



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:25 AM UTC

PDB ID : 1A5S / pdb_00001a5s
Title : CRYSTAL STRUCTURE OF WILD-TYPE TRYPTOPHAN SYNTHASE
COMPLEXED WITH 5-FLUOROINDOLE PROPANOL PHOSPHATE AND
L-SER BOUND AS AMINO ACRYLATE TO THE BETA SITE
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ing, I.
Deposited on : 1998-02-17
Resolution : 2.30 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](#) ①) 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

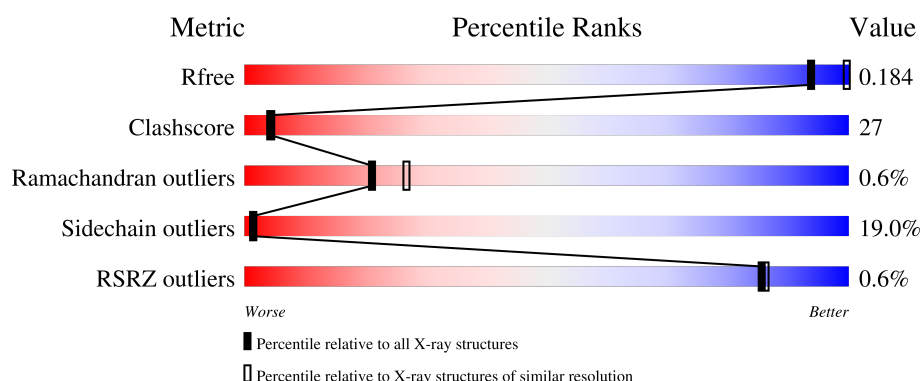
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	268	43% 39% 14% .
2	B	397	61% 29% 7% .

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
6	SER	B	902	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5032 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.

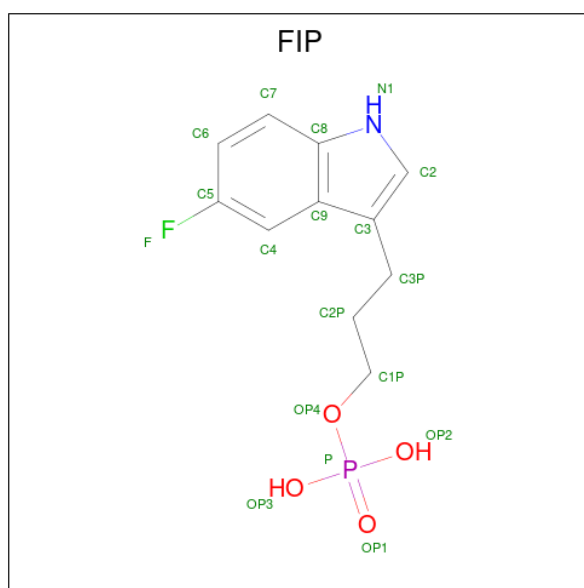
- Molecule 1 is a protein called TRYPTOPHAN SYNTHASE (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1942	1233	335	367	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	387	Total	C	N	O	S	0	0	0
			2934	1843	516	556	19			

- Molecule 3 is 5-FLUOROINDOLE PROPANOL PHOSPHATE (CCD ID: FIP) (formula: $C_{11}H_{13}FNO_4P$).

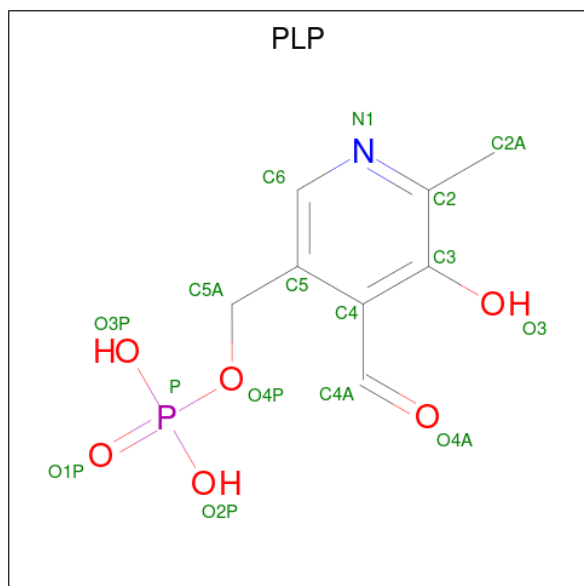


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	P	0	0
			18	11	1	1	4	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

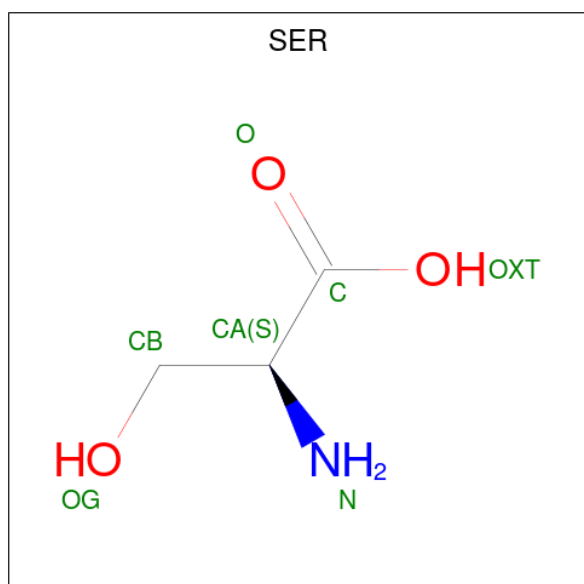
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 6 is SERINE (CCD ID: SER) (formula: C₃H₇NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			6	3	1	2		

