



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:58 PM UTC

PDB ID : 9FMM / pdb_00009fmm
Title : Structure of human ACE2 in complex with a fluorinated small molecule inhibitor
Authors : Benoit, R.B.; Rodrigues, M.J.; Wieser, M.M.
Deposited on : 2024-06-06
Resolution : 2.50 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

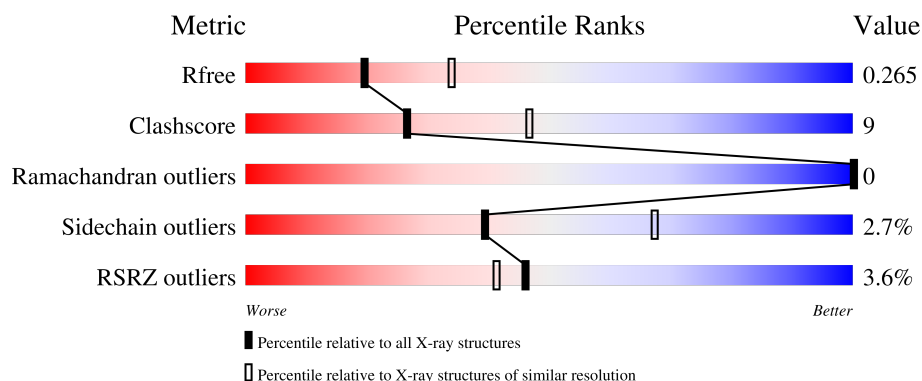
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

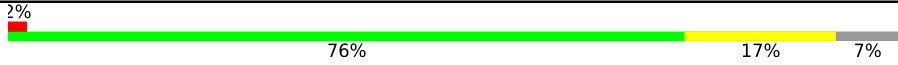
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	730	
1	B	730	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11357 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.

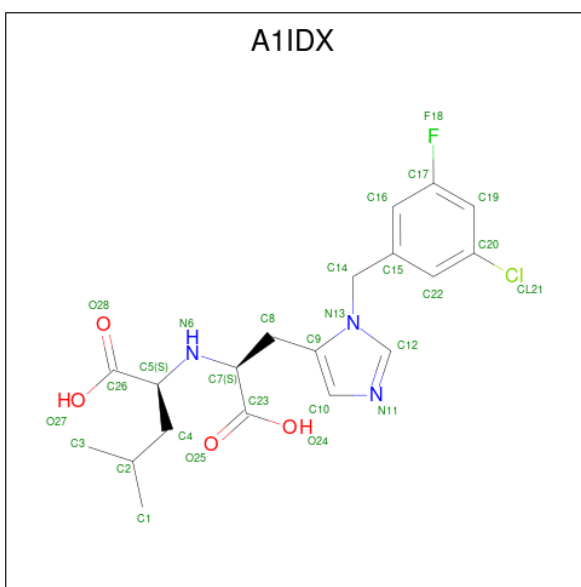
- Molecule 1 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	677	Total	C	N	O	S	170	0	0
			5541	3545	925	1038	33			
1	B	669	Total	C	N	O	S	248	0	0
			5481	3509	914	1025	33			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	741	HIS	-	expression tag	UNP Q9BYF1
A	742	HIS	-	expression tag	UNP Q9BYF1
A	743	HIS	-	expression tag	UNP Q9BYF1
A	744	HIS	-	expression tag	UNP Q9BYF1
A	745	HIS	-	expression tag	UNP Q9BYF1
A	746	HIS	-	expression tag	UNP Q9BYF1
A	747	HIS	-	expression tag	UNP Q9BYF1
A	748	HIS	-	expression tag	UNP Q9BYF1
B	741	HIS	-	expression tag	UNP Q9BYF1
B	742	HIS	-	expression tag	UNP Q9BYF1
B	743	HIS	-	expression tag	UNP Q9BYF1
B	744	HIS	-	expression tag	UNP Q9BYF1
B	745	HIS	-	expression tag	UNP Q9BYF1
B	746	HIS	-	expression tag	UNP Q9BYF1
B	747	HIS	-	expression tag	UNP Q9BYF1
B	748	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is (2 {S})-2-[[(2 {S})-3-[3-[(3-chloranyl-5-fluoranyl-phenyl)methyl]imidazol-4-yl]-1-oxidanyl-1-oxidanylidene-propan-2-yl]amino]-4-methyl-pentanoic acid (CCD ID: A1IDX) (formula: C₁₉H₂₃ClFN₃O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			28	19	1	1	3	4		
2	B	1	Total	C	Cl	F	N	O	0	0
			28	19	1	1	3	4		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



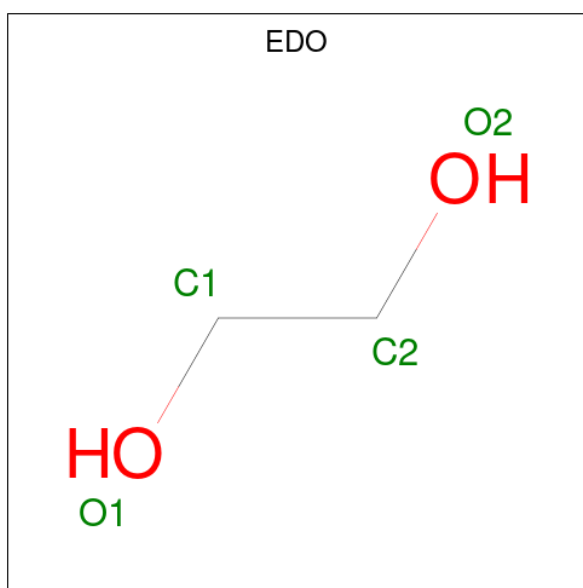
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	2	Total Cl 2 2	0	0

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0
6	B	1	Total Na 1 1	0	0

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Zn 1 1	0	0
7	B	1	Total Zn 1 1	0	0

