



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:45 PM UTC

PDB ID : 1EQB / pdb_00001eqb
Title : X-RAY CRYSTAL STRUCTURE AT 2.7 ANGSTROMS RESOLUTION OF
TERNARY COMPLEX BETWEEN THE Y65F MUTANT OF E-COLI SER-
INE HYDROXYMETHYLTRANSFERASE, GLYCINE AND 5-FORMYL
TETRAHYDROFOLATE
Authors : Contestabile, R.; Angelaccio, S.; Bossa, F.; Wright, H.T.; Scarsdale, N.;
Kazanina, G.; Schirch, V.
Deposited on : 2000-04-03
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	: 4-5-2 with Phenix2.0
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
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)

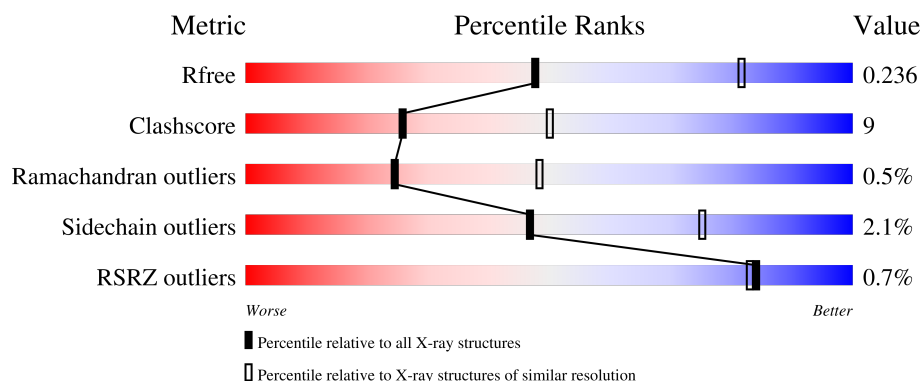
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	417	78% 19% .
1	B	417	79% 19% .
1	C	417	78% 20% .

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	417	80% 18%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13171 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	416	Total	C	N	O	S	0	0	0
			3161	2003	545	599	14			
1	B	417	Total	C	N	O	S	0	1	0
			3186	2017	547	607	15			
1	C	417	Total	C	N	O	S	0	0	0
			3161	2002	544	600	15			
1	D	417	Total	C	N	O	S	0	0	0
			3160	2003	541	601	15			

There are 4 discrepancies between the modelled and reference sequences:

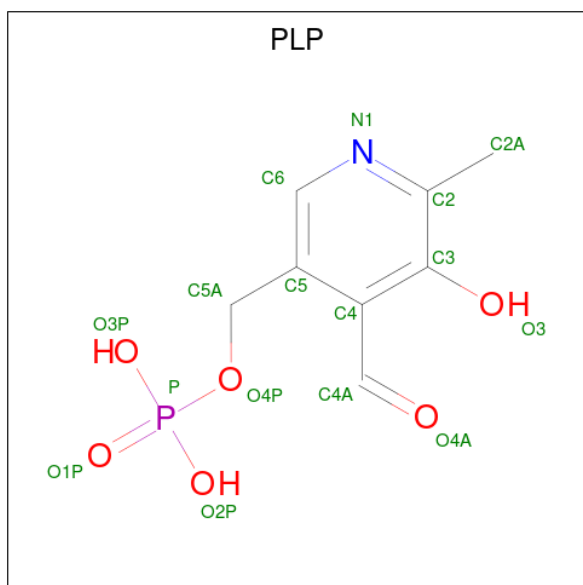
Chain	Residue	Modelled	Actual	Comment	Reference
A	65	PHE	TYR	engineered mutation	UNP P00477
B	65	PHE	TYR	engineered mutation	UNP P00477
C	65	PHE	TYR	engineered mutation	UNP P00477
D	65	PHE	TYR	engineered mutation	UNP P00477

- Molecule 2 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂).



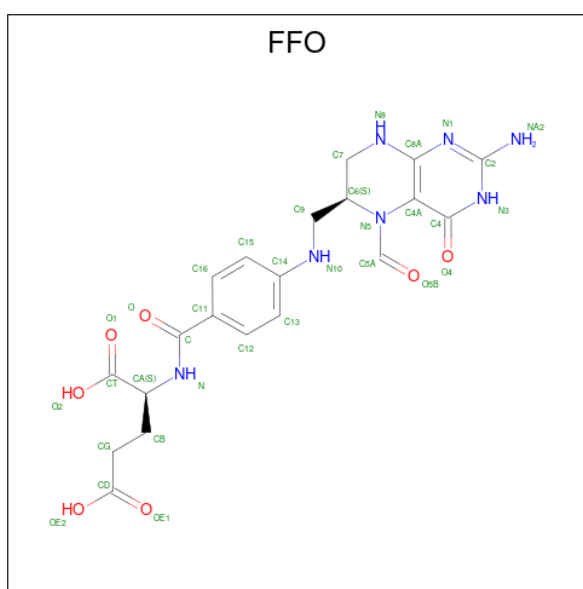
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	B	1	Total	C	N	O	0	0
			5	2	1	2		
2	C	1	Total	C	N	O	0	0
			5	2	1	2		
2	D	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 4 is N-[4-({[(6S)-2-amino-5-formyl-4-oxo-3,4,5,6,7,8-hexahydropteridin-6-yl]methyl}amino)benzoyl]-L-glutamic acid (CCD ID: FFO) (formula: C₂₀H₂₃N₇O₇).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	70	Total 70 O 70	0	0

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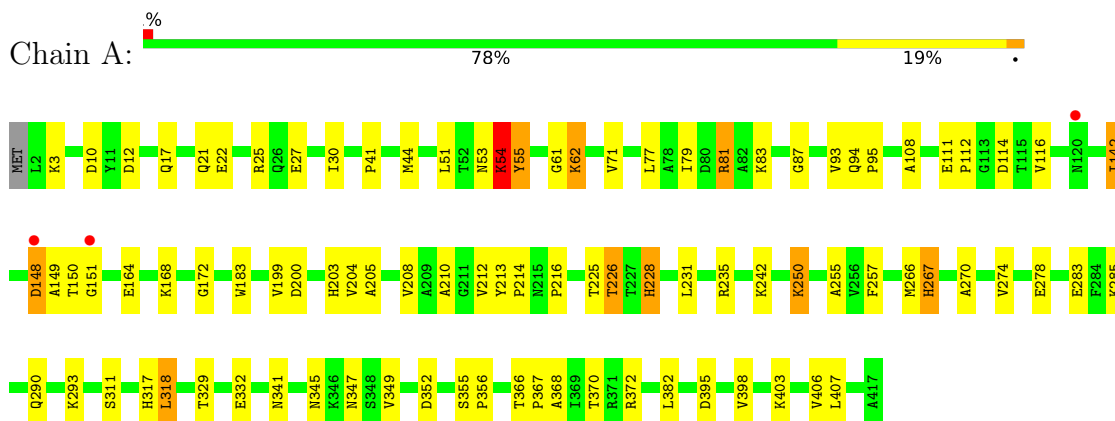
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	71	Total 71	O 71	0	0
5	C	73	Total 73	O 73	0	0
5	D	73	Total 73	O 73	0	0

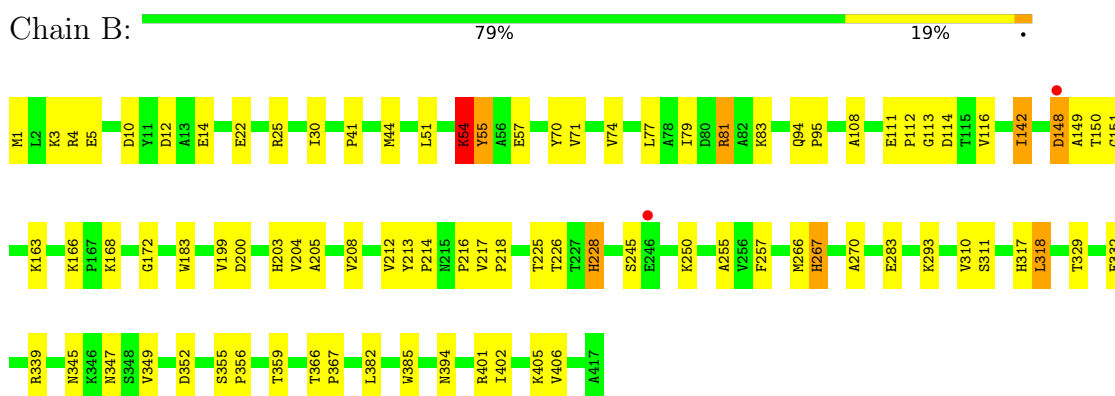
3 Residue-property plots [i](#)

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.

