



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:18 AM GMT

PDB ID : 2CLM  
Title : TRYPTOPHAN SYNTHASE (EXTERNAL ALDIMINE STATE) IN COM-  
PLEX WITH N-(4'-TRIFLUOROMETHOXYBENZOYL)-2-AMINO-1-ETH  
YLPHOSPHATE (F6F)  
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Deposited on : 2006-04-28  
Resolution : 1.51 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

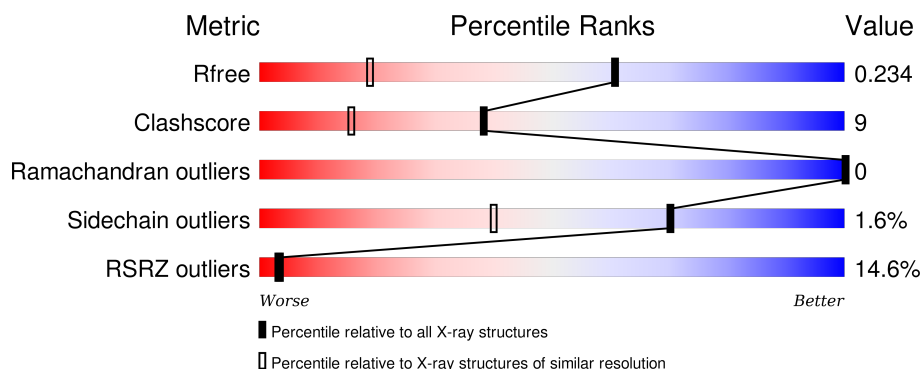
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.51 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2658 (1.54-1.50)
Clashscore	102246	2887 (1.54-1.50)
Ramachandran outliers	100387	2818 (1.54-1.50)
Sidechain outliers	100360	2816 (1.54-1.50)
RSRZ outliers	91569	2660 (1.54-1.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	268	
2	B	396	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5557 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
1	A	252	Total	C	N	O	S	0	0	1
			1902	1211	329	355	7			

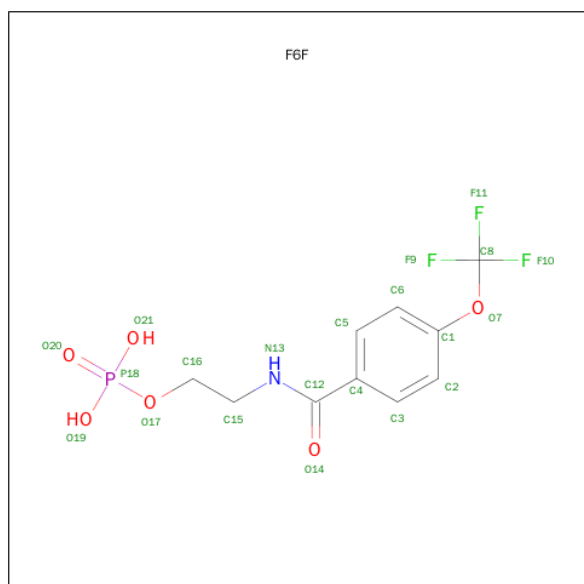
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	393	Total	C	N	O	S	0	0	1
			2968	1865	522	562	19			

There is a discrepancy between the modelled and reference sequences:

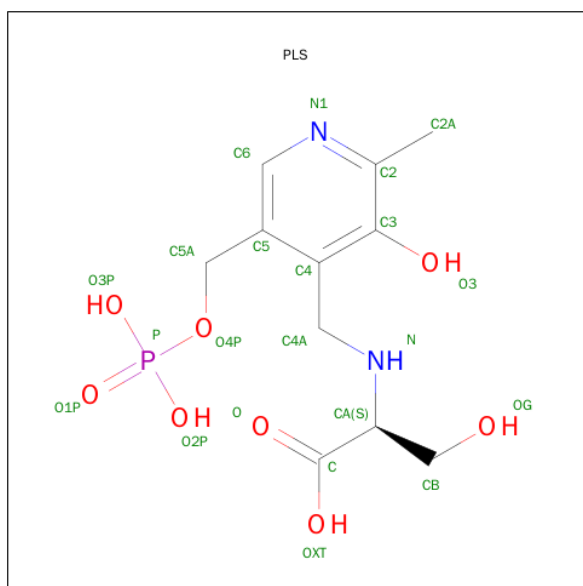
Chain	Residue	Modelled	Actual	Comment	Reference
B	34	ARG	SER	CONFLICT	UNP P0A2K1

