Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2023 – 02:38 PM EDT

|		
PDB ID	:	4PES
Title	:	Crystal structure of insulin degrading enzyme complexed with inhibitor tert-butyl [(2S)-2-(2,5-difluorophenyl)-3-(quinolin-3-yl)propyl]carbamate
Authors	:	Wang, Y.; Guo, S.
Deposited on	:	2014-04-24
Resolution	:	2.21 Å(reported)

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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 2.21 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	Percentile Ranks	Value
Rfree		0.258
Clashscore		3
Ramachandran outliers		0.3%
Sidechain outliers		2.5%
RSRZ outliers		2.2%

Worse   *Better*

▌ Percentile relative to all X-ray structures
◫ Percentile relative to X-ray structures of similar resolution
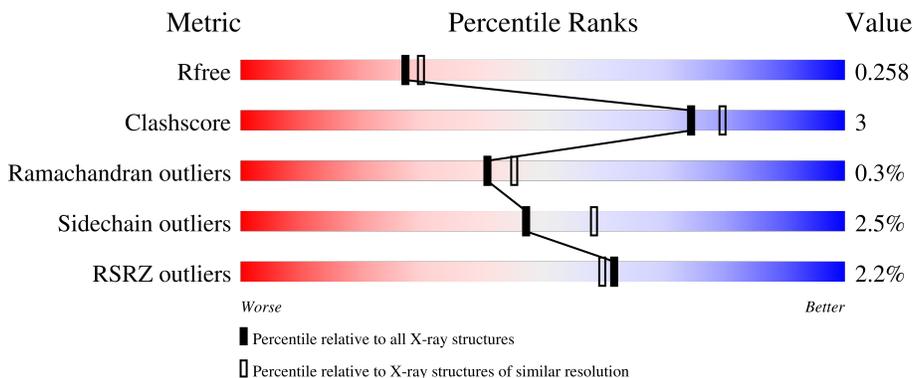
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 <=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	989	2% / 86% / 10% / ·
1	B	989	2% / 86% / 10% / ··
2	C	3	100%
2	D	3	100%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 16206 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	955	Total 7804	C 5029	N 1308	O 1445	S 22	0	1	0
1	B	959	Total 7840	C 5048	N 1315	O 1455	S 22	0	1	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	expression tag	UNP P14735
A	32	GLY	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	HIS	-	expression tag	UNP P14735
A	38	HIS	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ARG	-	expression tag	UNP P14735
A	41	ALA	-	expression tag	UNP P14735
A	110	LEU	CYS	engineered mutation	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735
A	974	ALA	CYS	engineered mutation	UNP P14735

WORLDWIDE
PDB
PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
B	31	MET	-	expression tag	UNP P14735
B	32	GLY	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	HIS	-	expression tag	UNP P14735
B	38	HIS	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ARG	-	expression tag	UNP P14735
B	41	ALA	-	expression tag	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is a protein called Ala-Ala-Ala.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total 15	C 9	N 3	O 3	0	0	0
2	D	3	Total 15	C 9	N 3	O 3	0	0	0

- Molecule 3 is tert-butyl [(2S)-2-(2,5-difluorophenyl)-3-(quinolin-3-yl)propyl]carbamate (three-letter code: 2PJ) (formula: $C_{23}H_{24}F_2N_2O_2$).
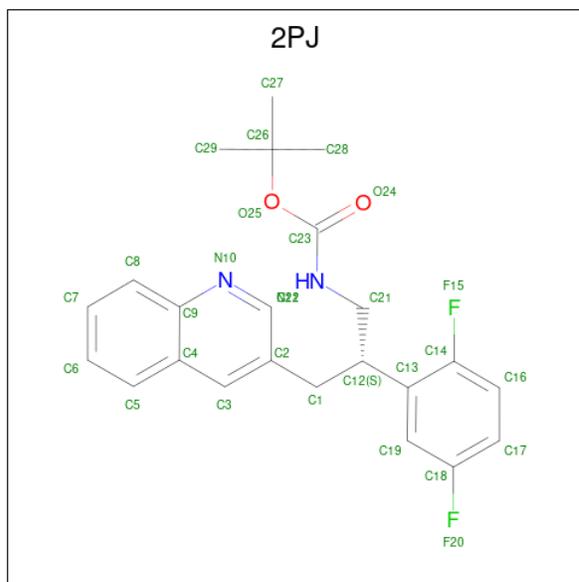
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 29	C 23	F 2	N 2	O 2	0	0
3	B	1	Total 29	C 23	F 2	N 2	O 2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	250	Total 250	O 250	0	0
5	B	222	Total 222	O 222	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Insulin-degrading enzyme

- Molecule 1: Insulin-degrading enzyme

M799 S803 L810 F811 A812 Q813 E817 P818 R824 L829 I843 Q844 A865 Q887 I891 W908 Y927 T932 K933 E934 D935 H952 S955 D964 S965 ASN PRO VAL VAL GLY GLU PHE PRO ALA GLN ASN D977 I978 N979 A983 P984 A985

