



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 08:25 PM UTC

PDB ID : 7NS5 / pdb_00007ns5
Title : Structure of yeast Fbp1 (Fructose-1,6-bisphosphatase 1)
Authors : Sherpa, D.; Chrustowicz, J.; Prabu, J.R.; Schulman, B.A.
Deposited on : 2021-03-05
Resolution : 1.95 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

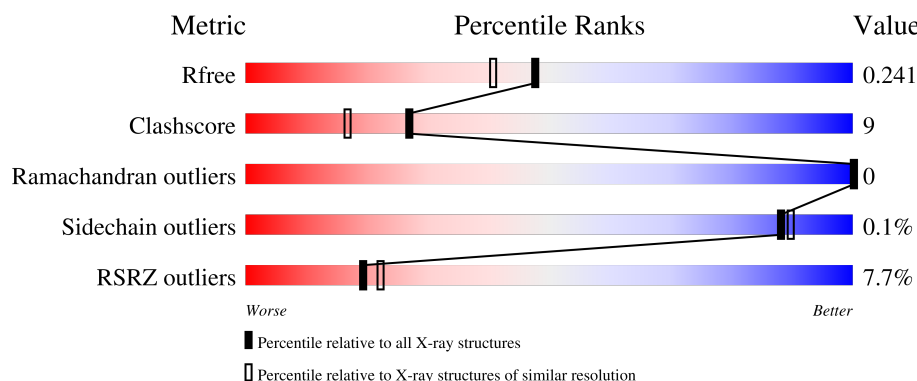
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	354	4% 79% 11% 10%
1	B	354	5% 77% 11% 12%
1	C	354	8% 67% 16% 17%
1	D	354	10% 66% 16% 18%

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	PO4	D	401	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9719 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 Fructose-1,6-bisphosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2467	1574	417	465	11			
1	D	290	Total	C	N	O	S	0	0	0
			2252	1450	378	413	11			
1	B	312	Total	C	N	O	S	0	0	0
			2421	1551	409	450	11			
1	C	293	Total	C	N	O	S	0	0	0
			2274	1462	383	418	11			

There are 24 discrepancies between the modelled and reference sequences:

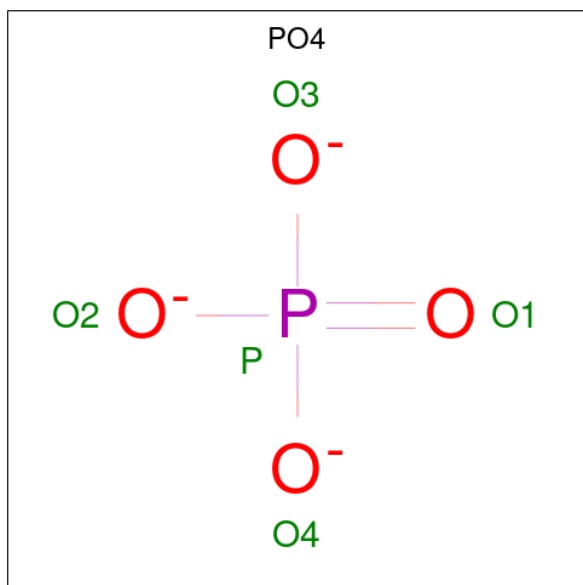
Chain	Residue	Modelled	Actual	Comment	Reference
A	349	HIS	-	expression tag	UNP P09201
A	350	HIS	-	expression tag	UNP P09201
A	351	HIS	-	expression tag	UNP P09201
A	352	HIS	-	expression tag	UNP P09201
A	353	HIS	-	expression tag	UNP P09201
A	354	HIS	-	expression tag	UNP P09201
D	349	HIS	-	expression tag	UNP P09201
D	350	HIS	-	expression tag	UNP P09201
D	351	HIS	-	expression tag	UNP P09201
D	352	HIS	-	expression tag	UNP P09201
D	353	HIS	-	expression tag	UNP P09201
D	354	HIS	-	expression tag	UNP P09201
B	349	HIS	-	expression tag	UNP P09201
B	350	HIS	-	expression tag	UNP P09201
B	351	HIS	-	expression tag	UNP P09201
B	352	HIS	-	expression tag	UNP P09201
B	353	HIS	-	expression tag	UNP P09201
B	354	HIS	-	expression tag	UNP P09201
C	349	HIS	-	expression tag	UNP P09201
C	350	HIS	-	expression tag	UNP P09201
C	351	HIS	-	expression tag	UNP P09201