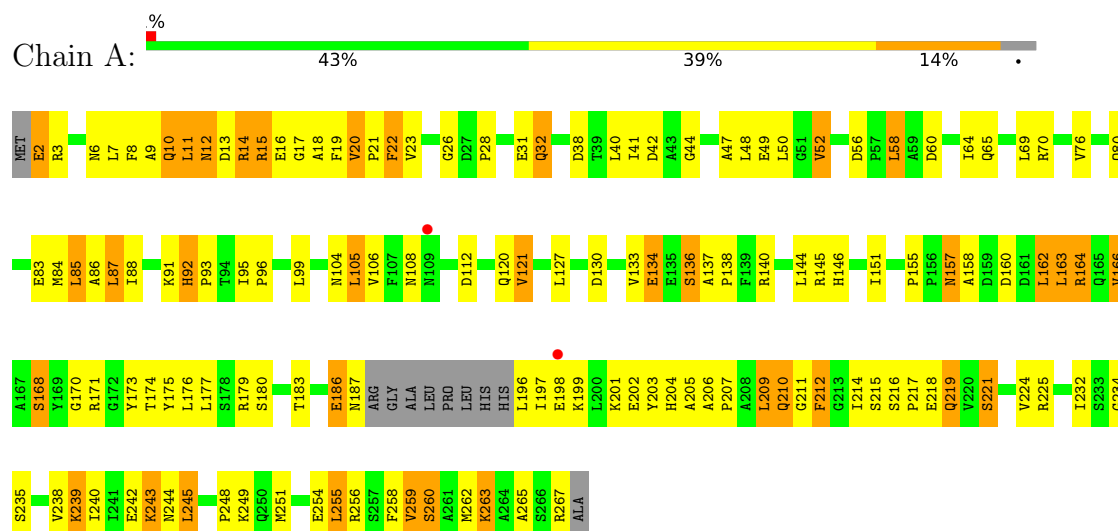
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	32	Total	O	0	0
			32	32		
7	B	84	Total	O	0	0
			84	84		

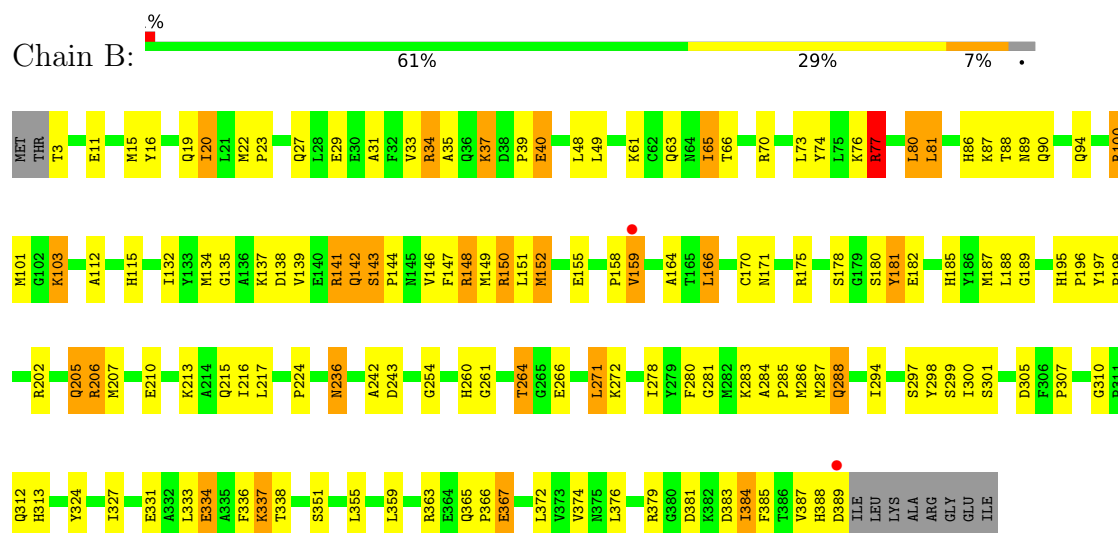
3 Residue-property plots [i](#)

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, α , β , γ	182.70Å 60.80Å 67.50Å 90.00° 94.60° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 10.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.8 (10.00-2.30) 92.7 (10.00-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.62 (at 2.29Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.177 , 0.247 0.171 , 0.184	Depositor DCC
R_{free} test set	3126 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.735	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5032	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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: FIP, NA, PLP

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	0.38	0/1978	0.92	5/2686 (0.2%)
2	B	0.44	0/2992	0.95	7/4042 (0.2%)
All	All	0.42	0/4970	0.94	12/6728 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	365	GLN	CA-C-N	8.30	128.02	119.56
2	B	365	GLN	C-N-CA	8.30	128.02	119.56
2	B	77	ARG	N-CA-C	6.54	119.78	109.39
1	A	92	HIS	CA-C-N	6.29	125.85	119.19
1	A	92	HIS	C-N-CA	6.29	125.85	119.19
1	A	20	VAL	N-CA-C	6.06	114.15	108.15
2	B	305	ASP	N-CA-C	5.94	120.15	113.02
1	A	136	SER	N-CA-C	5.78	120.33	113.28
2	B	90	GLN	N-CA-C	5.67	117.55	111.36
2	B	310	GLY	CA-C-N	5.61	125.72	119.32
2	B	310	GLY	C-N-CA	5.61	125.72	119.32
1	A	130	ASP	N-CA-C	5.30	118.56	112.57

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	1942	0	1946	136	0
2	B	2934	0	2904	131	0
3	A	18	0	11	1	0
4	B	1	0	0	0	0
5	B	15	0	7	2	0
6	B	6	0	1	1	0
7	A	32	0	0	4	0
7	B	84	0	0	5	1
All	All	5032	0	4869	260	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 27.

