



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:01 PM UTC

PDB ID : 6CZL / pdb_00006czl
Title : Crystal structure of Medicago truncatula ATP-phosphoribosyltransferase in relaxed form
Authors : Ruszkowski, M.
Deposited on : 2018-04-09
Resolution : 2.92 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

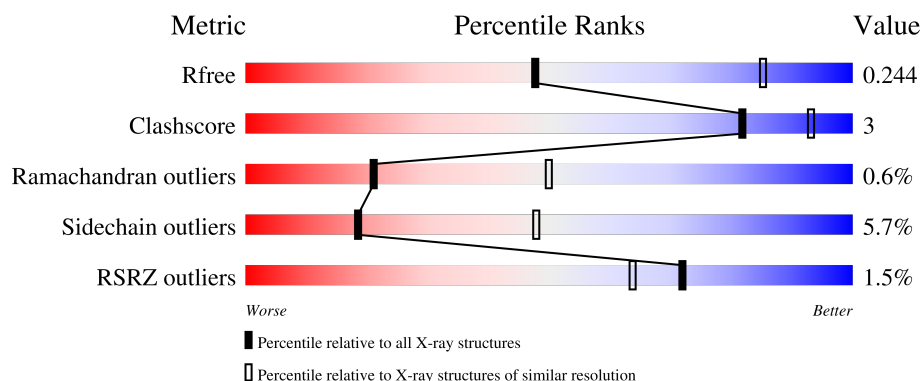
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	352	% 85% 9% • 5%
1	B	352	% 85% 11% 5%
1	C	352	 85% 9% • 5%
1	D	352	2% 84% 11% 5%
1	E	352	2% 86% 10% 5%

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Mol	Chain	Length	Quality of chain
1	F	352	% 82% 12% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15556 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 ATP phosphoribosyltransferase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2583	1634	446	491	12			
1	B	336	Total	C	N	O	S	0	0	0
			2583	1634	446	491	12			
1	C	334	Total	C	N	O	S	0	0	0
			2574	1627	446	489	12			
1	D	336	Total	C	N	O	S	0	0	0
			2583	1634	446	491	12			
1	E	336	Total	C	N	O	S	0	0	0
			2583	1634	446	491	12			
1	F	334	Total	C	N	O	S	0	0	0
			2574	1627	446	489	12			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	-	expression tag	UNP G7JFL4
A	23	ASN	-	expression tag	UNP G7JFL4
A	24	ALA	-	expression tag	UNP G7JFL4
B	22	SER	-	expression tag	UNP G7JFL4
B	23	ASN	-	expression tag	UNP G7JFL4
B	24	ALA	-	expression tag	UNP G7JFL4
C	22	SER	-	expression tag	UNP G7JFL4
C	23	ASN	-	expression tag	UNP G7JFL4
C	24	ALA	-	expression tag	UNP G7JFL4
D	22	SER	-	expression tag	UNP G7JFL4
D	23	ASN	-	expression tag	UNP G7JFL4
D	24	ALA	-	expression tag	UNP G7JFL4
E	22	SER	-	expression tag	UNP G7JFL4
E	23	ASN	-	expression tag	UNP G7JFL4
E	24	ALA	-	expression tag	UNP G7JFL4
F	22	SER	-	expression tag	UNP G7JFL4
F	23	ASN	-	expression tag	UNP G7JFL4

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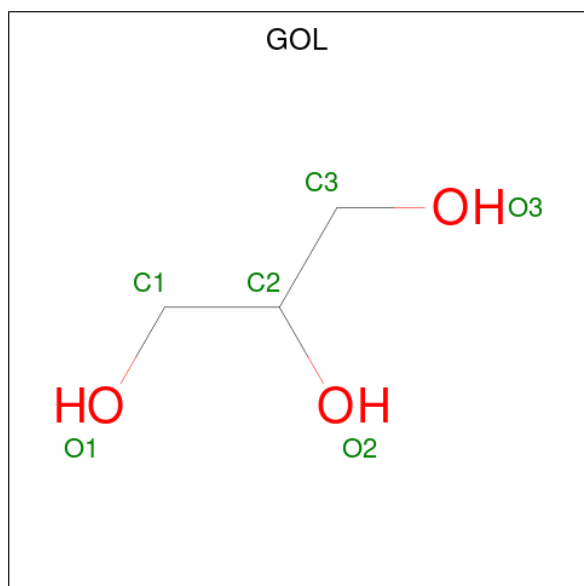
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Chain	Residue	Modelled	Actual	Comment	Reference
F	24	ALA	-	expression tag	UNP G7JFL4