Q988 E997 F998 K999 R1000 K1009 P1010 H1011 I1012 ASN PHE MET ALA ALA LYS LEU
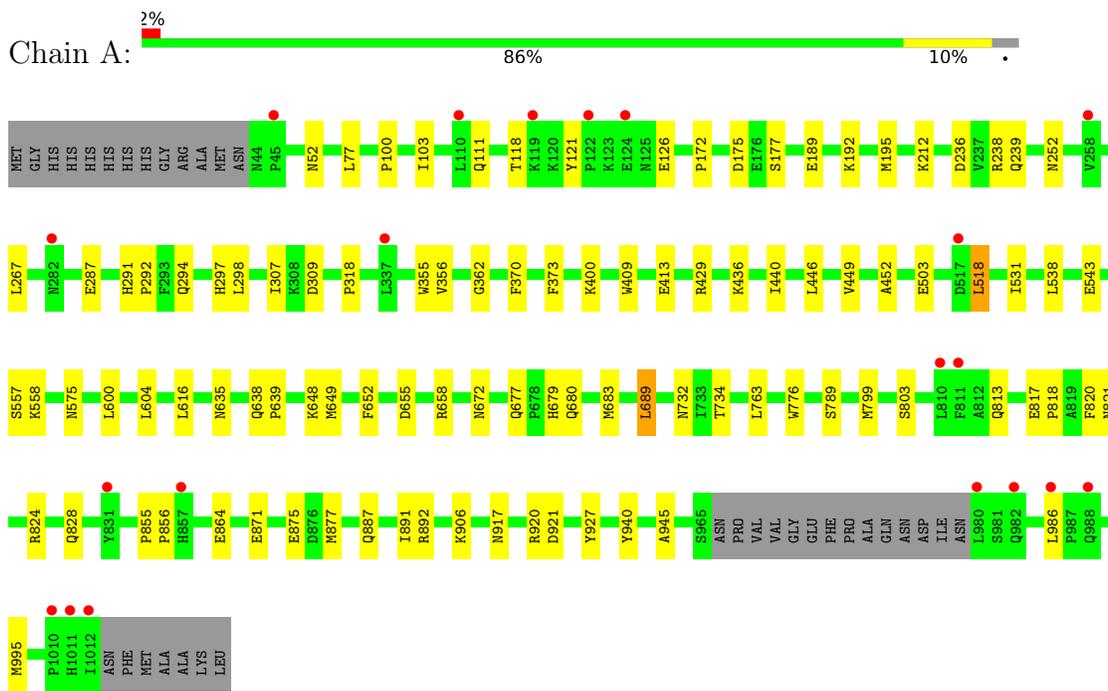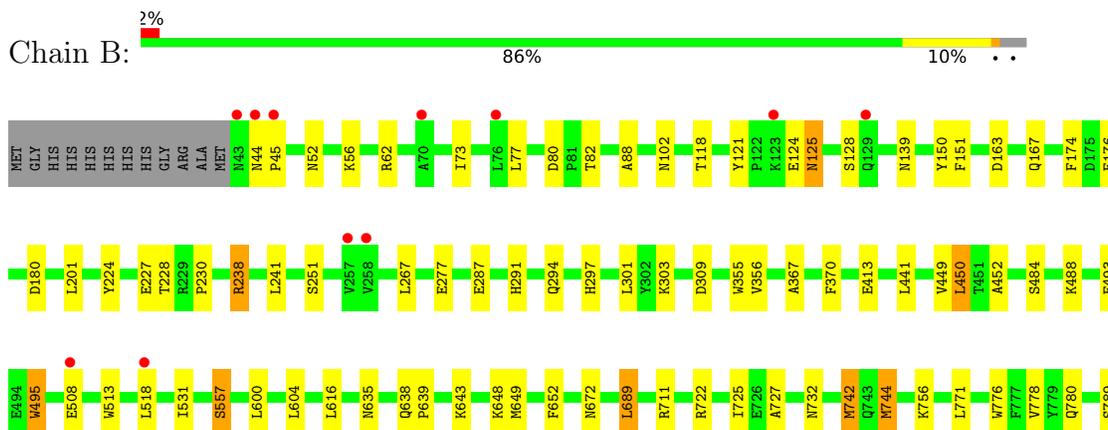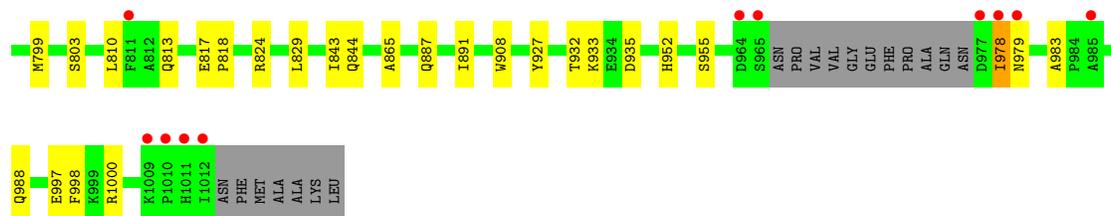
• Molecule 2: Ala-Ala-Ala

Chain C:

100%

There are no outlier residues recorded for this chain.