All (260) 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)
2:B:3:THR:HG21	2:B:15:MET:HE1	1.11	1.09
2:B:100:ARG:HG2	2:B:100:ARG:HH11	1.14	1.06
2:B:3:THR:HG21	2:B:15:MET:CE	1.90	1.02
1:A:14:ARG:HG2	1:A:14:ARG:O	1.59	1.01
1:A:19:PHE:HE2	1:A:259:VAL:HG12	1.28	0.95
2:B:65:ILE:HD11	2:B:338:THR:HG22	1.47	0.95
2:B:3:THR:CG2	2:B:15:MET:HE1	1.96	0.95
2:B:264:THR:HG23	2:B:266:GLU:H	1.30	0.93
1:A:157:ASN:H	1:A:157:ASN:HD22	1.12	0.92
2:B:31:ALA:HA	2:B:34:ARG:HE	1.36	0.90
2:B:70:ARG:NH1	2:B:367:GLU:HG3	1.86	0.90
2:B:112:ALA:O	2:B:142:GLN:HG2	1.73	0.89
2:B:70:ARG:HH12	2:B:367:GLU:HG3	1.37	0.88
1:A:16:GLU:HG3	1:A:267:ARG:HB3	1.53	0.88
2:B:142:GLN:O	2:B:146:VAL:HG23	1.74	0.87
1:A:255:LEU:O	1:A:259:VAL:HG22	1.73	0.87
1:A:249:LYS:H	1:A:249:LYS:HD2	1.40	0.86
1:A:133:VAL:H	2:B:19:GLN:HE22	1.14	0.86
1:A:183:THR:HG22	1:A:212:PHE:CE1	2.10	0.86
2:B:100:ARG:HG2	2:B:100:ARG:NH1	1.88	0.85
2:B:65:ILE:HG22	2:B:66:THR:HG23	1.57	0.84
1:A:174:THR:HG23	1:A:206:ALA:O	1.79	0.83
1:A:199:LYS:HD2	1:A:203:TYR:CE2	2.14	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLY:O	1:A:212:PHE:HB2	1.78	0.82
2:B:337:LYS:HB2	2:B:337:LYS:NZ	1.94	0.81
1:A:157:ASN:HD22	1:A:157:ASN:N	1.72	0.80
1:A:157:ASN:H	1:A:157:ASN:ND2	1.75	0.80
1:A:11:LEU:CD2	1:A:18:ALA:HB2	2.11	0.80
1:A:56:ASP:O	1:A:58:LEU:HD23	1.80	0.79
2:B:264:THR:CG2	2:B:266:GLU:H	1.94	0.79
1:A:87:LEU:HD22	1:A:87:LEU:O	1.82	0.79
1:A:183:THR:HG22	1:A:212:PHE:HE1	1.50	0.77
2:B:34:ARG:CG	2:B:100:ARG:HH12	1.98	0.77
1:A:242:GLU:HA	1:A:245:LEU:HD22	1.67	0.77
2:B:337:LYS:HB2	2:B:337:LYS:HZ3	1.50	0.76
1:A:8:PHE:CD2	1:A:207:PRO:HG2	2.21	0.76
2:B:385:PHE:O	2:B:388:HIS:HB3	1.86	0.76
2:B:271:LEU:HD12	2:B:271:LEU:O	1.85	0.75
2:B:135:GLY:HA2	2:B:159:VAL:HG22	1.69	0.74
1:A:249:LYS:HD2	1:A:249:LYS:N	2.00	0.74
1:A:137:ALA:HB3	1:A:138:PRO:CD	2.17	0.73
2:B:65:ILE:HD11	2:B:338:THR:CG2	2.17	0.73
1:A:243:LYS:HG3	1:A:244:ASN:N	2.03	0.72
1:A:162:LEU:O	1:A:166:VAL:HG13	1.89	0.71
1:A:19:PHE:CE2	1:A:259:VAL:HG12	2.19	0.71
2:B:138:ASP:HA	2:B:141:ARG:HD3	1.70	0.71
2:B:271:LEU:HD12	2:B:271:LEU:C	2.16	0.71
5:B:901:PLP:HO3	6:B:902:SER:N	1.87	0.70
2:B:182:GLU:OE1	2:B:182:GLU:HA	1.90	0.70
1:A:11:LEU:HD23	1:A:18:ALA:HB2	1.73	0.70
2:B:89:ASN:HD22	2:B:205:GLN:HE22	1.39	0.70
2:B:137:LYS:O	2:B:141:ARG:HG3	1.91	0.70
2:B:260:HIS:HB2	2:B:264:THR:HG21	1.73	0.70
1:A:76:VAL:HA	1:A:80:GLN:NE2	2.06	0.70
2:B:94:GLN:HB2	2:B:187:MET:HE2	1.75	0.69
2:B:202:ARG:HH11	2:B:312:GLN:HE22	1.37	0.69
2:B:76:LYS:NZ	2:B:215:GLN:HE22	1.91	0.68
2:B:260:HIS:HD2	2:B:266:GLU:OE1	1.76	0.68
1:A:234:GLY:O	1:A:238:VAL:HG23	1.94	0.68
1:A:174:THR:HG22	7:A:1042:HOH:O	1.93	0.68
2:B:132:ILE:HD13	2:B:149:MET:SD	2.33	0.68
1:A:221:SER:HB2	1:A:225:ARG:HH22	1.59	0.68
2:B:261:GLY:O	2:B:264:THR:HG22	1.94	0.68
1:A:6:ASN:O	1:A:10:GLN:HG2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:LYS:NZ	2:B:337:LYS:CB	2.57	0.66
1:A:160:ASP:O	1:A:164:ARG:HG3	1.95	0.66
1:A:210:GLN:HE21	1:A:214:ILE:HD11	1.61	0.66
1:A:22:PHE:CD1	1:A:22:PHE:C	2.73	0.66
1:A:221:SER:O	1:A:225:ARG:HB2	1.95	0.65
1:A:65:GLN:O	1:A:69:LEU:HD23	1.97	0.65
2:B:202:ARG:HD3	2:B:312:GLN:HE22	1.62	0.64
2:B:29:GLU:O	2:B:33:VAL:HG23	1.97	0.64
1:A:163:LEU:HD21	1:A:196:LEU:HD23	1.80	0.63
2:B:100:ARG:HD2	7:B:1075:HOH:O	1.98	0.63
2:B:334:GLU:HB3	7:B:1039:HOH:O	1.99	0.62
1:A:11:LEU:HD21	1:A:18:ALA:HB2	1.80	0.62
1:A:44:GLY:O	1:A:263:LYS:HG3	1.99	0.62
2:B:34:ARG:HG3	2:B:100:ARG:HH12	1.64	0.62
2:B:206:ARG:HD3	2:B:210:GLU:OE2	2.00	0.61
1:A:58:LEU:HD23	1:A:58:LEU:H	1.65	0.61
2:B:142:GLN:HG3	7:B:1139:HOH:O	2.00	0.61
1:A:137:ALA:HB3	1:A:138:PRO:HD3	1.81	0.61
2:B:195:HIS:HD2	7:B:1013:HOH:O	1.83	0.61
1:A:225:ARG:HG3	1:A:225:ARG:HH11	1.66	0.60
2:B:180:SER:C	2:B:182:GLU:N	2.59	0.60
2:B:379:ARG:HD2	2:B:381:ASP:OD2	2.01	0.59
1:A:134:GLU:HG3	2:B:22:MET:HE2	1.83	0.59
2:B:333:LEU:O	2:B:337:LYS:HG3	2.02	0.59
1:A:196:LEU:N	1:A:198:GLU:OE1	2.36	0.59