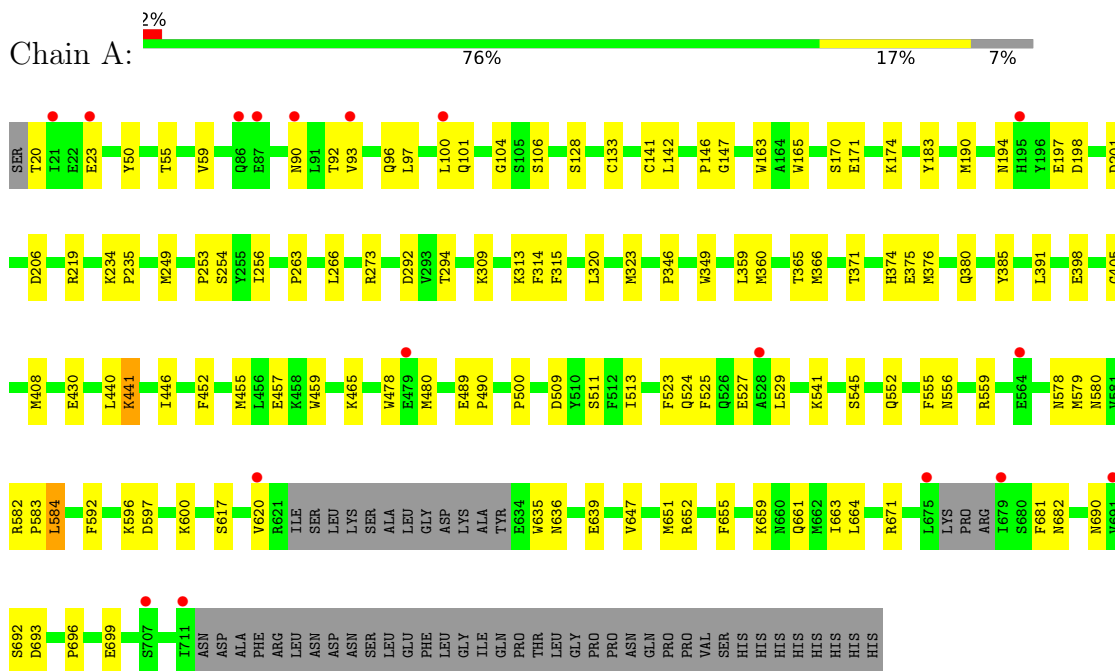
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	72	Total O 72 72	0	0
8	B	80	Total O 80 80	0	0

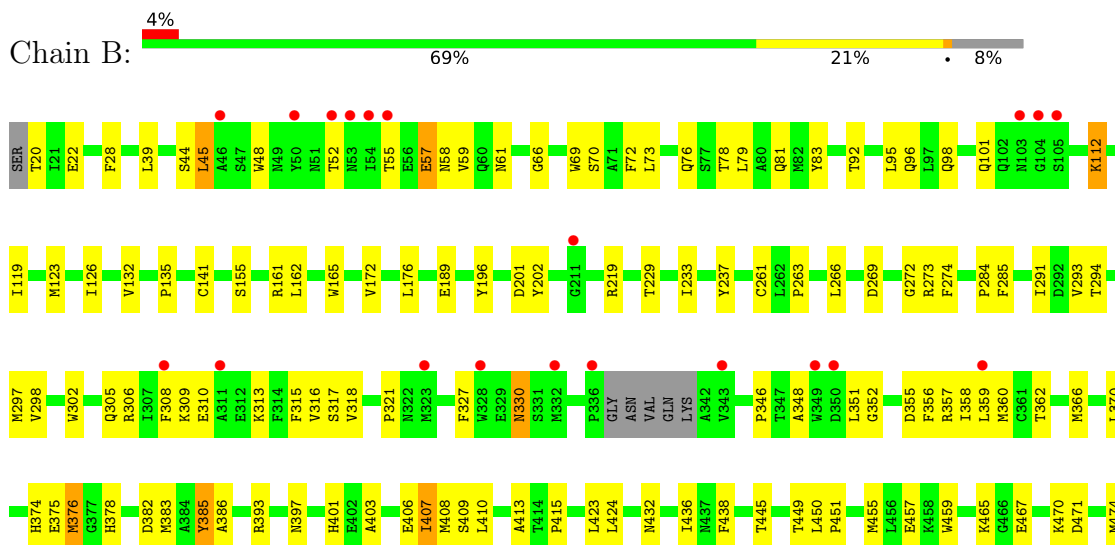
3 Residue-property plots [i](#)

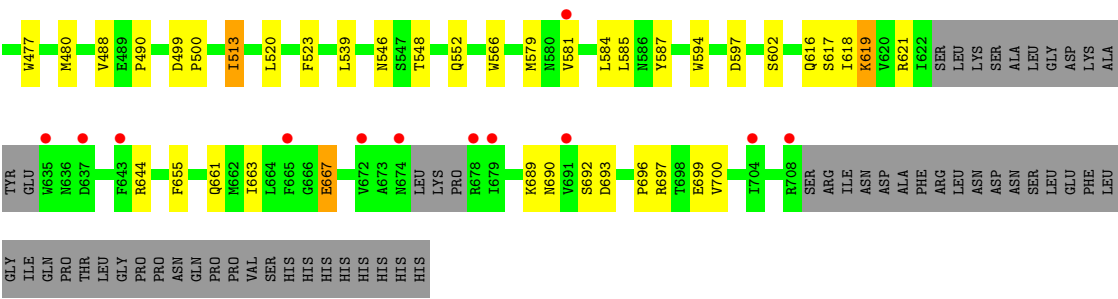
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Angiotensin-converting enzyme 2



• Molecule 1: Angiotensin-converting enzyme 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.30Å 82.90Å 105.50Å 90.00° 104.20° 90.00°	Depositor
Resolution (Å)	48.36 – 2.50 48.36 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.36-2.50) 98.1 (48.36-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20_4459, PHENIX 1.20_4459	Depositor
R, R_{free}	0.213 , 0.265 0.213 , 0.265	Depositor DCC
R_{free} test set	2854 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11357	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.69% 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: NAG, CL, EDO, A1IDX, NA, ZN

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	0.36	0/5689	0.53	0/7717
1	B	0.36	0/5628	0.54	0/7634
All	All	0.36	0/11317	0.53	0/15351

There are no bond length outliers.

There are no bond angle outliers.