- Molecule 3 is 2-{[4-(TRIFLUOROMETHOXY)BENZOYL]AMINO}ETHYL DIHYDROGEN PHOSPHATE (three-letter code: 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
3	A	1	Total	C	F	N	O	P	
			21	10	3	1	6	1	
								0	0

- Molecule 4 is [3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL METHYL]-SERINE (three-letter code: PLS) (formula:  $C_{11}H_{17}N_2O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P		
			22	11	2	8	1		
								0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na		
			1	1	0	0

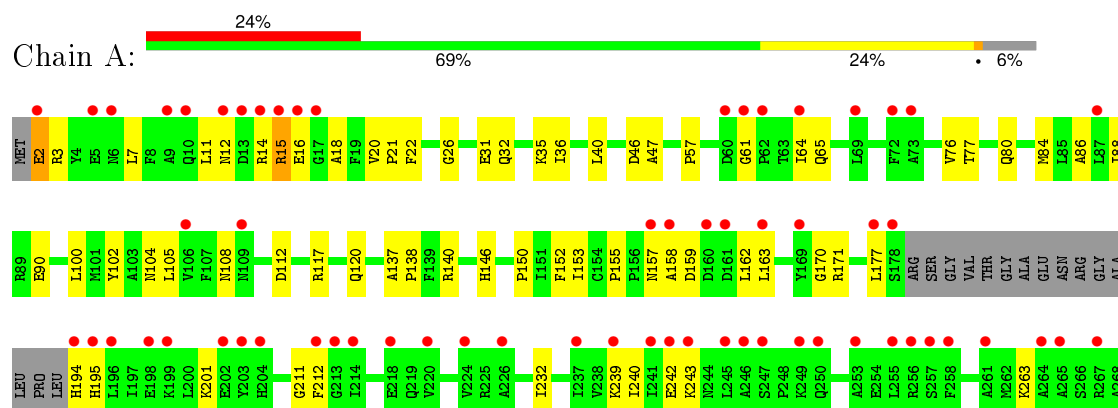
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	201	Total	O		
			201	201	0	0
6	B	442	Total	O		
			442	442	0	0

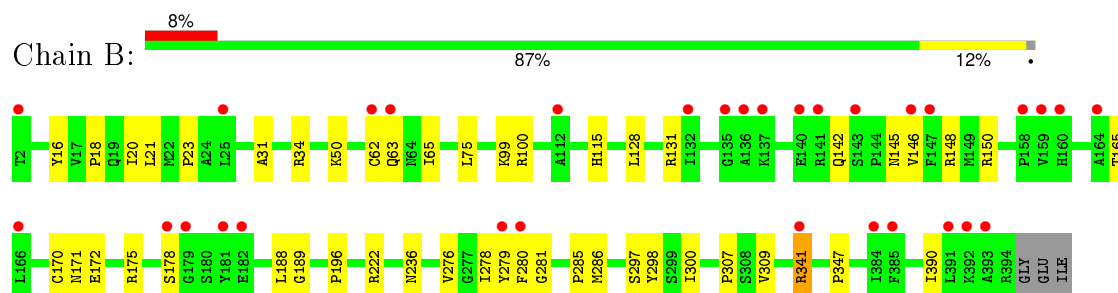
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: 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, $\alpha$ , $\beta$ , $\gamma$	182.51Å 59.54Å 67.71Å 90.00° 94.84° 90.00°	Depositor
Resolution (Å)	19.93 – 1.51 19.92 – 1.51	Depositor EDS
% Data completeness (in resolution range)	89.7 (19.93-1.51) 90.3 (19.92-1.51)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 1.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.218 , 0.239 0.216 , 0.234	Depositor DCC
$R_{free}$ test set	5137 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.9	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 45.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 102735 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5557	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, PLS, 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	0.29	0/1940	0.54	0/2636
2	B	0.31	0/3026	0.61	0/4090
All	All	0.30	0/4966	0.58	0/6726