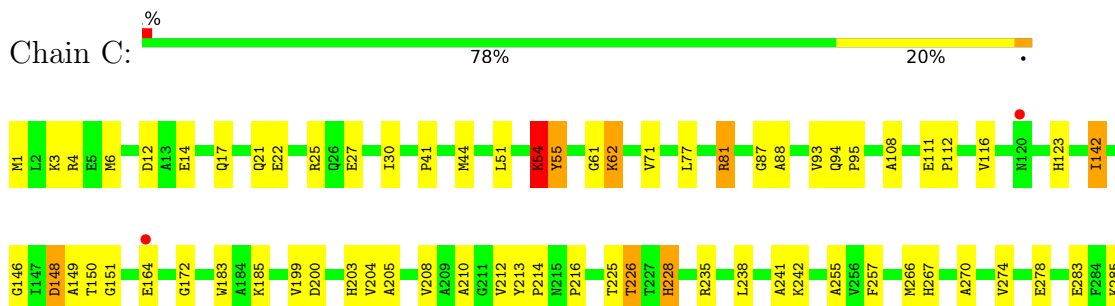
• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE



• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

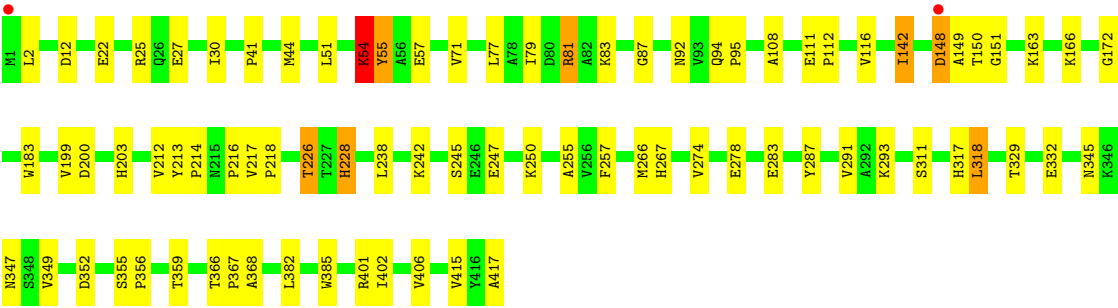
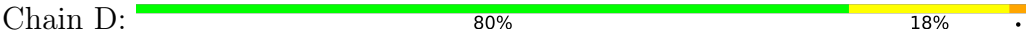


• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE





● Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.74Å 172.48Å 95.41Å 90.00° 104.28° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.00-2.70) 94.4 (20.00-2.70)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.236 0.204 , 0.236	Depositor DCC
R_{free} test set	6391 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13171	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.65% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FFO, 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	0.45	0/3229	0.91	11/4377 (0.3%)
1	B	0.44	0/3254	0.90	9/4409 (0.2%)
1	C	0.43	0/3229	0.92	9/4379 (0.2%)
1	D	0.45	0/3228	0.90	9/4377 (0.2%)
All	All	0.44	0/12940	0.91	38/17542 (0.2%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	ALA	N-CA-C	-9.84	101.27	113.28
1	D	149	ALA	N-CA-C	-9.73	101.41	113.28
1	B	149	ALA	N-CA-C	-9.53	101.66	113.28
1	A	149	ALA	N-CA-C	-9.11	102.17	113.28
1	A	228	HIS	N-CA-C	6.17	120.50	112.92
1	C	142	ILE	N-CA-C	6.14	117.13	108.36
1	A	142	ILE	N-CA-C	6.13	117.12	108.36
1	C	318	LEU	N-CA-C	6.12	117.86	109.18
1	D	54	LYS	N-CA-C	6.05	119.39	109.76
1	B	142	ILE	N-CA-C	6.05	117.01	108.36
1	D	228	HIS	N-CA-C	6.03	120.34	112.92
1	D	142	ILE	N-CA-C	5.90	116.80	108.36
1	B	318	LEU	N-CA-C	5.88	117.52	109.18
1	D	318	LEU	N-CA-C	5.85	117.49	109.18
1	B	228	HIS	N-CA-C	5.81	120.07	112.92
1	C	226	THR	N-CA-C	-5.79	101.89	110.46
1	C	54	LYS	N-CA-C	5.75	118.91	109.76
1	A	250	LYS	N-CA-C	-5.75	104.93	111.14
1	B	54	LYS	N-CA-C	5.74	118.89	109.76
1	A	54	LYS	N-CA-C	5.70	118.82	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ALA	N-CA-C	-5.66	105.19	111.36
1	A	355	SER	CA-C-N	5.66	126.03	119.47
1	A	355	SER	C-N-CA	5.66	126.03	119.47
1	C	228	HIS	N-CA-C	5.64	119.86	112.92
1	A	318	LEU	N-CA-C	5.57	117.09	109.18
1	C	355	SER	CA-C-N	5.57	125.93	119.47
1	C	355	SER	C-N-CA	5.57	125.93	119.47
1	B	355	SER	CA-C-N	5.42	125.76	119.47
1	B	355	SER	C-N-CA	5.42	125.76	119.47
1	D	355	SER	CA-C-N	5.41	125.75	119.47
1	D	355	SER	C-N-CA	5.41	125.75	119.47
1	A	226	THR	N-CA-C	-5.36	102.82	110.59
1	C	270	ALA	N-CA-C	-5.35	105.44	111.28
1	B	270	ALA	N-CA-C	-5.26	105.63	111.36
1	D	250	LYS	N-CA-C	-5.15	105.58	111.14
1	A	93	VAL	N-CA-C	5.14	117.12	112.29
1	D	226	THR	N-CA-C	-5.09	102.92	110.46
1	B	250	LYS	N-CA-C	-5.05	105.69	111.14

