



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:18 PM UTC

PDB ID : 6HCV / pdb_00006hcv
Title : Crystal Structure of Lysyl-tRNA Synthetase from Plasmodium falciparum complexed with a chromone ligand
Authors : Robinson, D.A.; Baragana, B.; Norcross, N.; Forte, B.; Walpole, C.; Gilbert, I.H.
Deposited on : 2018-08-16
Resolution : 2.20 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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

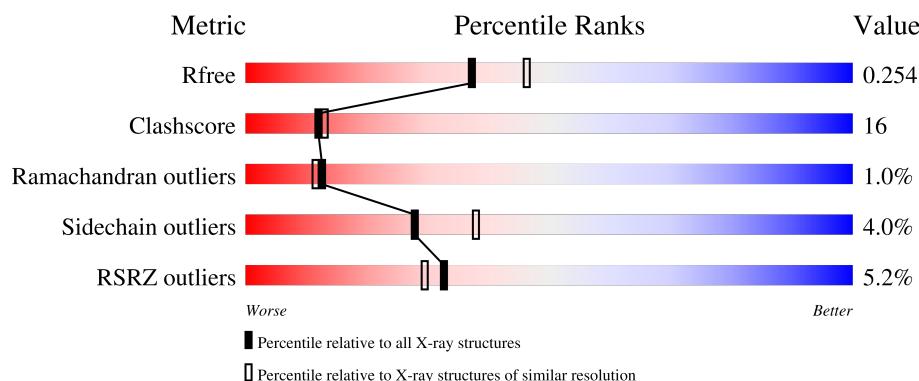
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	503	
1	B	503	

2 Entry composition [i](#)

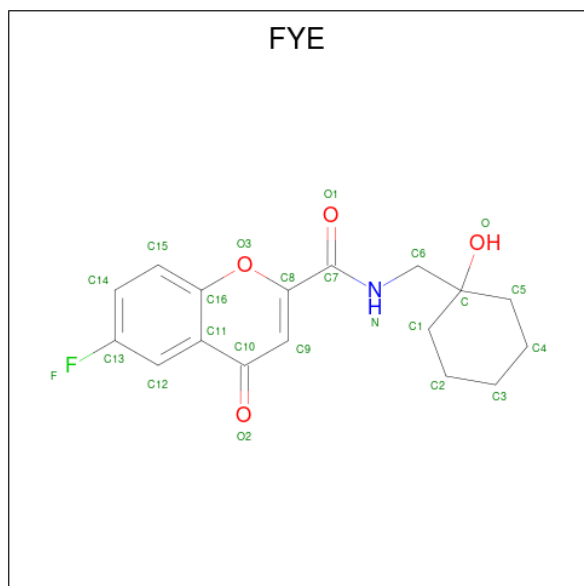
There are 3 unique types of molecules in this entry. The entry contains 8377 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lysine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3908	2525	649	717	17			
1	B	479	Total	C	N	O	S	0	0	0
			3884	2507	646	714	17			

- Molecule 2 is 6-fluoranyl- {N}-[(1-oxidanylcyclohexyl)methyl]-4-oxidanylidene-chromene-2-carboxamide (CCD ID: FYE) (formula: $C_{17}H_{18}FNO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			23	17	1	1	4		
2	B	1	Total	C	F	N	O	0	0
			23	17	1	1	4		

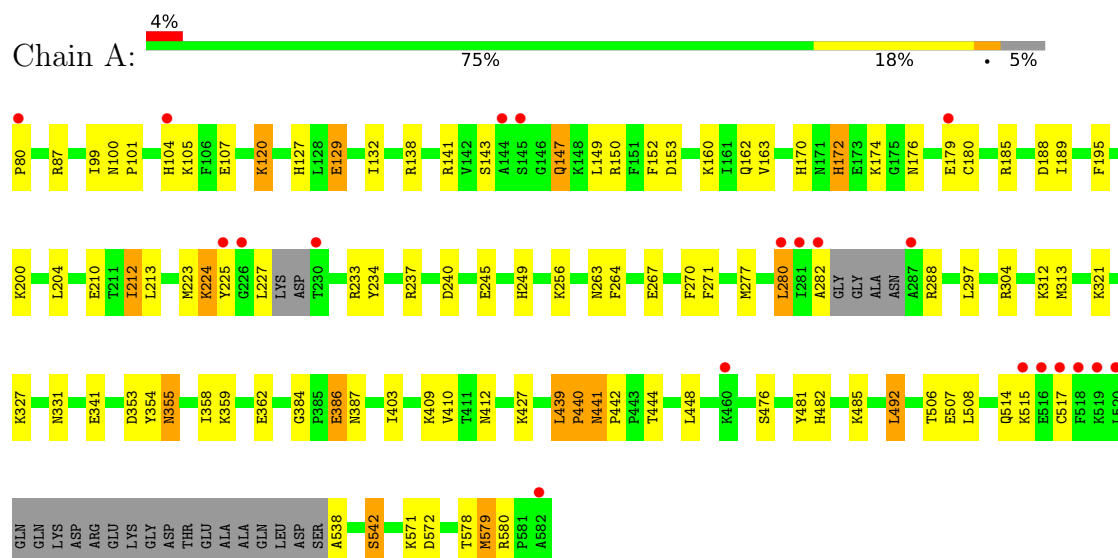
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	263	Total 263	O 263	0	0
3	B	276	Total 276	O 276	0	0