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	298	TYR	Sidechain

### 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	1902	0	1903	50	0
2	B	2968	0	2940	42	0
3	A	21	0	9	1	0
4	B	22	0	13	0	0
5	B	1	0	0	0	0
6	A	201	0	0	4	0
6	B	442	0	0	6	1
All	All	5557	0	4865	89	1

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 (89) 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:137:ALA:HB3	1:A:138:PRO:HD3	1.70	0.73
1:A:117:ARG:HH11	1:A:120:GLN:NE2	1.87	0.73
1:A:150:PRO:HD2	1:A:171:ARG:HB2	1.73	0.70
1:A:36:ILE:O	1:A:40:LEU:HD13	1.94	0.68
2:B:99:LYS:HD3	2:B:128:LEU:HD21	1.73	0.68
2:B:145:ASN:HD22	2:B:148:ARG:HE	1.44	0.65
2:B:34:ARG:HG3	2:B:100:ARG:HE	1.60	0.65
1:A:140:ARG:HD3	1:A:152:PHE:HZ	1.61	0.64
1:A:159:ASP:O	1:A:163:LEU:HD13	1.99	0.63
2:B:172:GLU:HA	2:B:175:ARG:HD2	1.80	0.63
1:A:240:ILE:HA	1:A:243:LYS:HE3	1.82	0.62
2:B:63:GLN:HG2	6:B:2403:HOH:O	1.98	0.62
2:B:171:ASN:O	2:B:175:ARG:HG2	2.00	0.61
1:A:117:ARG:NH1	1:A:120:GLN:NE2	2.48	0.61
2:B:341:ARG:HH11	2:B:341:ARG:HG3	1.66	0.61
1:A:194:HIS:CD2	1:A:195:HIS:H	2.21	0.59
2:B:150:ARG:NH1	6:B:2244:HOH:O	2.33	0.58
1:A:155:PRO:HG2	1:A:158:ALA:HB2	1.87	0.56
1:A:26:GLY:HA3	1:A:76:VAL:HG21	1.89	0.55
1:A:211:GLY:O	1:A:212:PHE:HB2	2.06	0.55
2:B:62:CYS:SG	2:B:75:LEU:HG	2.47	0.55
2:B:172:GLU:HA	2:B:175:ARG:CG	2.37	0.54
1:A:32:GLN:O	1:A:36:ILE:HG13	2.08	0.54
2:B:99:LYS:CD	2:B:128:LEU:HD21	2.39	0.53
1:A:140:ARG:HD3	1:A:152:PHE:CZ	2.44	0.53
2:B:172:GLU:HA	2:B:175:ARG:CD	2.39	0.53
1:A:155:PRO:HA	1:A:177:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:SER:OG	2:B:307:PRO:HA	2.08	0.52
1:A:2:GLU:HG2	1:A:3:ARG:N	2.25	0.51
2:B:34:ARG:HG3	2:B:100:ARG:NE	2.26	0.51
2:B:145:ASN:ND2	2:B:148:ARG:HH21	2.08	0.51
1:A:57:PRO:HA	1:A:102:TYR:CZ	2.45	0.51
1:A:170:GLY:O	1:A:171:ARG:HD2	2.11	0.50
2:B:222:ARG:NH2	6:B:2297:HOH:O	2.45	0.49
1:A:100:LEU:C	1:A:100:LEU:HD13	2.33	0.48
2:B:62:CYS:CB	2:B:65:ILE:HD11	2.43	0.48
1:A:46:ASP:OD2	1:A:263:LYS:HE2	2.13	0.48
1:A:117:ARG:O	1:A:120:GLN:HG2	2.13	0.48
2:B:62:CYS:HB3	2:B:65:ILE:HD11	1.96	0.48
1:A:12:ASN:O	1:A:15:ARG:HD2	2.14	0.47
2:B:341:ARG:NH1	2:B:341:ARG:HG3	2.28	0.47
