WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2023 – 01:17 AM EDT

PDB ID	:	1KL2
Title	:	Crystal Structure of Serine Hydroxymethyltransferase Complexed with Glycine and 5-formyl tetrahydrofolate
Authors	:	Trivedi, V.; Gupta, A.; Jala, V.R.; Saravanan, P.; Rao, G.S.J.; Rao, N.A.; Savithri, H.S.; Subramanya, H.S.
Deposited on	:	2001-12-11
Resolution	:	2.70 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.70 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.
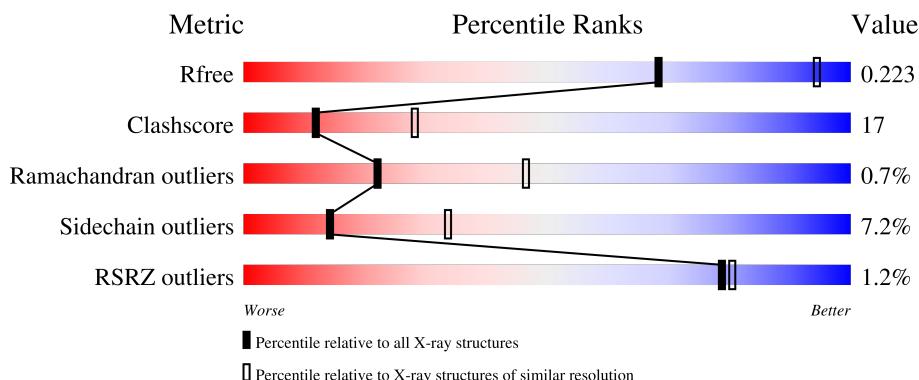
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	419	2% / 62% / 29% / 5% ·
1	B	419	65% / 28% · ·
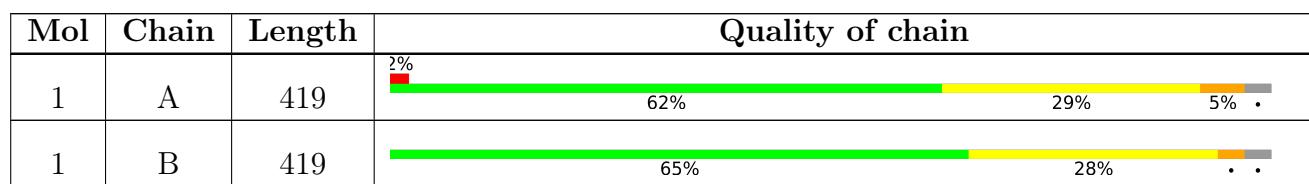
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	B	502	-	X	-	-
4	FON	A	505	X	-	-	-
4	FON	B	506	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6392 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 Serine Hydroxymethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3116	1970	551	584	11			
1	B	405	Total	C	N	O	S	0	0	0
			3116	1970	551	584	11			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).
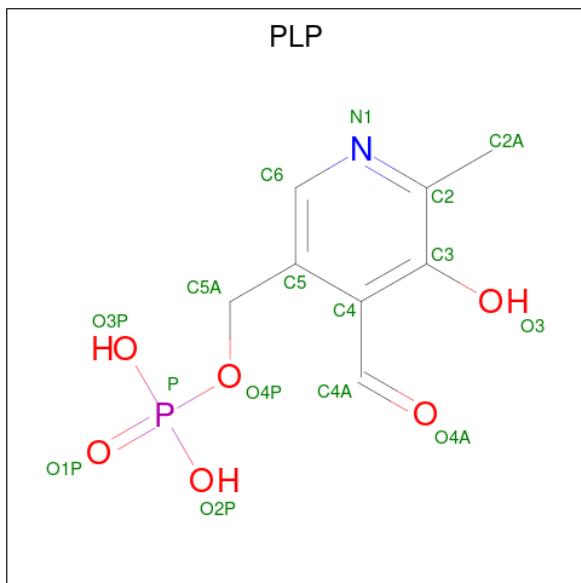
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).
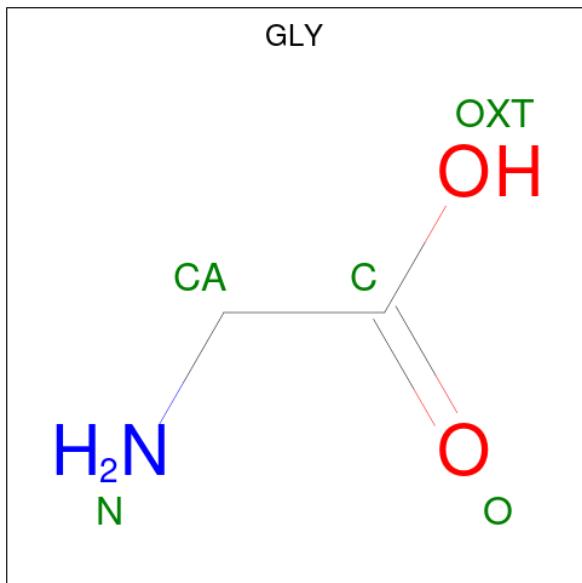
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 5	C 2	N 1	O 2	0	0
3	B	1	Total 5	C 2	N 1	O 2	0	0

- Molecule 4 is N-{[4-({[(6R)-2-amino-5-formyl-4-oxo-1,4,5,6,7,8-hexahydropteridin-6-yl]methyl}amino)phenyl]carbonyl}-L-glutamic acid (three-letter code: FON) (formula: $C_{20}H_{23}N_7O_7$).
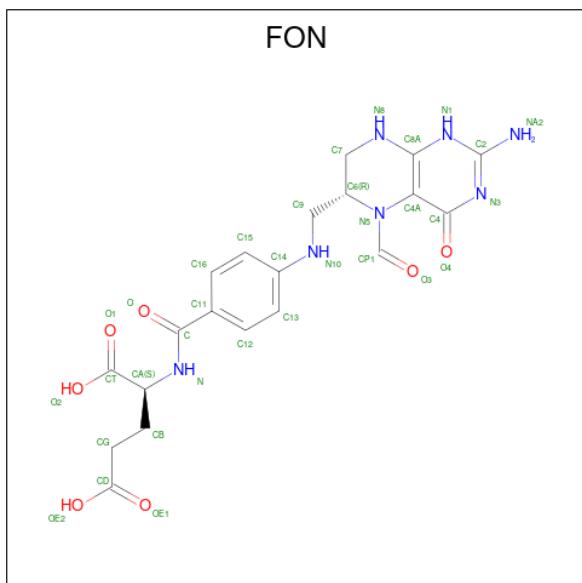
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 29	C 17	N 7	O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 34	C 20	N 7	O 7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total 24	O 24	0	0
5	B	33	Total 33	O 33	0	0