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

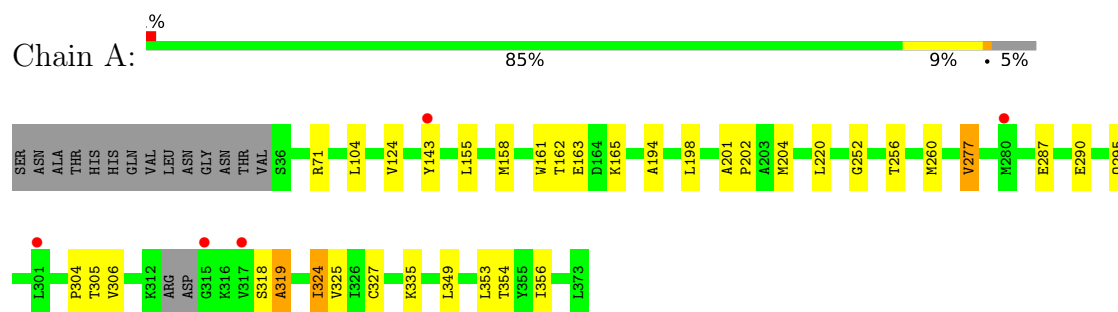
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	3	Total	O	0	0
			3	3		
4	C	8	Total	O	0	0
			8	8		
4	D	6	Total	O	0	0
			6	6		
4	E	8	Total	O	0	0
			8	8		
4	F	8	Total	O	0	0
			8	8		

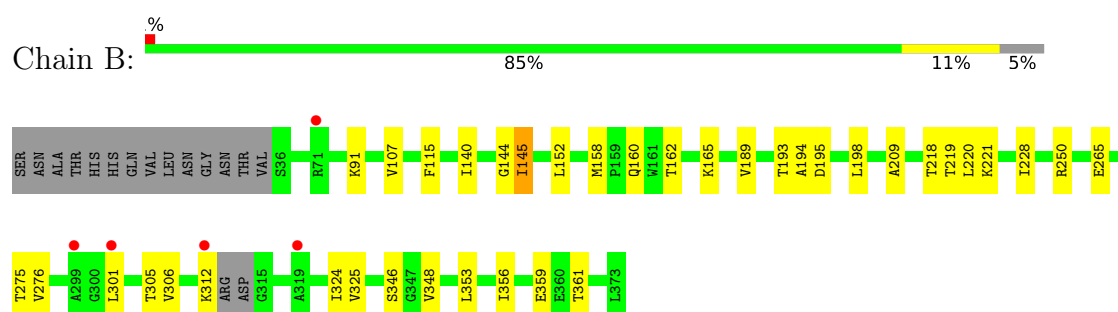
3 Residue-property plots [i](#)

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.

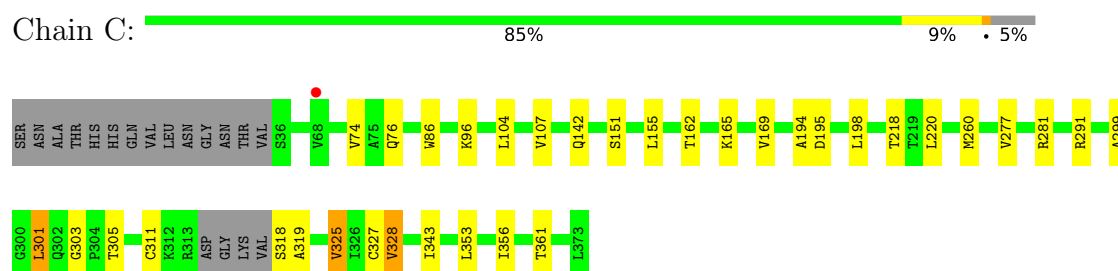
- Molecule 1: ATP phosphoribosyltransferase catalytic subunit