1:A:158:ALA:CB	1:A:162:LEU:HD23	2.45	0.46
2:B:142:GLN:O	2:B:146:VAL:HG23	2.15	0.46
1:A:15:ARG:N	1:A:15:ARG:HD2	2.31	0.46
2:B:21:LEU:HD21	2:B:178:SER:HA	1.98	0.46
1:A:20:VAL:HG22	1:A:47:ALA:HB3	1.97	0.46
2:B:34:ARG:CG	2:B:100:ARG:HE	2.25	0.46
2:B:31:ALA:O	2:B:34:ARG:HG2	2.16	0.46
2:B:131:ARG:NH1	6:B:2218:HOH:O	2.49	0.46
1:A:22:PHE:CD1	1:A:22:PHE:C	2.89	0.46
2:B:16:TYR:O	2:B:281:GLY:HA2	2.17	0.45
1:A:158:ALA:HB1	1:A:162:LEU:HD23	1.99	0.45
1:A:20:VAL:HB	1:A:232:ILE:HG12	1.99	0.45
1:A:11:LEU:CD1	1:A:18:ALA:HB2	2.46	0.45
1:A:16:GLU:HB3	6:A:2023:HOH:O	2.17	0.45
2:B:31:ALA:HA	2:B:34:ARG:HG2	1.99	0.44
2:B:150:ARG:HH11	2:B:150:ARG:HG2	1.82	0.44
2:B:34:ARG:CD	2:B:100:ARG:HE	2.30	0.43
1:A:61:GLY:O	1:A:65:GLN:HG3	2.18	0.43
1:A:108:ASN:HA	6:A:2099:HOH:O	2.18	0.43
1:A:77:THR:OG1	1:A:80:GLN:HG3	2.18	0.43
1:A:11:LEU:HD23	1:A:14:ARG:HH21	1.83	0.43
1:A:157:ASN:OD1	2:B:20:ILE:HD12	2.19	0.43
2:B:170:CYS:HB3	2:B:280:PHE:CE1	2.53	0.43
1:A:153:ILE:HG23	1:A:177:LEU:HG	1.99	0.43
1:A:157:ASN:ND2	2:B:23:PRO:HG2	2.33	0.43
1:A:7:LEU:O	1:A:11:LEU:HG	2.18	0.43
1:A:239:LYS:HA	1:A:242:GLU:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:LEU:CD2	2:B:178:SER:HA	2.48	0.42
2:B:276:VAL:HA	2:B:285:PRO:HA	2.01	0.42
2:B:18:PRO:HB2	2:B:20:ILE:HG22	2.02	0.42
1:A:86:ALA:O	1:A:90:GLU:HG3	2.19	0.42
1:A:194:HIS:HD2	1:A:195:HIS:H	1.67	0.42
2:B:300:ILE:HD11	2:B:390:ILE:CD1	2.50	0.42
2:B:50:LYS:HG3	6:B:2122:HOH:O	2.18	0.42
2:B:279:TYR:HB3	2:B:286:MET:SD	2.60	0.42
2:B:165:THR:CG2	6:B:2354:HOH:O	2.68	0.42
1:A:112:ASP:OD1	1:A:146:HIS:HE1	2.03	0.42
1:A:31:GLU:O	1:A:35:LYS:HG3	2.20	0.41
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.54	0.41
1:A:117:ARG:NH1	1:A:120:GLN:HE21	2.15	0.41
1:A:21:PRO:HD2	1:A:47:ALA:O	2.21	0.41
1:A:31:GLU:HG2	6:A:2035:HOH:O	2.19	0.41
1:A:64:ILE:CD1	3:A:1268:F6F:H151	2.51	0.41
2:B:285:PRO:C	2:B:286:MET:HG2	2.42	0.40
1:A:84:MET:O	1:A:88:ILE:HG13	2.21	0.40
1:A:104:ASN:HB2	2:B:278:ILE:O	2.21	0.40
2:B:285:PRO:HG2	2:B:309:VAL:HG12	2.04	0.40
1:A:201:LYS:HA	6:A:2166:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:2125:HOH:O	6:B:2125:HOH:O[2_655]	1.90	0.30