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Chain	Residue	Modelled	Actual	Comment	Reference
C	352	HIS	-	expression tag	UNP P09201
C	353	HIS	-	expression tag	UNP P09201
C	354	HIS	-	expression tag	UNP P09201

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

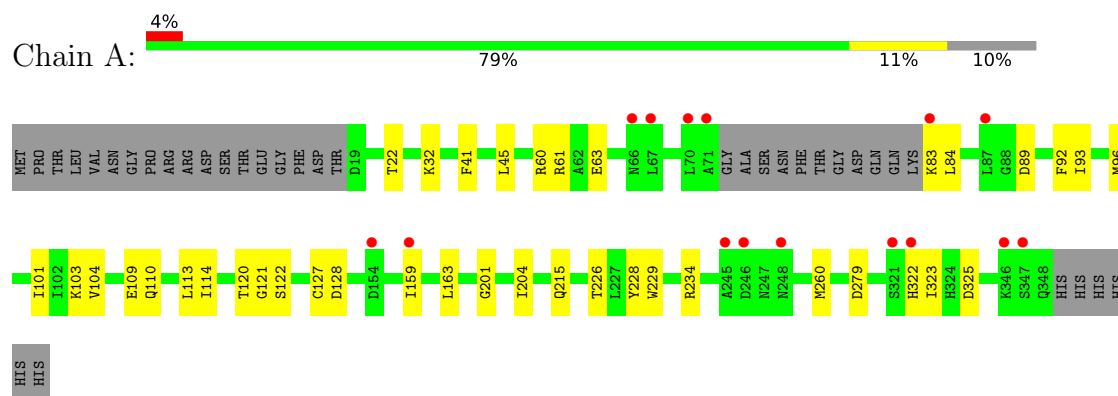
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	98	Total 98	O 98	0	0
4	D	45	Total 45	O 45	0	0
4	B	75	Total 75	O 75	0	0
4	C	59	Total 59	O 59	0	0

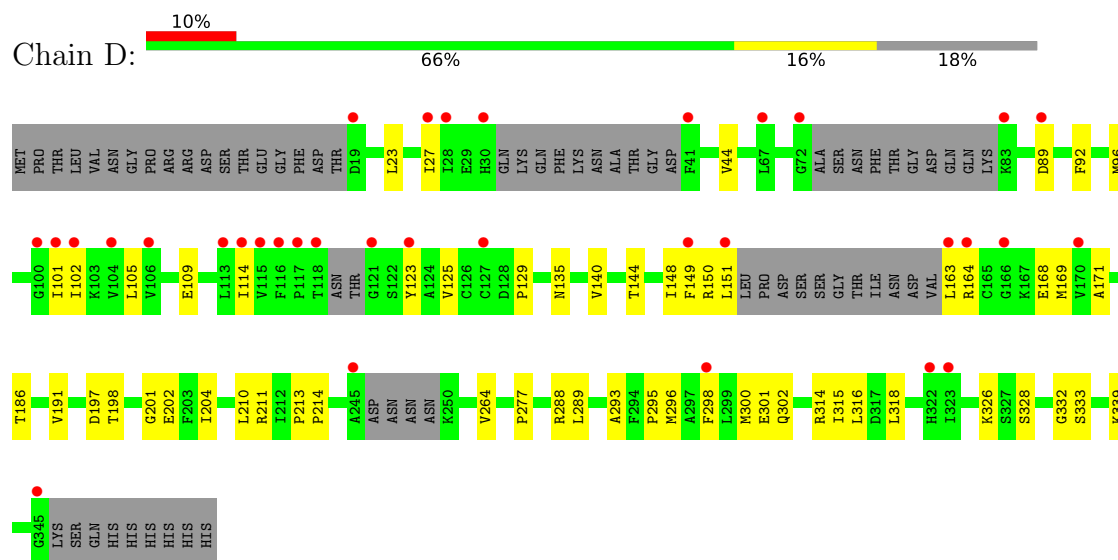
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

