B:470:LYS:HB3	1:B:646:ASP:HB2	1.94	0.49
1:A:600:GLN:HG3	1:B:137:LYS:HE3	1.92	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:B:170:VAL:C	1:B:173:PRO:HD2	2.33	0.49
1:A:640:LEU:C	1:A:640:LEU:HD23	2.32	0.49
1:A:473:PRO:HD3	1:A:645:VAL:HG13	1.95	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:B:640:LEU:C	1:B:640:LEU:HD23	2.33	0.48
1:A:522:LEU:HG	1:B:165:PRO:HD3	1.95	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:151:ARG:HD2	1:A:182:ILE:HD13	1.97	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:B:115:GLY:HA3	1:B:162:THR:HB	1.97	0.47
1:A:349:LEU:O	1:A:350:ASP:HB2	2.14	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:B:136:PRO:HG3	1:B:142:ALA:HB2	1.97	0.46
1:A:269:PRO:O	1:A:270:SER:HB2	2.15	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:B:136:PRO:HB3	1:B:145:MET:HE2	1.98	0.45
1:A:218:VAL:HG22	1:A:219:MET:N	2.30	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:555:MET:HE2	7:A:761:HOH:O	2.17	0.44
1:A:281:GLN:C	1:A:283:GLU:N	2.71	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:B:102:MET:HE3	1:B:107:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ALA:HB3	1:A:434:MET:CE	2.47	0.44
1:B:494:THR:HG22	1:B:517:ILE:HB	1.99	0.44
1:B:325:ASP:O	1:B:328:GLN:NE2	2.51	0.44
1:A:557:LEU:HD23	1:A:558:THR:N	2.32	0.44
1:A:457:GLU:C	1:A:459:PRO:HD3	2.38	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:329:ILE:HA	1:B:330:PRO:HD3	1.88	0.44
1:B:145:MET:HB2	1:B:145:MET:HE3	1.82	0.44
1:B:365:GLN:CA	1:B:390:PRO:HD2	2.39	0.43
1:B:336:GLN:HA	1:B:336:GLN:OE1	2.18	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:B:473:PRO:HG3	1:B:645:VAL:CG1	2.48	0.43
1:A:224:GLU:HG3	1:A:258:LEU:HD11	2.01	0.43
1:B:619:VAL:HG23	1:B:641:LEU:HD11	2.00	0.43
1:B:432:GLY:C	1:B:434:MET:H	2.21	0.43
1:A:458:TYR:N	1:A:459:PRO:CD	2.81	0.43
1:B:645:VAL:HG13	1:B:646:ASP:N	2.33	0.43
1:B:344:GLU:HG3	1:B:511:ARG:CZ	2.49	0.43
1:B:167:ALA:O	1:B:170:VAL:HG22	2.19	0.43
1:B:435:MET:CE	1:B:435:MET:HA	2.48	0.43
1:B:619:VAL:HG13	1:B:624:GLU:HG3	2.00	0.43
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: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:B:102:MET:CE	1:B:158:VAL:HG11	2.49	0.42
1:A:161:VAL:CG2	1:A:188:THR:HG22	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:582:MET:HE1	1:B:600:GLN:CG	2.50	0.41
1:B:111:PHE:O	1:B:159:VAL:HA	2.20	0.41
1:B:224:GLU:HG3	1:B:258:LEU:HD11	2.02	0.41
1:A:555:MET:HB3	1:A:555:MET:HE3	1.95	0.41