## 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%)	7 (3%)	0	100	100
2	B	391/396 (99%)	381 (97%)	10 (3%)	0	100	100
All	All	639/664 (96%)	622 (97%)	17 (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	197/208 (95%)	194 (98%)	3 (2%)	72	43
2	B	306/310 (99%)	301 (98%)	5 (2%)	70	40
All	All	503/518 (97%)	495 (98%)	8 (2%)	70	40

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	15	ARG
1	A	105	LEU
2	B	188	LEU
2	B	196	PRO
2	B	236	ASN
2	B	341	ARG
2	B	347	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	120	GLN
1	A	194	HIS
1	A	210	GLN
1	A	250	GLN

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Mol	Chain	Res	Type
2	B	26	ASN
2	B	64	ASN
2	B	142	GLN
2	B	145	ASN
2	B	236	ASN
2	B	317	ASN
2	B	375	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	F6F	A	1268	-	17,21,21	2.17	6 (35%)	21,30,30	2.27	4 (19%)
4	PLS	B	1394	-	19,22,22	4.46	11 (57%)	23,31,31	3.15	7 (30%)

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	F6F	A	1268	-	-	0/14/17/17	0/1/1/1
4	PLS	B	1394	-	-	0/13/17/17	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1394	PLS	C4A-N	-4.19	1.33	1.46
4	B	1394	PLS	P-O3P	-3.88	1.40	1.54
4	B	1394	PLS	P-O2P	-2.91	1.44	1.54
4	B	1394	PLS	P-O4P	-2.26	1.52	1.60
4	B	1394	PLS	CB-CA	2.05	1.56	1.52
4	B	1394	PLS	C6-N1	2.84	1.40	1.34
3	A	1268	F6F	C2-C1	3.02	1.44	1.38
3	A	1268	F6F	C3-C2	3.07	1.44	1.38
3	A	1268	F6F	C6-C1	3.36	1.45	1.38
4	B	1394	PLS	C2-N1	3.36	1.41	1.34
3	A	1268	F6F	C3-C4	3.42	1.45	1.39
3	A	1268	F6F	C6-C5	3.54	1.45	1.38
4	B	1394	PLS	C6-C5	3.62	1.45	1.37
3	A	1268	F6F	C5-C4	3.71	1.45	1.39
4	B	1394	PLS	C5-C4	4.23	1.46	1.40
4	B	1394	PLS	C3-C4	9.11	1.54	1.40
4	B	1394	PLS	C3-C2	13.67	1.50	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1268	F6F	C4-C12-N13	-8.87	97.18	117.12
4	B	1394	PLS	C4A-C4-C5	-2.99	117.04	119.71
3	A	1268	F6F	O14-C12-N13	-2.64	117.04	122.58
4	B	1394	PLS	C5-C6-N1	-2.53	119.46	123.86
3	A	1268	F6F	O14-C12-C4	-2.37	116.92	120.97
3	A	1268	F6F	O21-P18-O20	3.12	120.62	110.58
4	B	1394	PLS	C6-N1-C2	3.38	126.17	119.28
4	B	1394	PLS	O4P-C5A-C5	4.65	116.69	108.99
4	B	1394	PLS	O3-C3-C2	4.92	126.21	117.66
4	B	1394	PLS	O3P-P-O4P	6.78	126.10	106.56