• Molecule 2: Ala-Ala-Ala

Chain D:

100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.75Å 116.09Å 123.92Å 90.00° 98.09° 90.00°	Depositor
Resolution (Å)	122.69 – 2.21 19.95 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.6 (122.69-2.21) 98.8 (19.95-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.209 , 0.256 0.208 , 0.258	Depositor DCC
R_{free} test set	1008 reflections (0.93%)	wwPDB-VP
Wilson B-factor (Å^2)	37.9	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16206	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2PJ, 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	0.60	3/8000 (0.0%)	0.65	0/10827
1	B	0.61	5/8038 (0.1%)	0.64	0/10876
2	C	0.92	0/14	0.67	0/18
2	D	0.98	0/14	0.43	0/18
All	All	0.61	8/16066 (0.0%)	0.65	0/21739

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	776	TRP	CD2-CE2	6.00	1.48	1.41
1	A	355	TRP	CD2-CE2	5.40	1.47	1.41
1	B	495	TRP	CD2-CE2	5.40	1.47	1.41
1	B	355	TRP	CD2-CE2	5.32	1.47	1.41
1	B	908	TRP	CD2-CE2	5.30	1.47	1.41
1	A	409	TRP	CD2-CE2	5.27	1.47	1.41
1	B	776	TRP	CD2-CE2	5.20	1.47	1.41
1	B	513	TRP	CD2-CE2	5.11	1.47	1.41

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	7804	0	7719	44	0
1	B	7840	0	7769	56	0
2	C	15	0	17	0	0
2	D	15	0	17	0	0
3	A	29	0	24	0	0
3	B	29	0	24	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	250	0	0	1	0
5	B	222	0	0	2	0
All	All	16206	0	15570	99	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 3.