1:A:118:ILE:HG13	1:A:118:ILE:O	2.20	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:B:228:LEU:HB2	1:B:266:THR:HB	2.03	0.41
1:A:111:PHE:O	1:A:159:VAL:HA	2.20	0.41
1:A:450:GLN:HE21	1:A:450:GLN:CA	2.28	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:201:PHE:CE2	1:A:202:GLN:HG3	2.56	0.41
1:A:291:LYS:HA	1:A:291:LYS:HD3	1.90	0.41
1:B:115:GLY:HA3	1:B:162:THR:CB	2.51	0.41
1:A:409:SER:HA	1:A:410:PRO:HD3	1.93	0.41
1:A:600:GLN:NE2	1:B:565:GLN:OE1	2.55	0.40
1:A:119:LEU:HG	1:A:123:ASP:OD2	2.21	0.40
1:B:474:GLN:HG3	1:B:507:HIS:CD2	2.56	0.40
1:A:385:ILE:HD11	1:A:417:VAL:HG11	2.01	0.40
1:A:115:GLY:HA3	1:A:162:THR:CB	2.51	0.40
1:B:201:PHE:CE2	1:B:202:GLN:HG3	2.57	0.40
1:B:365:GLN:O	1:B:390:PRO:HG2	2.22	0.40
1:A:598:THR:HG23	1:B:135:LEU:HD11	2.03	0.40
1:B:595:TYR:CD1	1:B:595:TYR:N	2.89	0.40
1:A:335:LEU:HA	1:A:351:MET:HE2	2.02	0.40
1:A:201:PHE:CZ	1:A:202:GLN:HG3	2.57	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%)	30 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	536/630 (85%)	502 (94%)	29 (5%)	5 (1%)	21	42
All	All	1071/1260 (85%)	1019 (95%)	44 (4%)	8 (1%)	26	51

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 ⓘ

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%)	74	90
1	B	422/518 (82%)	415 (98%)	7 (2%)	68	88
All	All	856/1036 (83%)	843 (98%)	13 (2%)	72	90

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	1.30	0	6,6,6	0.77	0
5	TPP	A	700	3	20,27,27	1.60	5 (25%)	31,40,40	1.54	6 (19%)
6	FAD	A	701	-	48,58,58	2.40	23 (47%)	54,89,89	1.84	7 (12%)
4	2HP	B	1697	-	4,4,4	1.30	0	6,6,6	0.77	0
4	2HP	B	1698	-	4,4,4	1.30	0	6,6,6	0.76	0
5	TPP	B	1700	3	20,27,27	1.59	5 (25%)	31,40,40	1.59	6 (19%)
6	FAD	B	1701	-	48,58,58	2.42	23 (47%)	54,89,89	1.78	8 (14%)

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	-	-	0/30/50/50	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	-	-	0/30/50/50	0/6/6/6

All (56) 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	-2.33	1.46	1.54
5	B	1700	TPP	PB-O2B	-2.32	1.46	1.54
5	A	700	TPP	PA-O2A	-2.18	1.45	1.54
6	B	1701	FAD	P-O2P	-2.09	1.46	1.54
5	B	1700	TPP	PA-O2A	-2.06	1.46	1.54
5	B	1700	TPP	C6'-C5'	2.05	1.42	1.37
6	A	701	FAD	C4'-C3'	2.10	1.57	1.53
5	B	1700	TPP	C7'-C5'	2.15	1.55	1.51
6	A	701	FAD	C1'-N10	2.24	1.50	1.48
5	A	700	TPP	C6'-C5'	2.25	1.42	1.37
6	B	1701	FAD	O4'-C4'	2.26	1.48	1.43
6	B	1701	FAD	C10-N1	2.28	1.39	1.35
6	A	701	FAD	C10-N1	2.31	1.39	1.35
6	A	701	FAD	C10-N10	2.40	1.41	1.39
6	A	701	FAD	C5A-C4A	2.44	1.46	1.40
6	B	1701	FAD	C6-C5X	2.56	1.45	1.41
6	A	701	FAD	O4B-C1B	2.58	1.44	1.41