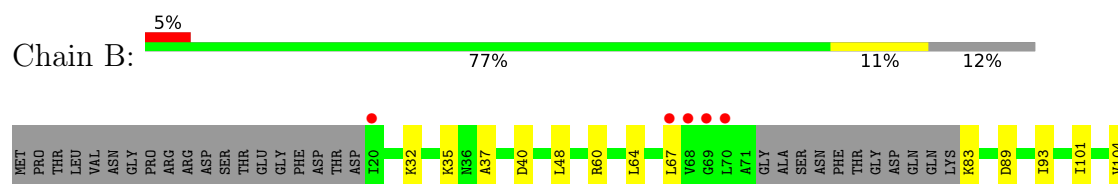
• Molecule 1: Fructose-1,6-bisphosphatase

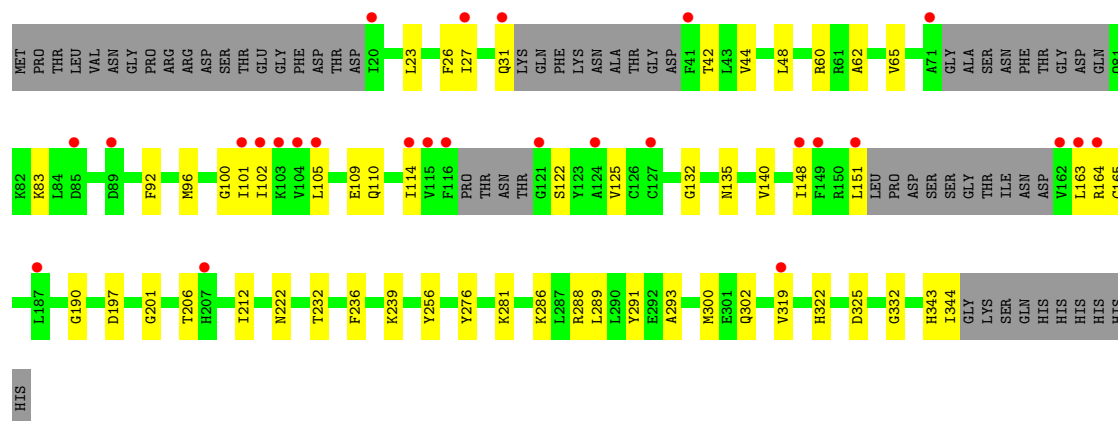


• Molecule 1: Fructose-1,6-bisphosphatase



• Molecule 1: Fructose-1,6-bisphosphatase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.02Å 133.79Å 171.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.22 – 1.95 45.22 – 1.95	Depositor EDS
% Data completeness (in resolution range)	91.4 (45.22-1.95) 90.7 (45.22-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.208 , 0.242 0.207 , 0.241	Depositor DCC
R_{free} test set	6158 reflections (6.23%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9719	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PO4

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	0.49	0/2517	0.73	1/3411 (0.0%)
1	B	0.47	0/2470	0.73	0/3344
1	C	0.42	0/2318	0.72	0/3135
1	D	0.43	0/2296	0.69	0/3102
All	All	0.45	0/9601	0.72	1/12992 (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	128	ASP	N-CA-CB	5.82	119.49	110.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2467	0	2447	30	0
1	B	2421	0	2420	45	0
1	C	2274	0	2270	54	0
1	D	2252	0	2259	57	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	98	0	0	3	0
4	B	75	0	0	3	0
4	C	59	0	0	1	0
4	D	45	0	0	2	0
All	All	9719	0	9396	173	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 9.