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	5541	0	5321	80	0
1	B	5481	0	5259	111	0
2	A	28	0	0	1	0
2	B	28	0	0	0	0
3	A	42	0	39	2	0
3	B	42	0	39	3	0
4	A	20	0	30	2	0
4	B	16	0	24	1	0
5	A	1	0	0	1	0
5	B	2	0	0	1	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	72	0	0	1	0
8	B	80	0	0	0	0
All	All	11357	0	10712	193	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 (193) 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:293:VAL:HG21	1:B:423:LEU:HB3	1.60	0.82
1:A:55:THR:HG21	3:A:802:NAG:H62	1.61	0.82
1:B:293:VAL:HG13	1:B:297:MET:HE2	1.64	0.79
1:A:104:GLY:HA2	1:A:194:ASN:HD21	1.50	0.75
1:B:315:PHE:CE2	1:B:408:MET:HG3	2.28	0.68
1:B:135:PRO:HB2	1:B:689:LYS:HB3	1.75	0.68
1:B:539:LEU:HD23	1:B:587:TYR:HD2	1.59	0.66
1:A:655:PHE:O	1:A:661:GLN:N	2.28	0.66
1:A:597:ASP:HA	1:A:600:LYS:HE2	1.77	0.66
1:B:445:THR:O	1:B:449:THR:HG23	1.95	0.66
1:A:455:MET:HE3	1:A:480:MET:HB2	1.79	0.65
1:B:305:GLN:O	1:B:309:LYS:HB2	1.97	0.64
1:B:162:LEU:HD23	1:B:692:SER:HB3	1.80	0.63
1:B:317:SER:HB3	1:B:546:ASN:H	1.66	0.61
1:B:308:PHE:HE1	1:B:362:THR:HG21	1.66	0.60
1:A:690:ASN:ND2	1:A:693:ASP:HB2	2.16	0.60
1:B:306:ARG:O	1:B:310:GLU:HB2	2.01	0.60
1:A:620:VAL:HG12	1:A:681:PHE:H	1.66	0.60
1:B:370:LEU:HD21	1:B:413:ALA:HB2	1.83	0.60
1:B:375:GLU:O	1:B:378:HIS:HB2	2.03	0.59
1:A:315:PHE:CE2	1:A:408:MET:HG3	2.38	0.58
1:A:104:GLY:O	1:A:106:SER:N	2.32	0.58
1:B:229:THR:HB	1:B:581:VAL:CG2	2.33	0.58
1:B:293:VAL:HG21	1:B:423:LEU:HD13	1.85	0.58
1:B:72:PHE:CE1	1:B:76:GLN:HG3	2.38	0.57
1:A:457:GLU:HG2	1:A:513:ILE:HG23	1.86	0.57
1:B:370:LEU:HG	1:B:409:SER:HB2	1.87	0.57
1:A:96:GLN:HB3	1:A:391:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ARG:HG3	1:A:452:PHE:CE2	2.40	0.56
1:A:617:SER:OG	1:A:682:ASN:HB3	2.05	0.56
1:B:229:THR:HB	1:B:581:VAL:HG21	1.89	0.55
1:A:696:PRO:HB2	1:A:699:GLU:HG2	1.88	0.55
1:A:142:LEU:HD22	1:A:147:GLY:HA3	1.88	0.55
1:B:308:PHE:CE1	1:B:362:THR:HG21	2.41	0.55
1:B:273:ARG:O	1:B:449:THR:HG22	2.08	0.55
1:B:356:PHE:CE2	1:B:383:MET:HG2	2.42	0.54
1:A:294:THR:HG23	1:A:365:THR:HA	1.89	0.54
1:A:647:VAL:O	1:A:651:MET:HG2	2.07	0.54
1:B:293:VAL:CG2	1:B:423:LEU:HB3	2.34	0.54
1:A:555:PHE:CE2	1:A:559:ARG:HD2	2.42	0.54
1:A:690:ASN:HD22	1:A:693:ASP:HB2	1.73	0.54
1:B:523:PHE:CE2	1:B:584:LEU:HD13	2.43	0.54
1:A:201:ASP:CG	1:A:219:ARG:HE	2.16	0.53
1:B:155:SER:O	1:B:161:ARG:HD2	2.09	0.53
3:A:805:NAG:H83	3:A:805:NAG:H3	1.90	0.53
1:B:690:ASN:ND2	1:B:693:ASP:HB2	2.23	0.53
1:B:269:ASP:OD1	1:B:272:GLY:N	2.41	0.52
1:A:104:GLY:HA2	1:A:194:ASN:ND2	2.23	0.52
1:B:294:THR:CG2	1:B:366:MET:H	2.23	0.51
1:A:374:HIS:HA	1:A:405:GLY:HA3	1.92	0.51
1:A:578:ASN:OD1	1:A:579:MET:N	2.38	0.51
1:B:327:PHE:HD1	1:B:357:ARG:HA	1.76	0.51
1:A:511:SER:HB3	4:A:809:EDO:H12	1.92	0.50
1:B:465:LYS:HG2	1:B:467:GLU:OE2	2.11	0.50
1:A:253:PRO:O	1:A:254:SER:OG	2.26	0.50
1:A:552:GLN:NE2	1:A:556:ASN:OD1	2.45	0.50
1:B:293:VAL:HG22	1:B:293:VAL:O	2.13	0.49
1:B:294:THR:HA	1:B:297:MET:HE3	1.93	0.49
1:B:55:THR:O	1:B:59:VAL:HG23	2.13	0.49
1:B:644:ARG:NH2	1:B:667:GLU:OE1	2.42	0.49
1:B:112:LYS:NZ	1:B:189:GLU:OE2	2.38	0.49