3 Residue-property plots ⓘ

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: Serine Hydroxymethyltransferase

Chain A:

- Molecule 1: Serine Hydroxymethyltransferase

Chain B:
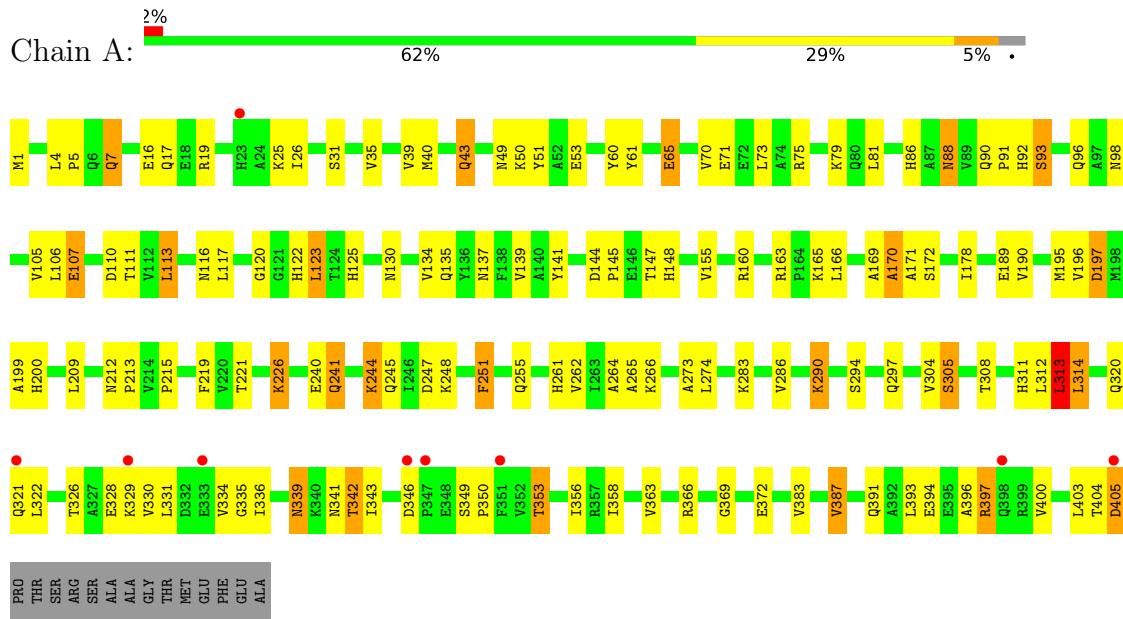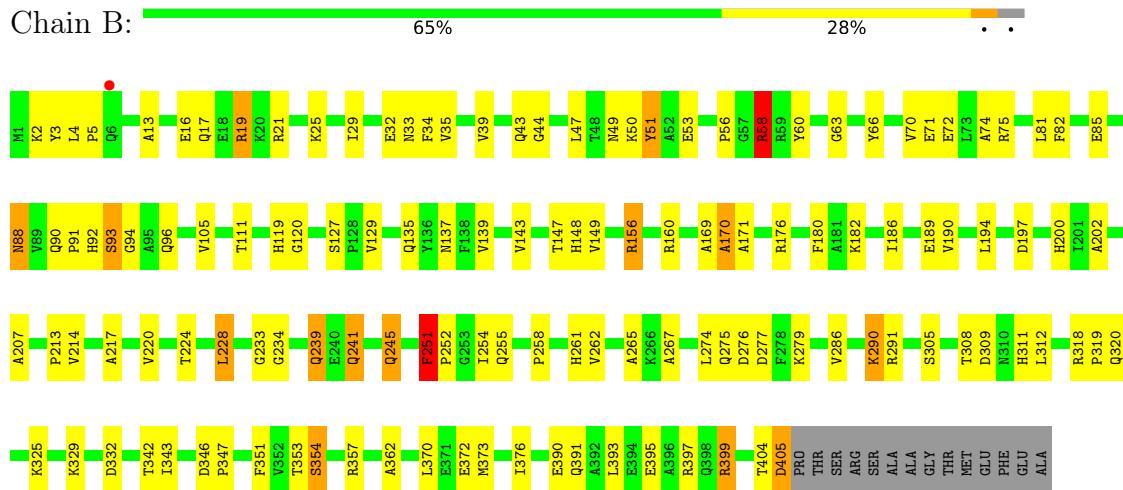
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.42Å 104.61Å 62.49Å 90.00° 91.43° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 14.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 95.3 (14.96-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.39 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.236 0.188 , 0.223	Depositor DCC
R_{free} test set	1007 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 64.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.068 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6392	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FON, 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	0.48	0/3179	1.04	6/4309 (0.1%)
1	B	0.49	0/3179	1.07	11/4309 (0.3%)
All	All	0.49	0/6358	1.06	17/8618 (0.2%)

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
1	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	156	ARG	CD-NE-CZ	13.21	142.09	123.60
1	B	239	GLN	CB-CG-CD	10.47	138.82	111.60
1	B	19	ARG	NE-CZ-NH1	-10.23	115.18	120.30
1	A	313	LEU	CA-CB-CG	7.03	131.46	115.30
1	A	251	PHE	CA-C-O	-6.90	105.61	120.10
1	B	357	ARG	NE-CZ-NH1	-6.73	116.93	120.30
1	B	251	PHE	CA-C-O	-6.67	106.10	120.10
1	B	19	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	A	197	ASP	CB-CG-OD1	6.50	124.15	118.30
1	B	58	ARG	CD-NE-CZ	6.14	132.19	123.60
1	B	156	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	B	58	ARG	CG-CD-NE	5.95	124.29	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	397	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	B	399	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	A	397	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	A	397	ARG	CD-NE-CZ	5.10	130.75	123.60
1	B	312	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	PHE	Mainchain,Peptide
1	B	251	PHE	Mainchain,Peptide

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	3116	0	3095	115	0
1	B	3116	0	3095	111	0
2	A	15	0	6	2	0
2	B	15	0	6	3	0
3	A	5	0	2	2	0
3	B	5	0	2	2	0
4	A	29	0	16	3	0
4	B	34	0	21	2	0
5	A	24	0	0	1	0
5	B	33	0	0	1	0
All	All	6392	0	6243	218	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 17.