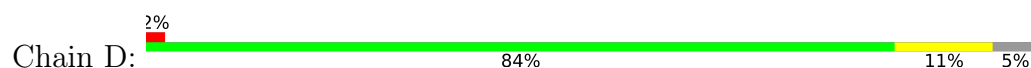
- Molecule 1: ATP phosphoribosyltransferase catalytic subunit

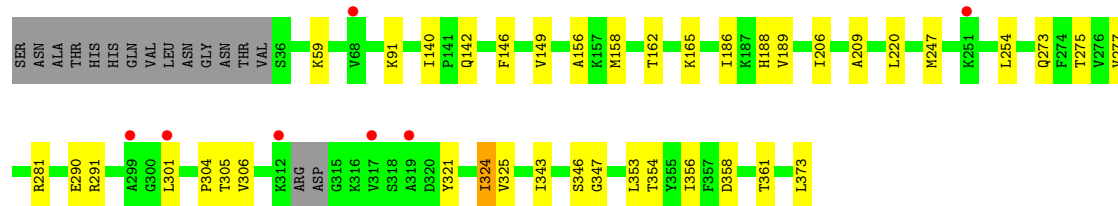


- Molecule 1: ATP phosphoribosyltransferase catalytic subunit

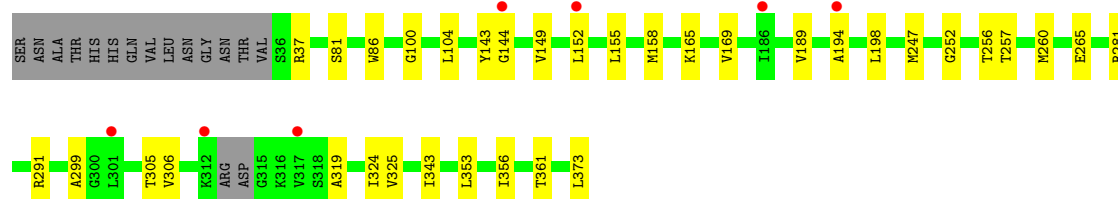
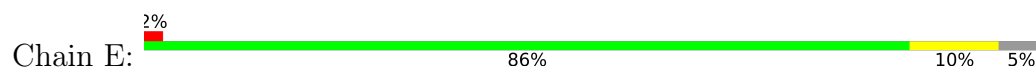


- Molecule 1: ATP phosphoribosyltransferase catalytic subunit

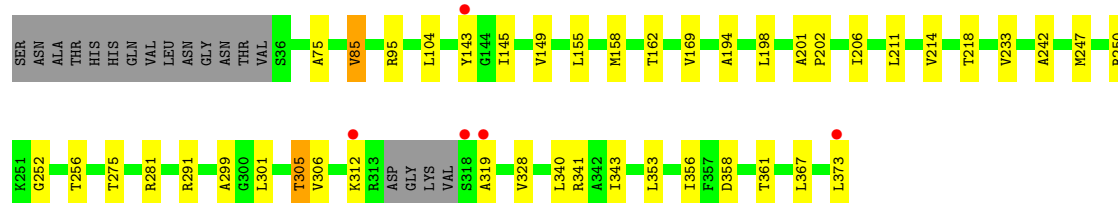
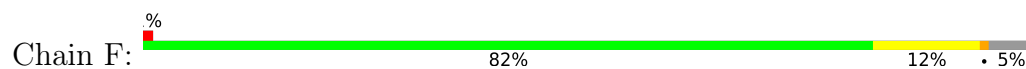




- Molecule 1: ATP phosphoribosyltransferase catalytic subunit



- Molecule 1: ATP phosphoribosyltransferase catalytic subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.83Å 195.62Å 100.21Å 90.00° 95.85° 90.00°	Depositor
Resolution (Å)	39.17 – 2.92 39.17 – 2.92	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.17-2.92) 99.5 (39.17-2.92)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.197 , 0.250 0.198 , 0.244	Depositor DCC
R_{free} test set	1237 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å ²)	84.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.058 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15556	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: GOL, CL