All (99) 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:294:GLN:H	1:A:297:HIS:HD2	1.26	0.82
1:B:125:ASN:HD22	1:B:125:ASN:H	1.30	0.76
1:B:887:GLN:O	1:B:891:ILE:HG12	1.90	0.71
1:B:294:GLN:H	1:B:297:HIS:HD2	1.40	0.69
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.77	0.66
1:B:643:LYS:HA	1:B:744:MET:HE1	1.77	0.65
1:A:294:GLN:H	1:A:297:HIS:CD2	2.15	0.61
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.35	0.61
1:B:174:PHE:O	1:B:238:ARG:NH2	2.35	0.60
5:A:1429:HOH:O	1:B:711:ARG:HD3	2.02	0.60
1:B:294:GLN:H	1:B:297:HIS:CD2	2.21	0.59
1:B:224:TYR:HA	1:B:228:THR:HB	1.83	0.59
1:B:176:GLU:HG3	1:B:238:ARG:HH21	1.70	0.57
1:B:643:LYS:HA	1:B:744:MET:CE	2.35	0.56
1:A:400:LYS:HD2	1:A:518:LEU:HD21	1.87	0.55
1:A:77:LEU:HD22	1:A:267:LEU:HB3	1.88	0.55
1:A:887:GLN:O	1:A:891:ILE:HG12	2.07	0.54
1:A:600:LEU:HD21	1:A:649:MET:HG2	1.90	0.54
1:A:189:GLU:O	1:A:192:LYS:HB3	2.08	0.53
1:A:291:HIS:ND1	1:A:292:PRO:HD2	2.24	0.53
1:A:195:MET:O	1:A:307:ILE:HD12	2.09	0.53
1:A:648:LYS:O	1:A:652:PHE:HB2	2.09	0.53
1:B:413:GLU:HG2	1:B:531:ILE:HD11	1.91	0.53
1:B:176:GLU:HG3	1:B:238:ARG:NH2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:LEU:HD21	1:B:649:MET:HG2	1.91	0.53
1:A:817:GLU:HB2	1:A:818:PRO:HD3	1.91	0.52
1:B:201:LEU:HB3	3:B:1101:2PJ:H3	1.91	0.52
1:B:413:GLU:HG2	1:B:531:ILE:CD1	2.38	0.52
1:B:118:THR:HG23	1:B:121:TYR:H	1.75	0.52
1:B:635:ASN:HD21	1:B:732:ASN:HD22	1.56	0.52
1:B:82:THR:HG22	5:B:1319:HOH:O	2.09	0.51
1:A:820:PHE:CE1	1:A:824:ARG:HD3	2.46	0.50
1:B:80:ASP:OD1	1:B:82:THR:HB	2.10	0.50
1:B:648:LYS:O	1:B:652:PHE:HB2	2.12	0.50
1:A:309:ASP:H	1:A:672:ASN:HD21	1.58	0.49
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.47	0.49
1:A:121:TYR:HB3	1:A:126:GLU:HG2	1.94	0.49
1:A:655:ASP:OD2	1:A:658:ARG:HG2	2.12	0.49
1:B:484:SER:O	1:B:488:LYS:HE2	2.13	0.49
1:B:638:GLN:HB3	1:B:639:PRO:HD3	1.95	0.48
1:B:810:LEU:O	1:B:813:GLN:HB3	2.12	0.48
1:A:309:ASP:H	1:A:672:ASN:ND2	2.11	0.48
1:B:309:ASP:H	1:B:672:ASN:HD21	1.61	0.48
1:B:727:ALA:HB3	1:B:742:MET:HE2	1.94	0.48
1:B:493:GLU:OE2	1:B:495:TRP:HB2	2.14	0.48
1:A:813:GLN:HE22	1:A:892:ARG:NH2	2.12	0.48
1:A:100:PRO:HG2	1:A:103:ILE:HB	1.95	0.47
1:B:865:ALA:HB2	1:B:983:ALA:HA	1.97	0.47
1:B:367:ALA:HB3	1:B:370:PHE:CE2	2.50	0.47
1:B:227:GLU:O	1:B:230:PRO:HD2	2.15	0.46
1:B:557:SER:HB3	1:B:725:ILE:HB	1.96	0.46
1:A:871:GLU:O	1:A:875:GLU:HG3	2.14	0.46
1:A:638:GLN:HB3	1:A:639:PRO:HD3	1.98	0.46
1:A:763:LEU:O	1:B:1000:ARG:NH2	2.49	0.46
1:B:77:LEU:HD22	1:B:267:LEU:HB3	1.98	0.46
1:A:538:LEU:HD13	1:A:734:THR:HG23	1.97	0.46
1:A:864:GLU:HG3	1:A:986:LEU:HD21	1.97	0.46
1:B:780:GLN:NE2	5:B:1247:HOH:O	2.49	0.46
1:A:118:THR:HG22	1:A:172:PRO:HA	1.98	0.45
1:B:449:VAL:HG23	1:B:450:LEU:HD13	1.98	0.45
1:A:635:ASN:HD21	1:A:732:ASN:HD22	1.64	0.45
1:A:803:SER:HA	1:A:927:TYR:CE2	2.51	0.45
1:A:413:GLU:HG2	1:A:531:ILE:HD11	1.98	0.45
1:B:635:ASN:ND2	1:B:732:ASN:HD22	2.15	0.45
1:B:616:LEU:HD11	1:B:638:GLN:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:ARG:O	1:A:828:GLN:HA	2.17	0.44
1:A:917:ASN:O	1:A:920:ARG:HB2	2.18	0.44
1:A:940:TYR:CE1	1:A:945:ALA:HB2	2.52	0.44
1:B:978:ILE:O	1:B:979:ASN:HB2	2.18	0.44
1:A:616:LEU:HD11	1:A:638:GLN:HG3	1.99	0.44
1:B:722:ARG:HA	1:B:756:LYS:O	2.17	0.44
1:B:689:LEU:HD23	1:B:998:PHE:CE2	2.52	0.44
1:B:817:GLU:HB2	1:B:818:PRO:HD3	2.00	0.44
1:A:298:LEU:HD21	1:A:318:PRO:HG2	2.00	0.44
1:A:855:PRO:HA	1:A:856:PRO:HD3	1.92	0.43
1:B:163:ASP:O	1:B:167:GLN:HG2	2.18	0.43
1:A:175:ASP:OD1	1:A:177:SER:HB3	2.18	0.43
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.53	0.43
1:A:906:LYS:CE	1:A:921:ASP:OD2	2.67	0.42
1:B:778:VAL:HG22	1:B:955:SER:HB2	2.00	0.42
1:A:436:LYS:O	1:A:440:ILE:HG12	2.19	0.42
1:A:689:LEU:HD13	1:A:995:MET:HG2	2.02	0.42
1:A:236:ASP:HB3	1:A:239:GLN:HG2	2.00	0.42
1:B:771:LEU:HB2	1:B:952:HIS:HB3	2.01	0.42
1:A:679:HIS:O	1:A:683:MET:HG3	2.19	0.42
1:B:56:LYS:NZ	1:B:62:ARG:O	2.48	0.42
1:B:139:ASN:HB3	1:B:150:TYR:CZ	2.54	0.42
1:A:677:GLN:O	1:A:680:GLN:HB2	2.19	0.42
1:B:73:ILE:HG13	1:B:251:SER:HB2	2.02	0.42
1:B:309:ASP:H	1:B:672:ASN:ND2	2.17	0.42
1:B:803:SER:HA	1:B:927:TYR:CE2	2.55	0.42
1:B:301:LEU:HD21	1:B:303:LYS:HE3	2.01	0.41
1:A:362:GLY:HA2	1:A:373:PHE:CZ	2.56	0.41
1:B:44:ASN:HA	1:B:45:PRO:HD3	1.97	0.41
1:B:932:THR:O	1:B:935:ASP:HB2	2.21	0.41
1:B:829:LEU:HD23	1:B:829:LEU:HA	1.97	0.40
1:A:575:ASN:N	1:A:575:ASN:HD22	2.19	0.40
1:B:843:ILE:HG22	1:B:844:GLN:N	2.36	0.40
1:A:813:GLN:HE22	1:A:892:ARG:CZ	2.34	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	952/989 (96%)	921 (97%)	28 (3%)	3 (0%)	41	45
1	B	956/989 (97%)	923 (96%)	30 (3%)	3 (0%)	41	45
2	C	1/3 (33%)	1 (100%)	0	0	100	100
2	D	1/3 (33%)	1 (100%)	0	0	100	100
All	All	1910/1984 (96%)	1846 (97%)	58 (3%)	6 (0%)	41	45

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	877	MET
1	A	452	ALA
1	B	452	ALA
1	A	52	ASN
1	B	52	ASN
1	B	978	ILE

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	847/878 (96%)	828 (98%)	19 (2%)	52	64
1	B	854/878 (97%)	830 (97%)	24 (3%)	43	54
All	All	1701/1756 (97%)	1658 (98%)	43 (2%)	47	58