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	3161	0	3107	65	0
1	B	3186	0	3132	62	0
1	C	3161	0	3097	68	0
1	D	3160	0	3097	60	0
2	A	5	0	2	1	0
2	B	5	0	2	1	0
2	C	5	0	2	1	0
2	D	5	0	2	1	0
3	A	15	0	6	1	0
3	B	15	0	6	1	0
3	C	15	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	15	0	6	1	0
4	A	34	0	21	4	0
4	B	34	0	21	2	0
4	C	34	0	21	3	0
4	D	34	0	21	2	0
5	A	70	0	0	1	0
5	B	71	0	0	3	0
5	C	73	0	0	3	0
5	D	73	0	0	4	0
All	All	13171	0	12549	241	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 (241) 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:B:339:ARG:HD2	5:B:1431:HOH:O	1.76	0.86
1:B:1:MET:HE3	1:B:3:LYS:HE3	1.62	0.78
1:A:108:ALA:HB2	1:A:255:ALA:HB2	1.75	0.68
1:B:77:LEU:O	1:B:81:ARG:HG2	1.94	0.68
1:B:14[B]:GLU:H	1:B:14[B]:GLU:CD	2.02	0.67
1:D:108:ALA:HB2	1:D:255:ALA:HB2	1.76	0.66
1:C:108:ALA:HB2	1:C:255:ALA:HB2	1.77	0.66
1:A:81:ARG:NH2	1:B:12:ASP:OD2	2.29	0.66
1:D:77:LEU:O	1:D:81:ARG:HG2	1.96	0.65
1:B:108:ALA:HB2	1:B:255:ALA:HB2	1.78	0.65
1:D:318:LEU:C	1:D:318:LEU:HD12	2.23	0.64
1:C:318:LEU:HD12	1:C:318:LEU:C	2.24	0.63
1:D:30:ILE:HG12	1:D:406:VAL:HG13	1.81	0.62
1:C:385:TRP:HB3	1:C:402:ILE:HD12	1.81	0.62
1:A:77:LEU:O	1:A:81:ARG:HG2	1.99	0.61
1:D:366:THR:N	1:D:367:PRO:CD	2.64	0.61
1:B:318:LEU:C	1:B:318:LEU:HD12	2.26	0.61
1:C:366:THR:N	1:C:367:PRO:CD	2.64	0.61
1:D:71:VAL:HB	1:D:266:MET:HE2	1.82	0.61
1:B:71:VAL:HB	1:B:266:MET:HE2	1.83	0.60
1:A:366:THR:N	1:A:367:PRO:CD	2.65	0.60
1:A:267:HIS:H	1:A:267:HIS:CD2	2.20	0.60
1:B:267:HIS:CD2	1:B:267:HIS:H	2.19	0.59
1:B:366:THR:N	1:B:367:PRO:CD	2.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ARG:HG3	1:B:4:ARG:HH11	1.66	0.59
1:B:77:LEU:O	1:B:81:ARG:CG	2.51	0.59
1:C:4:ARG:HG3	1:D:417:ALA:C	2.28	0.59
1:C:77:LEU:O	1:C:81:ARG:HG2	2.01	0.59
1:A:318:LEU:HD12	1:A:318:LEU:C	2.27	0.59
1:C:77:LEU:O	1:C:81:ARG:CG	2.51	0.59
1:D:366:THR:N	1:D:367:PRO:HD3	2.18	0.58
1:C:22:GLU:OE2	1:C:25:ARG:NH1	2.37	0.58
1:D:77:LEU:O	1:D:81:ARG:CG	2.52	0.58
1:B:203:HIS:HD2	1:B:317:HIS:NE2	2.03	0.57
1:C:366:THR:N	1:C:367:PRO:HD3	2.19	0.57
1:D:267:HIS:H	1:D:267:HIS:CD2	2.22	0.57
1:A:203:HIS:HD2	1:A:317:HIS:NE2	2.02	0.57
1:C:203:HIS:HD2	1:C:317:HIS:NE2	2.02	0.57
1:B:3:LYS:HB3	1:B:5:GLU:HG2	1.86	0.56
1:A:71:VAL:HB	1:A:266:MET:HE2	1.86	0.56
1:D:203:HIS:HD2	1:D:317:HIS:NE2	2.03	0.56
1:C:226:THR:HB	1:C:228:HIS:CE1	2.41	0.56
1:C:212:VAL:O	1:C:212:VAL:HG12	2.06	0.56
1:C:267:HIS:H	1:C:267:HIS:CD2	2.24	0.55
1:C:54:LYS:HD3	1:C:55:TYR:N	2.21	0.55
1:D:385:TRP:HB3	1:D:402:ILE:HD12	1.88	0.55
1:C:71:VAL:HB	1:C:266:MET:HE2	1.89	0.55
1:A:54:LYS:HD3	1:A:55:TYR:N	2.22	0.55
1:D:54:LYS:HD3	1:D:55:TYR:N	2.21	0.55
1:B:226:THR:HB	1:B:228:HIS:CE1	2.42	0.55
1:A:212:VAL:HG12	1:A:212:VAL:O	2.08	0.54
1:B:212:VAL:HG12	1:B:212:VAL:O	2.07	0.54
1:A:341:ASN:HB2	1:A:406:VAL:HG21	1.89	0.54
1:A:366:THR:N	1:A:367:PRO:HD3	2.22	0.54
1:B:113:GLY:HA2	5:B:1310:HOH:O	2.07	0.54
1:B:366:THR:N	1:B:367:PRO:HD3	2.22	0.53
1:A:77:LEU:O	1:A:81:ARG:CG	2.56	0.53
1:D:226:THR:HB	1:D:228:HIS:CE1	2.43	0.53
1:A:22:GLU:OE2	1:A:25:ARG:NH1	2.42	0.53
1:C:402:ILE:O	1:C:406:VAL:HG23	2.08	0.53
1:D:41:PRO:HA	1:D:44:MET:HE3	1.91	0.53
1:B:54:LYS:HD3	1:B:55:TYR:N	2.23	0.53
1:A:12:ASP:OD2	1:B:81:ARG:NH2	2.42	0.52
1:A:226:THR:HB	1:A:228:HIS:CE1	2.44	0.52
1:A:41:PRO:HA	1:A:44:MET:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:THR:OG1	1:B:332:GLU:HG3	2.10	0.52
1:C:3:LYS:HB2	1:C:6:MET:HG3	1.92	0.52
1:A:30:ILE:HG21	1:A:382:LEU:HD21	1.92	0.51
1:C:283:GLU:H	1:C:283:GLU:CD	2.18	0.51
1:C:12:ASP:OD2	1:D:81:ARG:NH2	2.42	0.51
1:D:27:GLU:HG2	5:D:554:HOH:O	2.09	0.51
1:D:212:VAL:HG12	1:D:212:VAL:O	2.09	0.51
1:A:61:GLY:C	1:A:62:LYS:HD2	2.35	0.51
1:C:185:LYS:NZ	5:C:1452:HOH:O	2.43	0.51
1:C:183:TRP:CE2	1:C:216:PRO:HB3	2.46	0.51
1:D:329:THR:OG1	1:D:332:GLU:HG3	2.11	0.51
1:C:329:THR:OG1	1:C:332:GLU:HG3	2.10	0.51
1:B:10:ASP:OD2	1:B:10:ASP:C	2.53	0.51
1:D:401:ARG:HG3	1:D:401:ARG:HH11	1.75	0.51
1:A:116:VAL:HB	1:A:142:ILE:HD13	1.92	0.50
1:A:329:THR:OG1	1:A:332:GLU:HG3	2.11	0.50
1:A:283:GLU:H	1:A:283:GLU:CD	2.20	0.50
1:C:274:VAL:O	1:C:278:GLU:HG3	2.11	0.50
1:B:116:VAL:HB	1:B:142:ILE:HD13	1.92	0.50
1:C:41:PRO:HA	1:C:44:MET:HE3	1.94	0.50
1:D:30:ILE:HG21	1:D:382:LEU:HD21	1.94	0.50
1:A:406:VAL:HG23	1:A:407:LEU:N	2.27	0.49
1:C:17:GLN:O	1:C:21:GLN:HG3	2.12	0.49
1:B:41:PRO:HA	1:B:44:MET:HE3	1.94	0.49
1:B:94:GLN:N	1:B:95:PRO:CD	2.75	0.49
1:D:349:VAL:O	1:D:352:ASP:HB2	2.12	0.49
1:B:385:TRP:HB3	1:B:402:ILE:HD12	1.93	0.49
1:D:22:GLU:OE2	1:D:25:ARG:NH1	2.45	0.49
1:C:30:ILE:HG21	1:C:382:LEU:HD21	1.92	0.49
1:B:30:ILE:HG21	1:B:382:LEU:HD21	1.94	0.49
1:C:61:GLY:C	1:C:62:LYS:HD2	2.38	0.49
1:C:81:ARG:NH2	1:D:12:ASP:OD2	2.45	0.49
1:D:94:GLN:N	1:D:95:PRO:CD	2.75	0.49
1:D:283:GLU:CD	1:D:283:GLU:H	2.21	0.49
1:C:366:THR:H	1:C:367:PRO:HD3	1.77	0.49
1:A:183:TRP:CE2	1:A:216:PRO:HB3	2.47	0.48
1:A:349:VAL:O	1:A:352:ASP:HB2	2.13	0.48
1:B:183:TRP:CE2	1:B:216:PRO:HB3	2.48	0.48
1:B:283:GLU:CD	1:B:283:GLU:H	2.21	0.48
1:A:274:VAL:O	1:A:278:GLU:HG3	2.14	0.48
1:A:368:ALA:HB3	5:A:555:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:ARG:O	1:B:405:LYS:HG3	2.14	0.48
1:C:116:VAL:HB	1:C:142:ILE:HD13	1.95	0.48
1:C:94:GLN:N	1:C:95:PRO:CD	2.77	0.48
1:D:183:TRP:CE2	1:D:216:PRO:HB3	2.49	0.48
1:D:242:LYS:N	5:D:654:HOH:O	2.44	0.48
1:B:148:ASP:HB3	1:B:150:THR:H	1.79	0.48
1:D:148:ASP:HB3	1:D:150:THR:H	1.79	0.48
4:A:1293:FFO:H13	1:B:257:PHE:HZ	1.78	0.47
1:C:148:ASP:HB3	1:C:150:THR:H	1.80	0.47
1:C:349:VAL:O	1:C:352:ASP:HB2	2.14	0.47
1:B:349:VAL:O	1:B:352:ASP:HB2	2.13	0.47
1:A:62:LYS:HD2	1:A:62:LYS:N	2.30	0.47
1:D:274:VAL:O	1:D:278:GLU:HG3	2.15	0.47