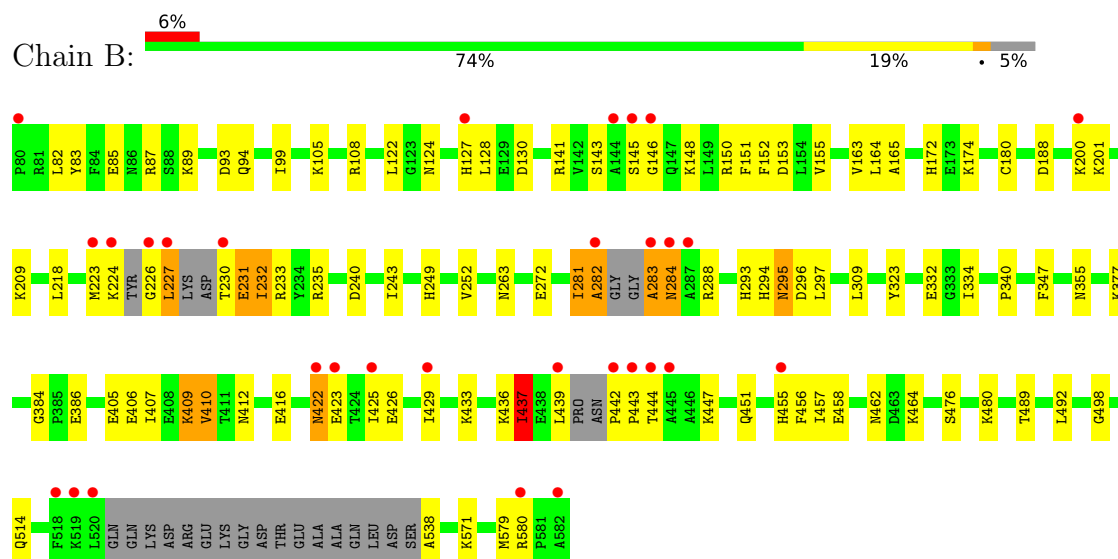
3 Residue-property plots [i](#)

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: Lysine-tRNA ligase



• Molecule 1: Lysine-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.56Å 95.19Å 166.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.20 48.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.00-2.20) 98.6 (48.00-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.213 , 0.254 0.215 , 0.254	Depositor DCC
R_{free} test set	2998 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8377	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: FYE

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	0.72	0/4004	0.91	5/5409 (0.1%)
1	B	0.81	2/3978 (0.1%)	0.89	5/5373 (0.1%)
All	All	0.77	2/7982 (0.0%)	0.90	10/10782 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	LEU	C-N	17.63	1.58	1.33
1	B	284	ASN	C-N	13.66	1.52	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	LEU	CA-C-N	9.19	129.79	119.32
1	A	439	LEU	C-N-CA	9.19	129.79	119.32
1	B	309	LEU	CA-C-N	-6.73	112.76	119.56
1	B	309	LEU	C-N-CA	-6.73	112.76	119.56
1	A	172	HIS	N-CA-C	5.66	118.99	111.75
1	A	403	ILE	N-CA-C	5.58	115.77	110.42
1	A	440	PRO	N-CA-C	5.47	121.89	113.75
1	B	284	ASN	CA-C-N	5.19	131.46	121.54
1	B	284	ASN	C-N-CA	5.19	131.46	121.54
1	B	437	ILE	N-CA-C	5.03	119.80	109.34

