



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:50 AM UTC

PDB ID : 4PV7 / pdb_00004pv7
Title : Cocrystal structure of dipeptidyl-peptidase 4 with an indole scaffold inhibitor
Authors : Xiao, P.; Guo, R.; Huang, S.; Cui, H.; Ye, S.; Zhang, Z.
Deposited on : 2014-03-15
Resolution : 3.24 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

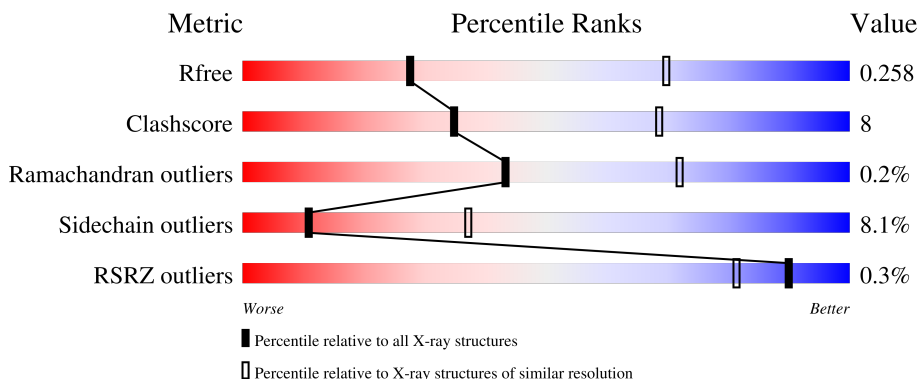
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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	752	 73% 21% . .
1	B	752	 75% 20% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11948 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 Dipeptidyl peptidase 4 soluble form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5951	3821	978	1126	26			
1	B	727	Total	C	N	O	S	0	0	0
			5951	3821	978	1126	26			

There are 48 discrepancies between the modelled and reference sequences:

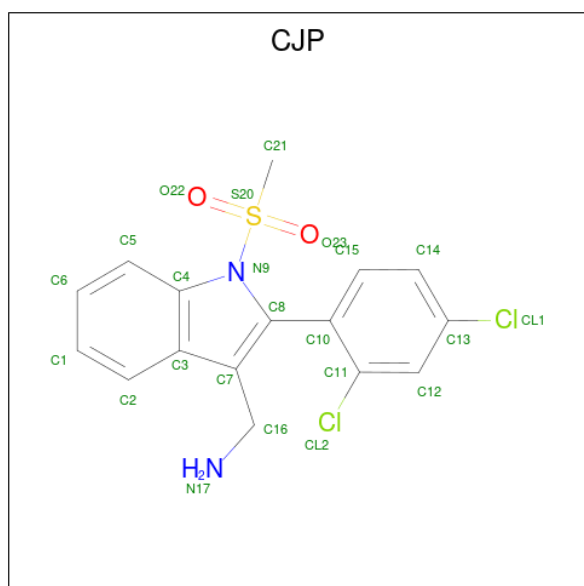
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	HIS	-	expression tag	UNP P27487
A	16	HIS	-	expression tag	UNP P27487
A	17	HIS	-	expression tag	UNP P27487
A	18	HIS	-	expression tag	UNP P27487
A	19	HIS	-	expression tag	UNP P27487
A	20	HIS	-	expression tag	UNP P27487
A	21	ASP	-	expression tag	UNP P27487
A	22	TYR	-	expression tag	UNP P27487
A	23	ASP	-	expression tag	UNP P27487
A	24	ILE	-	expression tag	UNP P27487
A	25	PRO	-	expression tag	UNP P27487
A	26	THR	-	expression tag	UNP P27487
A	27	THR	-	expression tag	UNP P27487
A	28	GLU	-	expression tag	UNP P27487
A	29	ASN	-	expression tag	UNP P27487
A	30	LEU	-	expression tag	UNP P27487
A	31	TYR	-	expression tag	UNP P27487
A	32	PHE	-	expression tag	UNP P27487
A	33	GLN	-	expression tag	UNP P27487
A	34	GLY	-	expression tag	UNP P27487
A	35	ALA	-	expression tag	UNP P27487
A	36	MET	-	expression tag	UNP P27487
A	37	GLY	-	expression tag	UNP P27487
A	38	SER	-	expression tag	UNP P27487
B	15	HIS	-	expression tag	UNP P27487