All (173) 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:D:109:GLU:OE1	4:D:501:HOH:O	1.59	1.17
1:D:164:ARG:NE	1:D:168:GLU:OE2	1.79	1.14
1:C:300:MET:HE3	1:C:332:GLY:HA2	1.22	1.12
1:A:215:GLN:NE2	4:A:501:HOH:O	1.79	1.11
1:D:164:ARG:NH2	1:D:168:GLU:OE2	1.85	1.09
1:D:164:ARG:CZ	1:D:168:GLU:OE2	2.05	1.04
1:C:322:HIS:ND1	1:C:325:ASP:OD1	2.05	0.90
1:B:162:VAL:HG13	1:B:290:LEU:HD21	1.54	0.89
1:B:110:GLN:HG3	1:B:114:ILE:HD11	1.55	0.88
1:C:300:MET:HE3	1:C:332:GLY:CA	2.01	0.88
1:C:100:GLY:C	1:C:101:ILE:HD13	1.99	0.87
1:C:125:VAL:HG12	1:C:148:ILE:HG12	1.58	0.85
1:D:201:GLY:HA3	1:C:201:GLY:HA3	1.57	0.85
1:D:164:ARG:HE	1:D:168:GLU:CD	1.85	0.85
1:C:190:GLY:H	1:C:302:GLN:HE21	1.26	0.83
1:B:60:ARG:HH11	1:C:60:ARG:NH2	1.76	0.83
1:B:145:ILE:HD13	1:B:296:MET:HE2	1.58	0.83
1:C:300:MET:CE	1:C:332:GLY:HA2	2.07	0.80
1:A:89:ASP:O	1:A:93:ILE:HG12	1.82	0.78
1:D:314:ARG:O	1:D:318:LEU:CD2	2.31	0.78
1:A:322:HIS:ND1	1:A:325:ASP:OD1	2.18	0.77
1:C:322:HIS:CE1	1:C:325:ASP:OD1	2.37	0.77
1:B:60:ARG:HH11	1:C:60:ARG:HH21	1.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:LEU:HD23	1:D:114:ILE:HD11	1.69	0.75
1:D:191:VAL:HG23	1:D:210:LEU:HB3	1.66	0.74
1:B:322:HIS:ND1	1:B:325:ASP:OD1	2.19	0.74
1:B:169:MET:CE	1:B:294:PHE:HB3	2.19	0.72
1:C:105:LEU:HB3	1:C:114:ILE:HB	1.71	0.72
1:C:26:PHE:HD1	1:C:27:ILE:HD13	1.56	0.70
1:B:344:ILE:HD12	4:B:554:HOH:O	1.93	0.69
1:B:60:ARG:NH1	1:C:60:ARG:HH21	1.91	0.69
1:B:169:MET:HE2	1:B:294:PHE:HB3	1.76	0.68
1:D:44:VAL:HG23	1:D:101:ILE:HD13	1.76	0.67
1:B:162:VAL:HG13	1:B:290:LEU:CD2	2.25	0.67
1:B:60:ARG:HD2	1:C:60:ARG:CZ	2.27	0.65
1:C:190:GLY:H	1:C:302:GLN:NE2	1.93	0.64
1:C:239:LYS:HE3	1:C:343:HIS:CE1	2.32	0.64
1:D:211:ARG:NH2	1:D:302:GLN:O	2.31	0.64
1:D:264:VAL:HG11	1:D:296:MET:HE2	1.78	0.63
1:C:48:LEU:HD11	1:C:148:ILE:HD11	1.81	0.63
1:A:201:GLY:HA3	1:B:201:GLY:HA3	1.81	0.63
1:D:300:MET:HE3	1:D:332:GLY:HA2	1.80	0.62
1:D:314:ARG:O	1:D:318:LEU:HD23	2.00	0.62
1:A:60:ARG:HH21	1:D:198:THR:HG21	1.64	0.61
1:C:110:GLN:HG3	1:C:114:ILE:HD11	1.81	0.61
1:C:44:VAL:HG22	1:C:102:ILE:HD11	1.83	0.61
