



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:44 AM UTC

PDB ID : 2CLE / pdb\_00002cle  
Title : Tryptophan Synthase in complex with N-(4'-trifluoromethoxybenzoyl)-2- amino-1-ethylphosphate (F6) - lowF6 complex  
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Deposited on : 2006-04-27  
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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 : ?? (??), CSD ??CSD?? (????)  
Xtrriage (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

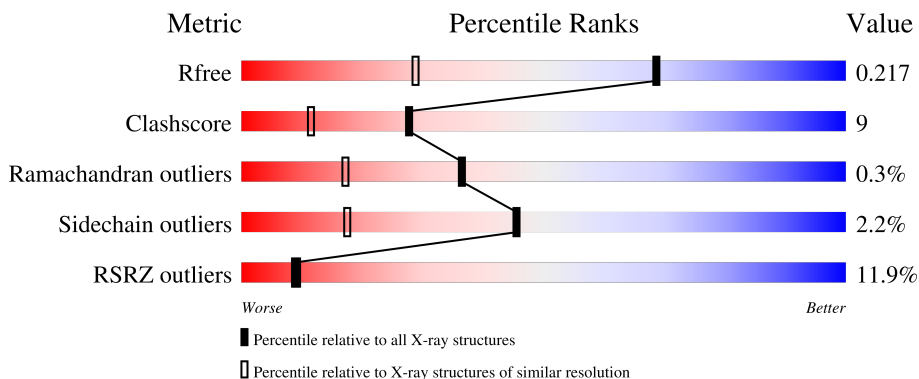
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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  $\geq 3$ , 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	268	
2	B	396	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5524 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 TRYPTOPHAN SYNTHASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	252	1899	1210	328	354	7	0	0	1

- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	395	2987	1876	528	564	19	0	0	1

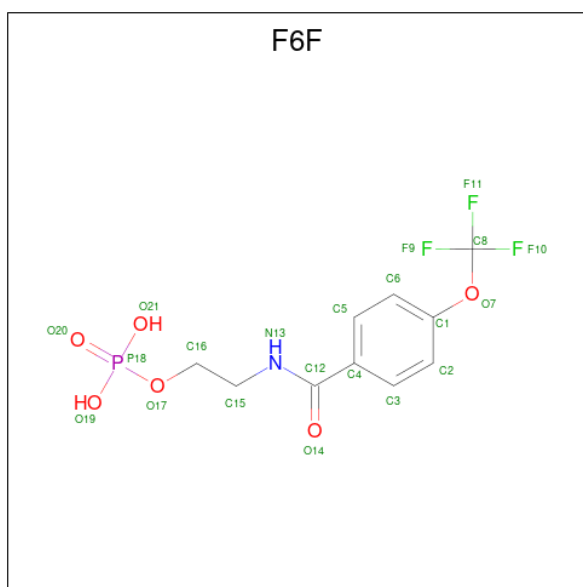
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	34	ARG	SER	conflict	UNP P0A2K1

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

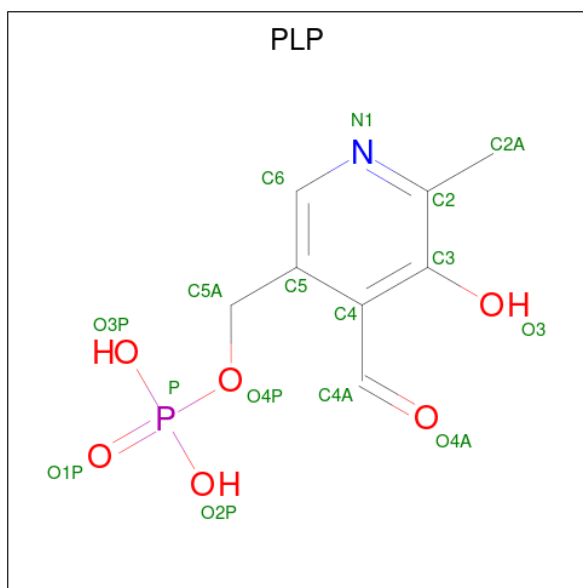
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	1	1	0	0

- Molecule 4 is 2-{[4-(TRIFLUOROMETHOXY)BENZOYL]AMINO}ETHYL DIHYDROGEN PHOSPHATE (CCD ID: F6F) (formula: C<sub>10</sub>H<sub>11</sub>F<sub>3</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			P
4	A	1	21	10	3	1	6	1	0	0