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Chain	Residue	Modelled	Actual	Comment	Reference
B	16	HIS	-	expression tag	UNP P27487
B	17	HIS	-	expression tag	UNP P27487
B	18	HIS	-	expression tag	UNP P27487
B	19	HIS	-	expression tag	UNP P27487
B	20	HIS	-	expression tag	UNP P27487
B	21	ASP	-	expression tag	UNP P27487
B	22	TYR	-	expression tag	UNP P27487
B	23	ASP	-	expression tag	UNP P27487
B	24	ILE	-	expression tag	UNP P27487
B	25	PRO	-	expression tag	UNP P27487
B	26	THR	-	expression tag	UNP P27487
B	27	THR	-	expression tag	UNP P27487
B	28	GLU	-	expression tag	UNP P27487
B	29	ASN	-	expression tag	UNP P27487
B	30	LEU	-	expression tag	UNP P27487
B	31	TYR	-	expression tag	UNP P27487
B	32	PHE	-	expression tag	UNP P27487
B	33	GLN	-	expression tag	UNP P27487
B	34	GLY	-	expression tag	UNP P27487
B	35	ALA	-	expression tag	UNP P27487
B	36	MET	-	expression tag	UNP P27487
B	37	GLY	-	expression tag	UNP P27487
B	38	SER	-	expression tag	UNP P27487

- Molecule 2 is 1-[2-(2,4-dichlorophenyl)-1-(methylsulfonyl)-1H-indol-3-yl]methanamine (CCD ID: CJP) (formula: C₁₆H₁₄Cl₂N₂O₂S).

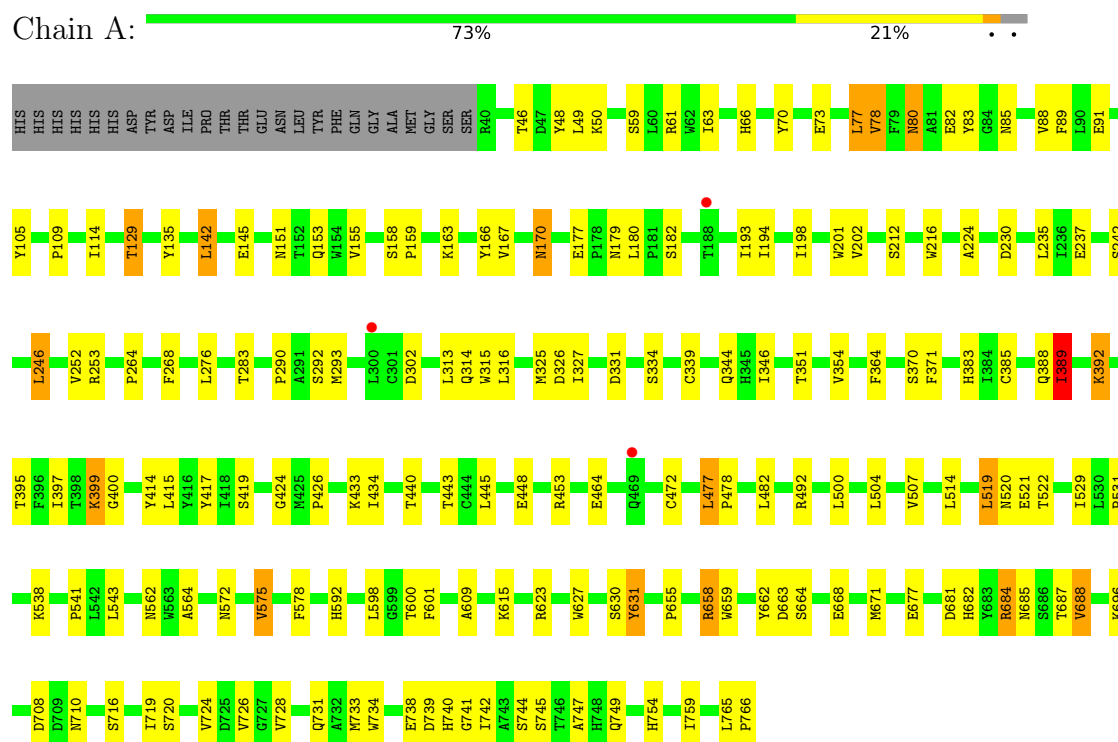


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 23	C 16	Cl 2	N 2	O 2	S 1	0	0
2	B	1	Total 23	C 16	Cl 2	N 2	O 2	S 1	0	0

