



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:10 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 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/ValidationPDFNotes.html>

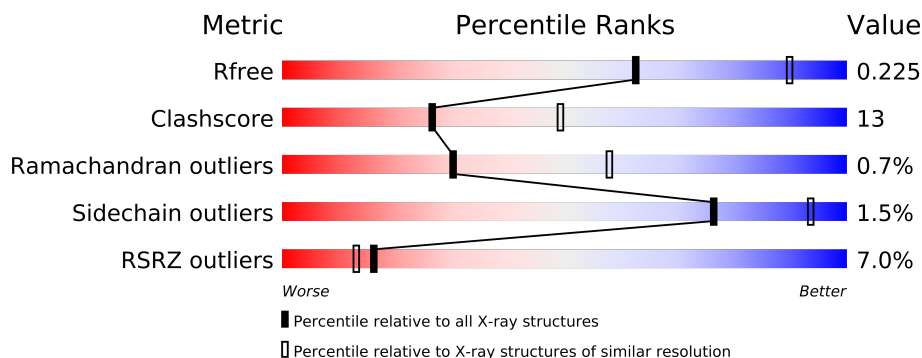
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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. 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	630	
1	B	630	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
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 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 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			

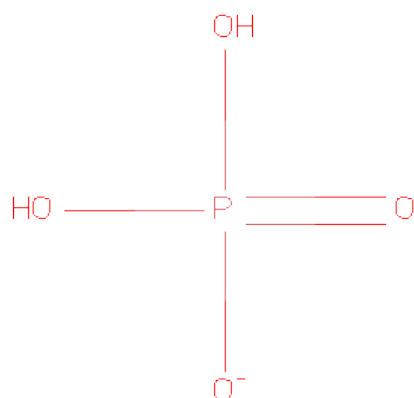
- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

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).

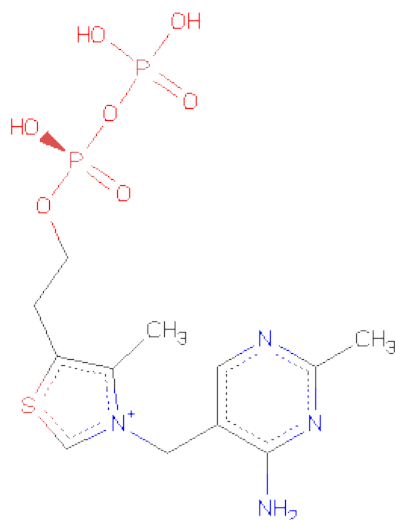
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- 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).



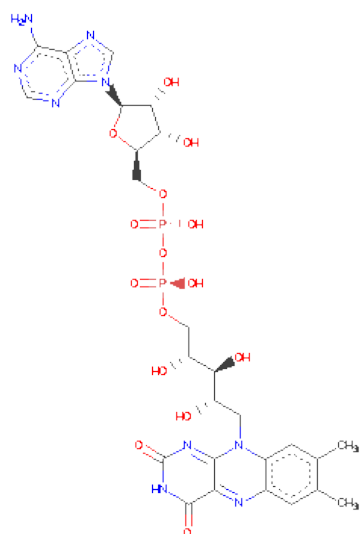
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

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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.