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	0.60	0/2623	0.88	1/3544 (0.0%)
1	B	0.61	1/2623 (0.0%)	0.86	0/3544
1	C	0.60	0/2614	0.88	2/3532 (0.1%)
1	D	0.60	0/2623	0.88	0/3544
1	E	0.61	0/2623	0.85	1/3544 (0.0%)
1	F	0.61	0/2614	0.89	1/3532 (0.0%)
All	All	0.61	1/15720 (0.0%)	0.88	5/21240 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	346	SER	CA-C	6.15	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	299	ALA	N-CA-C	5.98	118.26	110.43
1	F	305	THR	N-CA-C	-5.41	101.34	109.95
1	A	143	TYR	N-CA-C	5.25	117.42	111.02
1	C	303	GLY	CA-C-N	5.24	126.39	119.84
1	C	303	GLY	C-N-CA	5.24	126.39	119.84

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	2583	0	2643	13	0
1	B	2583	0	2643	13	0
1	C	2574	0	2631	13	0
1	D	2583	0	2643	15	0
1	E	2583	0	2643	12	0
1	F	2574	0	2631	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
4	A	7	0	0	0	0
4	B	3	0	0	0	0
4	C	8	0	0	0	0
4	D	6	0	0	0	0
4	E	8	0	0	0	0
4	F	8	0	0	0	0
All	All	15556	0	15874	79	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 3.