6	B	1701	FAD	C5A-C4A	2.62	1.46	1.40
6	B	1701	FAD	C4-C4X	2.64	1.46	1.41
6	B	1701	FAD	C5X-N5	2.72	1.39	1.35
6	A	701	FAD	C4-C4X	2.73	1.46	1.41
6	B	1701	FAD	C2A-N1A	2.73	1.39	1.33
6	A	701	FAD	O4'-C4'	2.75	1.49	1.43
6	A	701	FAD	C2A-N1A	2.79	1.39	1.33
6	B	1701	FAD	C4X-N5	2.81	1.37	1.33
6	A	701	FAD	C4A-N3A	2.82	1.39	1.35
5	A	700	TPP	C7'-C5'	2.87	1.57	1.51
6	A	701	FAD	C5X-N5	2.95	1.40	1.35
6	A	701	FAD	C6-C5X	2.99	1.46	1.41
6	B	1701	FAD	O4B-C1B	3.01	1.45	1.41
6	B	1701	FAD	C1'-N10	3.03	1.51	1.48
6	B	1701	FAD	C4A-N3A	3.04	1.40	1.35
6	A	701	FAD	C9-C9A	3.13	1.47	1.40
6	A	701	FAD	C2A-N3A	3.19	1.37	1.32
6	B	1701	FAD	C9-C9A	3.19	1.47	1.40
6	A	701	FAD	C4X-N5	3.21	1.38	1.33
6	A	701	FAD	C4X-C10	3.22	1.47	1.41
6	B	1701	FAD	C6-C7	3.27	1.46	1.37
6	A	701	FAD	C6-C7	3.38	1.47	1.37
6	B	1701	FAD	C4X-C10	3.43	1.47	1.41
6	B	1701	FAD	C2A-N3A	3.44	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	701	FAD	C9-C8	3.54	1.47	1.37
6	B	1701	FAD	C10-N10	3.55	1.43	1.39
6	B	1701	FAD	C9-C8	3.55	1.47	1.37
6	A	701	FAD	C7M-C7	3.59	1.58	1.51
6	B	1701	FAD	C7M-C7	3.69	1.58	1.51
6	B	1701	FAD	C9A-C5X	4.00	1.50	1.42
6	A	701	FAD	C9A-C5X	4.01	1.50	1.42
6	B	1701	FAD	C8-C7	4.15	1.52	1.41
6	A	701	FAD	C8-C7	4.31	1.52	1.41
6	A	701	FAD	C4-N3	5.13	1.42	1.33
6	B	1701	FAD	C4-N3	5.29	1.42	1.33
6	B	1701	FAD	C9A-N10	5.55	1.46	1.38
6	A	701	FAD	C9A-N10	5.82	1.46	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	701	FAD	C4X-C4-N3	-5.49	116.09	123.59
6	B	1701	FAD	C4X-C4-N3	-5.44	116.16	123.59
5	B	1700	TPP	CM4-C4-C5	-3.10	121.92	128.90
5	A	700	TPP	CM4-C4-C5	-3.04	122.07	128.90
5	B	1700	TPP	N1'-C2'-N3'	-2.78	120.45	125.60
5	A	700	TPP	N1'-C2'-N3'	-2.62	120.76	125.60
6	A	701	FAD	C1B-N9A-C4A	-2.49	123.19	126.94
5	B	1700	TPP	C5'-C6'-N1'	-2.47	119.57	123.86
5	A	700	TPP	C5'-C6'-N1'	-2.30	119.86	123.86
6	B	1701	FAD	C4X-C10-N10	-2.17	119.24	120.52
6	B	1701	FAD	C1B-N9A-C4A	-2.13	123.72	126.94
6	B	1701	FAD	C6-C5X-C9A	2.07	121.71	118.98
6	A	701	FAD	C6-C5X-C9A	2.09	121.72	118.98
6	B	1701	FAD	O3P-P-O5'	2.16	108.67	102.94
6	A	701	FAD	O3P-P-O5'	2.52	109.61	102.94
5	A	700	TPP	CM2-C2'-N1'	2.73	120.31	117.03
5	A	700	TPP	C5-C4-N3	2.79	113.83	107.69
6	B	1701	FAD	C1'-N10-C9A	2.82	122.03	118.86
5	B	1700	TPP	C5-C4-N3	2.83	113.91	107.69
5	B	1700	TPP	CM2-C2'-N1'	3.03	120.67	117.03
6	A	701	FAD	C1'-N10-C9A	3.47	122.75	118.86
5	B	1700	TPP	C6'-N1'-C2'	3.52	121.92	115.77
5	A	700	TPP	C6'-N1'-C2'	3.52	121.93	115.77
6	B	1701	FAD	C4X-N5-C5X	3.84	121.18	116.76