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula:  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	15	8	1	5	1	0	0

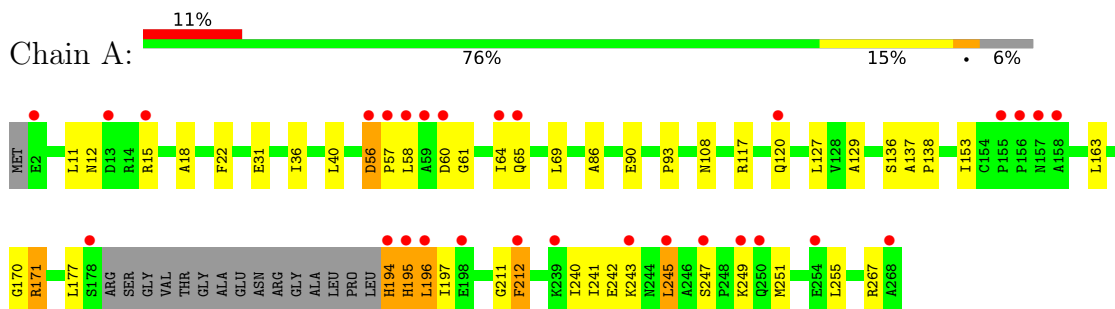
- Molecule 6 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	A	212	Total 212	O 212	0	0
6	B	389	Total 389	O 389	0	0

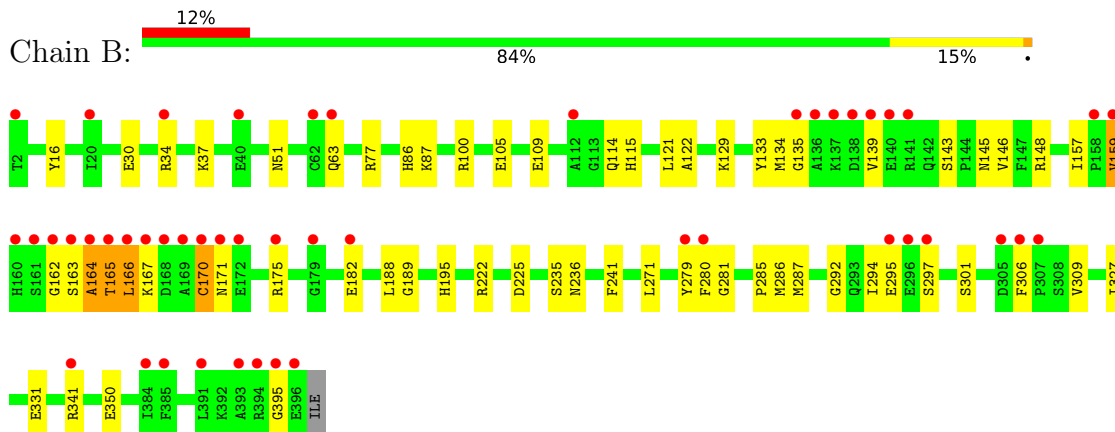
### 3 Residue-property plots [i](#)

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: TRYPTOPHAN SYNTHASE ALPHA CHAIN



- Molecule 2: TRYPTOPHAN SYNTHASE BETA CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.36Å 59.62Å 67.25Å 90.00° 94.73° 90.00°	Depositor
Resolution (Å)	19.92 – 1.50 19.92 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (19.92-1.50) 96.7 (19.92-1.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 1.42Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.194 , 0.210 (Not available) , 0.217	Depositor DCC
$R_{free}$ test set	6336 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.3	Xtrriage
Anisotropy	0.557	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PLP, F6F