2:B:137:LYS:HB2	2:B:164:ALA:O	2.03	0.59
2:B:363:ARG:O	2:B:366:PRO:HD3	2.03	0.59
2:B:29:GLU:OE2	2:B:195:HIS:HE1	1.85	0.58
2:B:101:MET:HE3	2:B:103:LYS:HE3	1.85	0.58
2:B:180:SER:O	2:B:182:GLU:N	2.37	0.58
1:A:199:LYS:HD2	1:A:203:TYR:HE2	1.66	0.57
1:A:11:LEU:HD12	1:A:14:ARG:NH1	2.19	0.57
2:B:34:ARG:HG3	2:B:100:ARG:HH22	1.70	0.57
2:B:31:ALA:HA	2:B:34:ARG:NE	2.15	0.57
2:B:76:LYS:HZ3	2:B:215:GLN:HE22	1.52	0.57
2:B:146:VAL:O	2:B:150:ARG:HG3	2.04	0.57
1:A:12:ASN:ND2	1:A:13:ASP:N	2.53	0.56
2:B:100:ARG:NH1	2:B:100:ARG:CG	2.59	0.56
2:B:94:GLN:CB	2:B:187:MET:HE2	2.35	0.56
2:B:175:ARG:O	2:B:178:SER:HB2	2.05	0.56
2:B:180:SER:C	2:B:182:GLU:H	2.11	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PHE:CE2	1:A:207:PRO:HB2	2.41	0.56
2:B:65:ILE:CG2	2:B:66:THR:HG23	2.32	0.56
1:A:26:GLY:HA3	1:A:76:VAL:HG21	1.86	0.55
1:A:267:ARG:HH11	1:A:267:ARG:HG2	1.70	0.55
2:B:363:ARG:HD2	7:B:1126:HOH:O	2.05	0.55
2:B:383:ASP:O	2:B:387:VAL:HG23	2.07	0.55
1:A:240:ILE:HG21	1:A:255:LEU:HD13	1.89	0.55
1:A:267:ARG:HG2	1:A:267:ARG:NH1	2.21	0.55
1:A:87:LEU:HD22	1:A:87:LEU:C	2.32	0.54
1:A:104:ASN:HD21	2:B:288:GLN:NE2	2.05	0.54
1:A:104:ASN:HB2	2:B:278:ILE:O	2.07	0.54
2:B:271:LEU:C	2:B:271:LEU:CD1	2.81	0.54
2:B:216:ILE:HG21	2:B:224:PRO:HD3	1.90	0.54
1:A:256:ARG:O	1:A:259:VAL:HG23	2.08	0.53
2:B:134:MET:O	2:B:158:PRO:HA	2.09	0.53
1:A:85:LEU:HB3	1:A:121:VAL:HG11	1.91	0.53
1:A:127:LEU:HB2	1:A:151:ILE:HB	1.91	0.53
1:A:11:LEU:HD12	1:A:14:ARG:HH12	1.72	0.53
1:A:170:GLY:C	1:A:171:ARG:HG2	2.34	0.53
2:B:34:ARG:CD	2:B:100:ARG:HH12	2.22	0.53
1:A:174:THR:HG21	1:A:205:ALA:HB1	1.90	0.52
1:A:235:SER:O	1:A:239:LYS:HG3	2.10	0.52
1:A:180:SER:HA	2:B:20:ILE:HD13	1.91	0.52
1:A:186:GLU:N	1:A:186:GLU:CD	2.67	0.52
1:A:197:ILE:O	1:A:201:LYS:HG3	2.09	0.52
2:B:195:HIS:CD2	2:B:196:PRO:HA	2.45	0.52
1:A:2:GLU:HG3	7:A:1097:HOH:O	2.10	0.52
1:A:196:LEU:N	1:A:198:GLU:CD	2.68	0.52
1:A:38:ASP:OD2	1:A:91:LYS:NZ	2.43	0.51
2:B:61:LYS:HB2	2:B:74:TYR:CE1	2.45	0.51
1:A:170:GLY:O	1:A:171:ARG:HD3	2.10	0.51
2:B:147:PHE:O	2:B:151:LEU:HB2	2.11	0.51
2:B:31:ALA:O	2:B:34:ARG:HG2	2.11	0.51
1:A:76:VAL:HA	1:A:80:GLN:HE22	1.76	0.50
1:A:133:VAL:HG13	2:B:19:GLN:NE2	2.26	0.50
1:A:212:PHE:HA	3:A:270:FIP:OP3	2.11	0.50
2:B:139:VAL:HG21	2:B:158:PRO:HB3	1.92	0.50
1:A:112:ASP:OD1	1:A:146:HIS:HE1	1.95	0.50
1:A:179:ARG:HH21	1:A:187:ASN:HB2	1.75	0.50
2:B:202:ARG:HH11	2:B:312:GLN:NE2	2.05	0.50
1:A:133:VAL:N	2:B:19:GLN:HE22	1.96	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ILE:HG12	1:A:95:ILE:HD13	1.93	0.50
2:B:81:LEU:HD13	2:B:88:THR:HB	1.94	0.49
1:A:145:ARG:NH2	7:A:1104:HOH:O	2.44	0.49
1:A:14:ARG:O	1:A:14:ARG:CG	2.44	0.49
2:B:148:ARG:O	2:B:152:MET:HE2	2.13	0.49
2:B:73:LEU:HD11	2:B:374:VAL:HG23	1.95	0.49
1:A:258:PHE:CE2	1:A:262:MET:HG3	2.47	0.49
1:A:177:LEU:HG	1:A:179:ARG:O	2.13	0.48
2:B:86:HIS:NE2	2:B:236:ASN:HB3	2.28	0.48
1:A:52:VAL:CG2	1:A:105:LEU:HD23	2.43	0.48
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.49	0.48
1:A:137:ALA:CB	1:A:138:PRO:CD	2.85	0.48
2:B:297:SER:OG	2:B:307:PRO:HA	2.14	0.48
2:B:336:PHE:CE1	2:B:387:VAL:HG11	2.48	0.48
2:B:264:THR:CG2	2:B:266:GLU:N	2.72	0.48
2:B:327:ILE:HG23	2:B:331:GLU:HB2	1.95	0.47
1:A:20:VAL:HG21	1:A:209:LEU:HD21	1.96	0.47
2:B:166:LEU:HD22	2:B:170:CYS:SG	2.54	0.47
1:A:221:SER:HB2	1:A:225:ARG:NH2	2.26	0.47
1:A:256:ARG:O	1:A:260:SER:OG	2.32	0.47
2:B:284:ALA:HB1	2:B:285:PRO:HD2	1.95	0.47
2:B:384:ILE:HG22	2:B:385:PHE:N	2.29	0.47
1:A:210:GLN:NE2	1:A:214:ILE:HD11	2.27	0.47
2:B:34:ARG:HG3	2:B:100:ARG:NH1	2.30	0.47
1:A:248:PRO:HA	1:A:251:MET:CE	2.44	0.47
2:B:260:HIS:CD2	2:B:266:GLU:OE1	2.64	0.47
1:A:134:GLU:CD	1:A:134:GLU:H	2.22	0.47
2:B:337:LYS:HZ3	2:B:337:LYS:CB	2.21	0.46
1:A:186:GLU:CD	1:A:186:GLU:H	2.22	0.46
2:B:298:TYR:CG	2:B:299:SER:N	2.83	0.46
1:A:206:ALA:O	1:A:207:PRO:C	2.58	0.46
2:B:16:TYR:O	2:B:281:GLY:HA2	2.16	0.46