6	A	701	FAD	C4X-N5-C5X	3.85	121.19	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	B	1701	FAD	C4-N3-C2	8.10	122.25	115.25
6	A	701	FAD	C4-N3-C2	8.34	122.45	115.25

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	541/630 (85%)	-0.14	21 (3%) 43 35	33, 48, 90, 140	0
1	B	550/630 (87%)	0.35	58 (10%) 8 5	33, 56, 136, 147	0
All	All	1091/1260 (86%)	0.11	79 (7%) 18 13	33, 50, 125, 147	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	649	VAL	8.1
1	B	590	PHE	6.6
1	B	82	GLU	6.5
1	B	396	ALA	6.3
1	B	593	HIS	5.6
1	B	595	TYR	5.4
1	A	463	MET	5.2
1	B	83	PRO	5.2
1	A	596	SER	4.9
1	B	298	LEU	4.8
1	A	461	ALA	4.7
1	B	466	THR	4.6
1	B	458	TYR	4.6
1	B	280	ALA	4.5
1	B	648	LYS	4.5
1	B	467	PRO	4.4
1	B	366	ASN	4.3
1	B	384	ASN	4.3
1	A	467	PRO	4.2
1	A	599	HIS	4.2
1	B	392	ALA	3.9
1	B	586	TRP	3.9
1	A	83	PRO	3.9
1	B	468	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	460	TYR	3.8
1	B	589	LEU	3.7
1	B	127	ASN	3.7
1	A	597	HIS	3.6
1	B	435	MET	3.5
1	B	389	ALA	3.4
1	B	587	GLN	3.4
1	B	441	VAL	3.3
1	B	283	GLU	3.3
1	A	456	LYS	3.3
1	A	462	TYR	3.3
1	B	369	LEU	3.2
1	A	281	GLN	3.2
1	B	391	GLU	3.2
1	B	364	VAL	3.2
1	B	447	TRP	3.2
1	B	464	GLU	3.1
1	B	588	SER	3.0
1	B	457	GLU	2.9
1	A	468	GLY	2.9
1	B	439	PHE	2.9
1	B	445	SER	2.8
1	B	278	SER	2.7
1	A	466	THR	2.7
1	B	647	LYS	2.7
1	B	418	GLN	2.7
1	B	448	PHE	2.6
1	B	326	ARG	2.6
1	A	598	THR	2.6
1	B	129	ASP	2.6
1	B	286	MET	2.6
1	B	450	GLN	2.6
1	B	579	GLU	2.5
1	B	328	GLN	2.5
1	A	458	TYR	2.5
1	B	451	ILE	2.5
1	B	436	SER	2.5
1	B	361	ASN	2.4
1	B	277	THR	2.4
1	B	393	ARG	2.4
1	A	270	SER	2.4
1	B	449	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	465	GLU	2.3
1	A	84	ASP	2.3
1	B	367	ALA	2.3
1	B	581	GLY	2.3
1	A	464	GLU	2.2
1	B	302	PRO	2.2
1	A	268	LEU	2.2
1	A	283	GLU	2.2
1	B	420	GLN	2.2
1	A	96	GLN	2.1
1	B	646	ASP	2.1
1	B	276	LEU	2.1
1	B	580	GLN	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	2HP	A	698	5/5	0.85	0.24	4.03	120,120,121,121	0
4	2HP	B	1698	5/5	0.83	0.26	3.59	133,133,133,133	0
2	K	B	1696	1/1	0.98	0.20	2.41	43,43,43,43	0
2	K	A	696	1/1	0.99	0.19	1.79	32,32,32,32	0
6	FAD	B	1701	53/53	0.95	0.19	0.46	54,60,86,87	0
6	FAD	A	701	53/53	0.98	0.16	0.01	40,49,73,74	0
5	TPP	B	1700	26/26	0.99	0.13	-0.92	35,42,45,47	0
5	TPP	A	700	26/26	0.98	0.13	-1.02	36,46,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	B	1699	1/1	0.99	0.06	-1.52	42,42,42,42	0
3	MG	A	699	1/1	0.98	0.06	-	47,47,47,47	0
4	2HP	B	1697	5/5	0.92	0.12	-	115,115,115,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.