All (218) 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)
4:B:506:FON:HCP1	4:B:506:FON:O4	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:505:FON:HCP1	4:A:505:FON:O4	1.63	0.94
1:A:199:ALA:HB1	1:A:226:LYS:HE2	1.53	0.89
1:B:148:HIS:HD2	1:B:305:SER:H	1.22	0.85
1:A:92:HIS:H	1:A:255:GLN:HE22	1.22	0.84
1:A:304:VAL:HG13	1:A:314:LEU:HB3	1.61	0.82
1:A:241:GLN:H	1:A:241:GLN:HE21	1.27	0.80
1:A:313:LEU:HD22	1:A:358:ILE:HB	1.62	0.79
1:B:404:THR:O	1:B:405:ASP:HB3	1.81	0.78
1:B:88:ASN:HD21	1:B:90:GLN:HB2	1.46	0.78
1:B:85:GLU:OE2	1:B:239:GLN:HG2	1.84	0.77
1:B:88:ASN:ND2	1:B:90:GLN:H	1.83	0.77
1:B:88:ASN:HD22	1:B:90:GLN:H	1.35	0.75
1:B:148:HIS:CD2	1:B:305:SER:H	2.04	0.74
1:A:49:ASN:HD21	1:B:35:VAL:H	1.37	0.73
1:B:92:HIS:H	1:B:255:GLN:HE22	1.37	0.72
1:A:113:LEU:HD23	1:A:139:VAL:HG23	1.73	0.70
1:B:346:ASP:OD2	1:B:354:SER:OG	2.07	0.70
1:A:328:GLU:OE1	1:A:339:ASN:HA	1.92	0.68
1:B:261:HIS:CD2	1:B:261:HIS:H	2.11	0.67
1:B:91:PRO:HA	1:B:255:GLN:HE22	1.59	0.66
1:A:241:GLN:HE21	1:A:241:GLN:N	1.93	0.65
1:A:88:ASN:ND2	1:A:91:PRO:HD3	2.11	0.65
4:B:506:FON:O4	4:B:506:FON:CP1	2.44	0.64
1:A:286:VAL:HG13	1:A:290:LYS:NZ	2.13	0.63
1:A:290:LYS:HE2	1:A:308:THR:O	1.98	0.63
4:A:505:FON:CP1	4:A:505:FON:HN0	2.11	0.62
1:A:53:GLU:HB2	1:A:61:TYR:HE2	1.64	0.62
1:B:39:VAL:HG13	1:B:265:ALA:HB1	1.81	0.62
1:A:26:ILE:HD12	1:A:400:VAL:HG13	1.82	0.62
1:A:92:HIS:H	1:A:255:GLN:NE2	1.96	0.62
1:B:346:ASP:OD2	1:B:347:PRO:HD2	2.01	0.61
1:A:90:GLN:N	1:A:91:PRO:HD2	2.16	0.60
1:A:349:SER:HB2	1:A:350:PRO:HD2	1.83	0.60
1:B:2:LYS:HD2	1:B:3:TYR:CZ	2.37	0.60
1:A:350:PRO:HA	1:A:353:THR:HG22	1.84	0.59
1:B:94:GLY:HA3	2:B:502:PLP:H5A2	1.84	0.59
1:B:197:ASP:OD2	2:B:502:PLP:N1	2.35	0.59
1:A:17:GLN:HE21	1:B:66:TYR:HE2	1.47	0.59
1:B:119:HIS:HB3	1:B:143:VAL:HG22	1.85	0.59
1:A:17:GLN:HB3	1:B:66:TYR:CE2	2.38	0.59
1:B:13:ALA:O	1:B:17:GLN:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:VAL:HG13	1:B:290:LYS:NZ	2.17	0.59
1:B:390:GLU:OE1	1:B:393:LEU:HD12	2.03	0.59
1:B:290:LYS:N	1:B:290:LYS:HE3	2.18	0.58
1:B:21:ARG:HG2	1:B:25:LYS:HG3	1.86	0.57
1:A:35:VAL:H	1:B:49:ASN:HD21	1.52	0.57
1:B:58:ARG:HH12	1:B:60:TYR:HE2	1.51	0.57
1:B:395:GLU:OE2	1:B:399:ARG:NH1	2.37	0.57
1:A:7:GLN:HE21	1:B:275:GLN:HE22	1.51	0.57
1:A:39:VAL:HG13	1:A:265:ALA:HB1	1.86	0.56
1:A:122:HIS:H	1:A:125:HIS:CD2	2.22	0.56
3:A:601:GLY:HA2	1:B:51:TYR:CZ	2.40	0.56
1:A:92:HIS:N	1:A:255:GLN:HE22	1.98	0.56
1:B:254:ILE:HG13	1:B:255:GLN:HG3	1.88	0.56
2:B:502:PLP:O3	3:B:602:GLY:N	2.38	0.56
1:B:88:ASN:ND2	1:B:91:PRO:HD3	2.21	0.56
1:B:290:LYS:HE2	1:B:308:THR:HG23	1.87	0.56
1:A:290:LYS:HE3	1:A:290:LYS:N	2.21	0.55
1:A:241:GLN:H	1:A:241:GLN:NE2	2.01	0.55
1:B:34:PHE:CE2	1:B:362:ALA:HB1	2.42	0.55
1:A:313:LEU:CD2	1:A:358:ILE:HB	2.35	0.55
1:A:166:LEU:HD11	1:A:195:MET:HB2	1.88	0.54
1:A:81:LEU:HD13	1:A:274:LEU:HG	1.88	0.54
1:B:53:GLU:HB3	1:B:251:PHE:CZ	2.42	0.54
1:B:58:ARG:NH1	1:B:60:TYR:CE2	2.75	0.54
1:B:92:HIS:H	1:B:255:GLN:NE2	2.03	0.54
1:A:326:THR:HG23	1:A:329:LYS:HD3	1.89	0.53
1:A:148:HIS:HD2	1:A:305:SER:H	1.54	0.53
1:A:79:LYS:HD2	5:A:618:HOH:O	2.09	0.53
1:A:90:GLN:N	1:A:91:PRO:CD	2.71	0.53
1:B:90:GLN:N	1:B:91:PRO:CD	2.71	0.52
1:A:330:VAL:HG21	1:A:387:VAL:CG2	2.40	0.52
1:A:331:LEU:HA	1:A:334:VAL:HG22	1.92	0.52