1:A:21:PRO:HD2	1:A:47:ALA:O	2.16	0.46
1:A:177:LEU:HD12	1:A:177:LEU:HA	1.81	0.46
1:A:28:PRO:HD2	1:A:32:GLN:HB3	1.98	0.46
1:A:60:ASP:HB3	1:A:64:ILE:HB	1.98	0.46
1:A:203:TYR:O	1:A:204:HIS:HB2	2.16	0.46
2:B:40:GLU:H	2:B:40:GLU:HG3	1.54	0.45
2:B:65:ILE:HD12	2:B:65:ILE:HA	1.79	0.45
2:B:287:MET:HE3	2:B:287:MET:HB3	1.87	0.45
1:A:22:PHE:CD1	1:A:23:VAL:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:VAL:CG2	1:A:52:VAL:O	2.63	0.45
1:A:155:PRO:HB2	1:A:157:ASN:ND2	2.32	0.45
1:A:217:PRO:O	1:A:265:ALA:HB1	2.16	0.45
2:B:171:ASN:O	2:B:175:ARG:HG3	2.17	0.45
1:A:240:ILE:CG2	1:A:255:LEU:HD13	2.46	0.45
1:A:17:GLY:HA3	1:A:224:VAL:HG11	1.99	0.45
1:A:155:PRO:HD2	1:A:158:ALA:HB2	1.99	0.45
2:B:87:LYS:HE2	5:B:901:PLP:C4A	2.47	0.45
2:B:37:LYS:O	2:B:39:PRO:HD3	2.16	0.44
2:B:76:LYS:HZ3	2:B:215:GLN:NE2	2.13	0.44
2:B:207:MET:HE3	2:B:207:MET:HB3	1.79	0.44
1:A:69:LEU:HD13	1:A:69:LEU:HA	1.85	0.44
1:A:85:LEU:HB3	1:A:121:VAL:CG1	2.48	0.44
1:A:112:ASP:CG	1:A:146:HIS:HE1	2.26	0.44
2:B:76:LYS:HZ2	2:B:215:GLN:HE22	1.64	0.44
1:A:84:MET:O	1:A:88:ILE:HG13	2.18	0.44
1:A:155:PRO:HB2	1:A:157:ASN:HD21	1.82	0.44
2:B:152:MET:HE3	2:B:152:MET:HB2	1.83	0.44
2:B:254:GLY:O	2:B:324:TYR:HA	2.17	0.43
1:A:86:ALA:HB2	1:A:121:VAL:HG22	2.00	0.43
1:A:7:LEU:HD22	1:A:96:PRO:HG2	2.00	0.43
1:A:179:ARG:NH2	1:A:187:ASN:HB2	2.33	0.43
1:A:255:LEU:O	1:A:259:VAL:CG2	2.55	0.43
1:A:64:ILE:HG12	7:A:1058:HOH:O	2.18	0.43
1:A:137:ALA:HB3	1:A:138:PRO:HD2	1.99	0.43
1:A:163:LEU:HD21	1:A:196:LEU:CD2	2.48	0.43
1:A:56:ASP:OD1	2:B:294:ILE:HB	2.19	0.43
1:A:95:ILE:HA	1:A:96:PRO:HD3	1.93	0.43
1:A:9:ALA:O	1:A:13:ASP:HB2	2.19	0.43
2:B:197:TYR:HB2	2:B:198:PRO:HD3	2.00	0.43
1:A:92:HIS:HA	1:A:93:PRO:HD2	1.88	0.42
2:B:272:LYS:HA	2:B:272:LYS:HD2	1.88	0.42
2:B:159:VAL:O	2:B:159:VAL:HG23	2.18	0.42
2:B:170:CYS:HB3	2:B:280:PHE:CE1	2.54	0.42
1:A:42:ASP:OD2	1:A:256:ARG:NH1	2.48	0.42
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.79	0.42
2:B:286:MET:HE2	2:B:286:MET:HB3	1.94	0.42
1:A:183:THR:CG2	1:A:212:PHE:CE1	2.94	0.42
2:B:22:MET:N	2:B:23:PRO:CD	2.83	0.42
1:A:12:ASN:CG	1:A:13:ASP:N	2.76	0.42
1:A:6:ASN:O	1:A:10:GLN:CG	2.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:SER:O	1:A:137:ALA:C	2.63	0.42
2:B:271:LEU:O	2:B:271:LEU:CD1	2.63	0.42
2:B:143:SER:N	2:B:144:PRO:CD	2.83	0.42
2:B:313:HIS:HD2	2:B:324:TYR:OH	2.03	0.42
1:A:164:ARG:O	1:A:168:SER:HB3	2.20	0.41
1:A:14:ARG:O	1:A:15:ARG:C	2.63	0.41
1:A:209:LEU:HD23	1:A:232:ILE:HD11	2.02	0.41
1:A:248:PRO:O	1:A:251:MET:HB3	2.20	0.41
1:A:22:PHE:HA	1:A:49:GLU:O	2.20	0.41
1:A:179:ARG:NE	1:A:187:ASN:HB3	2.35	0.41
2:B:77:ARG:HB3	2:B:80:LEU:HD22	2.01	0.41
1:A:216:SER:O	1:A:219:GLN:HB2	2.20	0.41
2:B:206:ARG:CD	2:B:210:GLU:OE2	2.68	0.41
2:B:180:SER:O	2:B:181:TYR:C	2.63	0.41
2:B:387:VAL:HG12	2:B:387:VAL:O	2.20	0.41
2:B:15:MET:HE2	2:B:195:HIS:ND1	2.36	0.41
2:B:34:ARG:CG	2:B:35:ALA:N	2.83	0.41
1:A:175:TYR:HE1	1:A:177:LEU:HD13	1.86	0.41
1:A:179:ARG:HE	1:A:187:ASN:HB3	1.86	0.41
2:B:34:ARG:HG3	2:B:100:ARG:NH2	2.34	0.41
2:B:94:GLN:OE1	2:B:185:HIS:HE1	2.04	0.41
2:B:159:VAL:O	2:B:159:VAL:CG2	2.68	0.41
2:B:205:GLN:HA	2:B:205:GLN:HE21	1.85	0.41
2:B:337:LYS:HB2	2:B:337:LYS:HZ2	1.83	0.41
2:B:376:LEU:HD12	2:B:376:LEU:HA	1.85	0.41
1:A:196:LEU:C	1:A:198:GLU:N	2.76	0.40
2:B:327:ILE:HD13	2:B:327:ILE:HA	1.97	0.40
2:B:336:PHE:CD1	2:B:387:VAL:HG11	2.56	0.40
1:A:112:ASP:OD1	1:A:145:ARG:NH1	2.55	0.40
1:A:173:TYR:HB2	1:A:207:PRO:O	2.21	0.40
1:A:105:LEU:HD12	1:A:105:LEU:HA	1.74	0.40
2:B:81:LEU:CD1	2:B:88:THR:HB	2.52	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)
7:B:1073:HOH:O	7:B:1073:HOH:O[2_655]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	254/268 (95%)	236 (93%)	16 (6%)	2 (1%)	16	20
2	B	385/397 (97%)	370 (96%)	13 (3%)	2 (0%)	24	31
All	All	639/665 (96%)	606 (95%)	29 (4%)	4 (1%)	21	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	212	PHE
2	B	181	TYR
2	B	242	ALA