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	3908	0	3866	129	0
1	B	3884	0	3832	125	0
2	A	23	0	0	0	0
2	B	23	0	0	0	0
3	A	263	0	0	82	1
3	B	276	0	0	79	0
All	All	8377	0	7698	244	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 16.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:GLU:HB2	3:A:710:HOH:O	1.36	1.22
1:B:233:ARG:HD3	3:B:908:HOH:O	1.38	1.20
1:A:327:LYS:HD2	3:A:771:HOH:O	1.51	1.10
1:A:386:GLU:HG2	3:A:851:HOH:O	1.53	1.08
1:B:235:ARG:HG2	3:B:724:HOH:O	1.55	1.07
1:B:580:ARG:HD2	3:B:943:HOH:O	1.56	1.05
1:A:127:HIS:HB3	3:A:889:HOH:O	1.54	1.05
1:A:341:GLU:HB2	3:A:771:HOH:O	1.55	1.04
1:A:264:PHE:CE1	3:A:873:HOH:O	2.11	1.03
1:A:180:CYS:SG	3:A:727:HOH:O	2.06	1.02
1:A:138:ARG:HG3	3:A:762:HOH:O	1.60	1.00
1:A:359:LYS:HA	3:A:710:HOH:O	1.59	1.00
1:B:201:LYS:H	1:B:201:LYS:HD2	1.28	0.99
1:A:264:PHE:HE1	3:A:873:HOH:O	1.44	0.98
1:A:143:SER:HA	3:A:940:HOH:O	1.65	0.97
1:B:386:GLU:HG2	3:B:719:HOH:O	1.64	0.97
1:A:280:LEU:HD23	3:A:717:HOH:O	1.65	0.96
1:B:409:LYS:CE	3:B:716:HOH:O	2.13	0.96
1:B:295:ASN:HD22	1:B:295:ASN:H	1.15	0.95
1:B:82:LEU:HD12	3:B:922:HOH:O	1.67	0.94
1:A:277:MET:SD	3:A:865:HOH:O	2.26	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:THR:CB	3:B:852:HOH:O	2.14	0.94
1:A:578:THR:HG22	3:B:934:HOH:O	1.68	0.93
1:A:189:ILE:CG1	3:A:762:HOH:O	2.18	0.91
1:A:189:ILE:HG12	3:A:762:HOH:O	1.71	0.90
1:B:232:ILE:HG23	3:B:799:HOH:O	1.69	0.90
1:B:232:ILE:HG13	3:B:852:HOH:O	1.73	0.89
1:A:160:LYS:HE3	3:A:943:HOH:O	1.73	0.88
1:A:481:TYR:CE1	3:A:730:HOH:O	2.26	0.88
1:B:174:LYS:CG	3:B:847:HOH:O	2.24	0.86
1:A:99:ILE:HG13	3:A:741:HOH:O	1.77	0.85
1:B:409:LYS:CD	3:B:716:HOH:O	2.24	0.85
1:B:174:LYS:HD3	3:B:847:HOH:O	1.77	0.85
1:B:130:ASP:HB2	3:B:720:HOH:O	1.75	0.84
1:A:313:MET:HE1	3:B:773:HOH:O	1.77	0.84
1:A:129:GLU:HG3	3:A:889:HOH:O	1.78	0.84
1:B:174:LYS:HG3	3:B:847:HOH:O	1.76	0.83
1:A:223:MET:SD	3:A:739:HOH:O	2.37	0.82
1:B:409:LYS:HD2	3:B:716:HOH:O	1.77	0.82
1:A:538:ALA:N	3:A:701:HOH:O	2.13	0.81
1:A:359:LYS:HE2	3:A:815:HOH:O	1.80	0.79
1:B:172:HIS:HE1	3:B:935:HOH:O	1.67	0.77
1:A:321:LYS:HD3	3:A:935:HOH:O	1.84	0.77
1:B:87:ARG:HG3	3:B:711:HOH:O	1.86	0.76
1:A:189:ILE:HA	3:A:762:HOH:O	1.85	0.76
1:A:99:ILE:CG1	3:A:741:HOH:O	2.33	0.76
1:B:180:CYS:SG	3:B:974:HOH:O	2.45	0.75
1:B:99:ILE:HD12	3:B:838:HOH:O	1.88	0.73
1:B:127:HIS:CE1	3:B:742:HOH:O	2.41	0.73
1:B:295:ASN:HD22	1:B:295:ASN:N	1.86	0.73
1:B:409:LYS:HE3	3:B:716:HOH:O	1.81	0.73
1:A:263:ASN:ND2	1:A:267:GLU:OE2	2.21	0.72
1:B:444:THR:HA	3:B:738:HOH:O	1.87	0.72
1:A:270:PHE:CE1	3:A:935:HOH:O	2.43	0.72
1:B:377:LYS:HE2	3:B:882:HOH:O	1.89	0.71
1:B:226:GLY:CA	3:B:718:HOH:O	2.37	0.71
1:B:231:GLU:O	1:B:231:GLU:HG3	1.90	0.71
1:A:277:MET:HA	3:A:865:HOH:O	1.91	0.70
1:B:439:LEU:CB	3:B:717:HOH:O	2.40	0.70
1:B:451:GLN:HE21	1:B:455:HIS:CD2	2.08	0.70
1:A:359:LYS:CE	3:A:815:HOH:O	2.39	0.69
1:B:174:LYS:CD	3:B:847:HOH:O	2.35	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ILE:CA	3:A:762:HOH:O	2.40	0.68
1:A:341:GLU:CB	3:A:771:HOH:O	2.27	0.67
1:A:282:ALA:HA	3:A:861:HOH:O	1.93	0.67
1:B:571:LYS:CG	3:B:728:HOH:O	2.42	0.67
1:A:353:ASP:HB3	1:B:105:LYS:HD3	1.78	0.66
1:A:507:GLU:HG2	3:A:748:HOH:O	1.95	0.66
1:A:105:LYS:HE3	1:A:107:GLU:HG3	1.78	0.66
1:A:99:ILE:CD1	3:A:741:HOH:O	2.44	0.65
1:A:353:ASP:CB	3:A:860:HOH:O	2.43	0.65
1:B:437:ILE:HA	3:B:831:HOH:O	1.96	0.65
1:B:444:THR:HG22	1:B:447:LYS:HD3	1.79	0.65
1:B:263:ASN:HB2	3:B:895:HOH:O	1.95	0.64
1:B:226:GLY:C	3:B:718:HOH:O	2.41	0.64
1:B:571:LYS:HG2	3:B:728:HOH:O	1.97	0.63
1:A:138:ARG:HA	3:A:762:HOH:O	1.97	0.63