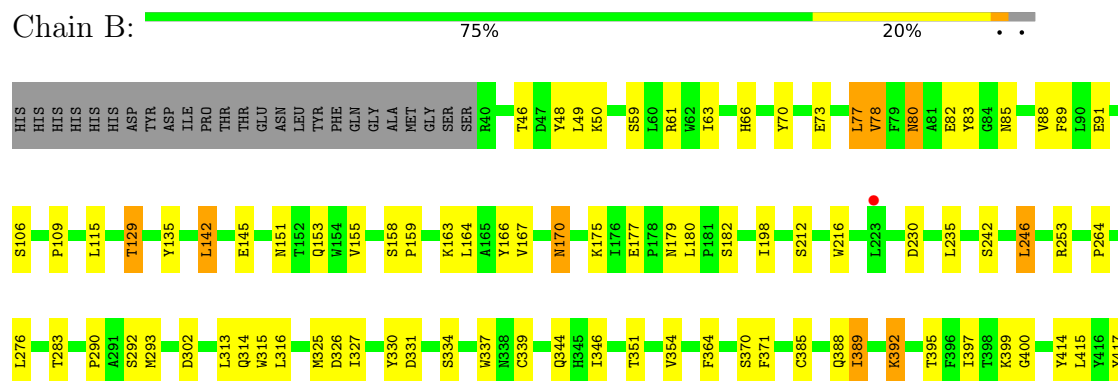
3 Residue-property plots

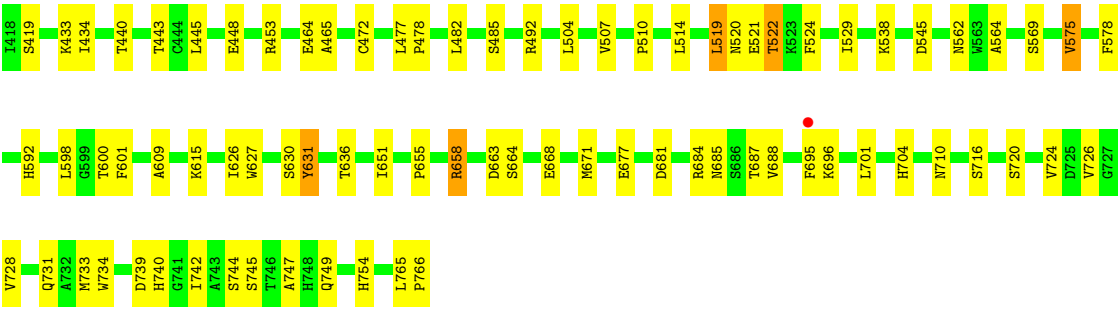
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dipeptidyl peptidase 4 soluble form



- Molecule 1: Dipeptidyl peptidase 4 soluble form





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	79.81Å 79.81Å 286.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.75 – 3.24 49.75 – 3.24	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.75-3.24) 99.9 (49.75-3.24)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.264 0.217 , 0.258	Depositor DCC
R_{free} test set	1332 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	114.4	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 90.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l 0.065 for h,-h-k,-l 0.043 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11948	wwPDB-VP
Average B, all atoms (Å ²)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CJP

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	0.54	0/6123	0.82	2/8329 (0.0%)
1	B	0.52	0/6123	0.82	2/8329 (0.0%)
All	All	0.53	0/12246	0.82	4/16658 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	400	GLY	N-CA-C	6.86	119.52	111.63
1	B	400	GLY	N-CA-C	5.38	117.82	111.63
1	A	631	TYR	N-CA-C	-5.02	105.72	111.14
1	B	631	TYR	N-CA-C	-5.00	105.74	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5951	0	5669	92	0
1	B	5951	0	5669	83	0
2	A	23	0	14	1	0
2	B	23	0	14	2	0
All	All	11948	0	11366	175	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 8.