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	201/208 (97%)	151 (75%)	50 (25%)	0	0
2	B	303/311 (97%)	257 (85%)	46 (15%)	3	3
All	All	504/519 (97%)	408 (81%)	96 (19%)	1	1

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	3	ARG

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Mol	Chain	Res	Type
1	A	10	GLN
1	A	11	LEU
1	A	12	ASN
1	A	14	ARG
1	A	15	ARG
1	A	22	PHE
1	A	31	GLU
1	A	32	GLN
1	A	40	LEU
1	A	48	LEU
1	A	50	LEU
1	A	52	VAL
1	A	58	LEU
1	A	70	ARG
1	A	83	GLU
1	A	85	LEU
1	A	87	LEU
1	A	99	LEU
1	A	105	LEU
1	A	106	VAL
1	A	120	GLN
1	A	121	VAL
1	A	134	GLU
1	A	140	ARG
1	A	144	LEU
1	A	157	ASN
1	A	162	LEU
1	A	163	LEU
1	A	164	ARG
1	A	166	VAL
1	A	168	SER
1	A	176	LEU
1	A	186	GLU
1	A	202	GLU
1	A	209	LEU
1	A	210	GLN
1	A	215	SER
1	A	218	GLU
1	A	219	GLN
1	A	221	SER
1	A	239	LYS
1	A	243	LYS