1:A:507:GLU:CG	3:A:748:HOH:O	2.46	0.63
1:B:180:CYS:HB3	3:B:929:HOH:O	1.98	0.62
1:A:538:ALA:N	3:A:703:HOH:O	2.31	0.62
1:B:108:ARG:HD2	3:B:725:HOH:O	2.00	0.62
1:A:132:ILE:HG12	3:A:776:HOH:O	1.99	0.61
1:B:151:PHE:CE2	1:B:164:LEU:HD11	2.35	0.61
1:A:147:GLN:OE1	1:A:150:ARG:NH2	2.34	0.61
1:B:422:ASN:HA	1:B:425:ILE:HB	1.82	0.60
1:B:422:ASN:O	1:B:426:GLU:HB2	2.01	0.60
1:B:209:LYS:HE2	3:B:789:HOH:O	1.99	0.60
1:A:354:TYR:HD2	1:A:355:ASN:OD1	1.85	0.60
1:B:405:GLU:HB2	3:B:946:HOH:O	2.01	0.60
1:B:224:LYS:O	1:B:226:GLY:N	2.35	0.60
1:B:412:ASN:HB2	3:B:963:HOH:O	2.01	0.59
1:A:331:ASN:ND2	1:B:295:ASN:HD21	1.99	0.59
1:B:83:TYR:HE2	3:B:711:HOH:O	1.84	0.59
1:B:143:SER:HB2	1:B:151:PHE:HB2	1.83	0.59
1:A:170:HIS:HD2	1:A:172:HIS:CD2	2.21	0.59
1:A:264:PHE:CZ	3:A:873:HOH:O	2.45	0.58
1:B:233:ARG:CD	3:B:908:HOH:O	2.18	0.58
1:A:99:ILE:HD12	3:A:741:HOH:O	2.01	0.58
1:A:481:TYR:HE1	3:A:730:HOH:O	1.76	0.58
1:B:226:GLY:HA3	3:B:718:HOH:O	2.02	0.58
1:B:99:ILE:CG1	3:B:838:HOH:O	2.51	0.58
1:B:172:HIS:HD2	3:B:822:HOH:O	1.86	0.58
1:B:99:ILE:HB	3:B:838:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:GLU:HG2	3:B:875:HOH:O	2.04	0.57
1:A:507:GLU:HG2	3:A:921:HOH:O	2.04	0.57
1:B:232:ILE:CG1	3:B:852:HOH:O	2.43	0.57
1:A:195:PHE:CE1	3:A:889:HOH:O	2.53	0.57
1:A:87:ARG:NH2	1:A:188:ASP:OD2	2.35	0.56
1:B:295:ASN:H	1:B:295:ASN:ND2	1.93	0.56
1:A:277:MET:HE2	3:B:800:HOH:O	2.05	0.55
1:B:355:ASN:HB3	3:B:721:HOH:O	2.05	0.55
1:B:281:ILE:HG13	3:B:769:HOH:O	2.06	0.55
1:A:210:GLU:HG3	3:A:770:HOH:O	2.06	0.55
1:B:82:LEU:CD1	3:B:922:HOH:O	2.40	0.55
1:B:87:ARG:HD2	3:B:949:HOH:O	2.06	0.55
1:A:288:ARG:NH2	3:A:705:HOH:O	2.40	0.55
1:B:218:LEU:C	3:B:711:HOH:O	2.49	0.55
1:A:439:LEU:HD12	1:A:440:PRO:HD2	1.89	0.54
1:B:227:LEU:CD2	1:B:233:ARG:HG3	2.38	0.54
1:A:313:MET:HG2	1:A:542:SER:OG	2.07	0.54
1:B:87:ARG:CD	3:B:949:HOH:O	2.54	0.54
1:B:85:GLU:HB3	3:B:961:HOH:O	2.07	0.54
1:B:150:ARG:HB2	1:B:165:ALA:HB3	1.89	0.53
1:B:444:THR:OG1	3:B:701:HOH:O	2.18	0.53
1:B:209:LYS:CE	3:B:789:HOH:O	2.55	0.53
1:A:152:PHE:HB2	1:A:163:VAL:HB	1.91	0.53
1:A:233:ARG:HG3	3:A:715:HOH:O	2.09	0.53
1:A:249:HIS:CD2	3:A:807:HOH:O	2.62	0.53
1:B:235:ARG:CG	3:B:724:HOH:O	2.31	0.52
1:A:580:ARG:NH1	1:B:297:LEU:O	2.43	0.51
1:B:442:PRO:HB2	3:B:968:HOH:O	2.09	0.51
1:B:230:THR:O	1:B:233:ARG:NH2	2.44	0.51
1:A:138:ARG:CB	3:A:762:HOH:O	2.57	0.50
1:A:245:GLU:HA	3:A:891:HOH:O	2.11	0.50
1:B:201:LYS:HD2	1:B:201:LYS:N	2.11	0.50
1:A:87:ARG:HH22	1:A:188:ASP:CG	2.18	0.50
1:A:571:LYS:HE2	3:A:777:HOH:O	2.10	0.50
1:B:94:GLN:HA	3:B:838:HOH:O	2.10	0.50
1:B:458:GLU:O	1:B:498:GLY:HA2	2.11	0.50
1:B:99:ILE:CD1	3:B:838:HOH:O	2.54	0.50
1:B:146:GLY:HA2	3:B:964:HOH:O	2.11	0.50
1:B:407:ILE:HG13	1:B:457:ILE:HD11	1.93	0.50
1:A:341:GLU:CG	3:A:771:HOH:O	2.59	0.49
1:B:334:ILE:HG12	1:B:340:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ASN:HB2	3:B:913:HOH:O	2.11	0.49
1:A:312:LYS:HD3	1:A:507:GLU:CD	2.37	0.49
1:B:124:ASN:ND2	1:B:200:LYS:O	2.46	0.49
1:A:578:THR:CG2	3:B:934:HOH:O	2.42	0.49
1:B:295:ASN:N	1:B:295:ASN:ND2	2.50	0.49
1:A:80:PRO:HA	3:A:955:HOH:O	2.11	0.49
1:B:406:GLU:O	1:B:410:VAL:HG13	2.13	0.49
1:B:218:LEU:HA	3:B:711:HOH:O	2.12	0.48
1:B:233:ARG:HG2	1:B:240:ASP:CG	2.38	0.48
1:A:270:PHE:CZ	3:A:935:HOH:O	2.64	0.48
1:A:138:ARG:CG	3:A:762:HOH:O	2.37	0.48
1:A:174:LYS:HG3	3:A:877:HOH:O	2.13	0.48
1:A:234:TYR:HB2	3:A:716:HOH:O	2.14	0.47
1:A:353:ASP:HB2	3:A:860:HOH:O	2.13	0.47
1:B:347:PHE:C	1:B:347:PHE:CD1	2.93	0.47
1:A:234:TYR:OH	1:A:572:ASP:OD1	2.31	0.47
1:B:87:ARG:NH2	1:B:188:ASP:OD1	2.47	0.47
1:B:355:ASN:CG	3:B:771:HOH:O	2.57	0.47