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	0.36	1/1937 (0.1%)	0.88	7/2632 (0.3%)
2	B	0.37	1/3045 (0.0%)	0.89	9/4113 (0.2%)
All	All	0.36	2/4982 (0.0%)	0.88	16/6745 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	ARG	C-N	-5.81	1.25	1.33
2	B	395	GLY	C-N	-5.70	1.25	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	HIS	N-CA-C	-11.27	98.14	112.90
1	A	136	SER	N-CA-C	6.96	121.52	112.89
2	B	77	ARG	N-CA-C	6.60	120.92	110.70
1	A	196	LEU	N-CA-C	-5.98	104.84	111.36
2	B	170	CYS	N-CA-C	-5.70	105.15	111.36
1	A	56	ASP	CA-C-N	5.63	126.88	119.84
1	A	56	ASP	C-N-CA	5.63	126.88	119.84
2	B	235	SER	N-CA-C	5.62	117.21	111.14
2	B	157	ILE	N-CA-C	5.46	112.95	107.55
1	A	93	PRO	N-CA-C	5.41	120.66	113.57
2	B	51	ASN	N-CA-C	5.40	119.58	112.89
2	B	225	ASP	N-CA-C	-5.25	105.61	112.23
1	A	129	ALA	N-CA-C	5.24	117.67	111.33
2	B	241	PHE	N-CA-C	5.15	116.97	111.36
2	B	195	HIS	N-CA-C	-5.10	102.75	109.84
2	B	292	GLY	N-CA-C	5.02	122.50	115.43