1:A:393:LEU:O	1:A:396:ALA:HB3	2.09	0.52
1:B:160:ARG:NH2	1:B:189:GLU:OE1	2.41	0.52
1:B:88:ASN:HD22	1:B:91:PRO:HD3	1.75	0.52
1:A:110:ASP:OD2	1:A:165:LYS:HD2	2.10	0.52
1:A:135:GLN:OE1	1:B:135:GLN:NE2	2.39	0.52
1:A:40:MET:HB3	1:B:44:GLY:O	2.09	0.52
1:A:304:VAL:HG11	1:A:314:LEU:HD13	1.92	0.52
1:A:17:GLN:HB3	1:B:66:TYR:CD2	2.45	0.51
1:B:4:LEU:HB3	1:B:5:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:PRO:HD3	5:B:610:HOH:O	2.11	0.51
1:B:90:GLN:HG2	1:B:258:PRO:HB3	1.92	0.51
1:A:170:ALA:HA	1:A:178:ILE:HD13	1.91	0.51
1:A:93:SER:HB2	1:A:96:GLN:NE2	2.24	0.51
1:A:93:SER:HB2	1:A:96:GLN:HE21	1.76	0.51
1:B:93:SER:O	1:B:234:GLY:HA3	2.11	0.51
1:B:186:ILE:O	1:B:190:VAL:HG22	2.11	0.50
1:B:239:GLN:HB3	1:B:241:GLN:CD	2.31	0.50
1:A:25:LYS:HD2	1:A:335:GLY:HA2	1.93	0.50
1:A:331:LEU:HB3	1:A:336:ILE:HB	1.94	0.50
1:B:286:VAL:HG13	1:B:290:LYS:HZ2	1.75	0.49
1:B:325:LYS:HE2	1:B:329:LYS:HZ3	1.77	0.49
1:B:261:HIS:CD2	1:B:261:HIS:N	2.80	0.49
1:A:88:ASN:HD22	1:A:91:PRO:HD3	1.76	0.49
1:A:160:ARG:HD3	1:A:189:GLU:OE1	2.13	0.49
1:B:2:LYS:HB3	1:B:3:TYR:CD2	2.48	0.48
1:B:47:LEU:HD21	1:B:70:VAL:HG21	1.95	0.48
1:A:1:MET:SD	1:A:4:LEU:HD23	2.52	0.48
1:A:169:ALA:O	1:A:170:ALA:HB3	2.14	0.48
1:A:286:VAL:HG13	1:A:290:LYS:HZ2	1.79	0.48
1:A:86:HIS:HE1	1:A:247:ASP:OD1	1.97	0.48
1:A:226:LYS:HZ1	2:A:501:PLP:C4A	2.27	0.48
1:A:261:HIS:H	1:A:261:HIS:CD2	2.32	0.48
1:B:291:ARG:HG2	1:B:370:LEU:HD22	1.94	0.48
1:A:98:ASN:HD22	1:A:221:THR:HG21	1.79	0.48
1:A:7:GLN:NE2	1:B:275:GLN:HE22	2.11	0.48
1:B:194:LEU:HD23	1:B:217:ALA:HA	1.96	0.48
1:A:105:VAL:HG23	1:A:106:LEU:CD2	2.44	0.48
1:A:244:LYS:O	1:A:248:LYS:HG3	2.13	0.48
1:A:286:VAL:HG13	1:A:290:LYS:HZ3	1.77	0.48
1:A:356:ILE:HD12	1:A:358:ILE:HD11	1.95	0.48
1:B:91:PRO:HA	1:B:255:GLN:NE2	2.27	0.48
1:A:290:LYS:HE3	1:A:290:LYS:CA	2.44	0.47
1:B:74:ALA:HB2	1:B:267:ALA:HB2	1.96	0.47
1:A:4:LEU:N	1:A:5:PRO:HD2	2.29	0.47
1:A:130:ASN:O	1:A:134:VAL:HG23	2.15	0.47
1:A:320:GLN:O	1:A:322:LEU:N	2.47	0.47
1:B:373:MET:CE	1:B:376:ILE:HD12	2.43	0.47
1:B:81:LEU:HD13	1:B:274:LEU:HG	1.97	0.47
1:A:111:THR:HA	1:A:137:ASN:O	2.15	0.47
1:A:294:SER:HA	1:A:297:GLN:HE21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:SER:OG	1:B:129:VAL:HG22	2.15	0.46
1:A:212:ASN:O	1:A:215:PRO:HD2	2.16	0.46
1:B:147:THR:O	1:B:149:VAL:HG23	2.15	0.46
1:A:363:VAL:O	1:A:366:ARG:HG2	2.15	0.46
1:A:16:GLU:OE2	1:A:19:ARG:NH1	2.48	0.46
1:A:60:TYR:CE1	1:B:351:PHE:HD2	2.33	0.46
1:B:92:HIS:N	1:B:255:GLN:HE22	2.07	0.46
1:A:123:LEU:HD11	1:B:252:PRO:HB2	1.97	0.46
1:A:343:ILE:O	1:A:346:ASP:HB2	2.16	0.46
1:A:91:PRO:HA	1:A:255:GLN:HE22	1.81	0.46
1:A:226:LYS:NZ	2:A:501:PLP:C4A	2.79	0.46
1:A:393:LEU:HD23	1:A:397:ARG:HH11	1.81	0.46
1:B:120:GLY:O	1:B:171:ALA:HB1	2.15	0.46
1:A:113:LEU:HD22	1:A:141:TYR:HD2	1.81	0.46
1:A:169:ALA:O	1:A:170:ALA:CB	2.63	0.46
1:B:96:GLN:HB3	1:B:255:GLN:HE21	1.81	0.46
1:A:71:GLU:O	1:A:75:ARG:HG3	2.16	0.46
1:B:88:ASN:HD22	1:B:88:ASN:C	2.19	0.46
1:B:93:SER:HB3	1:B:96:GLN:H	1.81	0.46
1:A:43:GLN:NE2	1:A:262:VAL:HG22	2.31	0.45
1:A:393:LEU:HD23	1:A:397:ARG:NH1	2.30	0.45
1:B:169:ALA:O	1:B:170:ALA:CB	2.64	0.45
1:B:200:HIS:HD2	1:B:311:HIS:NE2	2.15	0.45
1:B:16:GLU:CD	1:B:19:ARG:HH12	2.20	0.45
1:A:125:HIS:HE1	1:A:197:ASP:OD2	1.99	0.45
1:B:176:ARG:HD2	1:B:309:ASP:OD1	2.16	0.45