1:A:331:ASN:ND2	1:B:295:ASN:ND2	2.62	0.47
1:A:412:ASN:ND2	3:A:712:HOH:O	2.47	0.47
1:B:146:GLY:O	1:B:148:LYS:N	2.41	0.47
1:B:429:ILE:HG22	1:B:433:LYS:HE2	1.97	0.47
1:B:444:THR:CG2	1:B:447:LYS:HD3	2.44	0.46
1:B:249:HIS:CE1	3:B:705:HOH:O	2.67	0.46
1:B:355:ASN:CB	3:B:721:HOH:O	2.62	0.46
1:B:282:ALA:O	1:B:283:ALA:HB2	2.13	0.46
1:A:176:ASN:CB	3:A:735:HOH:O	2.64	0.46
1:A:271:PHE:CZ	1:B:252:VAL:HA	2.51	0.46
1:A:277:MET:CA	3:A:865:HOH:O	2.55	0.46
1:B:444:THR:HG22	1:B:447:LYS:HB2	1.98	0.46
1:A:331:ASN:HD21	1:B:295:ASN:ND2	2.14	0.46
1:A:313:MET:CE	3:B:773:HOH:O	2.50	0.46
1:A:99:ILE:HG21	3:A:741:HOH:O	2.15	0.46
1:A:297:LEU:HD22	1:B:580:ARG:HG2	1.97	0.45
1:A:120:LYS:HA	3:A:938:HOH:O	2.15	0.45
1:A:304:ARG:HG2	3:A:865:HOH:O	2.15	0.45
1:B:386:GLU:N	3:B:719:HOH:O	2.48	0.45
1:B:227:LEU:N	3:B:718:HOH:O	2.48	0.45
1:B:272:GLU:HB2	1:B:323:TYR:CZ	2.51	0.45
1:B:231:GLU:HA	3:B:856:HOH:O	2.17	0.45
1:A:256:LYS:HD3	3:A:806:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:MET:HE2	1:A:579:MET:HB3	1.79	0.45
1:A:141:ARG:HB3	1:A:153:ASP:HB2	1.98	0.45
1:A:189:ILE:HG13	3:A:762:HOH:O	2.03	0.44
1:A:358:ILE:HD13	1:A:492:LEU:HD13	1.98	0.44
1:A:444:THR:O	1:A:448:LEU:HG	2.16	0.44
1:B:538:ALA:N	3:B:730:HOH:O	2.50	0.44
1:B:122:LEU:HD21	1:B:128:LEU:HD11	1.99	0.44
1:A:508:LEU:HD11	3:A:730:HOH:O	2.17	0.44
1:A:100:ASN:HA	1:A:101:PRO:HD3	1.86	0.44
1:A:277:MET:CB	3:A:865:HOH:O	2.65	0.44
1:A:507:GLU:CB	3:A:748:HOH:O	2.66	0.44
1:B:282:ALA:C	3:B:769:HOH:O	2.60	0.44
1:A:200:LYS:HE2	3:A:774:HOH:O	2.18	0.43
1:B:293:HIS:HE1	3:B:948:HOH:O	2.01	0.43
1:A:120:LYS:HB3	1:A:120:LYS:HE2	1.86	0.43
1:B:451:GLN:NE2	1:B:455:HIS:CD2	2.82	0.43
1:B:130:ASP:CB	3:B:720:HOH:O	2.49	0.43
1:B:141:ARG:HB2	1:B:153:ASP:HB2	2.01	0.43
1:B:164:LEU:HA	1:B:164:LEU:HD12	1.58	0.43
1:A:185:ARG:HA	1:A:185:ARG:HD3	1.87	0.43
1:B:462:ASN:ND2	3:B:732:HOH:O	2.51	0.43
1:A:331:ASN:OD1	1:B:295:ASN:ND2	2.50	0.43
1:A:384:GLY:HA3	3:A:851:HOH:O	2.19	0.43
1:A:386:GLU:HG2	1:A:386:GLU:H	1.59	0.43
1:A:223:MET:HA	3:A:739:HOH:O	2.19	0.43
1:A:441:ASN:HA	1:A:442:PRO:HA	1.90	0.43
1:B:384:GLY:C	3:B:719:HOH:O	2.61	0.43
1:A:160:LYS:CE	3:A:943:HOH:O	2.50	0.42
1:A:179:GLU:CD	3:A:857:HOH:O	2.61	0.42
1:A:482:HIS:CE1	1:A:485:LYS:HG3	2.55	0.42
1:A:180:CYS:CB	3:A:727:HOH:O	2.59	0.42
1:A:129:GLU:CD	1:A:129:GLU:H	2.27	0.42
1:A:331:ASN:HD21	1:B:295:ASN:HD21	1.66	0.42
1:A:409:LYS:HB2	3:A:755:HOH:O	2.20	0.42
1:B:87:ARG:HD3	3:B:949:HOH:O	2.18	0.42
1:A:514:GLN:O	1:A:515:LYS:C	2.63	0.42
1:A:227:LEU:C	3:A:905:HOH:O	2.63	0.41
1:B:152:PHE:HB2	1:B:163:VAL:HB	2.02	0.41
1:B:476:SER:HB2	1:B:489:THR:HG21	2.01	0.41
1:A:87:ARG:NH2	1:A:185:ARG:HB2	2.35	0.41
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ASP:HB3	3:A:860:HOH:O	2.13	0.41
1:A:104:HIS:CD2	1:B:480:LYS:HE2	2.55	0.41
1:B:410:VAL:HG21	1:B:456:PHE:HB3	2.02	0.41
1:A:212:ILE:HD13	1:A:212:ILE:HA	1.70	0.41
1:A:224:LYS:O	1:A:225:TYR:HB2	2.21	0.41
1:A:87:ARG:HD3	1:A:87:ARG:HA	1.90	0.41
1:A:180:CYS:HB2	3:A:727:HOH:O	2.21	0.41
1:A:263:ASN:HB2	3:A:948:HOH:O	2.19	0.41
1:B:174:LYS:HE3	1:B:174:LYS:HB3	1.79	0.41
1:A:387:ASN:OD1	1:A:387:ASN:N	2.54	0.41
1:A:237:ARG:NH1	1:A:240:ASP:OD2	2.47	0.41
1:B:89:LYS:HE2	1:B:93:ASP:OD2	2.22	0.40
1:B:409:LYS:NZ	3:B:716:HOH:O	2.48	0.40
1:B:294:HIS:CE1	1:B:296:ASP:HB2	2.56	0.40
1:A:176:ASN:HB2	3:A:735:HOH:O	2.21	0.40
1:A:514:GLN:HB3	1:A:517:CYS:HB2	2.03	0.40
1:A:578:THR:HA	3:A:706:HOH:O	2.21	0.40
1:A:578:THR:HG23	3:A:864:HOH:O	2.21	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)
3:A:749:HOH:O	3:A:951:HOH:O[3_555]	2.14	0.06