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	212	LYS
1	A	238	ARG
1	A	252	ASN
1	A	287	GLU
1	A	356	VAL
1	A	429	ARG
1	A	446	LEU
1	A	449	VAL
1	A	503	GLU
1	A	518	LEU
1	A	543	GLU
1	A	557	SER
1	A	558	LYS
1	A	604	LEU
1	A	689	LEU
1	A	789	SER
1	A	799	MET
1	A	821	ASN
1	B	102	ASN
1	B	124	GLU
1	B	125	ASN
1	B	128	SER
1	B	180	ASP
1	B	238	ARG
1	B	241	LEU
1	B	277	GLU
1	B	287	GLU
1	B	356	VAL
1	B	450	LEU
1	B	508	GLU
1	B	518	LEU
1	B	557	SER
1	B	604	LEU
1	B	689	LEU
1	B	742	MET
1	B	744	MET
1	B	789	SER
1	B	799	MET
1	B	824	ARG
1	B	933	LYS
1	B	988	GLN

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Mol	Chain	Res	Type
1	B	997	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	A	157	HIS
1	A	231	ASN
1	A	232	GLN
1	A	297	HIS
1	A	312	ASN
1	A	575	ASN
1	A	635	ASN
1	A	672	ASN
1	A	788	ASN
1	A	813	GLN
1	A	887	GLN
1	A	922	ASN
1	B	102	ASN
1	B	125	ASN
1	B	157	HIS
1	B	231	ASN
1	B	297	HIS
1	B	575	ASN
1	B	635	ASN
1	B	672	ASN
1	B	922	ASN
1	B	988	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
3	2PJ	A	1101	-	31,31,31	1.11	2 (6%)	41,44,44	1.52	4 (9%)
3	2PJ	B	1101	-	31,31,31	1.16	2 (6%)	41,44,44	1.54	8 (19%)

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
3	2PJ	A	1101	-	-	6/18/18/18	0/3/3/3
3	2PJ	B	1101	-	-	6/18/18/18	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	2PJ	O25-C26	-2.20	1.44	1.48
3	B	1101	2PJ	C1-C12	-2.19	1.51	1.54
3	B	1101	2PJ	C8-C9	-2.14	1.38	1.41
3	A	1101	2PJ	C23-N22	2.12	1.38	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1101	2PJ	C12-C21-N22	-5.56	105.13	112.55
3	B	1101	2PJ	C19-C13-C12	-3.92	114.53	121.34
3	B	1101	2PJ	C19-C13-C14	3.14	119.09	116.48
3	A	1101	2PJ	C21-N22-C23	3.11	126.22	121.62
3	A	1101	2PJ	C19-C13-C12	-2.74	116.58	121.34
3	B	1101	2PJ	F15-C14-C13	2.68	122.57	118.23
3	B	1101	2PJ	C5-C4-C9	2.55	122.06	118.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1101	2PJ	C2-C1-C12	-2.54	110.52	113.81
3	B	1101	2PJ	C5-C4-C3	-2.32	117.92	122.02
3	B	1101	2PJ	C26-O25-C23	-2.31	117.43	120.99
3	B	1101	2PJ	C16-C14-C13	-2.18	121.29	123.72
3	A	1101	2PJ	C2-C1-C12	2.13	116.56	113.81

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1101	2PJ	C2-C1-C12-C21
3	B	1101	2PJ	C1-C12-C13-C14
3	A	1101	2PJ	C21-C12-C13-C14
3	A	1101	2PJ	C1-C12-C13-C14
3	A	1101	2PJ	O25-C23-N22-C21
3	B	1101	2PJ	O25-C23-N22-C21
3	A	1101	2PJ	O24-C23-N22-C21
3	B	1101	2PJ	O24-C23-N22-C21
3	B	1101	2PJ	C1-C12-C13-C19
3	A	1101	2PJ	C21-C12-C13-C19
3	A	1101	2PJ	C1-C12-C13-C19
3	B	1101	2PJ	C2-C1-C12-C13

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1101	2PJ	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 2PJ A 1101