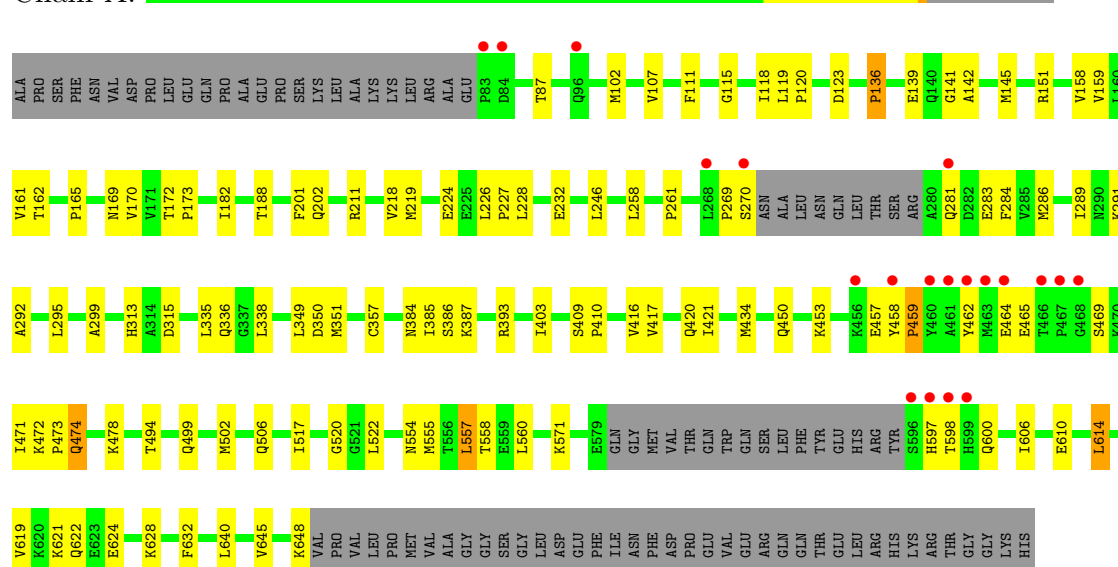
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	203	Total	O		
			203	203	0	0
7	B	122	Total	O		
			122	122	0	0

3 Residue-property plots

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.

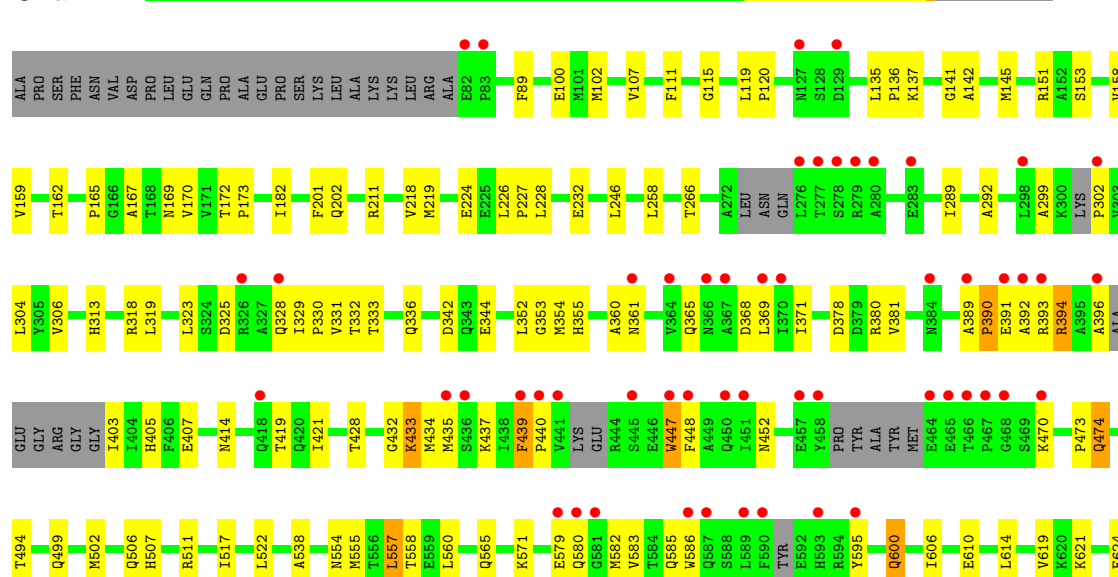
• Molecule 1: ACETOHYDROXY-ACID SYNTHASE

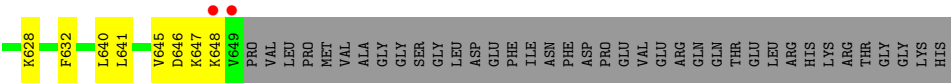
Chain A:



• Molecule 1: ACETOHYDROXY-ACID SYNTHASE

Chain B:





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 0.197 , 0.225	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 , 50.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.

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 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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	0	0
4	B	10	0	0	0	0
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

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 13.