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	472/503 (94%)	454 (96%)	17 (4%)	1 (0%)	43 51
1	B	471/503 (94%)	443 (94%)	20 (4%)	8 (2%)	7 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	943/1006 (94%)	897 (95%)	37 (4%)	9 (1%)	12 11

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	SER
1	B	283	ALA
1	B	284	ASN
1	B	437	ILE
1	B	436	LYS
1	B	282	ALA
1	A	441	ASN
1	B	288	ARG
1	B	443	PRO

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	430/453 (95%)	412 (96%)	18 (4%)	26 36
1	B	425/453 (94%)	409 (96%)	16 (4%)	29 40
All	All	855/906 (94%)	821 (96%)	34 (4%)	28 38

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	LYS
1	A	129	GLU
1	A	147	GLN
1	A	149	LEU
1	A	162	GLN
1	A	212	ILE
1	A	213	LEU
1	A	224	LYS
1	A	280	LEU

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Mol	Chain	Res	Type
1	A	355	ASN
1	A	386	GLU
1	A	410	VAL
1	A	427	LYS
1	A	476	SER
1	A	492	LEU
1	A	506	THR
1	A	542	SER
1	A	579	MET
1	B	155	VAL
1	B	223	MET
1	B	231	GLU
1	B	232	ILE
1	B	243	ILE
1	B	281	ILE
1	B	295	ASN
1	B	409	LYS
1	B	410	VAL
1	B	416	GLU
1	B	422	ASN
1	B	423	GLU
1	B	464	LYS
1	B	492	LEU
1	B	514	GLN
1	B	579	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	HIS
1	A	172	HIS
1	A	176	ASN
1	A	412	ASN
1	A	441	ASN
1	A	455	HIS
1	B	124	ASN
1	B	172	HIS
1	B	293	HIS
1	B	295	ASN
1	B	451	GLN
1	B	455	HIS
1	B	462	ASN

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Mol	Chain	Res	Type
1	B	473	GLN

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](#)

2 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	$\# Z > 2$
2	FYE	A	601	-	25,25,25	0.83	0	31,36,36	1.33	5 (16%)
2	FYE	B	601	-	25,25,25	0.94	1 (4%)	31,36,36	1.38	4 (12%)

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
2	FYE	A	601	-	-	0/10/20/20	0/3/3/3
2	FYE	B	601	-	-	0/10/20/20	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FYE	C9-C10	-2.63	1.39	1.44

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FYE	O3-C16-C15	3.20	120.51	116.25
2	B	601	FYE	C6-N-C7	2.95	126.47	122.73
2	A	601	FYE	O3-C8-C9	-2.51	120.31	123.84
2	B	601	FYE	O3-C16-C11	-2.41	119.38	121.57
2	B	601	FYE	O3-C16-C15	2.33	119.35	116.25
2	A	601	FYE	C12-C11-C16	2.32	121.42	118.28
2	A	601	FYE	C14-C13-C12	-2.20	120.32	123.23
2	B	601	FYE	C1-C2-C3	-2.09	108.10	111.35
2	A	601	FYE	C16-C11-C10	-2.01	118.44	119.74