1:B:311:ARG:NH1	1:B:313:GLU:OE2	2.35	0.60
1:B:67:LEU:HD13	1:C:206:THR:HG22	1.83	0.60
1:C:288:ARG:HG2	1:C:291:TYR:OH	2.02	0.59
1:B:169:MET:HE1	1:B:294:PHE:C	2.28	0.59
1:C:105:LEU:CD1	1:C:125:VAL:HG23	2.33	0.58
1:C:132:GLY:N	2:C:401:PO4:O4	2.35	0.58
1:D:148:ILE:HD12	1:D:171:ALA:HB3	1.87	0.57
1:B:174:TYR:CD2	1:B:296:MET:HE1	2.40	0.56
1:B:162:VAL:CG1	1:B:290:LEU:HD21	2.31	0.56
1:B:93:ILE:HD13	1:B:105:LEU:HD21	1.88	0.56
1:A:32:LYS:NZ	1:B:40:ASP:OD1	2.38	0.56
1:D:101:ILE:HD11	1:D:123:TYR:CD2	2.41	0.56
1:A:63:GLU:H	1:A:63:GLU:CD	2.13	0.56
1:D:289:LEU:HA	1:D:293:ALA:HB3	1.87	0.55
1:A:229:TRP:O	1:A:234:ARG:NH1	2.40	0.55
1:B:344:ILE:CD1	4:B:554:HOH:O	2.53	0.55
1:C:212:ILE:HD12	1:C:300:MET:HE1	1.89	0.55
1:A:103:LYS:HB2	1:A:121:GLY:HA2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:VAL:HG13	1:B:113:LEU:HD11	1.89	0.55
1:D:105:LEU:HB3	1:D:114:ILE:HG13	1.89	0.54
1:A:322:HIS:CE1	1:A:325:ASP:OD1	2.61	0.54
1:B:131:ASP:HA	2:B:401:PO4:O3	2.07	0.54
1:A:110:GLN:HG3	1:A:114:ILE:HD11	1.89	0.54
1:C:109:GLU:OE2	4:C:501:HOH:O	2.19	0.54
1:B:232:THR:CG2	1:B:344:ILE:HD13	2.39	0.53
1:D:105:LEU:O	1:D:114:ILE:HG12	2.08	0.53
1:C:163:LEU:O	1:C:164:ARG:HD3	2.09	0.52
1:D:339:LYS:NZ	4:D:503:HOH:O	2.41	0.52
1:D:105:LEU:CD1	1:D:125:VAL:HB	2.40	0.52
1:C:288:ARG:HG2	1:C:291:TYR:CZ	2.44	0.52
1:C:62:ALA:O	1:C:65:VAL:HG22	2.10	0.52
1:B:232:THR:HG21	1:B:344:ILE:HD13	1.92	0.51
1:B:89:ASP:O	1:B:93:ILE:HG12	2.11	0.51
1:C:276:TYR:CE2	1:C:286:LYS:HB2	2.45	0.51
1:B:105:LEU:HA	1:B:125:VAL:O	2.10	0.51
1:A:109:GLU:OE2	4:A:502:HOH:O	2.19	0.51
1:B:60:ARG:HD2	1:C:60:ARG:NE	2.25	0.50
1:C:135:ASN:HB3	1:C:140:VAL:HG23	1.92	0.50
1:D:277:PRO:HA	1:D:328:SER:HB2	1.94	0.50
1:A:104:VAL:CG1	1:A:113:LEU:HD11	2.42	0.50
1:C:26:PHE:HD1	1:C:27:ILE:CD1	2.23	0.49
1:D:186:THR:HB	1:D:191:VAL:HG12	1.95	0.49
1:C:101:ILE:HD13	1:C:101:ILE:N	2.25	0.49
1:D:202:GLU:O	1:D:204:ILE:HD12	2.12	0.49
1:B:147:SER:HB2	1:B:169:MET:SD	2.53	0.49
1:D:44:VAL:HG22	1:D:102:ILE:HD11	1.94	0.49
1:B:145:ILE:HD11	1:B:295:PRO:HB2	1.95	0.49