All (216) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:B:318:ARG:HH21	1:B:319:LEU:HD21	1.71	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	33	63
1	B	536/630 (85%)	502 (94%)	29 (5%)	5 (1%)	25	49
All	All	1071/1260 (85%)	1019 (95%)	44 (4%)	8 (1%)	30	58

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%)	78	94
1	B	422/518 (82%)	415 (98%)	7 (2%)	73	92
All	All	856/1036 (83%)	843 (98%)	13 (2%)	76	93

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
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 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 ⓘ

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	1.31	0	6,6,6	0.72	0
5	TPP	A	700	3	27,27,27	1.58	6 (22%)	40,40,40	1.68	8 (20%)
6	FAD	A	701	-	58,58,58	2.21	24 (41%)	85,89,89	1.37	11 (12%)
4	2HP	B	1697	-	4,4,4	1.31	0	6,6,6	0.72	0
4	2HP	B	1698	-	4,4,4	1.32	0	6,6,6	0.71	0
5	TPP	B	1700	3	27,27,27	1.44	5 (18%)	40,40,40	1.70	8 (20%)
6	FAD	B	1701	-	58,58,58	2.23	26 (44%)	85,89,89	1.33	8 (9%)

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	-	0/17/17/17	0/2/2/2
6	FAD	A	701	-	-	0/34/50/50	0/1/6/6
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	-	0/17/17/17	0/2/2/2
6	FAD	B	1701	-	-	0/34/50/50	0/1/6/6

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	701	FAD	C9A-N10	5.39	1.46	1.38
6	B	1701	FAD	C9A-N10	5.14	1.46	1.38
6	A	701	FAD	C8-C7	4.05	1.52	1.40
6	A	701	FAD	C9A-C5X	4.01	1.50	1.42
6	B	1701	FAD	C9A-C5X	3.99	1.50	1.42
6	B	1701	FAD	C1'-C2'	3.91	1.55	1.51
6	B	1701	FAD	C8-C7	3.90	1.52	1.40
6	A	701	FAD	C6-C5X	3.79	1.46	1.41
6	B	1701	FAD	C4X-C10	3.76	1.47	1.40
5	A	700	TPP	C5-S1	3.64	1.76	1.73
6	A	701	FAD	C8A-N9A	3.59	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1701	FAD	C9-C8	3.54	1.47	1.37
6	A	701	FAD	C4X-C10	3.54	1.47	1.40
6	A	701	FAD	C9-C8	3.53	1.47	1.37
6	B	1701	FAD	C9-C9A	3.53	1.47	1.40
6	B	1701	FAD	C7M-C7	3.48	1.58	1.51
6	A	701	FAD	C9-C9A	3.46	1.47	1.40
6	B	1701	FAD	C4-N3	3.40	1.42	1.37
6	A	701	FAD	C7M-C7	3.39	1.58	1.51
6	A	701	FAD	C6-C7	3.37	1.47	1.37
6	A	701	FAD	C4-C4X	3.36	1.46	1.41
6	B	1701	FAD	C8A-N9A	3.34	1.41	1.36
6	B	1701	FAD	C6-C7	3.26	1.46	1.37
6	B	1701	FAD	C4-C4X	3.26	1.46	1.41
6	B	1701	FAD	C6-C5X	3.24	1.45	1.41
6	A	701	FAD	C4-N3	3.23	1.42	1.37
6	B	1701	FAD	C2A-N3A	3.08	1.38	1.32
6	A	701	FAD	C5X-N5	3.07	1.40	1.35
6	A	701	FAD	C1'-C2'	3.03	1.54	1.51
6	B	1701	FAD	C1'-N10	3.03	1.51	1.48
6	B	1701	FAD	C4A-N3A	2.93	1.40	1.35
6	A	701	FAD	C2A-N3A	2.86	1.37	1.32
6	B	1701	FAD	C5X-N5	2.84	1.39	1.35
5	A	700	TPP	C7'-C5'	2.76	1.57	1.51
6	A	701	FAD	C4A-N3A	2.72	1.39	1.35
6	A	701	FAD	C2-N3	2.71	1.42	1.37
6	A	701	FAD	C2A-N1A	2.68	1.39	1.33
6	A	701	FAD	O4'-C4'	2.67	1.49	1.43
6	B	1701	FAD	C2A-N1A	2.63	1.39	1.33
6	B	1701	FAD	C5A-C4A	2.62	1.46	1.40
5	B	1700	TPP	C5-S1	2.59	1.75	1.73
6	B	1701	FAD	C2-N3	2.57	1.42	1.37
5	B	1700	TPP	C4-N3	-2.53	1.36	1.39
6	B	1701	FAD	P-O3P	-2.46	1.55	1.59
5	A	700	TPP	C2-S1	2.46	1.76	1.68
6	A	701	FAD	C5A-C4A	2.44	1.46	1.40
6	B	1701	FAD	O4B-C1B	2.38	1.45	1.41
6	A	701	FAD	C1'-N10	2.30	1.50	1.48
5	A	700	TPP	PB-O2B	-2.29	1.46	1.54
5	B	1700	TPP	PB-O2B	-2.28	1.46	1.54
5	B	1700	TPP	C2-S1	2.26	1.75	1.68
6	B	1701	FAD	O4'-C4'	2.20	1.48	1.43
5	A	700	TPP	C6'-C5'	2.14	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	701	FAD	C10-N1	2.12	1.39	1.35
5	A	700	TPP	PA-O2A	-2.11	1.45	1.55
6	B	1701	FAD	C10-N1	2.10	1.39	1.35
6	B	1701	FAD	C10-N10	2.08	1.43	1.38
5	B	1700	TPP	C7'-C5'	2.08	1.55	1.51
6	A	701	FAD	C4'-C3'	2.04	1.57	1.53
6	A	701	FAD	O4B-C1B	2.03	1.44	1.41
6	B	1701	FAD	P-O2P	-2.02	1.46	1.55