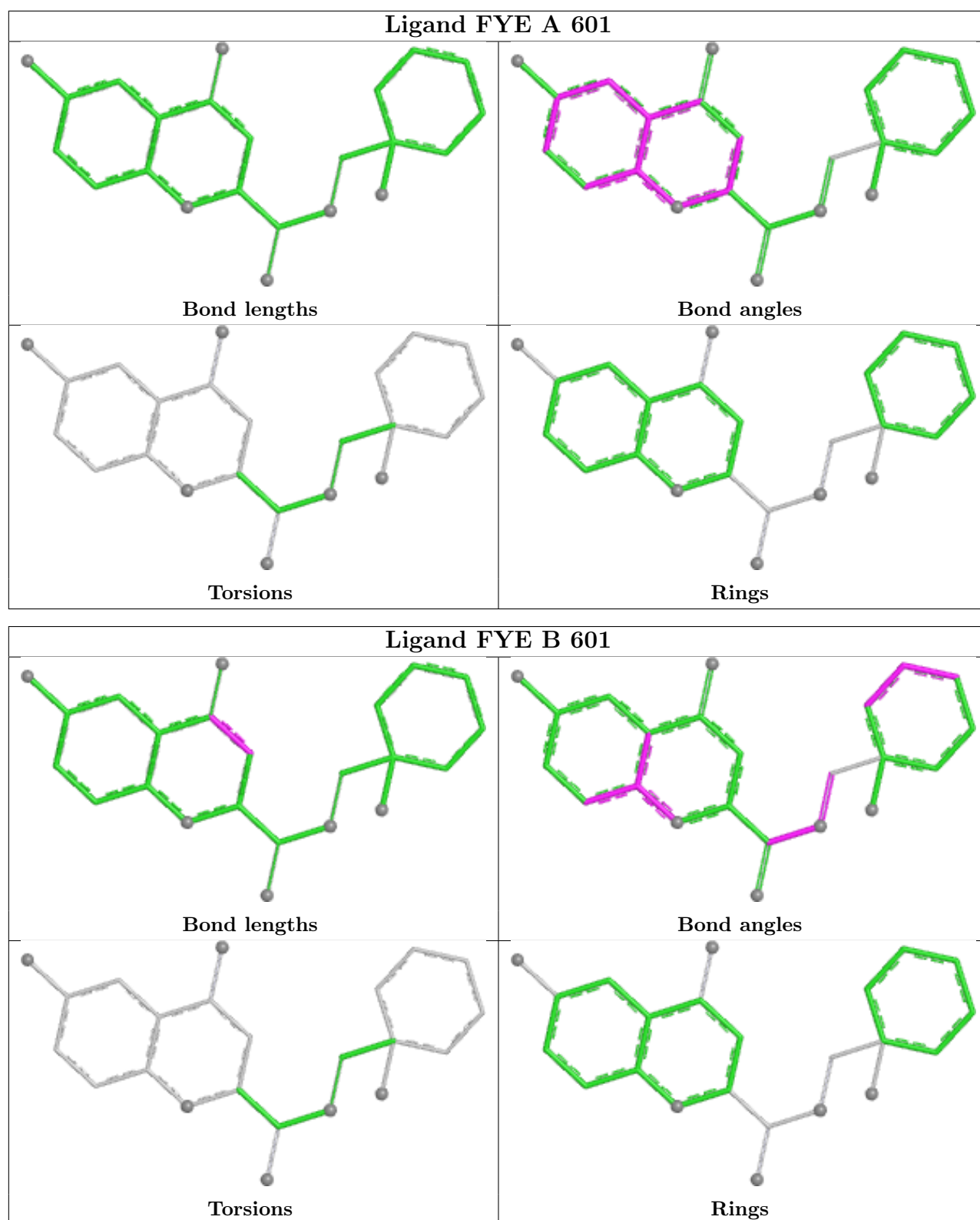
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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(Å ²)	Q < 0.9
1	A	480/503 (95%)	-0.02	20 (4%)	40	37	14, 26, 50, 101	0
1	B	479/503 (95%)	0.09	30 (6%)	26	23	12, 27, 56, 80	0
All	All	959/1006 (95%)	0.04	50 (5%)	33	29	12, 26, 54, 101	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	520	LEU	6.8
1	B	144	ALA	5.9
1	B	582	ALA	5.2
1	B	439	LEU	5.1
1	A	582	ALA	5.1
1	A	519	LYS	5.0
1	B	227	LEU	4.8
1	A	518	PHE	4.6
1	B	520	LEU	4.5
1	A	225	TYR	4.4
1	B	287	ALA	4.3
1	B	442	PRO	4.2
1	B	443	PRO	4.0
1	B	80	PRO	3.8
1	B	146	GLY	3.6
1	A	145	SER	3.4
1	B	226	GLY	3.4
1	B	422	ASN	3.3
1	A	80	PRO	3.2
1	A	282	ALA	3.2
1	A	517	CYS	3.1
1	B	518	PHE	3.1
1	B	284	ASN	3.0
1	B	519	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	516	GLU	3.0
1	A	226	GLY	2.8
1	B	444	THR	2.8
1	B	282	ALA	2.8
1	B	423	GLU	2.7
1	A	104	HIS	2.6
1	B	223	MET	2.6
1	B	127	HIS	2.6
1	A	515	LYS	2.5
1	B	429	ILE	2.5
1	B	224	LYS	2.5
1	A	281	ILE	2.4
1	B	283	ALA	2.4
1	A	230	THR	2.4
1	A	179	GLU	2.3
1	B	145	SER	2.3
1	A	144	ALA	2.2
1	A	287	ALA	2.2
1	B	455	HIS	2.2
1	A	280	LEU	2.2
1	A	460	LYS	2.2
1	B	230	THR	2.1
1	B	445	ALA	2.1
1	B	200	LYS	2.1
1	B	425	ILE	2.0
1	B	580	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