1:B:336:GLU:OE1	1:B:339:LYS:HE3	2.12	0.49
1:C:163:LEU:C	1:C:164:ARG:HD3	2.38	0.49
1:C:232:THR:HG21	1:C:344:ILE:HG22	1.95	0.48
1:D:105:LEU:HB3	1:D:114:ILE:CG1	2.44	0.48
1:A:61:ARG:HH12	1:D:197:ASP:CG	2.22	0.47
1:C:105:LEU:HD12	1:C:125:VAL:HG23	1.95	0.47
1:D:168:GLU:O	1:D:168:GLU:HG2	2.13	0.47
1:D:315:ILE:HA	1:D:318:LEU:HD23	1.96	0.47
1:B:169:MET:HE1	1:B:294:PHE:O	2.14	0.47
1:D:149:PHE:CE1	1:D:169:MET:HG2	2.48	0.47
1:C:31:GLN:OE1	1:C:42:THR:HG21	2.14	0.47
1:C:100:GLY:O	1:C:101:ILE:HD13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:ASP:OD2	1:D:109:GLU:HG3	2.15	0.46
1:B:60:ARG:HH11	1:C:60:ARG:CZ	2.28	0.46
1:A:113:LEU:HD22	1:A:159:ILE:HB	1.96	0.46
1:B:322:HIS:CE1	1:B:325:ASP:OD1	2.68	0.46
1:D:288:ARG:NH1	1:D:326:LYS:HE3	2.30	0.46
1:D:129:PRO:HA	1:D:144:THR:HG23	1.97	0.46
1:A:159:ILE:HD11	1:A:323:ILE:HG23	1.97	0.46
1:D:150:ARG:O	1:D:151:LEU:HB2	2.16	0.45
1:B:155:SER:OG	1:B:161:ASP:OD2	2.30	0.45
1:C:289:LEU:HA	1:C:293:ALA:HB3	1.98	0.45
1:D:23:LEU:O	1:D:27:ILE:HG12	2.17	0.45
1:B:48:LEU:HD11	1:B:148:ILE:HD11	1.98	0.45
1:D:163:LEU:C	1:D:164:ARG:HG3	2.42	0.45
1:D:186:THR:HG21	1:D:298:PHE:HD2	1.82	0.44
1:D:301:GLU:OE1	1:D:316:LEU:HD12	2.17	0.44
1:B:83:LYS:N	4:B:508:HOH:O	2.50	0.44
1:B:113:LEU:HD22	1:B:159:ILE:HG23	1.99	0.44
1:D:135:ASN:HB3	1:D:140:VAL:HG23	1.98	0.44
1:D:169:MET:HE1	1:D:295:PRO:HA	2.00	0.44
1:C:23:LEU:O	1:C:27:ILE:HG12	2.16	0.44
1:D:44:VAL:HG23	1:D:101:ILE:CD1	2.45	0.44
1:D:105:LEU:HD12	1:D:125:VAL:O	2.18	0.44
1:B:32:LYS:HB3	1:B:37:ALA:HB2	1.99	0.44
1:C:44:VAL:CG2	1:C:102:ILE:HD11	2.46	0.44
1:A:83:LYS:HG3	1:A:84:LEU:N	2.33	0.43
1:B:104:VAL:CG1	1:B:113:LEU:HD11	2.48	0.43
1:B:232:THR:HG21	1:B:344:ILE:CD1	2.49	0.43
1:A:22:THR:HG22	1:A:204:ILE:HD13	2.00	0.43
1:A:41:PHE:CZ	1:A:45:LEU:HD21	2.53	0.43
1:A:120:THR:HG22	1:A:122:SER:OG	2.18	0.43
1:D:197:ASP:HB2	1:D:204:ILE:HD13	2.00	0.43
1:D:264:VAL:CG1	1:D:296:MET:HE2	2.48	0.43
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.79	0.43
1:D:92:PHE:O	1:D:96:MET:HG2	2.18	0.43
1:B:35:LYS:HB3	1:B:35:LYS:HE3	1.77	0.43
1:A:260:MET:C	1:A:260:MET:SD	3.01	0.43