4	B	1394	PLS	C4A-N-CA	9.44	128.24	113.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1268	F6F	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, 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%)	1.32	63 (25%) 1 1	11, 27, 37, 44	0
2	B	393/396 (99%)	0.55	31 (7%) 15 15	9, 15, 32, 55	0
All	All	645/664 (97%)	0.85	94 (14%) 3 3	9, 20, 35, 55	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	HIS	8.0
1	A	69	LEU	6.4
2	B	393	ALA	6.2
1	A	13	ASP	5.6
1	A	245	LEU	5.3
2	B	140	GLU	5.2
1	A	158	ALA	5.0
2	B	2	THR	4.9
1	A	157	ASN	4.9
1	A	198	GLU	4.5
2	B	181	TYR	4.4
1	A	212	PHE	4.4
1	A	177	LEU	4.4
1	A	15	ARG	4.4
1	A	178	SER	4.3
1	A	249	LYS	4.3
2	B	385	PHE	4.2
1	A	204	HIS	4.1
1	A	14	ARG	4.1
1	A	72	PHE	4.0
1	A	194	HIS	4.0
1	A	247	SER	3.8
1	A	264	ALA	3.8
1	A	213	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	243	LYS	3.7
2	B	182	GLU	3.7
2	B	63	GLN	3.7
1	A	246	ALA	3.6
1	A	250	GLN	3.6
1	A	169	TYR	3.6
1	A	220	VAL	3.5
1	A	73	ALA	3.4
2	B	62	CYS	3.4
1	A	109	ASN	3.4
2	B	160	HIS	3.3
1	A	10	GLN	3.2
2	B	179	GLY	3.2
1	A	241	ILE	3.2
1	A	199	LYS	3.1
1	A	257	SER	3.0
2	B	391	LEU	3.0
1	A	226	ALA	2.9
1	A	203	TYR	2.9
1	A	196	LEU	2.8
1	A	242	GLU	2.8
1	A	2	GLU	2.8
1	A	5	GLU	2.7
1	A	224	VAL	2.7
1	A	214	ILE	2.7
1	A	163	LEU	2.6
2	B	166	LEU	2.6
1	A	87	LEU	2.6
2	B	137	LYS	2.6
1	A	60	ASP	2.6
2	B	158	PRO	2.6
2	B	132	ILE	2.5
1	A	261	ALA	2.5
2	B	164	ALA	2.5
1	A	258	PHE	2.5
2	B	159	VAL	2.5
2	B	143	SER	2.4
1	A	239	LYS	2.4
2	B	112	ALA	2.4
2	B	146	VAL	2.4
1	A	9	ALA	2.4
1	A	12	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	160	ASP	2.3
2	B	178	SER	2.3
1	A	6	ASN	2.3
1	A	265	ALA	2.3
1	A	161	ASP	2.3
1	A	106	VAL	2.3
1	A	64	ILE	2.3
1	A	17	GLY	2.3
1	A	237	ILE	2.2
2	B	392	LYS	2.2
1	A	61	GLY	2.2
2	B	280	PHE	2.2
2	B	136	ALA	2.2
2	B	384	ILE	2.2
1	A	256	ARG	2.1
2	B	141	ARG	2.1
1	A	253	ALA	2.1
1	A	62	PRO	2.1
2	B	135	GLY	2.1
1	A	218	GLU	2.1
2	B	147	PHE	2.1
1	A	16	GLU	2.1
2	B	25	LEU	2.1
1	A	202	GLU	2.0
2	B	279	TYR	2.0
1	A	267	ARG	2.0
1	A	255	LEU	2.0
2	B	341	ARG	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	F6F	A	1268	21/21	0.81	0.17	0.60	29,31,35,37	0
4	PLS	B	1394	22/22	0.96	0.11	0.14	10,16,23,24	0
5	NA	B	1395	1/1	0.96	0.10	-0.39	15,15,15,15	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.