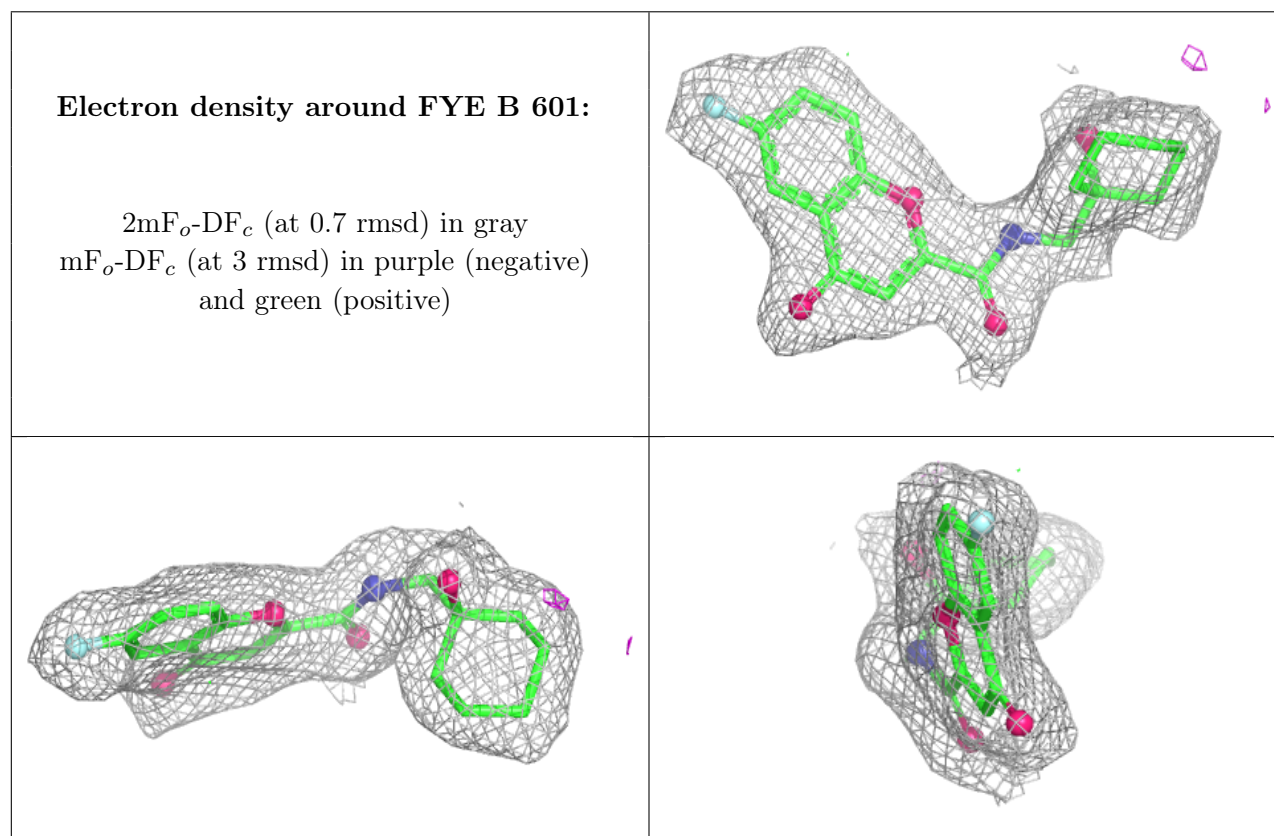
There are no oligosaccharides in this entry.

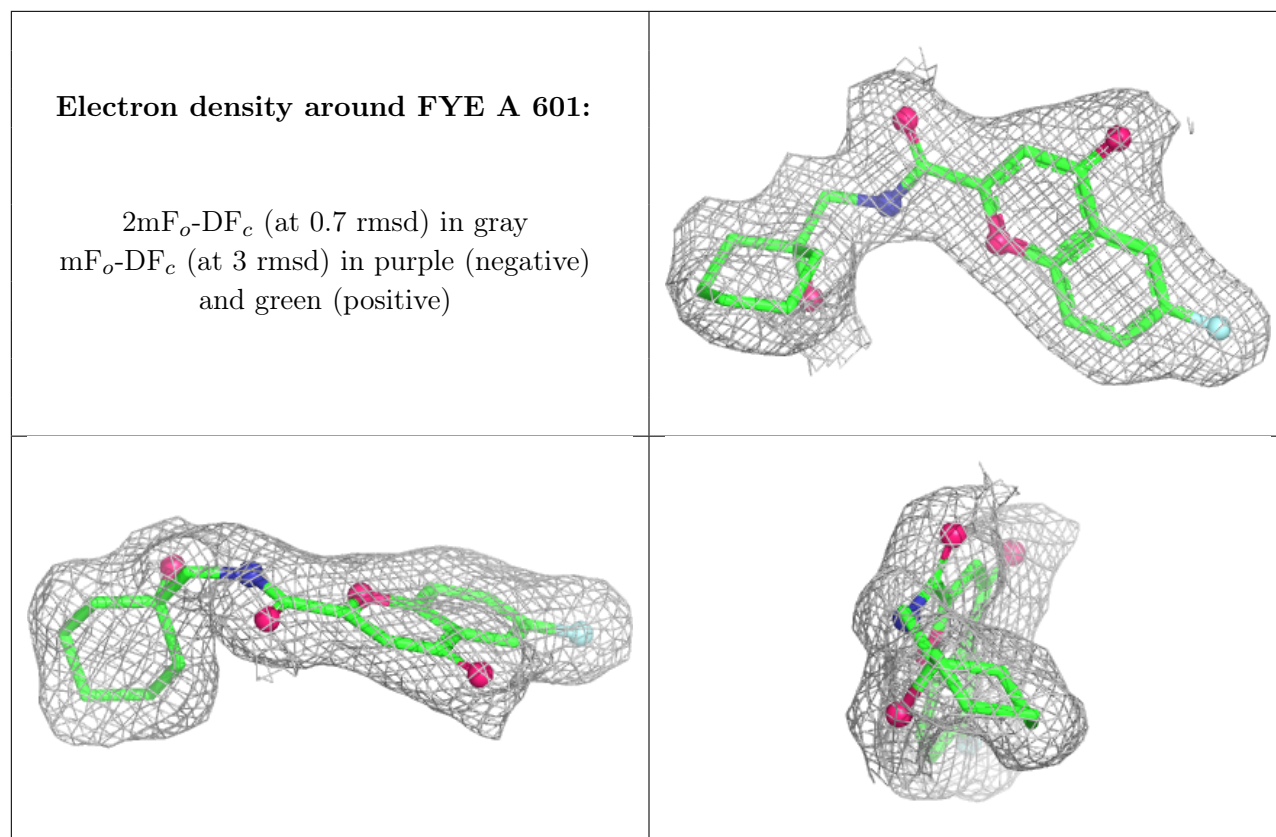
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	FYE	B	601	23/23	0.95	0.06	17,20,23,26	0
2	FYE	A	601	23/23	0.96	0.06	15,19,23,24	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.