1:A:314:PHE:CE2	1:A:408:MET:HE3	2.47	0.49
1:A:20:THR:HG23	1:A:23:GLU:H	1.77	0.49
1:A:206:ASP:OD2	1:A:398:GLU:HG2	2.12	0.49
1:A:620:VAL:HG11	1:A:681:PHE:CD2	2.48	0.49
1:B:294:THR:HG22	1:B:366:MET:H	1.78	0.49
1:B:455:MET:HE3	1:B:480:MET:HB2	1.94	0.49
1:B:321:PRO:HB2	1:B:383:MET:HE1	1.94	0.49
1:A:524:GLN:HG2	1:A:583:PRO:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LYS:O	1:A:313:LYS:HG3	2.14	0.48
1:A:170:SER:O	1:A:174:LYS:HD2	2.13	0.48
1:B:92:THR:O	1:B:96:GLN:HG3	2.13	0.48
1:B:20:THR:HG22	1:B:22:GLU:H	1.77	0.48
1:A:198:ASP:OD2	1:A:465:LYS:HA	2.13	0.48
1:A:459:TRP:CH2	1:A:500:PRO:HG2	2.48	0.48
1:B:291:ILE:HG22	1:B:424:LEU:HD11	1.96	0.48
1:B:477:TRP:CE3	1:B:500:PRO:HG3	2.49	0.48
1:B:330:ASN:HB2	1:B:357:ARG:CZ	2.44	0.47
1:B:123:MET:HG2	1:B:176:LEU:HD23	1.95	0.47
1:B:201:ASP:CG	1:B:219:ARG:HE	2.20	0.47
1:B:297:MET:HG2	1:B:302:TRP:CE3	2.49	0.47
1:A:446:ILE:HD13	1:A:523:PHE:HZ	1.78	0.47
1:B:57:GLU:OE2	1:B:58:ASN:ND2	2.48	0.47
1:B:78:THR:O	1:B:81:GLN:HB2	2.15	0.47
1:B:119:ILE:HG22	1:B:123:MET:HE2	1.97	0.47
1:B:382:ASP:HA	1:B:385:TYR:CE1	2.50	0.47
1:B:351:LEU:HD13	1:B:355:ASP:OD1	2.15	0.47
1:B:397:ASN:HD22	1:B:566:TRP:CG	2.33	0.47
1:A:97:LEU:O	1:A:101:GLN:HG3	2.14	0.47
1:A:671:ARG:HD2	8:A:932:HOH:O	2.15	0.46
1:B:126:ILE:HG22	1:B:172:VAL:HG13	1.97	0.46
1:B:432:ASN:HB2	3:B:801:NAG:H2	1.97	0.46
1:B:457:GLU:HG2	1:B:513:ILE:HB	1.97	0.46
1:A:55:THR:O	1:A:59:VAL:HG23	2.16	0.46
1:A:478:TRP:CD2	1:A:489:GLU:HB3	2.51	0.46
1:B:474:MET:HE1	1:B:500:PRO:CD	2.45	0.46
1:A:50:TYR:CE1	1:A:59:VAL:HG22	2.50	0.46
1:A:592:PHE:CZ	1:A:596:LYS:HE3	2.51	0.46
1:B:285:PHE:HZ	3:B:801:NAG:H82	1.81	0.45
1:B:293:VAL:HG21	1:B:423:LEU:CB	2.39	0.45
1:A:349:TRP:HA	4:A:807:EDO:H11	1.98	0.45
1:B:165:TRP:CH2	1:B:490:PRO:HD2	2.51	0.45
1:A:142:LEU:HD12	1:A:163:TRP:HH2	1.81	0.45
1:A:346:PRO:HB3	1:A:360:MET:HE2	1.98	0.45
1:B:95:LEU:O	1:B:98:GLN:HB3	2.16	0.45
1:B:360:MET:SD	1:B:362:THR:HG22	2.56	0.45
1:B:697:ARG:HA	1:B:700:VAL:HG12	1.98	0.45
1:B:233:ILE:HD13	1:B:450:LEU:HD13	1.98	0.45
1:B:581:VAL:HG12	1:B:585:LEU:HG	1.98	0.45
1:B:351:LEU:HD12	1:B:351:LEU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:PHE:O	1:A:529:LEU:HG	2.16	0.45
1:B:196:TYR:CD2	1:B:202:TYR:HA	2.51	0.45
1:B:165:TRP:CZ3	1:B:490:PRO:HD2	2.52	0.45
1:B:459:TRP:CH2	1:B:500:PRO:HG2	2.51	0.45
1:B:52:THR:HG22	1:B:359:LEU:HD13	1.99	0.45
1:B:346:PRO:HG3	1:B:360:MET:HG3	2.00	0.44
1:B:513:ILE:HD12	1:B:513:ILE:HA	1.80	0.44
1:A:165:TRP:CH2	1:A:490:PRO:HD2	2.53	0.44
1:A:320:LEU:HB3	1:A:380:GLN:OE1	2.18	0.44
1:B:284:PRO:HB3	1:B:594:TRP:CZ2	2.52	0.44
1:B:297:MET:HE1	1:B:366:MET:HA	1.98	0.44
1:A:197:GLU:HG3	1:A:201:ASP:OD2	2.16	0.44
1:A:346:PRO:HA	1:A:359:LEU:O	2.17	0.44
1:A:314:PHE:HE1	1:A:545:SER:HB2	1.82	0.44
1:B:132:VAL:O	1:B:141:CYS:HA	2.18	0.44
1:B:432:ASN:OD1	1:B:432:ASN:N	2.50	0.44
1:B:618:ILE:HD11	1:B:700:VAL:HG13	1.99	0.44
1:A:478:TRP:CE3	1:A:489:GLU:HB3	2.53	0.44
1:A:652:ARG:HG2	1:A:663:ILE:O	2.18	0.43
1:B:274:PHE:CD1	1:B:449:THR:HG21	2.53	0.43
1:A:371:THR:HG23	2:A:801:A1IDX:C10	2.48	0.43