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Mol	Chain	Res	Type
1	A	245	LEU
1	A	254	GLU
1	A	255	LEU
1	A	259	VAL
1	A	260	SER
1	A	263	LYS
2	B	11	GLU
2	B	20	ILE
2	B	27	GLN
2	B	34	ARG
2	B	37	LYS
2	B	40	GLU
2	B	48	LEU
2	B	49	LEU
2	B	63	GLN
2	B	65	ILE
2	B	77	ARG
2	B	80	LEU
2	B	81	LEU
2	B	100	ARG
2	B	103	LYS
2	B	141	ARG
2	B	142	GLN
2	B	143	SER
2	B	148	ARG
2	B	150	ARG
2	B	152	MET
2	B	155	GLU
2	B	159	VAL
2	B	166	LEU
2	B	188	LEU
2	B	205	GLN
2	B	206	ARG
2	B	213	LYS
2	B	217	LEU
2	B	236	ASN
2	B	243	ASP
2	B	264	THR
2	B	271	LEU
2	B	283	LYS
2	B	288	GLN
2	B	300	ILE

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Mol	Chain	Res	Type
2	B	301	SER
2	B	334	GLU
2	B	337	LYS
2	B	351	SER
2	B	355	LEU
2	B	359	LEU
2	B	367	GLU
2	B	372	LEU
2	B	384	ILE
2	B	389	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	12	ASN
1	A	32	GLN
1	A	66	ASN
1	A	68	ASN
1	A	80	GLN
1	A	146	HIS
1	A	157	ASN
1	A	204	HIS
1	A	210	GLN
2	B	19	GLN
2	B	64	ASN
2	B	114	GLN
2	B	142	GLN
2	B	185	HIS
2	B	195	HIS
2	B	205	GLN
2	B	215	GLN
2	B	260	HIS
2	B	288	GLN
2	B	312	GLN
2	B	313	HIS

5.3.3 RNA ⓘ

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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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$
6	SER	B	902	5	5,5,6	1.21	0	6,6,7	2.66	3 (50%)
5	PLP	B	901	6	15,15,16	1.73	4 (26%)	21,22,23	1.33	3 (14%)
3	FIP	A	270	-	19,19,19	0.84	0	27,27,27	1.27	3 (11%)

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
5	PLP	B	901	6	-	0/6/6/8	0/1/1/1
3	FIP	A	270	-	-	3/8/8/8	0/2/2/2
6	SER	B	902	5	1/1/2/2	2/4/4/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	901	PLP	C3-C2	-3.11	1.37	1.41
5	B	901	PLP	C5-C4	-2.95	1.37	1.40
5	B	901	PLP	C2A-C2	2.13	1.53	1.50
5	B	901	PLP	C4A-C4	2.12	1.55	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	902	SER	CB-CA-C	4.12	119.53	110.29
3	A	270	FIP	OP3-P-OP4	-3.71	96.99	106.67
6	B	902	SER	C-CA-N	3.33	119.70	107.93
6	B	902	SER	CB-CA-N	3.21	120.76	109.98
3	A	270	FIP	C7-C6-C5	3.18	121.64	118.38
5	B	901	PLP	C6-C5-C4	2.33	120.01	118.10
5	B	901	PLP	C5-C6-N1	-2.27	120.14	123.83
3	A	270	FIP	OP3-P-OP2	2.10	115.69	107.80
5	B	901	PLP	O2P-P-O4P	-2.06	101.29	106.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	902	SER	CA

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	270	FIP	C1P-OP4-P-OP2
3	A	270	FIP	C1P-OP4-P-OP3
6	B	902	SER	OXT-C-CA-N
3	A	270	FIP	C1P-OP4-P-OP1
6	B	902	SER	O-C-CA-N