1:B:111:THR:HA	1:B:137:ASN:O	2.17	0.45
1:B:202:ALA:HB1	1:B:228:LEU:HD22	1.99	0.45
1:A:262:VAL:O	1:A:266:LYS:HG3	2.17	0.45
1:A:196:VAL:HG11	1:A:213:PRO:CB	2.47	0.45
1:B:373:MET:HE1	1:B:376:ILE:HD12	1.99	0.45
1:A:26:ILE:HD11	1:A:403:LEU:HB2	1.98	0.44
4:A:505:FON:CP1	4:A:505:FON:N10	2.80	0.44
1:A:404:THR:O	1:A:405:ASP:C	2.56	0.44
1:A:329:LYS:HE2	1:A:330:VAL:CG2	2.47	0.44
1:B:50:LYS:HE3	1:B:63:GLY:O	2.17	0.44
1:B:169:ALA:O	1:B:170:ALA:HB3	2.17	0.44
1:B:58:ARG:NH1	1:B:60:TYR:HE2	2.12	0.44
1:A:107:GLU:HG3	1:A:110:ASP:OD2	2.16	0.44
1:A:144:ASP:HB3	1:A:147:THR:OG1	2.18	0.44
1:B:90:GLN:CD	1:B:258:PRO:HG3	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:GLN:HB3	1:B:241:GLN:CG	2.47	0.44
1:A:311:HIS:HD1	1:A:311:HIS:H	1.66	0.43
1:B:290:LYS:HE2	1:B:308:THR:O	2.18	0.43
1:A:200:HIS:HA	1:A:226:LYS:HD2	1.99	0.43
1:B:207:ALA:HA	1:B:279:LYS:HD3	2.00	0.43
1:B:81:LEU:HD23	1:B:82:PHE:CE2	2.53	0.43
1:B:214:VAL:HG22	1:B:220:VAL:HG21	2.01	0.43
1:A:329:LYS:HG2	1:A:330:VAL:N	2.32	0.43
1:B:239:GLN:HB3	1:B:241:GLN:HG2	2.01	0.43
1:A:311:HIS:CE1	1:A:312:LEU:HD23	2.54	0.43
1:A:120:GLY:O	1:A:171:ALA:HB1	2.19	0.43
1:A:53:GLU:HB2	1:A:61:TYR:CE2	2.49	0.42
1:A:81:LEU:HD21	1:A:273:ALA:HB3	2.00	0.42
1:A:369:GLY:N	1:A:372:GLU:OE2	2.38	0.42
1:B:72:GLU:CD	1:B:75:ARG:HH21	2.22	0.42
1:B:311:HIS:HD1	1:B:311:HIS:H	1.67	0.42
1:B:318:ARG:HB2	1:B:319:PRO:HD3	2.01	0.42
1:B:290:LYS:HE3	1:B:290:LYS:CA	2.48	0.42
1:A:163:ARG:NH1	1:A:190:VAL:HA	2.34	0.42
1:B:16:GLU:OE1	1:B:19:ARG:NH1	2.52	0.42
1:B:43:GLN:NE2	1:B:262:VAL:HG22	2.34	0.42
1:B:200:HIS:HE1	3:B:602:GLY:O	2.02	0.42
1:B:343:ILE:O	1:B:346:ASP:HB2	2.20	0.42
1:A:50:LYS:NZ	1:B:32:GLU:OE1	2.42	0.42
1:A:70:VAL:HG11	1:A:264:ALA:HB2	2.02	0.42
1:A:65:GLU:H	1:A:65:GLU:HG3	1.46	0.42
1:A:43:GLN:HE21	1:A:43:GLN:HB3	1.69	0.42
1:B:342:THR:HG22	1:B:353:THR:HG22	2.02	0.42
1:A:141:TYR:CD1	1:A:155:VAL:HG22	2.55	0.41
1:B:29:ILE:CG2	1:B:32:GLU:HG3	2.50	0.41
1:B:33:ASN:HA	1:B:362:ALA:HB2	2.02	0.41
1:B:393:LEU:O	1:B:397:ARG:HG3	2.19	0.41
1:A:342:THR:HA	1:A:353:THR:HB	2.01	0.41
1:A:349:SER:CB	1:A:350:PRO:HD2	2.48	0.41
1:B:182:LYS:O	1:B:186:ILE:HG13	2.21	0.41
1:B:372:GLU:O	1:B:376:ILE:HG13	2.20	0.41
1:B:245:GLN:H	1:B:245:GLN:HG3	1.58	0.41
1:A:105:VAL:HG11	1:A:219:PHE:CE1	2.55	0.41
1:A:123:LEU:HD11	1:B:252:PRO:CB	2.51	0.41
1:A:200:HIS:HE1	3:A:601:GLY:O	2.04	0.41
1:B:56:PRO:HG3	1:B:71:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASN:HB2	1:A:141:TYR:O	2.20	0.41
1:B:180:PHE:CE1	1:B:213:PRO:HB3	2.56	0.41
1:A:130:ASN:ND2	1:B:252:PRO:O	2.46	0.41
1:B:170:ALA:CB	1:B:197:ASP:O	2.69	0.41
1:B:92:HIS:O	1:B:233:GLY:HA2	2.20	0.41
1:B:93:SER:HB2	1:B:96:GLN:HE21	1.86	0.41
1:A:209:LEU:CD1	1:A:283:LYS:HA	2.51	0.40
1:A:290:LYS:CE	1:A:308:THR:HG23	2.51	0.40
1:A:330:VAL:HG12	1:A:383:VAL:CG1	2.51	0.40
1:B:58:ARG:HD3	1:B:58:ARG:O	2.20	0.40
1:A:144:ASP:HA	1:A:145:PRO:HD3	1.90	0.40
1:A:88:ASN:ND2	1:A:90:GLN:H	2.20	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	403/419 (96%)	381 (94%)	18 (4%)	4 (1%)	15	37
1	B	403/419 (96%)	385 (96%)	16 (4%)	2 (0%)	29	54
All	All	806/838 (96%)	766 (95%)	34 (4%)	6 (1%)	22	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	ALA
1	A	321	GLN
1	B	170	ALA
1	A	353	THR
1	B	241	GLN
1	A	226	LYS