Bond lengths

Bond angles

Torsions

Rings

Ligand 2PJ B 1101

Bond lengths

Bond angles

Torsions

Rings
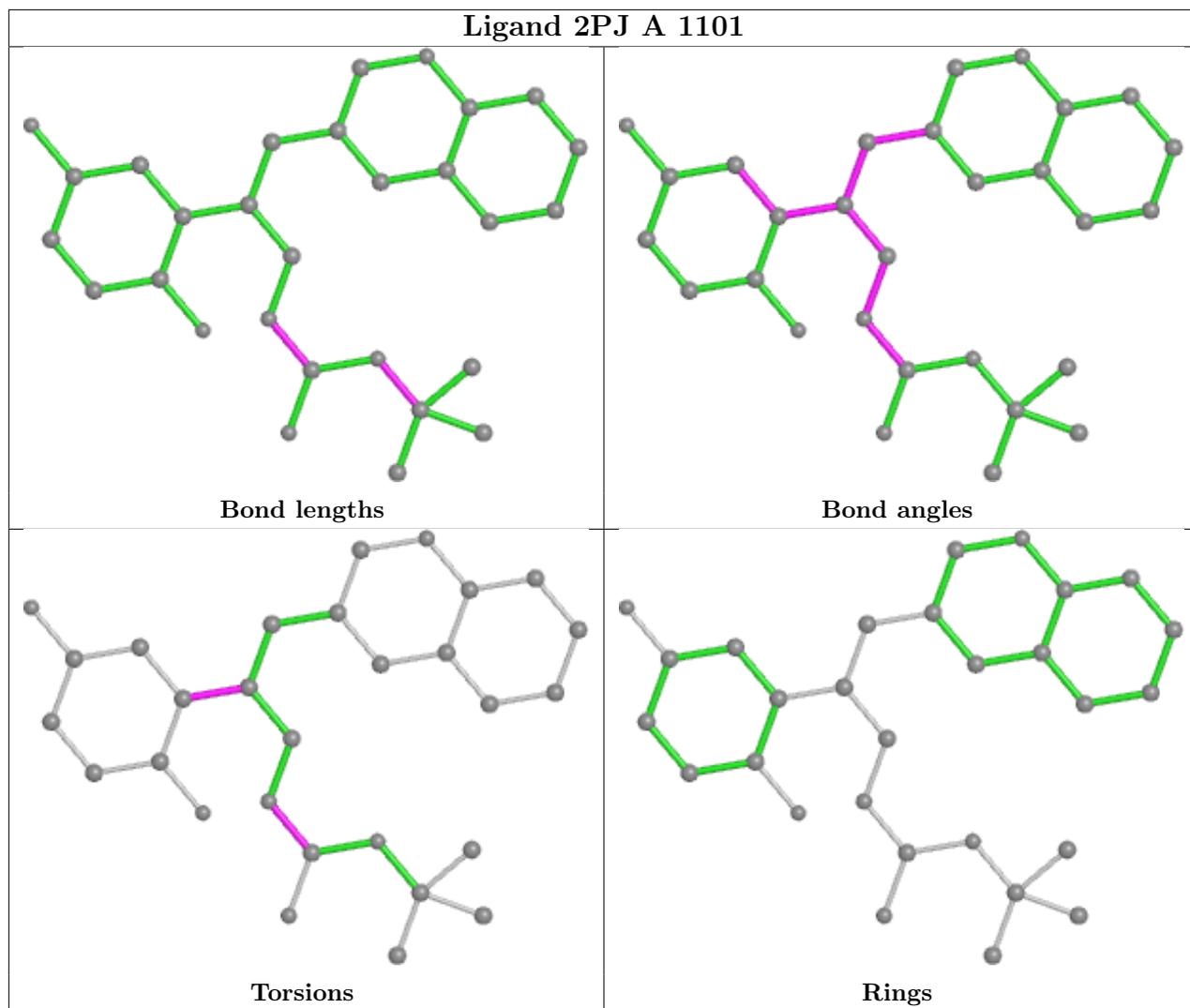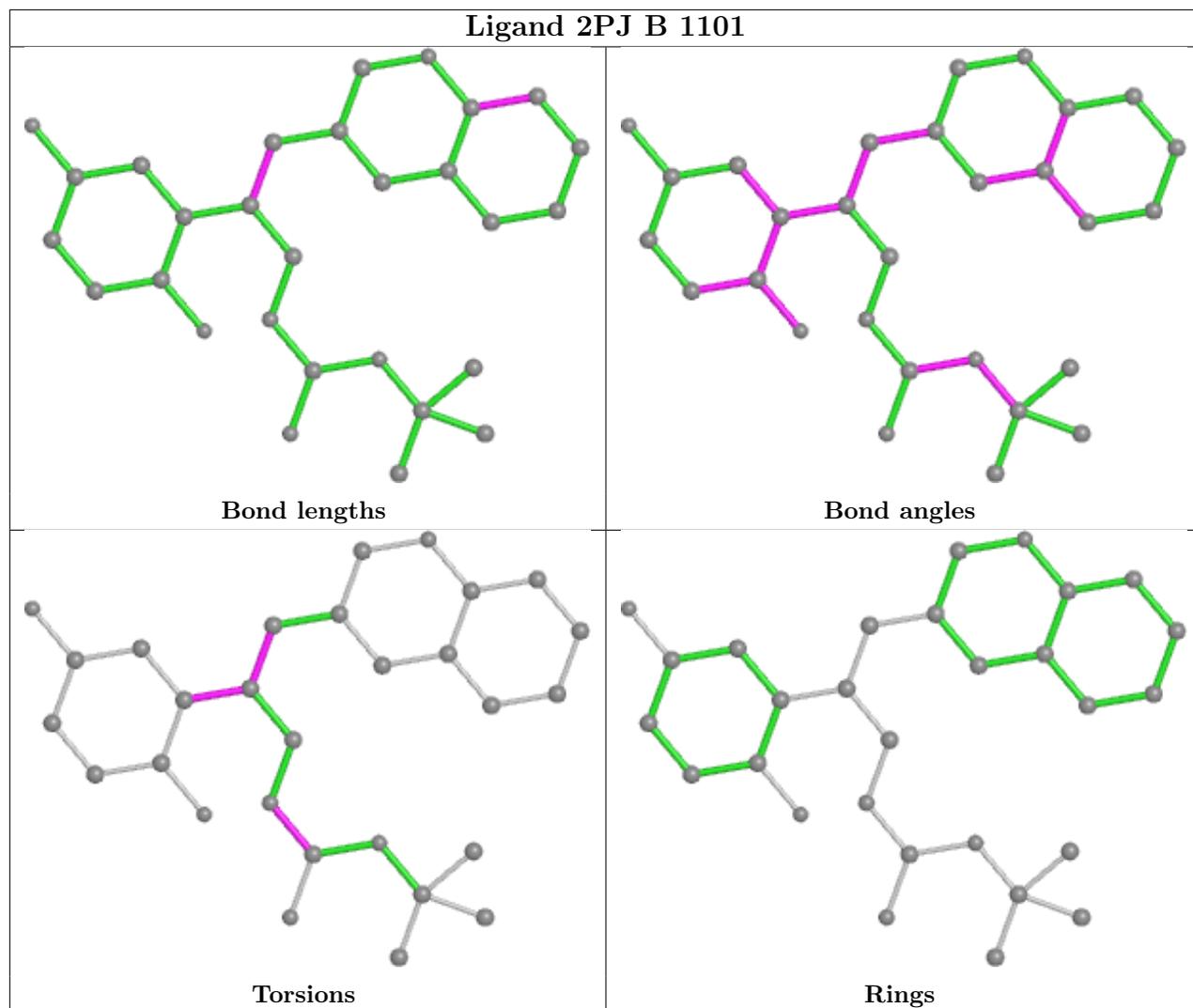
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6　Fit of model and data ⓘ