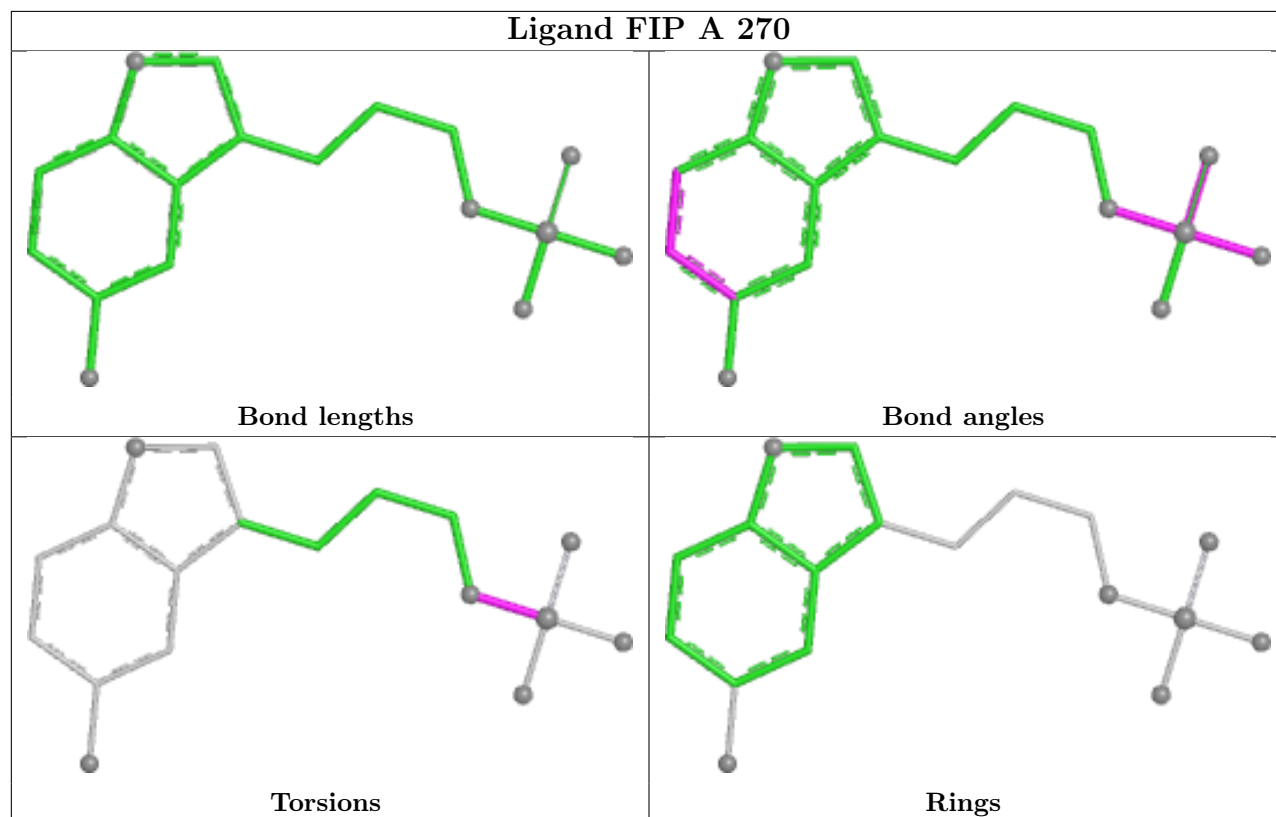
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	902	SER	1	0
5	B	901	PLP	2	0
3	A	270	FIP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	258/268 (96%)	-0.24	2 (0%) 82 83	10, 31, 55, 72	0
2	B	387/397 (97%)	-0.71	2 (0%) 87 87	5, 17, 40, 64	0
All	All	645/665 (96%)	-0.52	4 (0%) 85 86	5, 22, 49, 72	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	ASN	3.9
2	B	389	ASP	3.0
1	A	198	GLU	2.1
2	B	159	VAL	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.

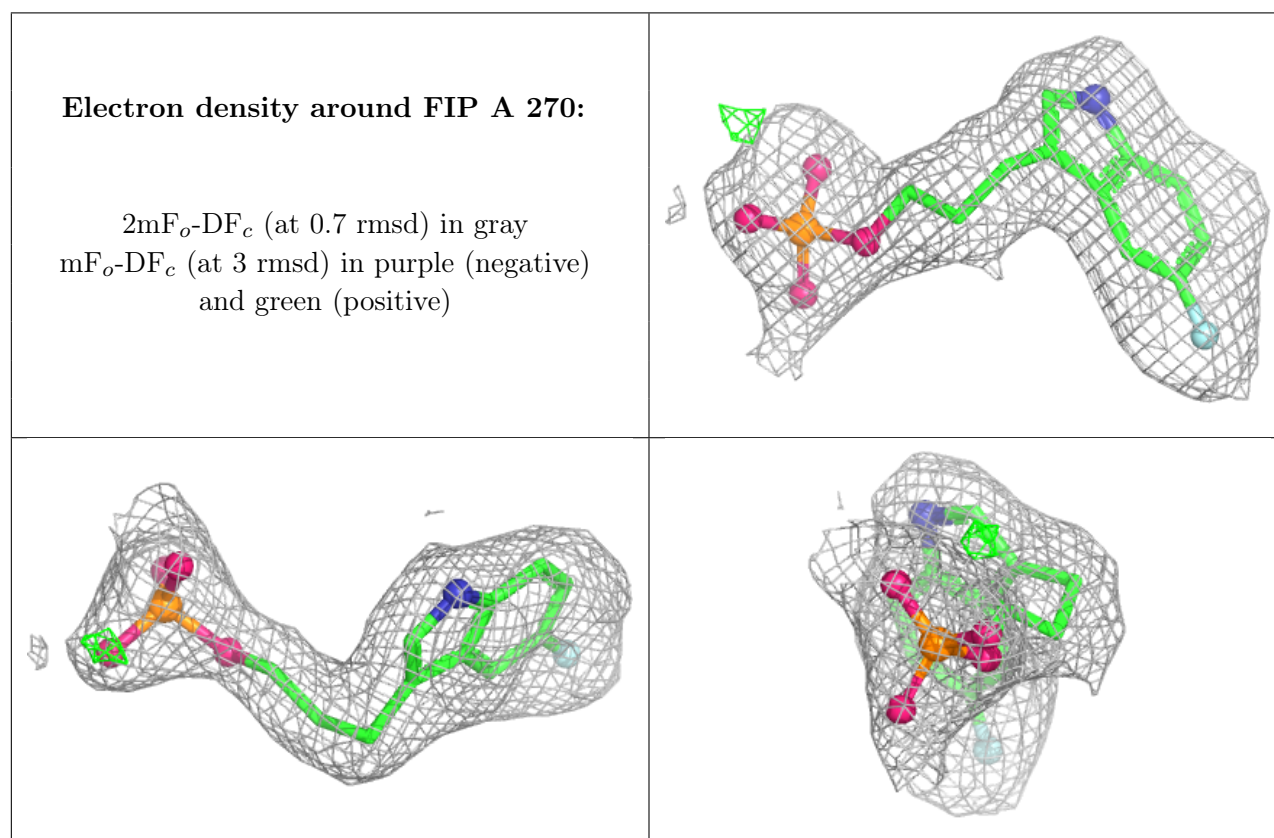
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NA	B	2000	1/1	0.81	0.26	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SER	B	902	6/7	0.81	0.14	23,35,46,47	0
3	FIP	A	270	18/18	0.96	0.05	17,25,37,39	0
5	PLP	B	901	15/16	0.99	0.05	7,22,28,32	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.