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	321/331 (97%)	293 (91%)	28 (9%)	10	23
1	B	321/331 (97%)	303 (94%)	18 (6%)	21	45
All	All	642/662 (97%)	596 (93%)	46 (7%)	14	34

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	31	SER
1	A	43	GLN
1	A	51	TYR
1	A	65	GLU
1	A	73	LEU
1	A	88	ASN
1	A	93	SER
1	A	107	GLU
1	A	113	LEU
1	A	117	LEU
1	A	123	LEU
1	A	172	SER
1	A	240	GLU
1	A	241	GLN
1	A	244	LYS
1	A	245	GLN
1	A	290	LYS
1	A	305	SER
1	A	313	LEU
1	A	314	LEU
1	A	339	ASN
1	A	341	ASN
1	A	342	THR
1	A	387	VAL
1	A	391	GLN
1	A	394	GLU

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Mol	Chain	Res	Type
1	A	405	ASP
1	B	51	TYR
1	B	58	ARG
1	B	88	ASN
1	B	93	SER
1	B	105	VAL
1	B	139	VAL
1	B	156	ARG
1	B	224	THR
1	B	228	LEU
1	B	245	GLN
1	B	276	ASP
1	B	277	ASP
1	B	290	LYS
1	B	320	GLN
1	B	332	ASP
1	B	354	SER
1	B	391	GLN
1	B	405	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	7	GLN
1	A	43	GLN
1	A	49	ASN
1	A	86	HIS
1	A	88	ASN
1	A	90	GLN
1	A	98	ASN
1	A	125	HIS
1	A	148	HIS
1	A	200	HIS
1	A	239	GLN
1	A	241	GLN
1	A	255	GLN
1	A	261	HIS
1	A	275	GLN
1	A	297	GLN
1	A	320	GLN
1	B	6	GLN

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Mol	Chain	Res	Type
1	B	7	GLN
1	B	43	GLN
1	B	49	ASN
1	B	86	HIS
1	B	88	ASN
1	B	90	GLN
1	B	96	GLN
1	B	125	HIS
1	B	148	HIS
1	B	200	HIS
1	B	239	GLN
1	B	245	GLN
1	B	255	GLN
1	B	261	HIS
1	B	297	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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
4	FON	B	506	-	34,36,36	2.54	13 (38%)	36,50,50	3.72	18 (50%)
4	FON	A	505	-	29,31,36	2.69	13 (44%)	29,43,50	3.85	14 (48%)
2	PLP	A	501	3	15,15,16	1.82	4 (26%)	20,22,23	2.93	10 (50%)
2	PLP	B	502	3	15,15,16	1.80	5 (33%)	20,22,23	2.61	8 (40%)
3	GLY	B	602	2	4,4,4	0.99	0	3,4,4	1.13	0
3	GLY	A	601	2	4,4,4	0.99	0	3,4,4	1.21	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
4	FON	B	506	-	1/1/6/10	11/24/37/37	0/2/3/3
4	FON	A	505	-	1/1/4/10	6/16/29/37	0/2/3/3
2	PLP	A	501	3	-	3/6/6/8	0/1/1/1
2	PLP	B	502	3	-	5/6/6/8	0/1/1/1
3	GLY	B	602	2	-	2/2/2/2	-
3	GLY	A	601	2	-	0/2/2/2	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	506	FON	C7-N8	-6.31	1.34	1.44
4	A	505	FON	C4A-C4	6.08	1.49	1.41
4	B	506	FON	C4A-C4	5.98	1.49	1.41
4	A	505	FON	C7-N8	-5.97	1.34	1.44
4	A	505	FON	C7-C6	-5.31	1.45	1.52
4	B	506	FON	C7-C6	-4.58	1.46	1.52
4	A	505	FON	C14-N10	4.41	1.51	1.38
4	A	505	FON	C4A-N5	4.20	1.47	1.41
2	A	501	PLP	C3-C2	3.65	1.44	1.40
4	B	506	FON	CB-CG	3.62	1.64	1.52
4	B	506	FON	C4A-N5	3.49	1.46	1.41
4	A	505	FON	C13-C14	3.41	1.45	1.39
4	B	506	FON	C4-N3	3.40	1.39	1.33
4	B	506	FON	C2-N3	3.35	1.41	1.35
4	A	505	FON	C4-N3	3.32	1.38	1.33
4	B	506	FON	C13-C14	3.27	1.44	1.39
2	B	502	PLP	C3-C2	3.21	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	505	FON	C2-N3	3.14	1.41	1.35
2	A	501	PLP	C4A-C4	-2.83	1.45	1.51
4	B	506	FON	C14-N10	2.81	1.46	1.38
2	B	502	PLP	C4A-C4	-2.81	1.45	1.51
2	A	501	PLP	C6-C5	2.65	1.43	1.37
4	B	506	FON	C15-C14	-2.60	1.34	1.39
4	B	506	FON	CG-CD	2.59	1.56	1.50
4	A	505	FON	C15-C14	-2.50	1.35	1.39
4	A	505	FON	C8A-N1	2.48	1.39	1.34
2	B	502	PLP	C3-C4	2.46	1.45	1.40
2	B	502	PLP	C6-C5	2.45	1.42	1.37
4	B	506	FON	C8A-N1	2.44	1.39	1.34
4	A	505	FON	C12-C11	2.33	1.43	1.39
2	B	502	PLP	P-O4P	-2.32	1.52	1.60
2	A	501	PLP	C3-C4	2.28	1.44	1.40
4	A	505	FON	C9-N10	2.15	1.49	1.45
4	B	506	FON	C9-C6	2.02	1.61	1.53
4	A	505	FON	C9-C6	2.00	1.61	1.53