1:A:146:PRO:HD2	5:A:810:CL:CL	2.56	0.43
1:B:39:LEU:HD12	1:B:72:PHE:CD2	2.54	0.43
1:B:57:GLU:OE2	1:B:58:ASN:CG	2.61	0.43
1:B:474:MET:HE1	1:B:500:PRO:HD2	2.01	0.43
1:B:284:PRO:HG2	1:B:436:ILE:HG22	2.01	0.43
1:A:92:THR:O	1:A:96:GLN:HG3	2.19	0.42
1:A:635:TRP:HA	1:A:639:GLU:HG3	2.01	0.42
1:B:28:PHE:HE2	1:B:79:LEU:HG	1.84	0.42
1:A:690:ASN:O	1:A:692:SER:N	2.47	0.42
1:B:45:LEU:HD13	1:B:45:LEU:HA	1.89	0.42
1:B:386:ALA:HA	1:B:393:ARG:HD3	2.01	0.42
1:A:292:ASP:HA	1:A:366:MET:CE	2.49	0.42
1:A:292:ASP:HA	1:A:366:MET:HE1	2.01	0.42
1:B:66:GLY:O	1:B:70:SER:N	2.44	0.42
1:B:697:ARG:NH2	4:B:807:EDO:H21	2.33	0.42
1:A:183:TYR:OH	1:A:509:ASP:OD1	2.23	0.42
3:B:801:NAG:O7	3:B:801:NAG:H3	2.20	0.42
1:A:523:PHE:CD2	1:A:584:LEU:HB2	2.55	0.42
1:B:499:ASP:HB3	5:B:809:CL:CL	2.57	0.42
1:A:234:LYS:HB2	1:A:235:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:TRP:CH2	1:B:359:LEU:HB2	2.55	0.41
1:B:83:TYR:O	1:B:101:GLN:NE2	2.51	0.41
1:B:261:CYS:HB2	1:B:488:VAL:HB	2.01	0.41
1:A:580:ASN:OD1	1:A:582:ARG:HB3	2.20	0.41
1:B:410:LEU:HA	1:B:410:LEU:HD23	1.81	0.41
1:B:690:ASN:HD22	1:B:693:ASP:HB2	1.84	0.41
1:B:696:PRO:HB2	1:B:699:GLU:HG3	2.02	0.41
1:A:366:MET:HE3	1:A:441:LYS:HE3	2.01	0.41
1:B:274:PHE:CE1	1:B:449:THR:HG21	2.56	0.41
1:B:352:GLY:O	1:B:355:ASP:N	2.41	0.41
1:A:655:PHE:HA	1:A:659:LYS:HB2	2.03	0.41
1:B:403:ALA:O	1:B:407:ILE:HG23	2.21	0.41
1:A:90:ASN:O	1:A:93:VAL:N	2.45	0.41
1:A:323:MET:HA	1:A:323:MET:HE2	2.02	0.41
1:A:584:LEU:O	1:A:584:LEU:HD12	2.20	0.41
1:B:520:LEU:HD12	1:B:579:MET:SD	2.61	0.41
1:B:655:PHE:HB3	1:B:661:GLN:HB2	2.02	0.41
1:B:263:PRO:HB2	1:B:266:LEU:HD12	2.02	0.41
1:B:415:PRO:HD3	1:B:438:PHE:CD1	2.56	0.41
1:A:263:PRO:HB2	1:A:266:LEU:HD12	2.03	0.41
1:A:375:GLU:OE1	1:A:375:GLU:HA	2.20	0.41
1:A:636:ASN:H	1:A:639:GLU:HG2	1.85	0.41
1:A:652:ARG:NH1	1:A:664:LEU:HD22	2.36	0.41
1:B:330:ASN:HB2	1:B:357:ARG:NH1	2.35	0.41
1:B:348:ALA:HA	1:B:358:ILE:HG12	2.03	0.41
1:B:351:LEU:HB2	1:B:355:ASP:HB3	2.02	0.41
1:A:314:PHE:CD2	1:A:408:MET:HE3	2.56	0.41
1:A:636:ASN:OD1	1:A:639:GLU:HG2	2.21	0.41
1:B:44:SER:HB3	1:B:351:LEU:HG	2.03	0.41
1:B:315:PHE:CE1	1:B:376:MET:HG2	2.56	0.41
1:A:133:CYS:HA	1:A:141:CYS:HA	2.03	0.40
1:B:237:TYR:CZ	1:B:451:PRO:HG2	2.55	0.40
1:B:374:HIS:ND1	1:B:406:GLU:OE2	2.54	0.40
1:A:376:MET:HE3	1:A:376:MET:HB2	1.98	0.40
1:B:294:THR:O	1:B:298:VAL:HG23	2.21	0.40
1:A:430:GLU:HG3	1:A:541:LYS:HZ2	1.87	0.40
1:A:651:MET:O	1:A:655:PHE:HD1	2.03	0.40
1:B:69:TRP:CZ2	1:B:73:LEU:HD21	2.57	0.40
1:B:313:LYS:O	1:B:316:VAL:HG22	2.20	0.40
1:A:249:MET:HE3	1:A:256:ILE:O	2.21	0.40
1:B:618:ILE:HG22	1:B:619:LYS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:ARG:HA	1:B:700:VAL:CG1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	671/730 (92%)	642 (96%)	29 (4%)	0	100	100
1	B	661/730 (90%)	633 (96%)	28 (4%)	0	100	100
All	All	1332/1460 (91%)	1275 (96%)	57 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	601/648 (93%)	592 (98%)	9 (2%)	57	80
1	B	594/648 (92%)	571 (96%)	23 (4%)	28	55
All	All	1195/1296 (92%)	1163 (97%)	32 (3%)	39	67