1:B:200:ASP:OD2	3:B:2291:PLP:N1	2.48	0.47
1:D:317:HIS:H	1:D:317:HIS:HD1	1.63	0.47
1:A:200:ASP:OD2	3:A:1291:PLP:N1	2.48	0.47
1:B:293:LYS:HE3	1:B:293:LYS:HB2	1.79	0.47
1:C:62:LYS:HD2	1:C:62:LYS:N	2.30	0.46
1:A:94:GLN:N	1:A:95:PRO:CD	2.78	0.46
1:D:367:PRO:HB2	5:D:534:HOH:O	2.15	0.46
1:C:293:LYS:HB2	1:C:293:LYS:HE3	1.77	0.46
1:C:317:HIS:HD1	1:C:317:HIS:H	1.64	0.46
1:D:213:TYR:CD1	1:D:214:PRO:HD2	2.50	0.46
1:D:368:ALA:HB3	5:D:552:HOH:O	2.15	0.46
1:B:22:GLU:OE2	1:B:25:ARG:NH1	2.49	0.46
1:C:203:HIS:HE1	2:C:3292:GLY:O	1.99	0.45
1:C:77:LEU:O	1:C:81:ARG:HG3	2.16	0.45
1:B:108:ALA:HB2	1:B:255:ALA:CB	2.46	0.45
1:C:371:ARG:NH2	5:C:936:HOH:O	2.40	0.45
1:A:203:HIS:HE1	2:A:1292:GLY:O	1.99	0.45
1:C:204:VAL:O	1:C:208:VAL:HG23	2.16	0.45
1:A:317:HIS:HD1	1:A:317:HIS:H	1.64	0.45
1:D:116:VAL:HB	1:D:142:ILE:HD13	1.97	0.45
1:B:317:HIS:HD1	1:B:317:HIS:H	1.65	0.45
1:A:148:ASP:HB3	1:A:150:THR:H	1.81	0.45
1:B:203:HIS:HE1	2:B:2292:GLY:O	1.99	0.45
1:A:87:GLY:O	1:A:242:LYS:HD2	2.17	0.45
1:C:54:LYS:HD3	1:C:55:TYR:H	1.81	0.45
1:C:148:ASP:HB2	1:C:150:THR:OG1	2.17	0.45
1:C:257:PHE:HZ	4:D:4293:FFO:H13	1.82	0.45
1:A:172:GLY:O	1:A:199:VAL:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:GLY:HA3	1:B:311:SER:HA	2.00	0.44
1:C:200:ASP:OD2	3:C:3291:PLP:N1	2.51	0.44
1:D:57:GLU:HB3	1:D:257:PHE:CZ	2.52	0.44
1:C:108:ALA:HB2	1:C:255:ALA:CB	2.46	0.44
1:A:22:GLU:HG2	1:B:51:LEU:CD2	2.47	0.44
1:B:213:TYR:CD1	1:B:214:PRO:HD2	2.53	0.44
1:C:213:TYR:CD1	1:C:214:PRO:HD2	2.53	0.44
1:C:356:PRO:HB3	4:C:3293:FFO:H16	2.00	0.44
1:A:204:VAL:O	1:A:208:VAL:HG23	2.16	0.44
1:C:27:GLU:OE2	1:C:415:VAL:HB	2.17	0.44
1:A:54:LYS:HD3	1:A:55:TYR:H	1.81	0.44
1:A:228:HIS:CG	1:A:235:ARG:HA	2.52	0.44
1:A:403:LYS:HA	1:A:406:VAL:HG22	2.00	0.44
1:B:356:PRO:HB3	4:B:2293:FFO:H16	2.00	0.44
1:B:366:THR:H	1:B:367:PRO:HD3	1.82	0.44
1:D:79:ILE:O	1:D:83:LYS:HG3	2.18	0.44
1:A:151:GLY:HA3	1:A:311:SER:HA	2.00	0.44
1:D:203:HIS:HE1	2:D:4292:GLY:O	2.01	0.44
1:D:366:THR:H	1:D:367:PRO:HD3	1.81	0.44
1:A:257:PHE:HZ	4:B:2293:FFO:H13	1.83	0.44
1:B:114:ASP:OD2	1:B:168:LYS:HD3	2.18	0.44
1:C:318:LEU:C	1:C:318:LEU:CD1	2.91	0.44
1:D:151:GLY:HA3	1:D:311:SER:HA	2.00	0.44
1:D:200:ASP:OD2	3:D:4291:PLP:N1	2.51	0.43
1:A:53:ASN:HA	5:B:642:HOH:O	2.18	0.43
1:B:79:ILE:O	1:B:83:LYS:HG3	2.17	0.43
1:A:108:ALA:HB2	1:A:255:ALA:CB	2.45	0.43
1:D:27:GLU:OE2	1:D:415:VAL:HB	2.17	0.43
1:A:293:LYS:HB2	1:A:293:LYS:HE3	1.76	0.43
1:D:356:PRO:HB3	4:D:4293:FFO:H16	2.01	0.43
4:C:3293:FFO:H13	1:D:257:PHE:HZ	1.82	0.43
1:C:93:VAL:HG12	1:C:238:LEU:CD1	2.49	0.43
1:C:205:ALA:HB2	1:C:225:THR:OG1	2.19	0.43
1:B:172:GLY:O	1:B:199:VAL:HA	2.18	0.43
1:C:22:GLU:HG2	1:D:51:LEU:CD2	2.48	0.43
1:B:394:ASN:HD22	1:B:394:ASN:HA	1.63	0.43
1:C:172:GLY:O	1:C:199:VAL:HA	2.18	0.43
1:D:287:TYR:O	1:D:291:VAL:HG23	2.19	0.43
1:B:204:VAL:O	1:B:208:VAL:HG23	2.19	0.42
1:A:10:ASP:C	1:A:10:ASP:OD1	2.61	0.42
1:A:164:GLU:OE1	1:D:163:LYS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:HIS:CG	1:C:235:ARG:HA	2.54	0.42
1:D:54:LYS:HD3	1:D:55:TYR:H	1.84	0.42
1:A:210:ALA:O	1:A:285:LYS:HE2	2.19	0.42
1:B:57:GLU:HB3	1:B:257:PHE:CZ	2.55	0.42
1:A:250:LYS:HE3	1:A:250:LYS:HB2	1.82	0.42
1:A:356:PRO:HB3	4:A:1293:FFO:H16	2.01	0.42
1:C:1:MET:SD	1:D:417:ALA:CB	3.07	0.42
1:A:12:ASP:CG	1:B:81:ARG:HH22	2.27	0.42
1:B:163:LYS:HB3	1:C:164:GLU:OE1	2.18	0.42
1:C:27:GLU:O	1:C:372:ARG:NH2	2.42	0.42
1:A:81:ARG:HH22	1:B:12:ASP:CG	2.28	0.42
1:A:111:GLU:O	1:A:112:PRO:C	2.63	0.42
1:A:366:THR:H	1:A:367:PRO:HD3	1.82	0.42
1:C:87:GLY:O	1:C:242:LYS:HD2	2.20	0.42
1:D:87:GLY:O	1:D:242:LYS:HD2	2.20	0.42
1:A:213:TYR:CD1	1:A:214:PRO:HD2	2.55	0.42
1:C:210:ALA:O	1:C:285:LYS:HE2	2.20	0.42
1:C:394:ASN:HD22	1:C:394:ASN:HA	1.63	0.42
4:A:1293:FFO:CD	1:D:245:SER:HB2	2.50	0.41
1:C:151:GLY:HA3	1:C:311:SER:HA	2.02	0.41
1:D:217:VAL:N	1:D:218:PRO:HD2	2.35	0.41
1:A:17:GLN:O	1:A:21:GLN:HG3	2.19	0.41
1:A:114:ASP:OD2	1:A:168:LYS:HD3	2.20	0.41
1:D:92:ASN:O	1:D:238:LEU:HD12	2.20	0.41
1:D:318:LEU:C	1:D:318:LEU:CD1	2.91	0.41
1:A:318:LEU:C	1:A:318:LEU:CD1	2.94	0.41
1:B:54:LYS:HD3	1:B:55:TYR:H	1.84	0.41
1:C:111:GLU:O	1:C:112:PRO:C	2.63	0.41
1:D:293:LYS:HE3	1:D:293:LYS:HB2	1.79	0.41
1:A:51:LEU:CD2	1:B:22:GLU:HG2	2.51	0.41
1:B:310:VAL:O	1:B:311:SER:HB2	2.20	0.41
1:C:212:VAL:O	1:C:212:VAL:CG1	2.68	0.41
1:B:70:TYR:O	1:B:74:VAL:HG23	2.21	0.41
1:B:205:ALA:HB2	1:B:225:THR:OG1	2.20	0.41
1:B:217:VAL:N	1:B:218:PRO:HD2	2.36	0.41
1:C:88:ALA:HB1	1:C:241:ALA:O	2.21	0.41
1:C:395:ASP:CG	1:C:398:VAL:HG23	2.46	0.41
1:D:111:GLU:O	1:D:112:PRO:C	2.62	0.41
1:D:172:GLY:O	1:D:199:VAL:HA	2.21	0.41
1:A:79:ILE:O	1:A:83:LYS:HG3	2.20	0.41
1:A:290:GLN:HB3	1:A:370:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ASP:CG	1:A:398:VAL:HG23	2.46	0.41
1:A:27:GLU:O	1:A:372:ARG:NH2	2.42	0.40
1:A:205:ALA:HB2	1:A:225:THR:OG1	2.20	0.40
1:B:245:SER:HB2	4:C:3293:FFO:CD	2.52	0.40
1:A:231:LEU:HD12	1:A:231:LEU:HA	1.92	0.40
4:A:1293:FFO:O2	1:D:247:GLU:HG3	2.21	0.40
1:B:111:GLU:O	1:B:112:PRO:C	2.65	0.40
1:B:212:VAL:O	1:B:212:VAL:CG1	2.69	0.40
1:C:51:LEU:CD2	1:D:22:GLU:HG2	2.51	0.40
1:C:123:HIS:ND1	1:C:146:GLY:HA3	2.37	0.40
1:C:14:GLU:HB2	5:C:713:HOH:O	2.21	0.40
1:D:108:ALA:HB2	1:D:255:ALA:CB	2.47	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	414/417 (99%)	398 (96%)	14 (3%)	2 (0%)	24	48
1	B	416/417 (100%)	402 (97%)	12 (3%)	2 (0%)	24	48
1	C	415/417 (100%)	399 (96%)	15 (4%)	1 (0%)	43	68
1	D	415/417 (100%)	398 (96%)	14 (3%)	3 (1%)	18	41
All	All	1660/1668 (100%)	1597 (96%)	55 (3%)	8 (0%)	24	48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	148	ASP
1	B	148	ASP