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	505	FON	NA2-C2-N1	9.14	131.46	117.25
4	B	506	FON	NA2-C2-N1	9.09	131.38	117.25
2	A	501	PLP	O4P-C5A-C5	7.68	123.98	109.35
4	A	505	FON	C15-C14-C13	7.47	129.25	119.03
4	B	506	FON	C15-C14-C13	7.37	129.12	119.03
4	A	505	FON	N1-C2-N3	-7.25	114.05	125.42
4	A	505	FON	C2-N3-C4	7.18	127.34	115.93
4	B	506	FON	N1-C2-N3	-6.97	114.48	125.42
4	B	506	FON	C2-N3-C4	6.94	126.96	115.93
4	B	506	FON	O3-CP1-N5	-6.90	115.37	125.36
4	A	505	FON	C16-C15-C14	-6.70	112.56	120.30
4	B	506	FON	C16-C15-C14	-5.94	113.43	120.30
2	B	502	PLP	O4P-C5A-C5	5.43	119.70	109.35
4	A	505	FON	C13-C14-N10	-5.34	109.91	120.97
2	B	502	PLP	C2A-C2-C3	5.05	127.12	120.89
2	A	501	PLP	C5A-C5-C6	-4.81	111.45	119.37
4	B	506	FON	CB-CG-CD	4.75	125.11	112.51
4	A	505	FON	C2-N1-C8A	4.40	124.41	114.54
4	B	506	FON	C12-C13-C14	-4.30	115.33	120.30
2	A	501	PLP	C6-N1-C2	4.29	127.11	119.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	506	FON	C2-N1-C8A	4.23	124.01	114.54
2	B	502	PLP	C6-N1-C2	4.13	126.82	119.17
4	A	505	FON	C12-C13-C14	-3.96	115.73	120.30
4	B	506	FON	C4A-C4-N3	-3.93	115.07	123.14
4	A	505	FON	C4A-C4-N3	-3.91	115.10	123.14
4	B	506	FON	O-C-N	-3.87	115.32	122.45
2	B	502	PLP	C5A-C5-C6	-3.86	113.02	119.37
2	A	501	PLP	C2A-C2-C3	3.84	125.62	120.89
4	B	506	FON	C13-C14-N10	-3.81	113.07	120.97
4	B	506	FON	C9-N10-C14	3.67	131.62	122.14
4	B	506	FON	C8A-C4A-C4	3.64	117.29	114.44
2	A	501	PLP	C3-C2-N1	-3.62	116.09	120.77
4	A	505	FON	O-C-N	-3.57	115.50	122.61
4	A	505	FON	C8A-C4A-C4	3.56	117.22	114.44
2	A	501	PLP	C3-C4-C5	3.42	122.43	118.74
4	B	506	FON	C16-C11-C12	3.31	123.31	118.59
2	B	502	PLP	C3-C2-N1	-3.29	116.52	120.77
4	B	506	FON	OE1-CD-CG	-3.17	112.91	123.08
2	B	502	PLP	C3-C4-C5	3.13	122.12	118.74
2	B	502	PLP	C5-C6-N1	-3.04	118.75	123.82
2	A	501	PLP	C5-C6-N1	-2.72	119.29	123.82
2	B	502	PLP	C4A-C4-C3	-2.62	116.05	120.50
4	A	505	FON	C16-C11-C12	2.59	122.27	118.59
4	A	505	FON	C13-C12-C11	-2.58	117.77	120.78
4	B	506	FON	C13-C12-C11	-2.47	117.90	120.78
2	A	501	PLP	C4A-C4-C3	-2.29	116.62	120.50
2	A	501	PLP	O3-C3-C4	2.23	123.97	118.10
2	A	501	PLP	C6-C5-C4	-2.22	116.41	118.16
4	A	505	FON	O2-CT-O1	-2.08	118.12	123.30
4	B	506	FON	NA2-C2-N3	-2.01	114.13	117.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	505	FON	C6
4	B	506	FON	C6

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PLP	C5A-O4P-P-O2P
2	A	501	PLP	C5A-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
2	B	502	PLP	C4-C5-C5A-O4P
2	B	502	PLP	C6-C5-C5A-O4P
2	B	502	PLP	C5A-O4P-P-O1P
2	B	502	PLP	C5A-O4P-P-O2P
2	B	502	PLP	C5A-O4P-P-O3P
4	A	505	FON	N5-C6-C9-N10
4	A	505	FON	C7-C6-C9-N10
4	B	506	FON	N5-C6-C9-N10
4	A	505	FON	O-C-N-CA
4	B	506	FON	N-CA-CB-CG
4	A	505	FON	C15-C14-N10-C9
4	B	506	FON	C13-C14-N10-C9
4	A	505	FON	C13-C14-N10-C9
4	B	506	FON	C15-C14-N10-C9
3	B	602	GLY	OXT-C-CA-N
4	B	506	FON	CT-CA-CB-CG
4	B	506	FON	C7-C6-C9-N10
4	B	506	FON	CA-CB-CG-CD
4	B	506	FON	C6-C9-N10-C14
2	A	501	PLP	C6-C5-C5A-O4P
4	B	506	FON	N-C-C11-C12
4	B	506	FON	OE1-CD-CG-CB
4	A	505	FON	C11-C-N-CA
4	B	506	FON	OE2-CD-CG-CB
3	B	602	GLY	O-C-CA-N

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	506	FON	2	0
4	A	505	FON	3	0
2	A	501	PLP	2	0
2	B	502	PLP	3	0
3	B	602	GLY	2	0
3	A	601	GLY	2	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 then 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.