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	128	SER
1	A	171	GLU
1	A	190	MET
1	A	385	TYR
1	A	440	LEU
1	A	441	LYS
1	A	527	GLU
1	A	584	LEU
1	B	45	LEU
1	B	57	GLU
1	B	61	ASN
1	B	112	LYS
1	B	318	VAL
1	B	330	ASN
1	B	376	MET
1	B	385	TYR
1	B	401	HIS
1	B	407	ILE
1	B	470	LYS
1	B	471	ASP
1	B	513	ILE
1	B	548	THR
1	B	552	GLN
1	B	597	ASP
1	B	602	SER
1	B	616	GLN
1	B	617	SER
1	B	619	LYS
1	B	621	ARG
1	B	663	ILE
1	B	667	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	154	ASN
1	A	340	GLN
1	B	58	ASN
1	B	98	GLN
1	B	210	ASN
1	B	330	ASN

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Mol	Chain	Res	Type
1	B	442	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](#)

Of 24 ligands modelled in this entry, 7 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	EDO	A	809	-	3,3,3	0.64	0	2,2,2	0.22	0
2	A1IDX	B	802	7	29,29,29	0.60	0	36,40,40	0.53	0
3	NAG	B	803	1	14,14,15	0.45	0	17,19,21	0.44	0
3	NAG	A	802	1	14,14,15	0.73	1 (7%)	17,19,21	0.81	1 (5%)
4	EDO	A	808	-	3,3,3	0.54	0	2,2,2	0.23	0
4	EDO	B	806	-	3,3,3	0.41	0	2,2,2	0.48	0
3	NAG	A	805	1	14,14,15	0.44	0	17,19,21	1.40	2 (11%)
4	EDO	A	807	-	3,3,3	0.54	0	2,2,2	0.12	0
3	NAG	B	801	1	14,14,15	0.58	0	17,19,21	0.91	0
4	EDO	B	807	-	3,3,3	0.42	0	2,2,2	0.39	0
2	A1IDX	A	801	7	29,29,29	0.66	0	36,40,40	0.50	0
4	EDO	A	804	-	3,3,3	0.56	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	806	-	3,3,3	0.40	0	2,2,2	0.49	0
3	NAG	A	803	1	14,14,15	1.00	1 (7%)	17,19,21	0.61	0
4	EDO	B	808	-	3,3,3	0.52	0	2,2,2	0.26	0
3	NAG	B	805	1	14,14,15	0.41	0	17,19,21	0.60	0
4	EDO	B	804	-	3,3,3	0.42	0	2,2,2	0.50	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	EDO	A	809	-	-	0/1/1/1	-
2	A1IDX	B	802	7	-	5/24/24/24	0/2/2/2
3	NAG	B	803	1	-	1/6/23/26	0/1/1/1
3	NAG	A	802	1	-	0/6/23/26	0/1/1/1
4	EDO	A	808	-	-	0/1/1/1	-
4	EDO	B	806	-	-	1/1/1/1	-
3	NAG	A	805	1	-	6/6/23/26	0/1/1/1
4	EDO	A	807	-	-	0/1/1/1	-
3	NAG	B	801	1	-	2/6/23/26	0/1/1/1
4	EDO	B	807	-	-	0/1/1/1	-
2	A1IDX	A	801	7	-	4/24/24/24	0/2/2/2
4	EDO	A	804	-	-	0/1/1/1	-
4	EDO	A	806	-	-	0/1/1/1	-
3	NAG	A	803	1	-	3/6/23/26	0/1/1/1
4	EDO	B	808	-	-	0/1/1/1	-
3	NAG	B	805	1	-	4/6/23/26	0/1/1/1
4	EDO	B	804	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	NAG	O5-C1	3.17	1.49	1.43
3	A	802	NAG	O5-C1	2.43	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	805	NAG	C2-N2-C7	4.72	129.22	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	NAG	C1-O5-C5	2.70	115.81	112.19
3	A	805	NAG	C1-C2-N2	2.09	113.73	110.43

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	A1IDX	C2-C4-C5-C26
2	B	802	A1IDX	C26-C5-N6-C7
3	B	805	NAG	O5-C5-C6-O6
3	B	805	NAG	C4-C5-C6-O6
2	A	801	A1IDX	C2-C4-C5-N6
3	A	803	NAG	C8-C7-N2-C2
3	A	803	NAG	O7-C7-N2-C2
3	A	805	NAG	C8-C7-N2-C2
3	A	805	NAG	O7-C7-N2-C2
3	A	805	NAG	O5-C5-C6-O6
3	A	803	NAG	O5-C5-C6-O6
3	B	803	NAG	O5-C5-C6-O6
3	B	801	NAG	C3-C2-N2-C7
3	B	801	NAG	O5-C5-C6-O6
2	B	802	A1IDX	O27-C26-C5-N6
2	A	801	A1IDX	O27-C26-C5-N6
2	B	802	A1IDX	O28-C26-C5-N6
3	B	805	NAG	C1-C2-N2-C7
2	A	801	A1IDX	O28-C26-C5-N6
3	A	805	NAG	C1-C2-N2-C7
4	B	806	EDO	O1-C1-C2-O2
3	A	805	NAG	C3-C2-N2-C7
3	B	805	NAG	C3-C2-N2-C7
2	B	802	A1IDX	C2-C4-C5-C26
2	B	802	A1IDX	C2-C4-C5-N6
3	A	805	NAG	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	809	EDO	1	0
3	A	802	NAG	1	0
3	A	805	NAG	1	0

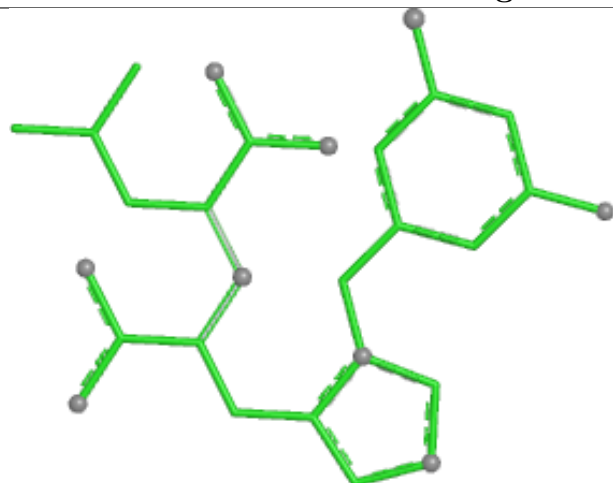
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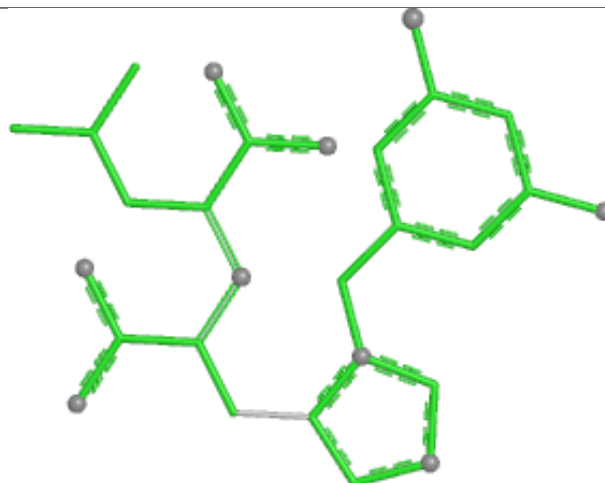
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	807	EDO	1	0
3	B	801	NAG	3	0
4	B	807	EDO	1	0
2	A	801	A1IDX	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