1:D:315:ILE:CA	1:D:318:LEU:HD23	2.48	0.43
1:A:120:THR:HG21	4:A:505:HOH:O	2.18	0.42
1:D:105:LEU:HD12	1:D:125:VAL:HB	2.01	0.42
1:D:129:PRO:O	1:D:144:THR:OG1	2.34	0.42
1:C:236:PHE:HB2	1:C:343:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ILE:C	1:B:101:ILE:HD12	2.44	0.42
1:D:214:PRO:O	1:D:333:SER:HB3	2.20	0.42
1:D:315:ILE:C	1:D:318:LEU:HD23	2.45	0.42
1:C:83:LYS:HD3	1:C:83:LYS:N	2.35	0.42
1:D:213:PRO:HA	1:D:214:PRO:HD3	1.90	0.42
1:C:122:SER:HA	1:C:151:LEU:HD12	2.02	0.42
1:A:63:GLU:CD	1:A:63:GLU:N	2.77	0.42
1:D:89:ASP:CG	1:D:109:GLU:HG3	2.44	0.42
1:D:318:LEU:HD22	1:D:318:LEU:N	2.35	0.42
1:A:101:ILE:HG22	1:A:120:THR:HB	2.03	0.41
1:D:105:LEU:HB3	1:D:114:ILE:HD11	2.03	0.41
1:A:226:THR:HA	1:A:229:TRP:CE3	2.55	0.41
1:C:222:ASN:HB2	1:C:256:TYR:CE2	2.56	0.41
1:D:164:ARG:HB3	1:D:168:GLU:OE1	2.20	0.41
1:A:92:PHE:O	1:A:96:MET:HG2	2.21	0.41
1:B:344:ILE:HD13	1:B:344:ILE:HA	1.81	0.41
1:C:239:LYS:HE3	1:C:343:HIS:ND1	2.35	0.41
1:C:92:PHE:O	1:C:96:MET:HG2	2.21	0.41
1:C:165:CYS:HA	1:C:319:VAL:HG22	2.03	0.41
1:D:191:VAL:CG2	1:D:210:LEU:HB3	2.45	0.40
1:A:228:TYR:CB	1:A:279:ASP:HB2	2.51	0.40
1:A:92:PHE:CE1	1:A:127:CYS:SG	3.09	0.40
1:C:281:LYS:HE2	1:C:281:LYS:HA	2.04	0.40
1:A:32:LYS:HB2	1:A:32:LYS:HE3	1.82	0.40
1:B:64:LEU:HD13	1:C:197:ASP:HB2	2.04	0.40
1:C:48:LEU:CD1	1:C:148:ILE:HD11	2.50	0.40
1:C:300:MET:HE3	1:C:332:GLY:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	315/354 (89%)	305 (97%)	10 (3%)	0	100	100
1	B	306/354 (86%)	292 (95%)	14 (5%)	0	100	100
1	C	283/354 (80%)	275 (97%)	8 (3%)	0	100	100
1	D	278/354 (78%)	271 (98%)	7 (2%)	0	100	100
All	All	1182/1416 (84%)	1143 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	269/301 (89%)	269 (100%)	0	100	100
1	B	264/301 (88%)	263 (100%)	1 (0%)	84	85
1	C	246/301 (82%)	246 (100%)	0	100	100
1	D	244/301 (81%)	244 (100%)	0	100	100
All	All	1023/1204 (85%)	1022 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	162	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	215	GLN
1	D	242	GLN
1	D	244	GLN
1	B	31	GLN
1	B	207	HIS