Ligand FON B 506

Bond lengths

Bond angles

Torsions

Rings

Ligand FON A 505

Bond lengths

Bond angles

Torsions

Rings
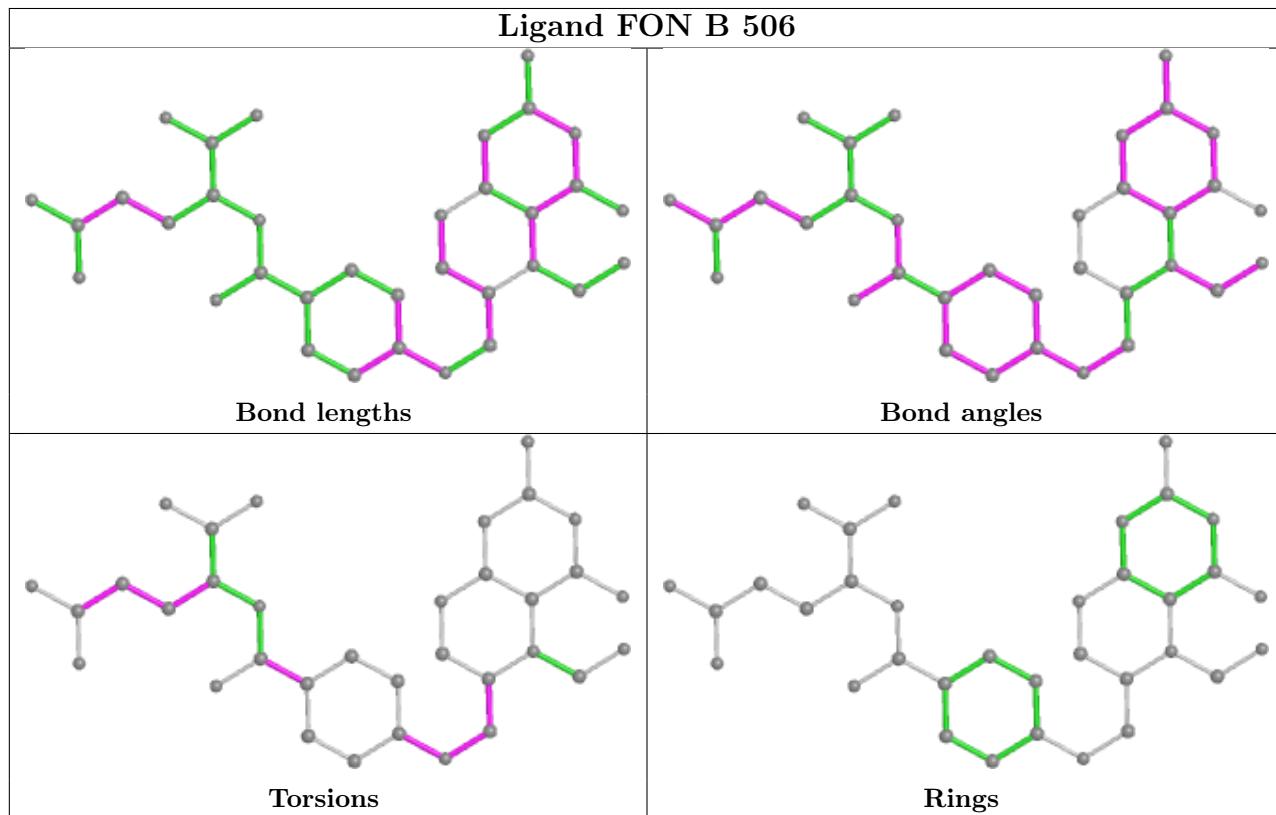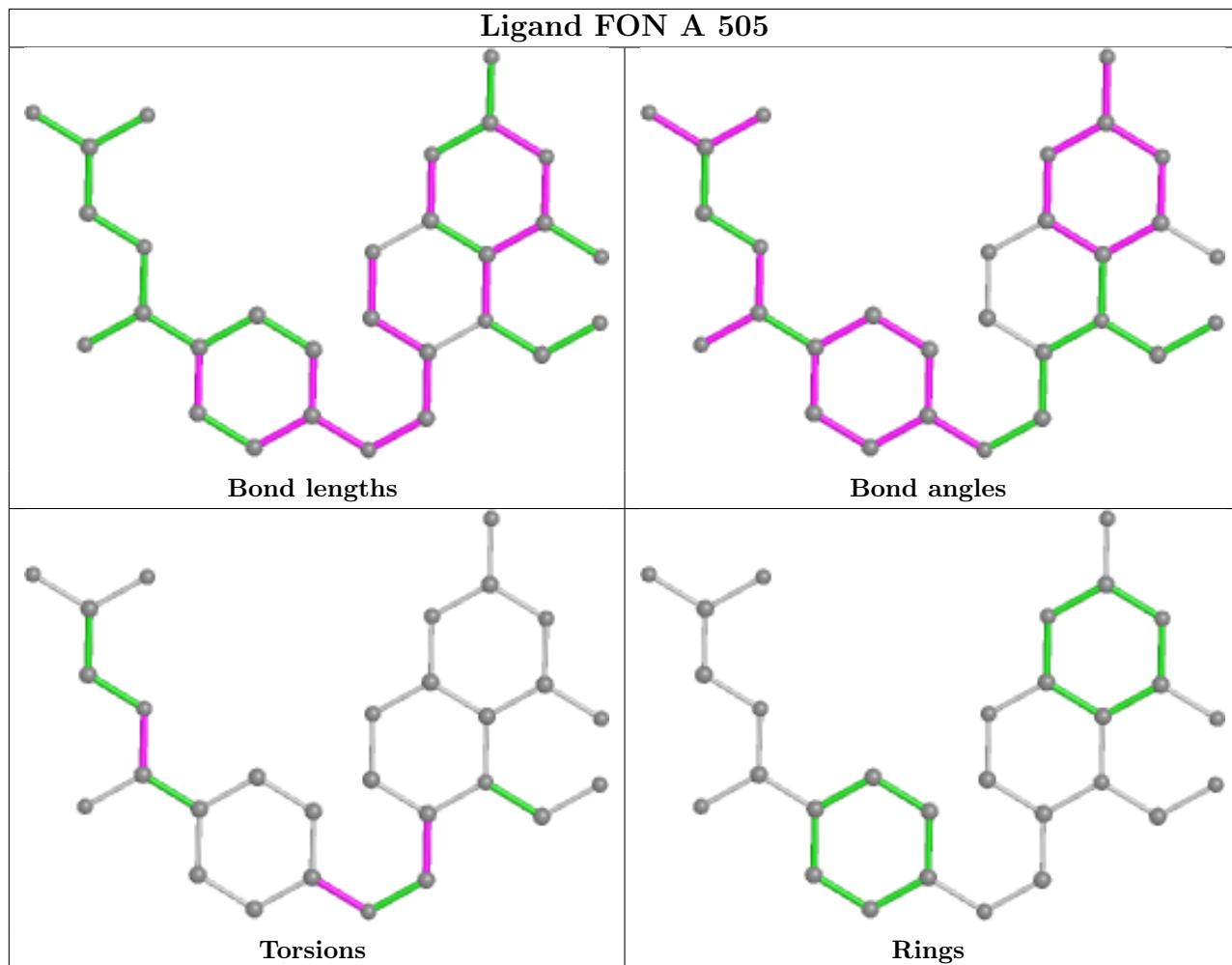
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	405/419 (96%)	-0.20	9 (2%)	62	63	12, 31, 52, 61	0
1	B	405/419 (96%)	-0.39	1 (0%)	95	96	13, 28, 43, 53	0
All	All	810/838 (96%)	-0.29	10 (1%)	79	80	12, 29, 48, 61	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	347	PRO	4.4
1	A	321	GLN	3.9
1	A	333	GLU	3.7
1	B	6	GLN	3.6
1	A	405	ASP	3.1
1	A	398	GLN	2.7
1	A	346	ASP	2.5
1	A	329	LYS	2.4
1	A	23	HIS	2.3
1	A	351	PHE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4　Ligands　ⓘ

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	FON	A	505	29/34	0.80	0.25	42,44,46,47	0
4	FON	B	506	34/34	0.89	0.18	33,37,44,45	0
2	PLP	A	501	15/16	0.93	0.23	36,38,39,39	0
3	GLY	A	601	5/5	0.94	0.19	37,37,38,38	0
2	PLP	B	502	15/16	0.95	0.17	30,32,33,33	0
3	GLY	B	602	5/5	0.97	0.18	30,31,31,32	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.

Electron density around FON A 505:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

Electron density around FON B 506:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.