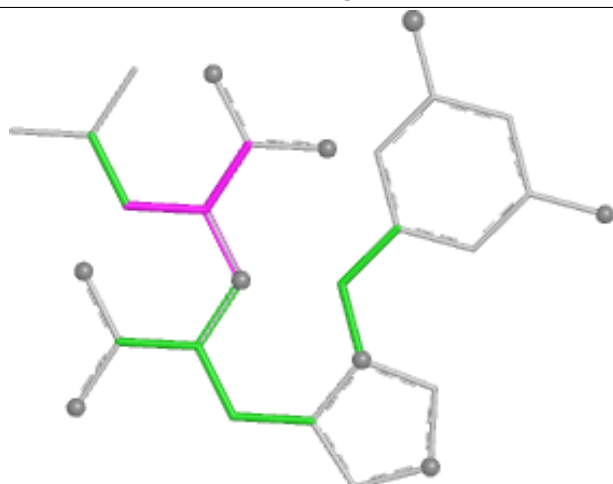
Ligand A1IDX B 802



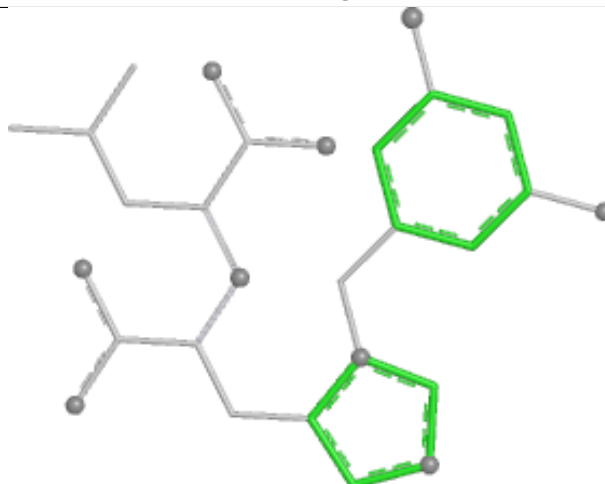
Bond lengths



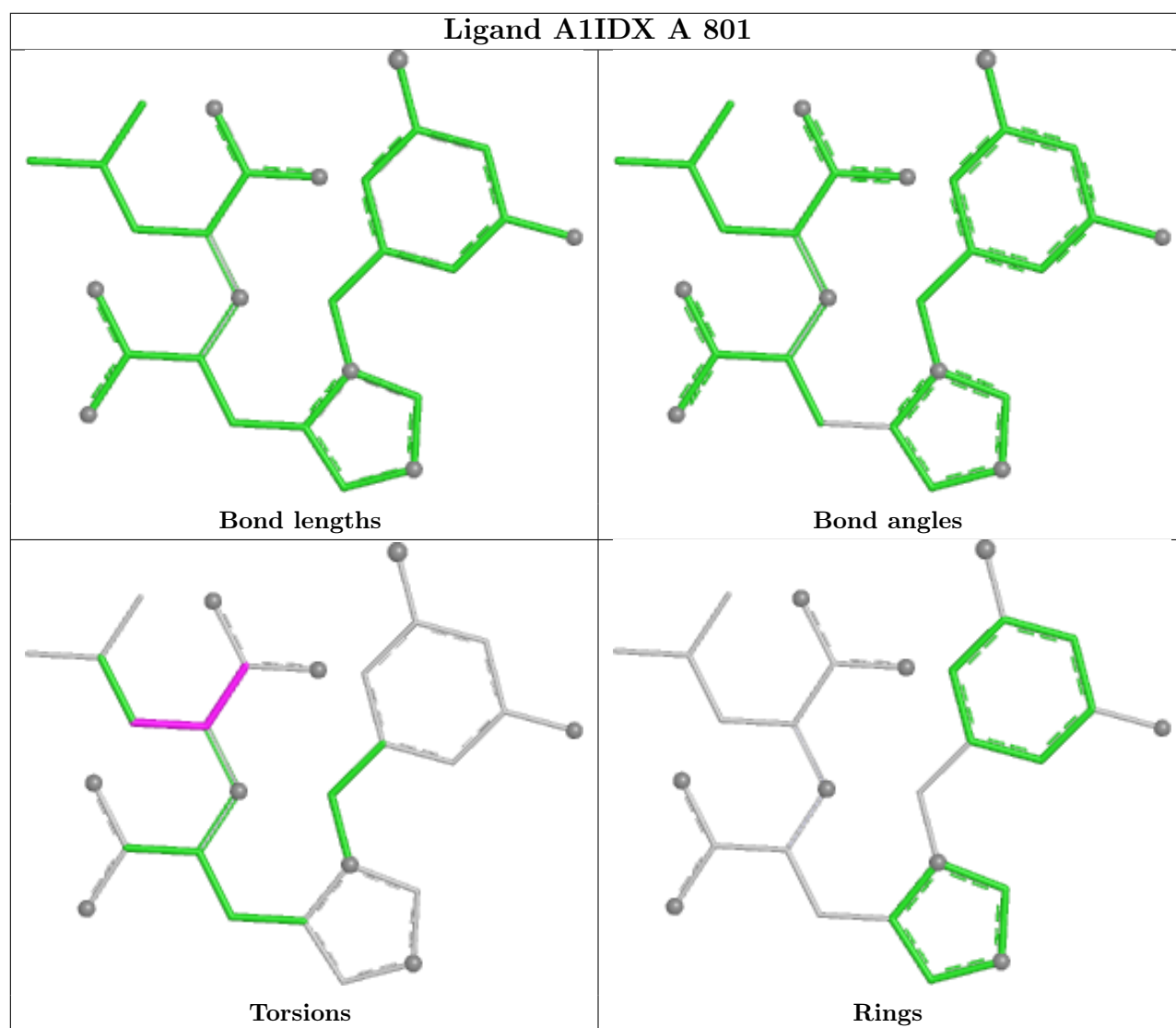
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	674/730 (92%)	0.30	17 (2%) 58 54	30, 53, 84, 111	41 (6%)
1	B	669/730 (91%)	0.44	32 (4%) 35 31	27, 55, 87, 102	67 (10%)
All	All	1343/1460 (91%)	0.37	49 (3%) 46 41	27, 54, 86, 111	108 (8%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	GLU	4.6
1	A	711	ILE	4.5
1	A	86	GLN	4.3
1	A	707	SER	4.0
1	B	103	ASN	4.0
1	B	55	THR	4.0
1	B	708	ARG	3.7
1	B	349	TRP	3.6
1	B	637	ASP	3.3
1	A	691	VAL	3.2
1	B	50	TYR	3.1
1	B	105	SER	3.0
1	A	675	LEU	2.9
1	B	635	TRP	2.9
1	A	620	VAL	2.8
1	B	323	MET	2.8
1	B	691	VAL	2.8
1	B	336	PRO	2.6
1	B	52	THR	2.6
1	A	21	ILE	2.6
1	B	54	ILE	2.6
1	B	665	PHE	2.6
1	B	53	ASN	2.6
1	B	311	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	672	VAL	2.4
1	B	350	ASP	2.4
1	A	100	LEU	2.4
1	A	195	HIS	2.4
1	B	104	GLY	2.3
1	B	211	GLY	2.3
1	A	93	VAL	2.3
1	B	46	ALA	2.3
1	A	528	ALA	2.2
1	B	679	ILE	2.2
1	A	564	GLU	2.2
1	B	332	MET	2.1
1	B	674	ASN	2.1
1	B	359	LEU	2.1
1	A	479	GLU	2.1
1	A	23	GLU	2.1
1	B	308	PHE	2.1
1	B	643	PHE	2.1
1	B	343	VAL	2.1
1	B	328	TRP	2.1
1	B	581	VAL	2.0
1	B	678	ARG	2.0
1	A	90	ASN	2.0
1	A	679	ILE	2.0
1	B	704	ILE	2.0