All (79) 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:277:VAL:HG22	1:D:325:VAL:HG12	1.68	0.75
1:F:149:VAL:HG21	1:F:158:MET:HE2	1.73	0.69
1:B:275:THR:HG23	1:B:353:LEU:HD21	1.78	0.66
1:F:281:ARG:O	1:F:291:ARG:NH2	2.30	0.64
1:D:149:VAL:HG21	1:D:158:MET:HE2	1.81	0.63
1:C:311:CYS:HG	1:C:318:SER:N	2.00	0.60
1:B:306:VAL:HG22	1:B:324:ILE:HG22	1.85	0.59
1:F:75:ALA:HB3	1:F:85:VAL:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:194:ALA:HB3	1:E:198:LEU:CD2	2.36	0.55
1:D:146:PHE:CD1	1:D:158:MET:HE1	2.42	0.55
1:C:74:VAL:HG12	1:C:86:TRP:CH2	2.42	0.55
1:D:149:VAL:HG11	1:D:158:MET:HE2	1.89	0.53
1:B:194:ALA:HB3	1:B:198:LEU:HD21	1.90	0.53
1:C:281:ARG:O	1:C:291:ARG:NH2	2.42	0.52
1:B:145:ILE:HD13	1:B:160:GLN:HE22	1.74	0.52
1:F:299:ALA:HB3	1:F:328:VAL:HG23	1.92	0.52
1:E:306:VAL:HG22	1:E:324:ILE:HG22	1.90	0.52
1:F:299:ALA:CB	1:F:328:VAL:HG23	2.40	0.52
1:C:194:ALA:HB3	1:C:198:LEU:CD2	2.40	0.52
1:A:158:MET:HE3	1:A:161:TRP:CH2	2.45	0.51
1:E:149:VAL:HG11	1:E:158:MET:HE3	1.91	0.51
1:C:299:ALA:HB3	1:C:328:VAL:HG22	1.92	0.51
1:C:277:VAL:HG22	1:C:325:VAL:HG12	1.93	0.51
1:D:346:SER:OG	1:D:347:GLY:N	2.45	0.50
1:A:306:VAL:HG22	1:A:324:ILE:HD12	1.94	0.50
1:C:343:ILE:HG22	1:C:343:ILE:O	2.11	0.50
1:F:194:ALA:HB3	1:F:198:LEU:CD1	2.41	0.50
1:F:252:GLY:O	1:F:256:THR:HG23	2.12	0.49
1:B:194:ALA:HB3	1:B:198:LEU:CD2	2.43	0.48
1:C:74:VAL:HG12	1:C:86:TRP:CZ3	2.49	0.48
1:A:353:LEU:HD13	1:A:356:ILE:HD11	1.95	0.48
1:E:194:ALA:HB3	1:E:198:LEU:HD23	1.96	0.47
1:E:281:ARG:O	1:E:291:ARG:NH2	2.48	0.47
1:A:277:VAL:HG22	1:A:349:LEU:HB2	1.95	0.47
1:A:194:ALA:HB3	1:A:198:LEU:CD2	2.45	0.47
1:B:353:LEU:HD13	1:B:356:ILE:HD11	1.97	0.47
1:D:247:MET:HE2	1:D:254:LEU:HD12	1.97	0.47
1:A:252:GLY:O	1:A:256:THR:HG23	2.15	0.47
1:A:304:PRO:HB2	1:A:324:ILE:HD11	1.97	0.47
1:D:156:ALA:HB2	1:D:186:ILE:CD1	2.44	0.47
1:F:211:LEU:HD11	1:F:233:VAL:HG21	1.96	0.46
1:A:104:LEU:HD13	1:A:260:MET:HE2	1.96	0.46
1:D:304:PRO:CB	1:D:324:ILE:HD11	2.46	0.46
1:E:194:ALA:HB3	1:E:198:LEU:HD21	1.97	0.46
1:F:353:LEU:HD13	1:F:356:ILE:HD11	1.98	0.46
1:E:37:ARG:NH2	1:E:100:GLY:O	2.49	0.45
1:E:252:GLY:O	1:E:256:THR:HG23	2.17	0.45
1:B:145:ILE:HD11	1:B:158:MET:CE	2.46	0.45
1:B:275:THR:CG2	1:B:353:LEU:HD21	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:ASP:O	1:F:341:ARG:NH2	2.50	0.45
1:B:140:ILE:HD11	1:B:228:ILE:HD11	1.99	0.45
1:D:273:GLN:HG3	1:D:356:ILE:CD1	2.47	0.45
1:C:194:ALA:HB3	1:C:198:LEU:HD23	1.99	0.44
1:E:247:MET:HE1	1:E:257:THR:HG21	1.99	0.44
1:F:155:LEU:HD12	1:F:158:MET:HE3	2.00	0.44
1:E:353:LEU:HD13	1:E:356:ILE:HD11	2.00	0.43
1:A:201:ALA:HB3	1:A:202:PRO:HD3	2.00	0.43
1:C:353:LEU:HD13	1:C:356:ILE:HD11	2.01	0.43
1:D:140:ILE:HD13	1:D:209:ALA:HB2	2.00	0.43
1:D:277:VAL:HG22	1:D:325:VAL:CG1	2.44	0.43
1:C:104:LEU:HD13	1:C:260:MET:HE2	2.00	0.43
1:D:281:ARG:O	1:D:291:ARG:NH2	2.51	0.42
1:A:318:SER:O	1:A:319:ALA:HB3	2.19	0.42
1:F:343:ILE:HG22	1:F:343:ILE:O	2.19	0.42
1:B:91:LYS:HG3	1:B:115:PHE:CZ	2.55	0.42
1:C:96:LYS:HE3	1:F:206:ILE:HD13	2.01	0.42
1:A:194:ALA:HB3	1:A:198:LEU:HD21	2.01	0.42
1:B:276:VAL:HG13	1:B:348:VAL:HG13	2.02	0.42
1:F:201:ALA:HB3	1:F:202:PRO:HD3	2.02	0.42
1:D:343:ILE:HG22	1:D:343:ILE:O	2.20	0.41
1:F:104:LEU:HD23	1:F:242:ALA:HB2	2.02	0.41
1:D:353:LEU:HD13	1:D:356:ILE:HD11	2.03	0.41
1:F:247:MET:HE1	1:F:367:LEU:HD21	2.03	0.41
1:B:145:ILE:HD11	1:B:158:MET:HE1	2.03	0.41
1:B:140:ILE:HG22	1:B:209:ALA:HB2	2.02	0.41
1:E:104:LEU:HD13	1:E:260:MET:CE	2.51	0.41
1:A:124:VAL:O	1:A:124:VAL:HG23	2.22	0.40
1:A:204:MET:HE3	1:E:86:TRP:CG	2.56	0.40
1:C:301:LEU:HD13	1:C:327:CYS:HB3	2.04	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	332/352 (94%)	314 (95%)	17 (5%)	1 (0%)	36	64
1	B	332/352 (94%)	317 (96%)	13 (4%)	2 (1%)	21	50
1	C	330/352 (94%)	313 (95%)	16 (5%)	1 (0%)	36	64
1	D	332/352 (94%)	316 (95%)	16 (5%)	0	100	100
1	E	332/352 (94%)	314 (95%)	14 (4%)	4 (1%)	10	32
1	F	330/352 (94%)	315 (96%)	12 (4%)	3 (1%)	14	40
All	All	1988/2112 (94%)	1889 (95%)	88 (4%)	11 (1%)	21	50