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Mol	Chain	Res	Type
1	C	148	ASP
1	D	2	LEU
1	B	359	THR
1	D	359	THR
1	D	148	ASP

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	323/329 (98%)	316 (98%)	7 (2%)	45	74
1	B	327/329 (99%)	319 (98%)	8 (2%)	43	72
1	C	322/329 (98%)	316 (98%)	6 (2%)	50	77
1	D	322/329 (98%)	316 (98%)	6 (2%)	50	77
All	All	1294/1316 (98%)	1267 (98%)	27 (2%)	47	75

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	55	TYR
1	A	62	LYS
1	A	81	ARG
1	A	267	HIS
1	A	345	ASN
1	A	347	ASN
1	B	54	LYS
1	B	55	TYR
1	B	81	ARG
1	B	166	LYS
1	B	267	HIS
1	B	345	ASN
1	B	347	ASN
1	B	406	VAL
1	C	54	LYS

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Mol	Chain	Res	Type
1	C	55	TYR
1	C	62	LYS
1	C	81	ARG
1	C	345	ASN
1	C	347	ASN
1	D	54	LYS
1	D	55	TYR
1	D	81	ARG
1	D	166	LYS
1	D	345	ASN
1	D	347	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	161	GLN
1	A	203	HIS
1	A	219	HIS
1	A	267	HIS
1	A	289	GLN
1	A	345	ASN
1	A	394	ASN
1	B	21	GLN
1	B	141	ASN
1	B	161	GLN
1	B	203	HIS
1	B	219	HIS
1	B	267	HIS
1	B	289	GLN
1	B	290	GLN
1	B	345	ASN
1	B	394	ASN
1	C	17	GLN
1	C	21	GLN
1	C	161	GLN
1	C	203	HIS
1	C	219	HIS
1	C	267	HIS
1	C	289	GLN
1	C	345	ASN
1	C	394	ASN

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Mol	Chain	Res	Type
1	D	17	GLN
1	D	21	GLN
1	D	50	GLN
1	D	141	ASN
1	D	161	GLN
1	D	203	HIS
1	D	219	HIS
1	D	267	HIS
1	D	289	GLN
1	D	290	GLN
1	D	394	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](#)

12 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	FFO	D	4293	-	33,36,36	2.69	11 (33%)	35,50,50	2.84	13 (37%)
3	PLP	A	1291	2	15,15,16	1.62	5 (33%)	21,22,23	2.60	9 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLY	D	4292	3	4,4,4	1.07	0	3,4,4	0.88	0
4	FFO	A	1293	-	33,36,36	2.68	12 (36%)	35,50,50	2.84	14 (40%)
3	PLP	D	4291	2	15,15,16	1.52	4 (26%)	21,22,23	2.60	9 (42%)
2	GLY	C	3292	3	4,4,4	1.02	0	3,4,4	1.06	0
2	GLY	B	2292	3	4,4,4	1.04	0	3,4,4	0.99	0
4	FFO	C	3293	-	33,36,36	2.61	11 (33%)	35,50,50	2.84	14 (40%)
2	GLY	A	1292	3	4,4,4	1.01	0	3,4,4	1.11	0
3	PLP	C	3291	2	15,15,16	1.56	5 (33%)	21,22,23	2.59	9 (42%)
3	PLP	B	2291	2	15,15,16	1.63	5 (33%)	21,22,23	2.58	9 (42%)
4	FFO	B	2293	-	33,36,36	2.70	10 (30%)	35,50,50	2.83	14 (40%)

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	FFO	D	4293	-	-	4/24/37/37	0/3/3/3
3	PLP	A	1291	2	-	1/6/6/8	0/1/1/1
2	GLY	D	4292	3	-	0/2/2/2	-
4	FFO	A	1293	-	-	4/24/37/37	0/3/3/3
3	PLP	D	4291	2	-	1/6/6/8	0/1/1/1
2	GLY	C	3292	3	-	0/2/2/2	-
2	GLY	B	2292	3	-	0/2/2/2	-
4	FFO	C	3293	-	-	4/24/37/37	0/3/3/3
2	GLY	A	1292	3	-	0/2/2/2	-
3	PLP	C	3291	2	-	1/6/6/8	0/1/1/1
3	PLP	B	2291	2	-	1/6/6/8	0/1/1/1
4	FFO	B	2293	-	-	4/24/37/37	0/3/3/3

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4293	FFO	C7-N8	-10.18	1.36	1.46
4	B	2293	FFO	C7-N8	-10.12	1.36	1.46
4	A	1293	FFO	C7-N8	-9.87	1.36	1.46
4	C	3293	FFO	C7-N8	-9.45	1.37	1.46
4	C	3293	FFO	C4A-N5	5.97	1.47	1.38
4	B	2293	FFO	C4A-N5	5.52	1.46	1.38
4	A	1293	FFO	C4A-N5	5.47	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4293	FFO	C4A-N5	5.23	1.46	1.38
4	B	2293	FFO	CB-CG	4.30	1.65	1.52
4	A	1293	FFO	CB-CG	4.24	1.65	1.52
4	D	4293	FFO	CB-CG	4.15	1.65	1.52
4	C	3293	FFO	CB-CG	4.02	1.64	1.52
4	D	4293	FFO	C13-C14	3.83	1.45	1.39
4	B	2293	FFO	C13-C14	3.70	1.45	1.39
4	A	1293	FFO	C13-C14	3.68	1.45	1.39
4	C	3293	FFO	C13-C14	3.47	1.45	1.39
4	D	4293	FFO	C12-C11	3.41	1.44	1.39
4	A	1293	FFO	C9-N10	3.36	1.51	1.45
4	B	2293	FFO	C12-C11	3.36	1.44	1.39
4	A	1293	FFO	C12-C11	3.35	1.44	1.39
4	B	2293	FFO	C9-N10	3.30	1.51	1.45
4	C	3293	FFO	C9-N10	3.28	1.51	1.45
4	D	4293	FFO	C7-C6	-3.21	1.48	1.52
4	C	3293	FFO	C7-C6	-3.18	1.48	1.52
4	D	4293	FFO	C9-N10	3.11	1.50	1.45
4	A	1293	FFO	C7-C6	-3.00	1.48	1.52
4	B	2293	FFO	C7-C6	-2.98	1.48	1.52
4	C	3293	FFO	C12-C11	2.91	1.43	1.39
4	B	2293	FFO	CG-CD	2.87	1.57	1.50
3	C	3291	PLP	C4A-C4	-2.84	1.45	1.51
3	A	1291	PLP	O3-C3	-2.65	1.30	1.36
4	C	3293	FFO	CG-CD	2.60	1.56	1.50
3	B	2291	PLP	C4A-C4	-2.60	1.46	1.51
3	D	4291	PLP	C4A-C4	-2.59	1.46	1.51
4	D	4293	FFO	CG-CD	2.48	1.56	1.50
3	A	1291	PLP	C4A-C4	-2.48	1.46	1.51
4	A	1293	FFO	CG-CD	2.45	1.56	1.50
3	B	2291	PLP	C6-C5	2.43	1.42	1.37
3	B	2291	PLP	C3-C4	2.43	1.44	1.40
3	B	2291	PLP	C3-C2	2.36	1.43	1.41
3	D	4291	PLP	C3-C2	2.34	1.43	1.41
3	B	2291	PLP	O3-C3	-2.32	1.31	1.36
3	C	3291	PLP	O3-C3	-2.30	1.31	1.36
3	D	4291	PLP	O3-C3	-2.29	1.31	1.36
4	B	2293	FFO	O4-C4	2.27	1.27	1.23
3	A	1291	PLP	C3-C2	2.26	1.43	1.41
4	D	4293	FFO	O4-C4	2.22	1.27	1.23
4	C	3293	FFO	C15-C14	-2.20	1.35	1.39
3	A	1291	PLP	C6-C5	2.20	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1291	PLP	C3-C4	2.19	1.44	1.40
4	D	4293	FFO	C4A-C4	2.19	1.49	1.43
3	C	3291	PLP	C6-C5	2.18	1.42	1.37
3	D	4291	PLP	C6-C5	2.18	1.42	1.37
3	C	3291	PLP	C3-C2	2.15	1.43	1.41
4	A	1293	FFO	C8A-N1	2.12	1.39	1.36
4	A	1293	FFO	C4A-C4	2.10	1.48	1.43
4	C	3293	FFO	C4A-C4	2.10	1.48	1.43
4	A	1293	FFO	O4-C4	2.04	1.27	1.23
3	C	3291	PLP	C3-C4	2.03	1.44	1.40
4	B	2293	FFO	C4A-C4	2.03	1.48	1.43
4	A	1293	FFO	C16-C15	2.01	1.42	1.38
4	C	3293	FFO	C8A-N1	2.01	1.39	1.36
4	D	4293	FFO	C16-C15	2.00	1.42	1.38