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	1899	0	1899	34	0
2	B	2987	0	2965	63	0
3	A	1	0	0	0	0
4	A	21	0	9	0	0
5	B	15	0	7	0	0
6	A	212	0	0	4	0
6	B	389	0	0	13	0
All	All	5524	0	4880	88	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 (88) 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:58:LEU:HA	2:B:171:ASN:ND2	1.82	0.95
2:B:165:THR:HG23	2:B:167:LYS:HG2	1.46	0.94
2:B:279:TYR:HB3	2:B:286:MET:HE1	1.57	0.86
2:B:87:LYS:HD2	2:B:114:GLN:HG3	1.59	0.84
2:B:134:MET:HE3	2:B:139:VAL:HG22	1.62	0.80
2:B:34:ARG:HH21	2:B:34:ARG:HG2	1.47	0.80
1:A:194:HIS:ND1	1:A:195:HIS:N	2.29	0.78
1:A:58:LEU:HA	2:B:171:ASN:CG	2.11	0.75
1:A:211:GLY:O	1:A:212:PHE:HB2	1.90	0.71
1:A:64:ILE:HD12	6:A:2065:HOH:O	1.89	0.71
1:A:240:ILE:HA	1:A:243:LYS:HE2	1.74	0.69
1:A:86:ALA:O	1:A:90:GLU:HG3	1.93	0.69
1:A:56:ASP:HB3	2:B:279:TYR:CE1	2.28	0.68
2:B:171:ASN:ND2	2:B:175:ARG:NH2	2.42	0.67
2:B:134:MET:HE1	2:B:146:VAL:HG22	1.77	0.67
2:B:100:ARG:HD3	6:B:2135:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ALA:HB3	1:A:138:PRO:HD3	1.78	0.65
2:B:145:ASN:HD22	2:B:148:ARG:HH21	1.45	0.65
1:A:65:GLN:O	1:A:69:LEU:HD13	1.97	0.64
2:B:34:ARG:HG2	2:B:34:ARG:NH2	2.13	0.63
1:A:242:GLU:HA	1:A:245:LEU:HD13	1.82	0.62
1:A:60:ASP:O	2:B:175:ARG:NH2	2.34	0.60
2:B:100:ARG:CG	6:B:2135:HOH:O	2.48	0.60
2:B:162:GLY:C	2:B:164:ALA:H	2.10	0.60
1:A:247:SER:HB2	6:A:2192:HOH:O	2.03	0.58
2:B:100:ARG:CD	6:B:2135:HOH:O	2.50	0.58
1:A:31:GLU:HG2	6:A:2032:HOH:O	2.03	0.57
2:B:163:SER:O	2:B:165:THR:N	2.37	0.57
1:A:56:ASP:OD1	2:B:167:LYS:HD2	2.05	0.56
1:A:69:LEU:HD21	2:B:162:GLY:HA2	1.87	0.56
1:A:163:LEU:HD21	1:A:196:LEU:HD22	1.88	0.56
1:A:56:ASP:OD2	2:B:294:ILE:HB	2.07	0.55
2:B:165:THR:CG2	2:B:167:LYS:HG2	2.29	0.55
1:A:57:PRO:O	2:B:171:ASN:ND2	2.40	0.55
1:A:117:ARG:HA	1:A:120:GLN:HG2	1.90	0.54
2:B:297:SER:HB2	6:B:2311:HOH:O	2.08	0.53
1:A:61:GLY:O	1:A:65:GLN:HG3	2.09	0.52
2:B:100:ARG:HG3	6:B:2137:HOH:O	2.10	0.51
1:A:12:ASN:O	1:A:15:ARG:HD2	2.10	0.51
2:B:145:ASN:ND2	2:B:148:ARG:HH21	2.08	0.51
1:A:194:HIS:N	1:A:197:ILE:HG13	2.27	0.50
2:B:16:TYR:O	2:B:281:GLY:HA2	2.11	0.50
2:B:163:SER:OG	2:B:165:THR:HG22	2.12	0.50
2:B:37:LYS:HG2	6:B:2063:HOH:O	2.12	0.49
2:B:171:ASN:CG	2:B:175:ARG:CZ	2.86	0.49
2:B:145:ASN:ND2	2:B:148:ARG:NH2	2.62	0.48
1:A:56:ASP:HB3	2:B:279:TYR:CZ	2.50	0.47
2:B:159:VAL:O	2:B:159:VAL:HG23	2.13	0.47
2:B:121:LEU:HD12	2:B:122:ALA:N	2.30	0.47
1:A:11:LEU:CD1	1:A:18:ALA:HB2	2.45	0.47
2:B:63:GLN:HG2	6:B:2347:HOH:O	2.15	0.47
1:A:194:HIS:CG	1:A:195:HIS:H	2.27	0.46
2:B:285:PRO:HG2	2:B:309:VAL:HG12	1.97	0.46
2:B:297:SER:CB	6:B:2311:HOH:O	2.62	0.46
1:A:22:PHE:CD1	1:A:22:PHE:C	2.92	0.46
1:A:108:ASN:HA	6:A:2097:HOH:O	2.16	0.46
2:B:166:LEU:C	2:B:166:LEU:HD12	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:ARG:NH2	6:B:2236:HOH:O	2.48	0.45
2:B:34:ARG:HG3	2:B:100:ARG:HH21	1.82	0.45
1:A:127:LEU:C	1:A:127:LEU:HD23	2.42	0.45
2:B:171:ASN:HD21	2:B:175:ARG:NH2	2.11	0.45
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.52	0.44
2:B:100:ARG:HG2	6:B:2135:HOH:O	2.15	0.44
2:B:135:GLY:HA3	2:B:164:ALA:O	2.18	0.44
2:B:159:VAL:O	2:B:159:VAL:CG2	2.66	0.44
2:B:171:ASN:ND2	2:B:175:ARG:CZ	2.80	0.44
1:A:170:GLY:O	1:A:171:ARG:HD3	2.18	0.44
2:B:271:LEU:HD23	2:B:271:LEU:C	2.43	0.44
2:B:182:GLU:HG3	6:B:2205:HOH:O	2.17	0.43
2:B:301:SER:OG	2:B:350:GLU:HG3	2.17	0.43
2:B:34:ARG:CG	2:B:100:ARG:HH21	2.32	0.43
2:B:109:GLU:HA	2:B:133:TYR:O	2.19	0.43
2:B:279:TYR:CG	2:B:280:PHE:N	2.86	0.43
2:B:86:HIS:CE1	2:B:236:ASN:HB3	2.54	0.42
1:A:194:HIS:CG	1:A:195:HIS:N	2.84	0.42
2:B:30:GLU:HG2	6:B:2060:HOH:O	2.19	0.42
2:B:341:ARG:HG3	2:B:341:ARG:HH11	1.84	0.42
2:B:279:TYR:CD1	2:B:280:PHE:N	2.87	0.42
2:B:287:MET:HB3	2:B:295:GLU:HB3	2.02	0.41
2:B:306:PHE:HB2	6:B:2309:HOH:O	2.19	0.41
2:B:134:MET:CE	2:B:146:VAL:HG22	2.47	0.41
1:A:153:ILE:HG23	1:A:177:LEU:HG	2.02	0.41
2:B:105:GLU:HG2	2:B:129:LYS:HB2	2.03	0.41
1:A:36:ILE:HG23	1:A:255:LEU:HD13	2.03	0.40
2:B:165:THR:OG1	2:B:166:LEU:N	2.55	0.40
2:B:285:PRO:HG2	2:B:309:VAL:CG1	2.51	0.40
2:B:327:ILE:HG23	2:B:331:GLU:HB2	2.02	0.40
1:A:241:ILE:O	1:A:251:MET:HE2	2.21	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	248/268 (92%)	241 (97%)	6 (2%)	1 (0%)	30	12
2	B	393/396 (99%)	384 (98%)	8 (2%)	1 (0%)	36	17
All	All	641/664 (96%)	625 (98%)	14 (2%)	2 (0%)	36	17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	164	ALA
1	A	212	PHE