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	701	FAD	C2-N1-C10	5.86	120.89	114.98
6	B	1701	FAD	C2-N1-C10	5.78	120.80	114.98
5	A	700	TPP	C2-S1-C5	-4.53	88.59	91.63
5	B	1700	TPP	C2-S1-C5	-4.20	88.81	91.63
6	A	701	FAD	C4X-N5-C5X	4.00	121.19	116.69
6	B	1701	FAD	C4X-N5-C5X	4.00	121.18	116.69
6	A	701	FAD	C1'-N10-C9A	3.99	122.75	118.87
5	A	700	TPP	C6'-N1'-C2'	3.56	121.93	115.68
5	B	1700	TPP	C6'-N1'-C2'	3.55	121.92	115.68
6	B	1701	FAD	C1'-N10-C9A	3.24	122.03	118.87
5	B	1700	TPP	C5-C4-N3	3.14	113.91	107.53
5	A	700	TPP	C5-C4-N3	3.10	113.83	107.53
5	A	700	TPP	C7'-N3-C2	-3.08	118.52	125.05
5	B	1700	TPP	CM2-C2'-N1'	3.06	120.67	117.02
5	B	1700	TPP	C7'-N3-C2	-3.03	118.62	125.05
5	B	1700	TPP	N1'-C2'-N3'	-2.88	120.45	125.65
5	B	1700	TPP	CM4-C4-C5	-2.87	121.92	129.10
5	A	700	TPP	CM4-C4-C5	-2.81	122.07	129.10
5	A	700	TPP	CM2-C2'-N1'	2.76	120.31	117.02
5	A	700	TPP	N1'-C2'-N3'	-2.71	120.76	125.65
6	B	1701	FAD	C4X-C10-N10	-2.55	119.24	120.51
6	B	1701	FAD	C4X-C10-N1	-2.49	120.24	122.73
6	A	701	FAD	C2'-C1'-N10	-2.38	109.30	112.45
5	B	1700	TPP	C5'-C6'-N1'	-2.38	119.57	123.86
6	B	1701	FAD	N3A-C4A-N9A	2.30	129.59	125.43
6	A	701	FAD	C4X-C10-N1	-2.27	120.46	122.73
5	A	700	TPP	C5'-C6'-N1'	-2.21	119.86	123.86
6	A	701	FAD	C4X-C10-N10	-2.18	119.42	120.51
6	A	701	FAD	C9-C9A-N10	2.16	126.23	121.59
6	B	1701	FAD	C4A-C5A-N7A	-2.12	107.70	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	701	FAD	C8A-N9A-C1B	2.10	130.51	126.38
6	A	701	FAD	N3A-C4A-N9A	2.09	129.20	125.43
6	B	1701	FAD	C9-C9A-N10	2.06	126.04	121.59
6	A	701	FAD	C4A-C5A-N7A	-2.03	107.78	109.52
6	A	701	FAD	C1'-N10-C10	-2.00	116.32	119.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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%)	-0.13	20 (3%) 39 35	33, 48, 90, 140	0
1	B	550/630 (87%)	0.36	56 (10%) 7 5	33, 56, 136, 147	0
All	All	1091/1260 (86%)	0.12	76 (6%) 16 13	33, 50, 125, 147	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	590	PHE	8.2