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	144	GLY
1	F	143	TYR
1	A	319	ALA
1	C	319	ALA
1	B	144	GLY
1	E	319	ALA
1	F	301	LEU
1	F	319	ALA
1	E	143	TYR
1	B	301	LEU
1	E	343	ILE

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	282/296 (95%)	266 (94%)	16 (6%)	18	48
1	B	282/296 (95%)	263 (93%)	19 (7%)	15	41
1	C	281/296 (95%)	265 (94%)	16 (6%)	18	48
1	D	282/296 (95%)	263 (93%)	19 (7%)	15	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	282/296 (95%)	271 (96%)	11 (4%)	28	61
1	F	281/296 (95%)	265 (94%)	16 (6%)	18	48
All	All	1690/1776 (95%)	1593 (94%)	97 (6%)	18	48

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ARG
1	A	155	LEU
1	A	162	THR
1	A	163	GLU
1	A	165	LYS
1	A	220	LEU
1	A	277	VAL
1	A	287	GLU
1	A	290	GLU
1	A	295	GLN
1	A	305	THR
1	A	324	ILE
1	A	325	VAL
1	A	327	CYS
1	A	335	LYS
1	A	354	THR
1	B	107	VAL
1	B	145	ILE
1	B	152	LEU
1	B	162	THR
1	B	165	LYS
1	B	189	VAL
1	B	193	THR
1	B	195	ASP
1	B	218	THR
1	B	219	THR
1	B	220	LEU
1	B	221	LYS
1	B	250	ARG
1	B	265	GLU
1	B	305	THR
1	B	312	LYS
1	B	325	VAL
1	B	359	GLU

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Mol	Chain	Res	Type
1	B	361	THR
1	C	76	GLN
1	C	107	VAL
1	C	142	GLN
1	C	151	SER
1	C	155	LEU
1	C	162	THR
1	C	165	LYS
1	C	169	VAL
1	C	195	ASP
1	C	218	THR
1	C	220	LEU
1	C	301	LEU
1	C	305	THR
1	C	325	VAL
1	C	328	VAL
1	C	361	THR
1	D	59	LYS
1	D	91	LYS
1	D	142	GLN
1	D	162	THR
1	D	165	LYS
1	D	188	HIS
1	D	189	VAL
1	D	206	ILE
1	D	220	LEU
1	D	275	THR
1	D	290	GLU
1	D	301	LEU
1	D	305	THR
1	D	306	VAL
1	D	321	TYR
1	D	324	ILE
1	D	354	THR
1	D	361	THR
1	D	373	LEU
1	E	81	SER
1	E	152	LEU
1	E	155	LEU
1	E	165	LYS
1	E	169	VAL
1	E	189	VAL

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Mol	Chain	Res	Type
1	E	265	GLU
1	E	305	THR
1	E	325	VAL
1	E	361	THR
1	E	373	LEU
1	F	85	VAL
1	F	95	ARG
1	F	145	ILE
1	F	162	THR
1	F	169	VAL
1	F	214	VAL
1	F	218	THR
1	F	250	ARG
1	F	275	THR
1	F	305	THR
1	F	306	VAL
1	F	312	LYS
1	F	340	LEU
1	F	358	ASP
1	F	361	THR
1	F	373	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	88	GLN
1	A	223	ASN
1	A	267	HIS
1	A	273	GLN
1	A	279	ASN
1	B	302	GLN
1	C	76	GLN
1	C	188	HIS
1	C	267	HIS
1	C	273	GLN
1	D	62	GLN
1	D	273	GLN
1	E	188	HIS
1	E	273	GLN
1	F	82	ASN
1	F	224	ASN