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/208 (94%)	191 (97%)	5 (3%)	40	13
2	B	308/310 (99%)	302 (98%)	6 (2%)	50	22
All	All	504/518 (97%)	493 (98%)	11 (2%)	45	17

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	171	ARG
1	A	194	HIS
1	A	245	LEU
1	A	249	LYS
2	B	143	SER
2	B	159	VAL
2	B	165	THR
2	B	166	LEU
2	B	170	CYS
2	B	188	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	65	GLN
1	A	68	ASN
1	A	165	GLN
1	A	244	ASN
1	A	250	GLN
2	B	26	ASN
2	B	44	GLN
2	B	64	ASN
2	B	145	ASN
2	B	375	ASN

### 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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	252/268 (94%)	0.60	29 (11%) 9 10	10, 19, 29, 41	0
2	B	395/396 (99%)	0.34	48 (12%) 8 9	7, 13, 31, 53	0
All	All	647/664 (97%)	0.44	77 (11%) 9 9	7, 15, 30, 53	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	164	ALA	7.2
2	B	161	SER	6.4
2	B	166	LEU	6.0
2	B	171	ASN	5.9
2	B	170	CYS	5.4
2	B	391	LEU	4.8
1	A	195	HIS	4.8
2	B	112	ALA	4.8
2	B	169	ALA	4.7
2	B	160	HIS	4.7
2	B	159	VAL	4.7
2	B	165	THR	4.6
2	B	162	GLY	4.6
2	B	136	ALA	4.5
1	A	58	LEU	4.3
2	B	163	SER	4.3
1	A	194	HIS	4.2
1	A	196	LEU	4.0
2	B	297	SER	4.0
2	B	306	PHE	4.0
2	B	141	ARG	4.0
1	A	57	PRO	4.0
2	B	305	ASP	3.9
1	A	64	ILE	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	279	TYR	3.8
2	B	2	THR	3.8
2	B	135	GLY	3.7
2	B	396	GLU	3.7
2	B	384	ILE	3.7
1	A	268	ALA	3.6
2	B	167	LYS	3.4
2	B	393	ALA	3.4
2	B	139	VAL	3.4
1	A	60	ASP	3.4
1	A	243	LYS	3.3
2	B	137	LYS	3.3
2	B	175	ARG	3.3
2	B	140	GLU	3.2
2	B	63	GLN	3.2
1	A	157	ASN	3.1
1	A	15	ARG	3.0
2	B	385	PHE	3.0
1	A	56	ASP	3.0
2	B	138	ASP	3.0
2	B	395	GLY	2.9
2	B	168	ASP	2.9
1	A	239	LYS	2.9
1	A	245	LEU	2.9
2	B	296	GLU	2.9
1	A	178	SER	2.9
1	A	247	SER	2.9
2	B	158	PRO	2.8
1	A	156	PRO	2.8
1	A	212	PHE	2.8
2	B	307	PRO	2.7
2	B	40	GLU	2.7
2	B	280	PHE	2.7
2	B	341	ARG	2.6
2	B	182	GLU	2.6
1	A	198	GLU	2.6
2	B	179	GLY	2.6
1	A	158	ALA	2.5
1	A	2	GLU	2.5
2	B	394	ARG	2.4
2	B	172	GLU	2.4
1	A	65	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	155	PRO	2.3
1	A	59	ALA	2.3
2	B	62	CYS	2.2
2	B	34	ARG	2.1
1	A	254	GLU	2.1
1	A	249	LYS	2.1
2	B	20	ILE	2.1
1	A	13	ASP	2.1
2	B	295	GLU	2.0
1	A	120	GLN	2.0
1	A	250	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	F6F	A	1268	21/21	0.87	0.12	21,24,33,34	0
3	NA	A	1263	1/1	0.94	0.07	11,11,11,11	0
5	PLP	B	1396	15/16	0.99	0.04	6,9,11,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.