1	B	649	VAL	7.6
1	A	596	SER	6.5
1	B	82	GLU	6.4
1	B	396	ALA	6.3
1	B	593	HIS	5.8
1	A	463	MET	5.5
1	B	595	TYR	5.3
1	A	460	TYR	4.9
1	B	83	PRO	4.9
1	B	366	ASN	4.7
1	B	458	TYR	4.6
1	B	280	ALA	4.5
1	B	467	PRO	4.5
1	B	298	LEU	4.4
1	A	83	PRO	4.3
1	A	461	ALA	4.2
1	B	466	THR	4.2
1	B	439	PHE	3.9
1	B	648	LYS	3.9
1	A	467	PRO	3.9
1	A	281	GLN	3.9
1	A	597	HIS	3.9
1	B	384	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	369	LEU	3.8
1	B	441	VAL	3.7
1	B	364	VAL	3.6
1	A	599	HIS	3.6
1	B	447	TRP	3.6
1	B	468	GLY	3.6
1	B	435	MET	3.5
1	B	589	LEU	3.5
1	B	392	ALA	3.5
1	B	389	ALA	3.4
1	A	462	TYR	3.3
1	B	127	ASN	3.3
1	B	391	GLU	3.3
1	A	456	LYS	3.3
1	B	302	PRO	3.3
1	B	464	GLU	3.3
1	B	586	TRP	3.2
1	B	283	GLU	3.1
1	B	276	LEU	3.0
1	B	278	SER	3.0
1	B	326	ARG	2.9
1	B	448	PHE	2.8
1	B	277	THR	2.8
1	B	457	GLU	2.8
1	A	598	THR	2.7
1	B	445	SER	2.7
1	B	581	GLY	2.7
1	B	129	ASP	2.7
1	A	468	GLY	2.6
1	B	418	GLN	2.6
1	B	450	GLN	2.6
1	B	587	GLN	2.5
1	B	451	ILE	2.5
1	B	361	ASN	2.5
1	B	465	GLU	2.5
1	B	436	SER	2.5
1	A	458	TYR	2.5
1	A	270	SER	2.4
1	B	367	ALA	2.4
1	B	370	ILE	2.3
1	B	470	LYS	2.3
1	B	579	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	466	THR	2.2
1	B	393	ARG	2.2
1	B	328	GLN	2.2
1	B	580	GLN	2.2
1	B	279	ARG	2.2
1	A	464	GLU	2.1
1	A	84	ASP	2.1
1	A	96	GLN	2.1
1	A	268	LEU	2.1
1	B	440	PRO	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	2HP	B	1698	5/5	0.26	4.57	133,133,133,133	0
4	2HP	A	698	5/5	0.23	3.98	120,120,121,121	0
2	K	B	1696	1/1	0.18	0.81	43,43,43,43	0
6	FAD	B	1701	53/53	0.19	0.49	54,60,86,87	0
2	K	A	696	1/1	0.16	0.34	32,32,32,32	0
6	FAD	A	701	53/53	0.17	0.13	40,49,73,74	0
5	TPP	A	700	26/26	0.13	-0.83	36,46,49,50	0
5	TPP	B	1700	26/26	0.12	-0.85	35,42,45,47	0
3	MG	B	1699	1/1	0.07	-1.52	42,42,42,42	0
3	MG	A	699	1/1	0.07	-2.67	47,47,47,47	0
4	2HP	B	1697	5/5	0.10	-3.64	115,115,115,115	0

6.5 Other polymers ⓘ

There are no such residues in this entry.