6.1　Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	955/989 (96%)	-0.05	20 (2%)	63	61	24, 44, 74, 97	0
1	B	959/989 (96%)	-0.05	22 (2%)	60	58	26, 44, 71, 118	0
2	C	3/3 (100%)	-0.39	0	100	100	40, 40, 44, 45	0
2	D	3/3 (100%)	0.89	0	100	100	39, 39, 51, 52	0
All	All	1920/1984 (96%)	-0.05	42 (2%)	62	60	24, 44, 73, 118	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1012	ILE	8.0
1	B	979	ASN	7.3
1	B	1012	ILE	5.1
1	B	518	LEU	5.0
1	A	1011	HIS	4.8
1	B	977	ASP	4.7
1	A	982	GLN	4.5
1	B	978	ILE	4.4
1	A	45	PRO	4.1
1	B	45	PRO	4.1
1	A	119	LYS	3.9
1	B	1010	PRO	3.8
1	B	43	ASN	3.5
1	B	1009	LYS	3.4
1	A	988	GLN	3.2
1	B	985	ALA	2.9
1	A	980	LEU	2.9
1	B	964	ASP	2.9
1	A	517	ASP	2.8
1	B	965	SER	2.8
1	B	129	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	1011	HIS	2.6
1	A	282	ASN	2.6
1	B	508	GLU	2.5
1	A	986	LEU	2.5
1	A	810	LEU	2.4
1	A	122	PRO	2.4
1	B	811	PHE	2.3
1	B	44	ASN	2.3
1	B	258	VAL	2.2
1	A	258	VAL	2.2
1	A	857	HIS	2.2
1	B	70	ALA	2.2
1	A	337	LEU	2.1
1	B	123	LYS	2.1
1	A	110	LEU	2.1
1	B	257	VAL	2.1
1	A	811	PHE	2.1
1	A	1010	PRO	2.1
1	B	76	LEU	2.0
1	A	831	TYR	2.0
1	A	124	GLU	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 monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	2PJ	B	1101	29/29	0.84	0.18	56,61,66,69	0
3	2PJ	A	1101	29/29	0.88	0.14	34,40,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	A	1102	1/1	0.98	0.02	76,76,76,76	0
4	ZN	B	1102	1/1	0.98	0.04	88,88,88,88	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 2PJ B 1101:

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

Electron density around 2PJ A 1101:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
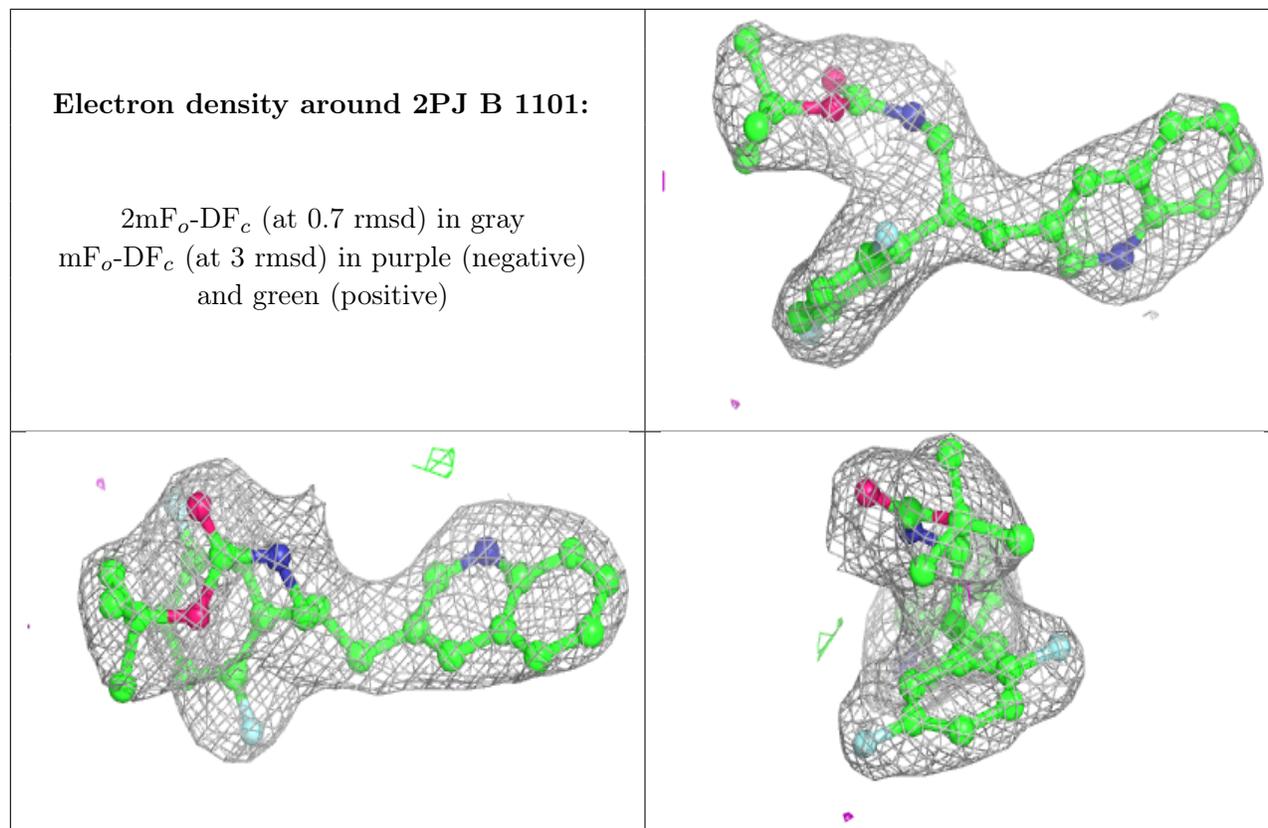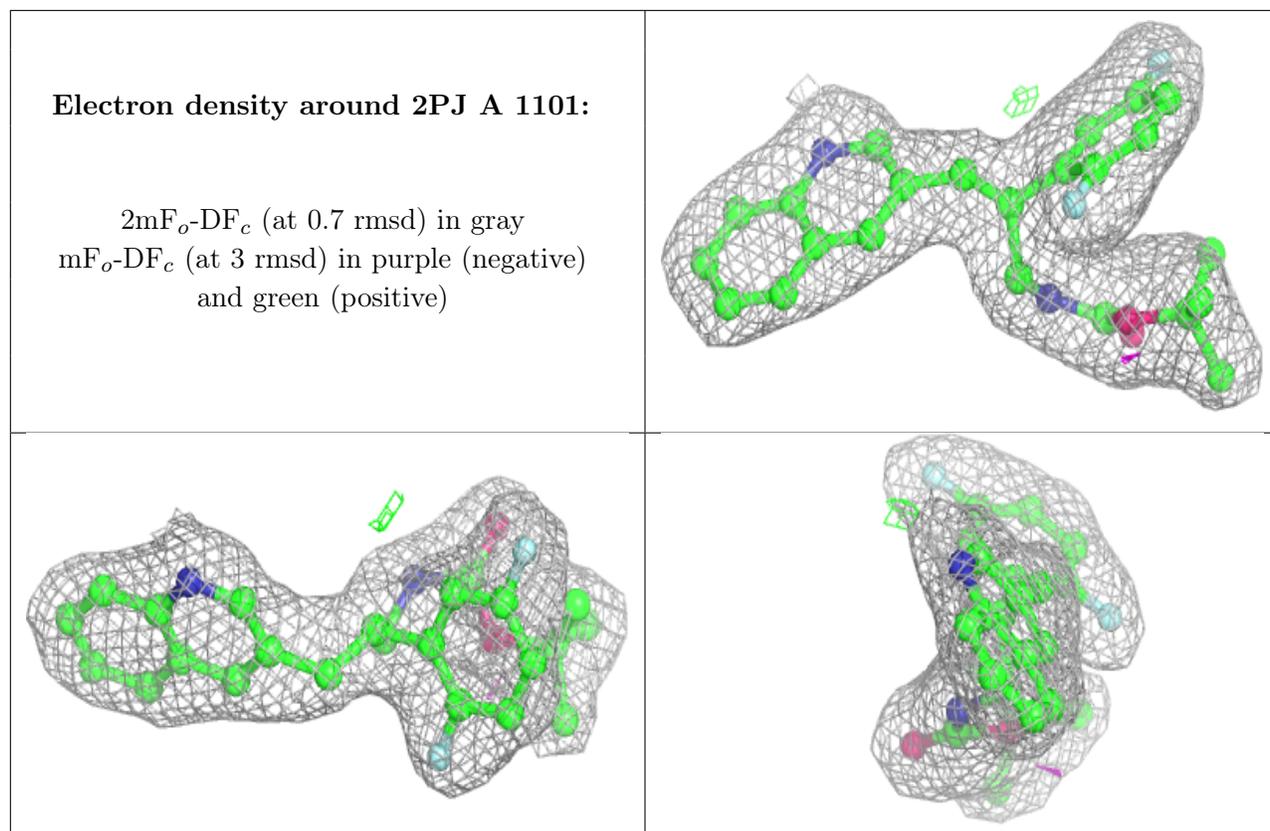
6.5 Other polymers (i)

There are no such residues in this entry.