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Mol	Chain	Res	Type
1	B	209	ASN
1	C	66	ASN
1	C	247	ASN
1	C	302	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z > 2$
2	PO4	B	401	3	4,4,4	1.83	2 (50%)	6,6,6	2.78	1 (16%)
2	PO4	C	401	3	4,4,4	1.95	1 (25%)	6,6,6	3.35	2 (33%)
2	PO4	A	401	3	4,4,4	1.58	1 (25%)	6,6,6	2.92	1 (16%)
2	PO4	D	401	3	4,4,4	1.84	2 (50%)	6,6,6	2.94	2 (33%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	PO4	P-O3	-3.35	1.44	1.54
2	B	401	PO4	P-O3	-2.54	1.47	1.54
2	D	401	PO4	P-O1	-2.49	1.44	1.50
2	A	401	PO4	P-O2	-2.24	1.48	1.54
2	B	401	PO4	P-O2	-2.21	1.48	1.54
2	D	401	PO4	P-O2	-2.16	1.48	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	PO4	O3-P-O1	-7.39	84.83	110.95
2	A	401	PO4	O2-P-O1	-6.38	88.40	110.95
2	D	401	PO4	O2-P-O1	-6.25	88.84	110.95
2	B	401	PO4	O3-P-O2	-6.06	89.06	107.91
2	D	401	PO4	O4-P-O3	2.52	115.75	107.91
2	C	401	PO4	O4-P-O2	2.22	114.82	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	PO4	1	0
2	C	401	PO4	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	319/354 (90%)	0.23	15 (4%) 36 42	26, 38, 61, 94	0
1	B	312/354 (88%)	0.34	17 (5%) 31 37	27, 40, 62, 94	0
1	C	293/354 (82%)	0.72	27 (9%) 14 16	30, 50, 71, 98	0
1	D	290/354 (81%)	0.88	34 (11%) 9 11	31, 55, 83, 106	0
All	All	1214/1416 (85%)	0.53	93 (7%) 19 22	26, 46, 73, 106	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	162	VAL	7.1
1	D	151	LEU	6.2
1	C	163	LEU	5.9
1	B	118	THR	5.6
1	C	115	VAL	5.2
1	D	245	ALA	4.9
1	D	101	ILE	4.4
1	B	344	ILE	4.4
1	B	345	GLY	4.3
1	D	27	ILE	4.3
1	D	30	HIS	4.2
1	D	163	LEU	4.1
1	C	121	GLY	3.8
1	D	118	THR	3.7
1	C	103	LYS	3.6
1	D	115	VAL	3.6
1	D	298	PHE	3.6
1	C	151	LEU	3.6
1	D	345	GLY	3.5
1	D	114	ILE	3.5
1	D	127	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	245	ALA	3.4
1	B	165	CYS	3.3
1	A	246	ASP	3.2
1	D	89	ASP	3.2
1	C	27	ILE	3.1
1	B	117	PRO	3.1
1	D	322	HIS	3.0
1	D	166	GLY	3.0
1	B	20	ILE	3.0
1	D	104	VAL	3.0
1	D	28	ILE	2.9
1	A	70	LEU	2.9
1	D	67	LEU	2.9
1	C	116	PHE	2.8
1	C	127	CYS	2.8
1	D	100	GLY	2.8
1	C	41	PHE	2.8
1	B	154	ASP	2.8
1	A	154	ASP	2.7
1	D	117	PRO	2.7
1	C	105	LEU	2.7
1	C	71	ALA	2.6
1	D	149	PHE	2.6
1	B	122	SER	2.6
1	C	20	ILE	2.6
1	C	89	ASP	2.6
1	C	114	ILE	2.6
1	C	164	ARG	2.6
1	D	121	GLY	2.5
1	C	148	ILE	2.5
1	C	124	ALA	2.4
1	B	246	ASP	2.4
1	A	347	SER	2.4
1	D	72	GLY	2.4
1	D	83	LYS	2.4
1	D	113	LEU	2.4
1	C	187	LEU	2.4
1	A	322	HIS	2.4
1	C	104	VAL	2.3
1	C	149	PHE	2.3
1	C	101	ILE	2.3
1	A	67	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	248	ASN	2.3
1	D	116	PHE	2.3
1	A	159	ILE	2.3
1	A	71	ALA	2.2
1	B	322	HIS	2.2
1	B	127	CYS	2.2
1	B	69	GLY	2.2
1	C	207	HIS	2.2
1	B	68	VAL	2.2
1	A	87	LEU	2.2
1	D	164	ARG	2.2
1	A	66	ASN	2.1
1	D	170	VAL	2.1
1	A	83	LYS	2.1
1	C	31	GLN	2.1
1	D	102	ILE	2.1
1	D	323	ILE	2.1
1	B	67	LEU	2.1
1	B	70	LEU	2.1
1	B	209	ASN	2.1
1	D	123	TYR	2.1
1	A	321	SER	2.1
1	A	346	LYS	2.1
1	D	106	VAL	2.1
1	B	167	LYS	2.0
1	C	102	ILE	2.0
1	C	319	VAL	2.0
1	D	19	ASP	2.0
1	C	85	ASP	2.0
1	D	41	PHE	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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
3	MG	B	403	1/1	0.70	0.13	45,45,45,45	1
2	PO4	D	401	5/5	0.72	0.17	59,60,63,66	5
3	MG	A	403	1/1	0.73	0.12	48,48,48,48	1
2	PO4	B	401	5/5	0.76	0.15	37,42,46,49	5
2	PO4	A	401	5/5	0.77	0.14	61,61,63,64	5
2	PO4	C	401	5/5	0.77	0.16	48,50,52,55	5
3	MG	D	403	1/1	0.84	0.11	59,59,59,59	1
3	MG	C	403	1/1	0.89	0.09	54,54,54,54	1
3	MG	A	402	1/1	0.97	0.06	45,45,45,45	0
3	MG	C	402	1/1	0.97	0.06	52,52,52,52	0
3	MG	B	402	1/1	0.97	0.04	44,44,44,44	0
3	MG	D	402	1/1	0.98	0.04	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.