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Mol	Chain	Res	Type
1	F	273	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 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	D	402	-	5,5,5	0.40	0	5,5,5	0.16	0
3	GOL	E	402	-	5,5,5	0.39	0	5,5,5	0.07	0
3	GOL	F	402	-	5,5,5	0.34	0	5,5,5	0.48	0
3	GOL	C	402	-	5,5,5	0.33	0	5,5,5	0.40	0
3	GOL	B	402	-	5,5,5	0.43	0	5,5,5	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	402	-	-	2/4/4/4	-
3	GOL	E	402	-	-	2/4/4/4	-
3	GOL	F	402	-	-	1/4/4/4	-
3	GOL	C	402	-	-	1/4/4/4	-
3	GOL	B	402	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	402	GOL	O1-C1-C2-C3
3	E	402	GOL	O1-C1-C2-C3
3	D	402	GOL	O1-C1-C2-O2
3	E	402	GOL	O1-C1-C2-O2
3	B	402	GOL	O1-C1-C2-O2
3	C	402	GOL	O2-C2-C3-O3
3	F	402	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	336/352 (95%)	-0.12	5 (1%)	72 64	69, 99, 152, 178	0
1	B	336/352 (95%)	-0.08	5 (1%)	72 64	69, 99, 159, 178	0
1	C	334/352 (94%)	-0.21	1 (0%)	90 87	65, 91, 138, 163	0
1	D	336/352 (95%)	-0.15	7 (2%)	63 54	65, 94, 142, 179	0
1	E	336/352 (95%)	-0.16	7 (2%)	63 54	65, 95, 152, 164	0
1	F	334/352 (94%)	-0.16	5 (1%)	72 64	64, 92, 146, 163	0
All	All	2012/2112 (95%)	-0.15	30 (1%)	72 64	64, 95, 151, 179	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	LEU	3.7
1	C	68	VAL	3.3
1	F	373	LEU	2.9
1	D	312	LYS	2.8
1	D	68	VAL	2.8
1	F	318	SER	2.7
1	B	299	ALA	2.7
1	B	312	LYS	2.7
1	F	312	LYS	2.6
1	E	317	VAL	2.6
1	D	301	LEU	2.5
1	D	251	LYS	2.4
1	A	317	VAL	2.4
1	D	317	VAL	2.3
1	D	299	ALA	2.3
1	B	319	ALA	2.2
1	E	144	GLY	2.2
1	A	280	MET	2.2
1	E	301	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	143	TYR	2.1
1	F	143	TYR	2.1
1	B	301	LEU	2.1
1	D	319	ALA	2.1
1	F	319	ALA	2.1
1	B	71	ARG	2.1
1	E	186	ILE	2.1
1	E	152	LEU	2.0
1	E	194	ALA	2.0
1	E	312	LYS	2.0
1	A	315	GLY	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	GOL	B	402	6/6	0.89	0.18	115,122,124,124	0
2	CL	A	401	1/1	0.90	0.10	108,108,108,108	0
3	GOL	E	402	6/6	0.90	0.14	111,119,120,121	0
3	GOL	F	402	6/6	0.90	0.15	115,118,119,119	0
2	CL	F	401	1/1	0.92	0.09	111,111,111,111	0
3	GOL	C	402	6/6	0.92	0.14	109,114,115,115	0
3	GOL	D	402	6/6	0.94	0.15	112,118,121,122	0
2	CL	E	401	1/1	0.94	0.07	112,112,112,112	0
2	CL	D	401	1/1	0.94	0.07	102,102,102,102	0
2	CL	B	401	1/1	0.95	0.05	100,100,100,100	0
2	CL	C	401	1/1	0.96	0.05	93,93,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.