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2293	FFO	C2-N1-C8A	6.21	124.33	113.36
4	C	3293	FFO	C15-C14-C13	6.20	127.27	119.04
4	D	4293	FFO	C15-C14-C13	6.17	127.23	119.04
4	A	1293	FFO	C15-C14-C13	6.15	127.21	119.04
4	D	4293	FFO	C2-N1-C8A	6.12	124.17	113.36
4	C	3293	FFO	C2-N1-C8A	6.12	124.17	113.36
4	A	1293	FFO	C2-N1-C8A	6.12	124.16	113.36
4	B	2293	FFO	C15-C14-C13	6.07	127.09	119.04
4	D	4293	FFO	NA2-C2-N1	5.97	131.32	119.67
4	C	3293	FFO	NA2-C2-N1	5.97	131.31	119.67
4	A	1293	FFO	NA2-C2-N1	5.88	131.15	119.67
4	B	2293	FFO	NA2-C2-N1	5.87	131.13	119.67
4	C	3293	FFO	C16-C15-C14	-5.50	113.97	120.30
4	D	4293	FFO	C16-C15-C14	-5.48	113.99	120.30
3	B	2291	PLP	O4P-C5A-C5	5.43	119.54	109.36
4	A	1293	FFO	C16-C15-C14	-5.36	114.13	120.30
4	B	2293	FFO	C16-C15-C14	-5.29	114.21	120.30
3	A	1291	PLP	O4P-C5A-C5	5.26	119.22	109.36
3	D	4291	PLP	O4P-C5A-C5	5.21	119.12	109.36
3	C	3291	PLP	O4P-C5A-C5	5.07	118.86	109.36
3	A	1291	PLP	C2A-C2-C3	5.05	126.70	120.80
3	D	4291	PLP	C2A-C2-C3	4.99	126.64	120.80
3	C	3291	PLP	C2A-C2-C3	4.94	126.58	120.80
4	A	1293	FFO	N3-C2-N1	-4.90	114.36	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2293	FFO	N3-C2-N1	-4.86	114.43	123.32
3	B	2291	PLP	C2A-C2-C3	4.84	126.47	120.80
4	D	4293	FFO	N3-C2-N1	-4.84	114.46	123.32
4	C	3293	FFO	N3-C2-N1	-4.81	114.52	123.32
4	B	2293	FFO	CB-CG-CD	4.46	124.38	112.49
4	A	1293	FFO	CB-CG-CD	4.37	124.16	112.49
4	D	4293	FFO	CB-CG-CD	4.35	124.09	112.49
4	C	3293	FFO	CB-CG-CD	4.25	123.82	112.49
3	A	1291	PLP	C5A-C5-C6	-3.86	113.07	119.36
4	D	4293	FFO	C13-C14-N10	-3.86	112.24	120.96
4	C	3293	FFO	C13-C14-N10	-3.85	112.25	120.96
3	C	3291	PLP	C5A-C5-C6	-3.84	113.11	119.36
3	C	3291	PLP	C6-N1-C2	3.83	126.14	119.20
3	D	4291	PLP	C6-N1-C2	3.81	126.11	119.20
4	A	1293	FFO	O5B-C5A-N5	-3.81	118.23	124.67
4	A	1293	FFO	C13-C14-N10	-3.79	112.38	120.96
4	B	2293	FFO	O5B-C5A-N5	-3.78	118.28	124.67
3	D	4291	PLP	C5A-C5-C6	-3.78	113.19	119.36
4	B	2293	FFO	C13-C14-N10	-3.77	112.44	120.96
3	A	1291	PLP	C6-N1-C2	3.76	126.03	119.20
3	C	3291	PLP	C5A-C5-C4	3.74	130.02	122.64
3	D	4291	PLP	C5A-C5-C4	3.72	129.97	122.64
3	B	2291	PLP	C6-N1-C2	3.68	125.87	119.20
3	A	1291	PLP	C5A-C5-C4	3.67	129.88	122.64
4	A	1293	FFO	C12-C13-C14	-3.67	116.08	120.30
3	D	4291	PLP	C3-C2-N1	-3.65	116.36	120.96
3	B	2291	PLP	C5A-C5-C6	-3.64	113.42	119.36
4	B	2293	FFO	C12-C13-C14	-3.59	116.16	120.30
3	B	2291	PLP	C5A-C5-C4	3.58	129.71	122.64
3	C	3291	PLP	C3-C2-N1	-3.56	116.47	120.96
3	A	1291	PLP	C3-C2-N1	-3.55	116.48	120.96
3	B	2291	PLP	C3-C2-N1	-3.53	116.51	120.96
4	D	4293	FFO	C12-C13-C14	-3.52	116.25	120.30
4	D	4293	FFO	O5B-C5A-N5	-3.47	118.82	124.67
4	C	3293	FFO	C12-C13-C14	-3.46	116.31	120.30
4	C	3293	FFO	O5B-C5A-N5	-3.43	118.88	124.67
3	B	2291	PLP	O3P-P-O4P	3.14	114.87	106.67
3	D	4291	PLP	O3P-P-O4P	2.88	114.17	106.67
3	C	3291	PLP	O3P-P-O4P	2.86	114.13	106.67
3	A	1291	PLP	O3P-P-O4P	2.83	114.05	106.67
4	D	4293	FFO	OE1-CD-CG	-2.75	114.37	123.09
4	A	1293	FFO	OE1-CD-CG	-2.72	114.46	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3291	PLP	C3-C4-C5	2.72	121.85	118.59
3	D	4291	PLP	C3-C4-C5	2.67	121.79	118.59
4	C	3293	FFO	OE1-CD-CG	-2.66	114.65	123.09
4	B	2293	FFO	OE1-CD-CG	-2.66	114.67	123.09
3	C	3291	PLP	C5-C6-N1	-2.61	119.58	123.83
4	C	3293	FFO	C4A-C4-N3	2.59	115.50	110.94
4	A	1293	FFO	C11-C-N	2.57	121.81	117.04
4	C	3293	FFO	C11-C-N	2.56	121.79	117.04
3	A	1291	PLP	C5-C6-N1	-2.55	119.68	123.83
3	A	1291	PLP	C3-C4-C5	2.54	121.64	118.59
3	B	2291	PLP	C3-C4-C5	2.53	121.63	118.59
3	D	4291	PLP	C5-C6-N1	-2.52	119.73	123.83
4	D	4293	FFO	C11-C-N	2.51	121.69	117.04
4	B	2293	FFO	C4A-C4-N3	2.48	115.31	110.94
4	B	2293	FFO	C11-C-N	2.48	121.64	117.04
4	A	1293	FFO	C4A-C4-N3	2.44	115.23	110.94
3	B	2291	PLP	C5-C6-N1	-2.39	119.94	123.83
4	D	4293	FFO	C4A-C4-N3	2.39	115.15	110.94
4	D	4293	FFO	C15-C16-C11	2.14	123.08	120.80
4	C	3293	FFO	O4-C4-C4A	-2.10	122.48	127.62
4	B	2293	FFO	O4-C4-C4A	-2.09	122.48	127.62
4	A	1293	FFO	C15-C16-C11	2.06	123.00	120.80
4	B	2293	FFO	C15-C16-C11	2.06	123.00	120.80
4	A	1293	FFO	O4-C4-C4A	-2.04	122.62	127.62
4	C	3293	FFO	C15-C16-C11	2.04	122.97	120.80

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1293	FFO	N-CA-CB-CG
4	B	2293	FFO	N-CA-CB-CG
4	C	3293	FFO	N-CA-CB-CG
4	D	4293	FFO	N-CA-CB-CG
4	A	1293	FFO	CT-CA-CB-CG
4	B	2293	FFO	CT-CA-CB-CG
4	C	3293	FFO	CT-CA-CB-CG
4	D	4293	FFO	CT-CA-CB-CG
4	A	1293	FFO	OE1-CD-CG-CB
4	D	4293	FFO	OE1-CD-CG-CB
4	B	2293	FFO	OE2-CD-CG-CB
4	C	3293	FFO	OE1-CD-CG-CB