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

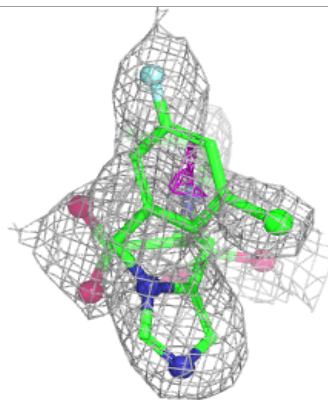
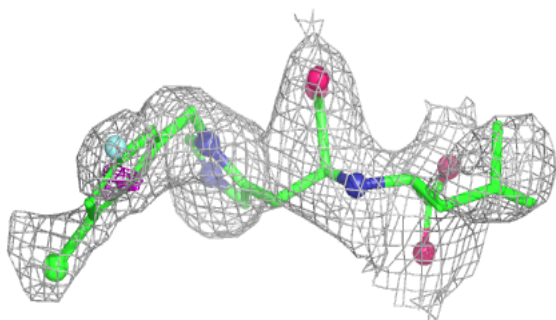
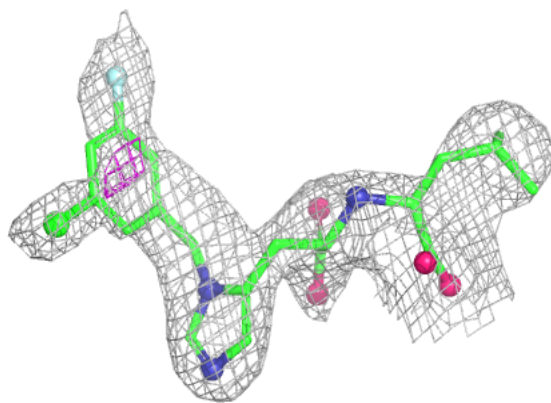
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	NAG	B	801	14/15	0.63	0.12	68,83,89,94	0
3	NAG	A	803	14/15	0.68	0.13	82,86,92,92	0
4	EDO	B	807	4/4	0.72	0.17	81,85,85,89	0
3	NAG	B	805	14/15	0.73	0.10	93,101,104,107	0
3	NAG	A	805	14/15	0.75	0.10	63,82,93,96	0
3	NAG	A	802	14/15	0.75	0.09	82,86,89,94	0
4	EDO	A	804	4/4	0.76	0.20	60,65,66,70	0
3	NAG	B	803	14/15	0.78	0.12	81,88,94,97	0
4	EDO	A	807	4/4	0.79	0.18	65,68,68,71	0
4	EDO	A	809	4/4	0.84	0.14	53,56,56,58	0
2	A1IDX	B	802	28/28	0.84	0.14	53,67,82,98	0
4	EDO	B	808	4/4	0.84	0.13	55,55,57,61	0
4	EDO	B	804	4/4	0.87	0.14	54,55,56,57	0
4	EDO	A	806	4/4	0.89	0.11	51,53,55,56	0
2	A1IDX	A	801	28/28	0.90	0.11	44,54,68,86	0
4	EDO	B	806	4/4	0.91	0.10	53,57,58,58	0
6	NA	A	811	1/1	0.91	0.11	45,45,45,45	0
5	CL	B	810	1/1	0.92	0.14	74,74,74,74	0
4	EDO	A	808	4/4	0.93	0.11	53,53,53,54	0
6	NA	B	811	1/1	0.94	0.08	37,37,37,37	0
7	ZN	A	812	1/1	0.94	0.08	45,45,45,45	1
5	CL	A	810	1/1	0.97	0.05	58,58,58,58	0
5	CL	B	809	1/1	0.97	0.05	46,46,46,46	0
7	ZN	B	812	1/1	0.97	0.06	56,56,56,56	1

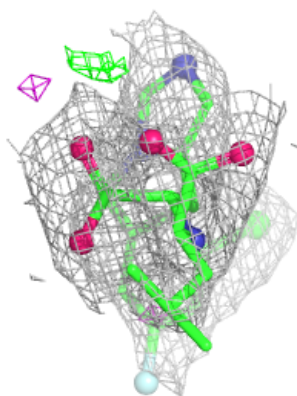
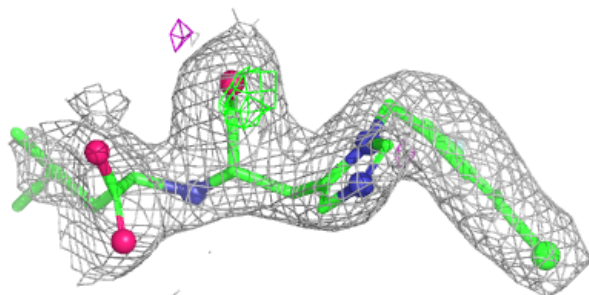
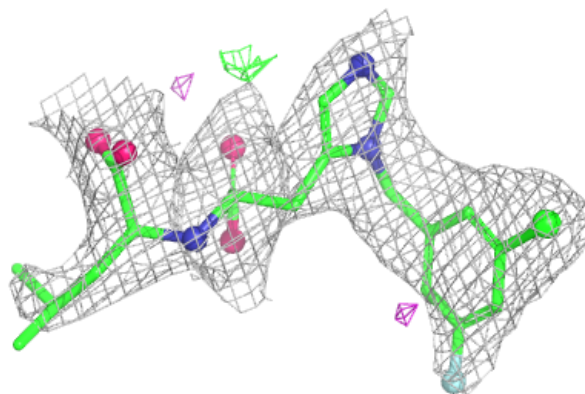
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1IDX B 802:

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

**Electron density around A1IDX A 801:**

$2mF_o-DF_c$ (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.