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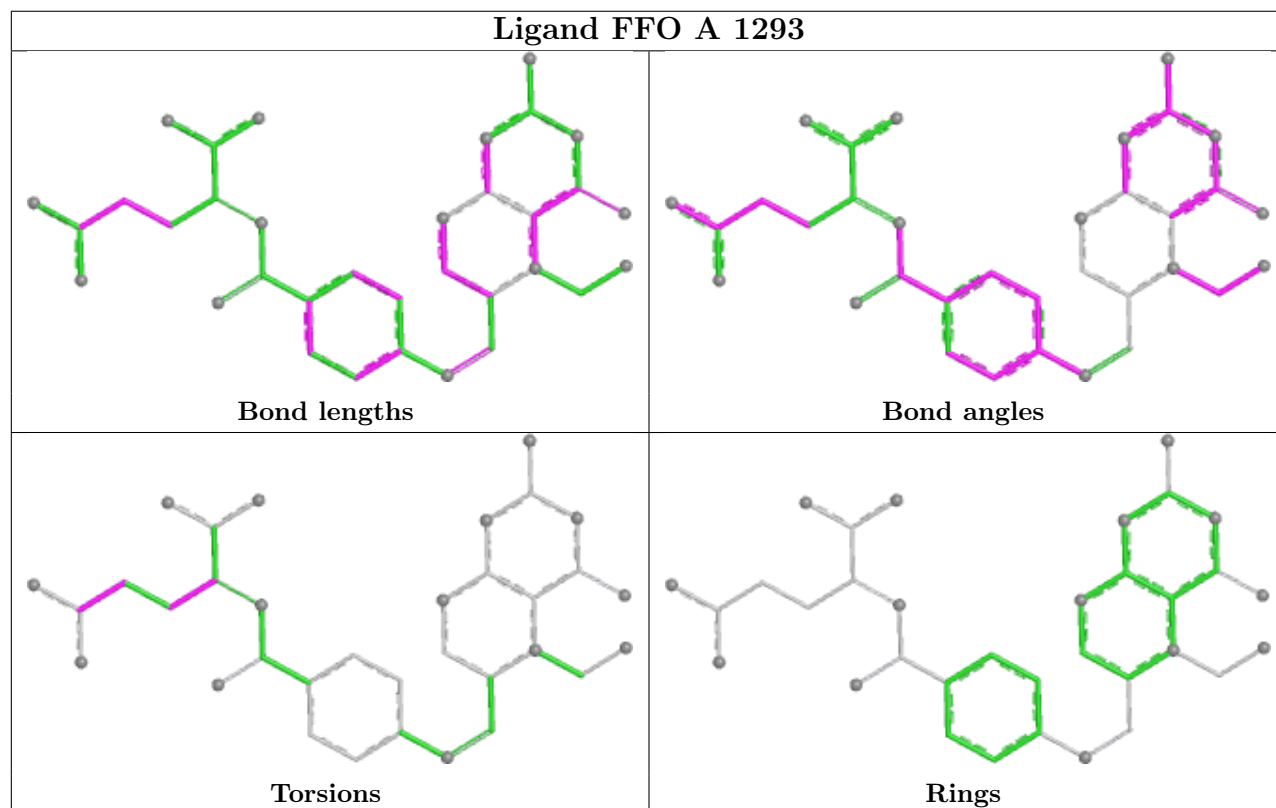
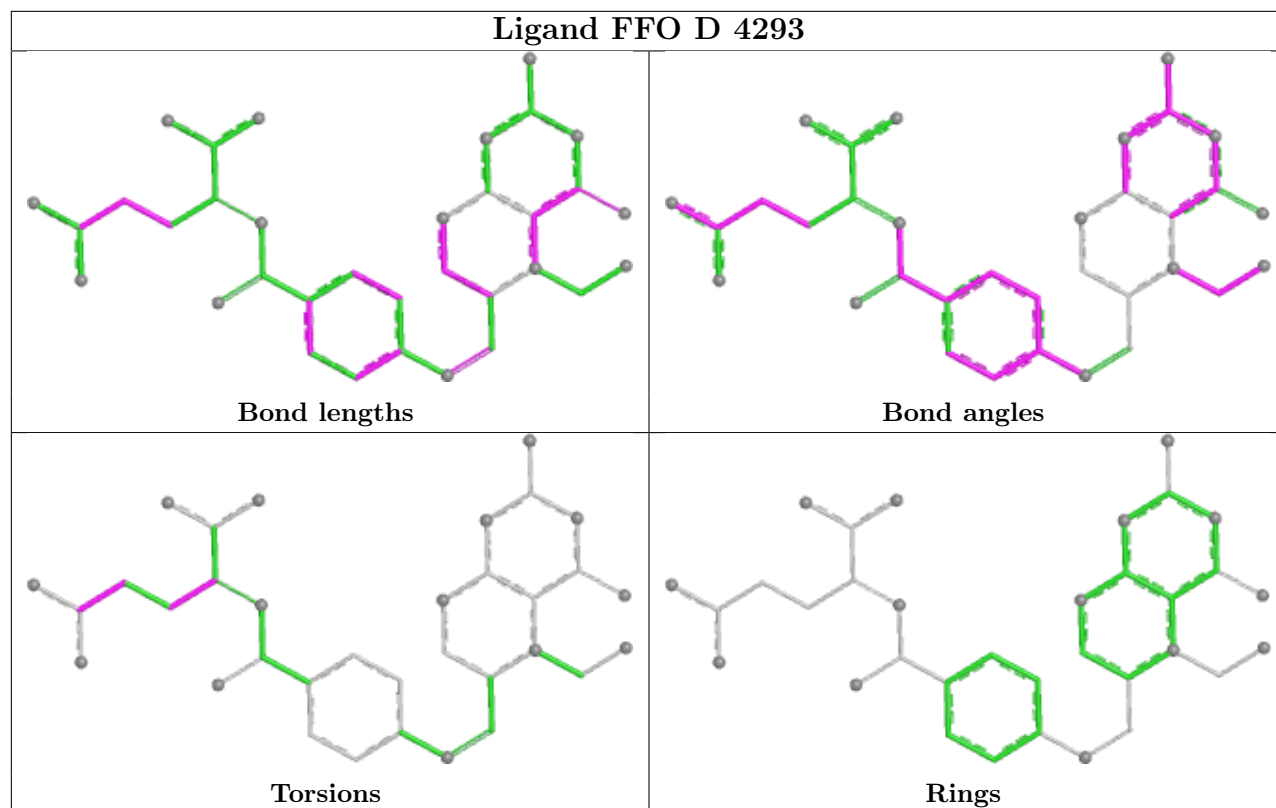
Mol	Chain	Res	Type	Atoms
4	C	3293	FFO	OE2-CD-CG-CB
4	D	4293	FFO	OE2-CD-CG-CB
3	A	1291	PLP	C5A-O4P-P-O3P
3	B	2291	PLP	C5A-O4P-P-O3P
3	C	3291	PLP	C5A-O4P-P-O3P
3	D	4291	PLP	C5A-O4P-P-O3P
4	A	1293	FFO	OE2-CD-CG-CB
4	B	2293	FFO	OE1-CD-CG-CB

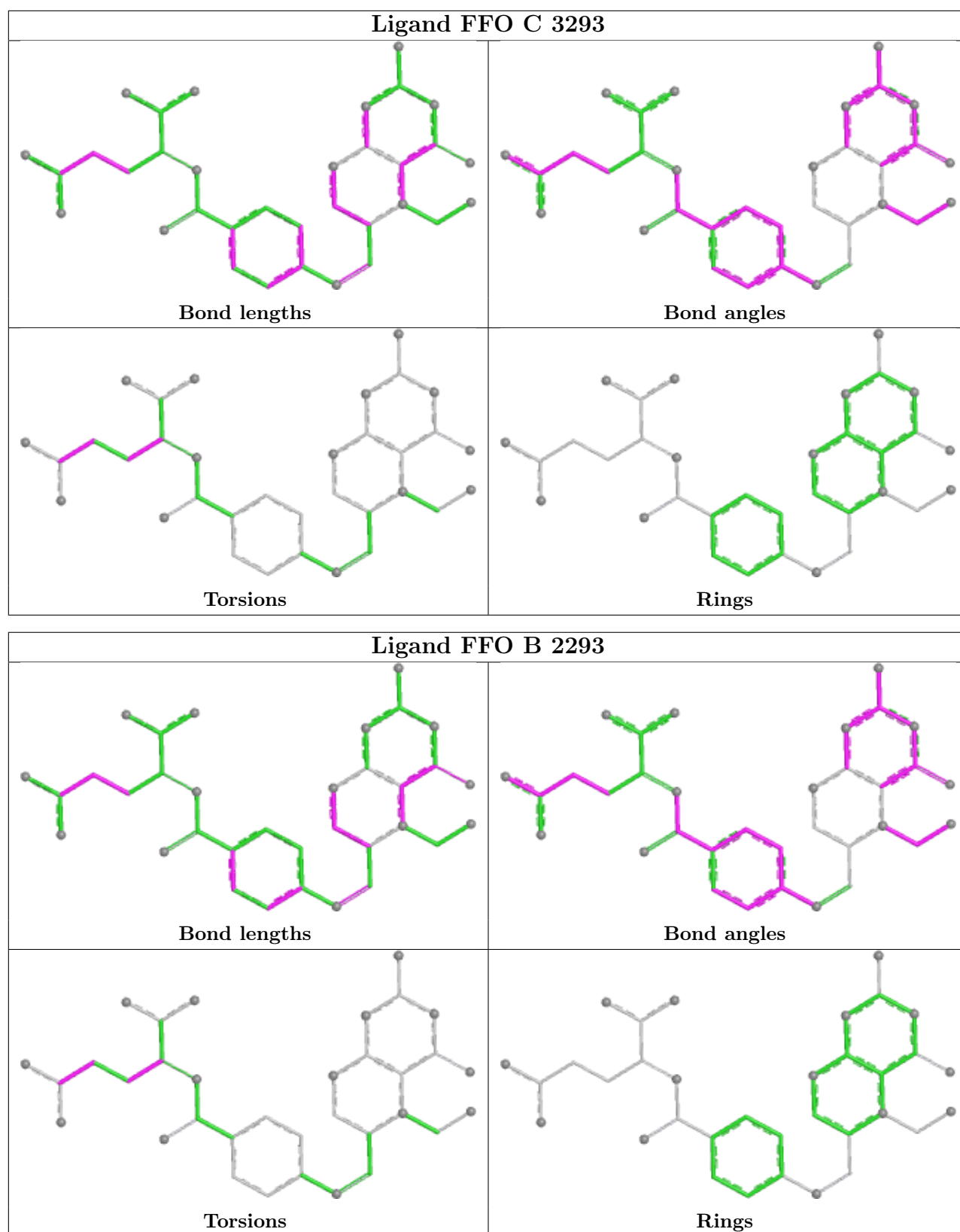
There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	4293	FFO	2	0
3	A	1291	PLP	1	0
2	D	4292	GLY	1	0
4	A	1293	FFO	4	0
3	D	4291	PLP	1	0
2	C	3292	GLY	1	0
2	B	2292	GLY	1	0
4	C	3293	FFO	3	0
2	A	1292	GLY	1	0
3	C	3291	PLP	1	0
3	B	2291	PLP	1	0
4	B	2293	FFO	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 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 ⓘ

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 [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	416/417 (99%)	-0.16	3 (0%) 84 83	16, 34, 59, 93	0
1	B	417/417 (100%)	-0.20	2 (0%) 87 86	13, 32, 59, 84	1 (0%)
1	C	417/417 (100%)	-0.12	4 (0%) 79 78	15, 37, 67, 87	0
1	D	417/417 (100%)	-0.19	2 (0%) 87 86	15, 31, 62, 99	0
All	All	1667/1668 (99%)	-0.17	11 (0%) 84 83	13, 33, 62, 99	1 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	3.7
1	D	148	ASP	3.3
1	B	148	ASP	2.6
1	A	151	GLY	2.4
1	C	164	GLU	2.4
1	C	120	ASN	2.4
1	A	120	ASN	2.2
1	A	148	ASP	2.2
1	C	394	ASN	2.1
1	C	304	GLU	2.0
1	B	246	GLU	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

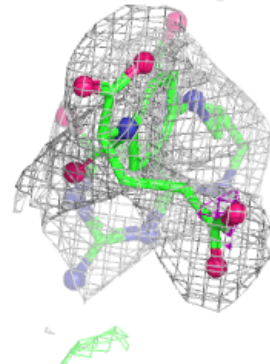
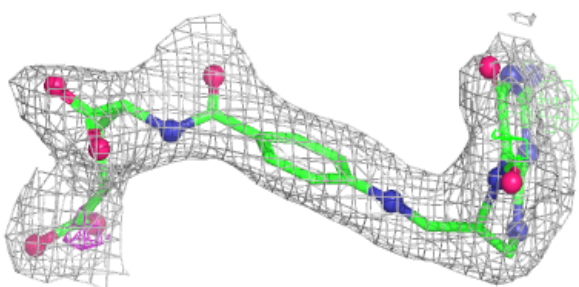
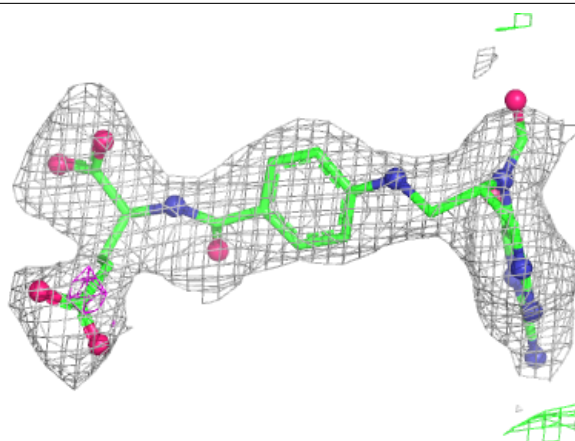
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FFO	B	2293	34/34	0.89	0.12	49,49,49,49	0
4	FFO	C	3293	34/34	0.90	0.11	43,43,43,43	0
4	FFO	D	4293	34/34	0.90	0.12	46,46,46,46	0
4	FFO	A	1293	34/34	0.92	0.09	37,37,37,37	0
2	GLY	B	2292	5/5	0.93	0.11	32,46,46,46	0
2	GLY	A	1292	5/5	0.95	0.07	24,31,31,31	0
2	GLY	C	3292	5/5	0.96	0.07	19,31,31,31	0
2	GLY	D	4292	5/5	0.96	0.06	26,39,39,39	0
3	PLP	A	1291	15/16	0.97	0.07	26,26,26,26	0
3	PLP	B	2291	15/16	0.97	0.07	31,31,31,31	0
3	PLP	C	3291	15/16	0.97	0.07	32,32,32,32	0
3	PLP	D	4291	15/16	0.97	0.08	34,34,34,34	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.

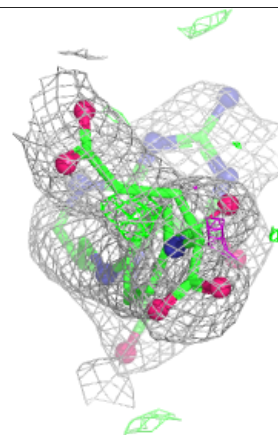
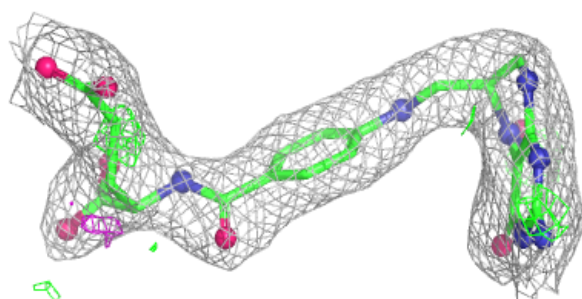
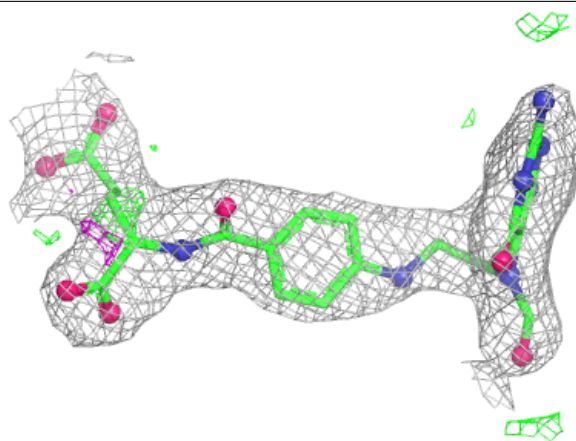
Electron density around FFO B 2293:

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



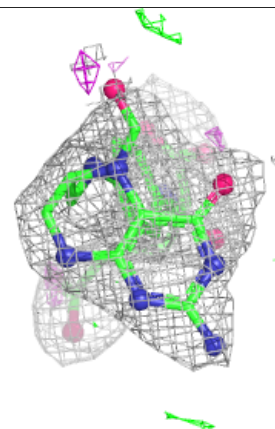
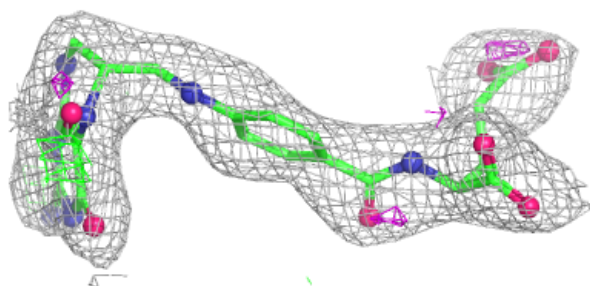
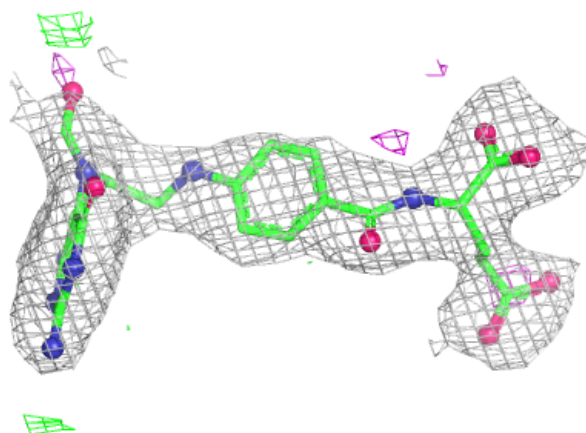
Electron density around FFO C 3293:

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

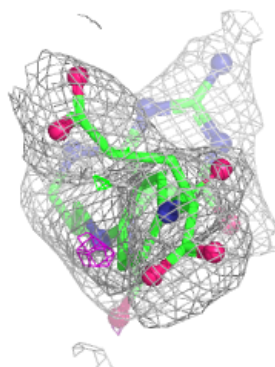
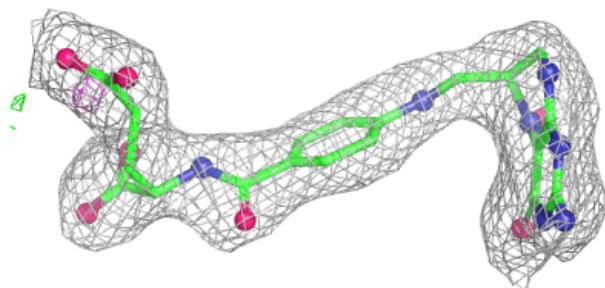
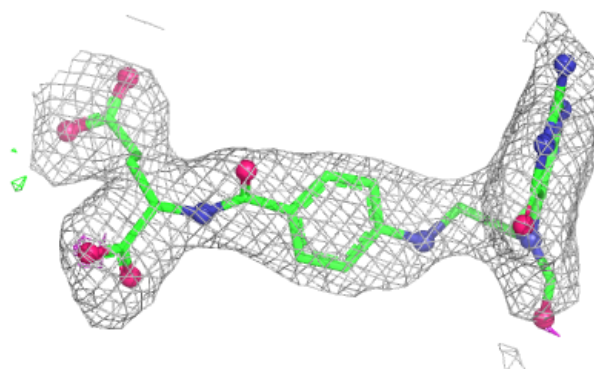


Electron density around FFO D 4293:

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

**Electron density around FFO A 1293:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.