All (175) 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:253:ARG:HH21	1:B:253:ARG:HH21	1.11	0.92
1:B:153:GLN:HE22	1:B:170:ASN:H	1.26	0.83
1:A:153:GLN:HE22	1:A:170:ASN:H	1.27	0.78
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.67	0.75
1:A:80:ASN:HD22	1:A:82:GLU:H	1.36	0.73
1:B:80:ASN:HD22	1:B:82:GLU:H	1.33	0.73
1:B:564:ALA:HB1	1:B:575:VAL:HG21	1.70	0.73
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.69	0.73
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.73	0.70
1:B:664:SER:HB2	1:B:668:GLU:OE2	1.91	0.69
1:A:564:ALA:HB1	1:A:575:VAL:HG21	1.75	0.69
1:B:242:SER:HB3	1:B:246:LEU:HD12	1.75	0.68
1:A:664:SER:HB2	1:A:668:GLU:OE2	1.96	0.66
1:B:351:THR:OG1	1:B:592:HIS:HD2	1.77	0.66
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.79	0.65
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.80	0.64
1:B:314:GLN:HG3	1:B:325:MET:HG3	1.80	0.64
2:B:1000:CJP:H1	2:B:1000:CJP:H4	1.80	0.63
1:B:733:MET:HE3	1:B:754:HIS:CE1	2.34	0.63
1:B:230:ASP:OD1	1:B:264:PRO:HB3	2.00	0.62
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.80	0.62
1:A:155:VAL:HG12	1:A:166:TYR:HB3	1.83	0.61
1:A:331:ASP:HB3	1:A:334:SER:HB2	1.82	0.61
1:B:109:PRO:HG2	1:B:158:SER:O	2.00	0.61
1:A:433:LYS:HD2	1:A:445:LEU:HD21	1.83	0.60
1:A:158:SER:OG	1:A:163:LYS:HB2	2.01	0.60
1:B:155:VAL:HG12	1:B:166:TYR:HB3	1.83	0.60
1:A:290:PRO:HG3	1:A:326:ASP:OD1	2.02	0.59
2:A:1000:CJP:H1	2:A:1000:CJP:H4	1.82	0.59
1:B:158:SER:OG	1:B:163:LYS:HB2	2.03	0.59
1:A:314:GLN:HG3	1:A:325:MET:HG3	1.83	0.59
1:B:327:ILE:HD13	1:B:389:ILE:CD1	2.34	0.58
1:A:46:THR:O	1:A:50:LYS:HB2	2.04	0.57
1:A:733:MET:HE3	1:A:754:HIS:CE1	2.40	0.57
1:B:46:THR:O	1:B:50:LYS:HB2	2.05	0.56
1:B:433:LYS:HD2	1:B:445:LEU:HD21	1.86	0.56
1:A:230:ASP:OD1	1:A:264:PRO:HB3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:PHE:CD2	1:A:609:ALA:HB2	2.40	0.56
1:A:325:MET:HE1	1:A:371:PHE:CZ	2.39	0.56
1:A:327:ILE:HD13	1:A:389:ILE:CD1	2.35	0.56
1:B:564:ALA:CB	1:B:575:VAL:HG21	2.36	0.56
1:A:109:PRO:HG2	1:A:158:SER:O	2.06	0.55
1:B:83:TYR:HB2	1:B:85:ASN:OD1	2.07	0.55
1:B:325:MET:HE1	1:B:371:PHE:CZ	2.42	0.54
1:A:83:TYR:HB2	1:A:85:ASN:OD1	2.07	0.54
1:A:417:TYR:HE1	1:A:419:SER:HB3	1.73	0.54
1:B:330:TYR:HB2	1:B:337:TRP:CZ3	2.42	0.53
1:B:331:ASP:HB3	1:B:334:SER:HB2	1.90	0.53
1:A:630:SER:OG	1:A:740:HIS:NE2	2.42	0.53
1:B:49:LEU:HD22	1:B:749:GLN:HA	1.92	0.52
1:B:600:THR:OG1	1:B:601:PHE:N	2.43	0.52
1:B:364:PHE:CD2	1:B:371:PHE:HB3	2.46	0.51
1:B:177:GLU:HB2	1:B:180:LEU:HD12	1.93	0.51
1:B:397:ILE:HD12	1:B:434:ILE:HD13	1.93	0.51
1:A:397:ILE:HD12	1:A:434:ILE:HD13	1.92	0.51
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.92	0.51
1:B:744:SER:HB2	1:B:747:ALA:HB3	1.93	0.51
1:A:48:TYR:CE1	1:A:562:ASN:HA	2.46	0.50
1:B:433:LYS:HB3	1:B:445:LEU:HD11	1.93	0.50
1:A:433:LYS:HB3	1:A:445:LEU:HD11	1.93	0.50
1:A:564:ALA:CB	1:A:575:VAL:HG21	2.41	0.50
1:B:710:ASN:C	1:B:710:ASN:HD22	2.21	0.49
1:A:364:PHE:CD2	1:A:371:PHE:HB3	2.47	0.49
1:B:290:PRO:HG3	1:B:326:ASP:OD1	2.12	0.49
1:A:177:GLU:HB2	1:A:180:LEU:HD12	1.93	0.49
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.43	0.49
1:B:48:TYR:CE1	1:B:562:ASN:HA	2.47	0.49
1:B:681:ASP:O	1:B:685:ASN:HB2	2.13	0.49
1:A:688:VAL:HG22	1:A:719:ILE:HG12	1.95	0.48
1:A:472:CYS:O	1:A:478:PRO:HA	2.13	0.48
1:A:600:THR:OG1	1:A:601:PHE:N	2.45	0.48
1:A:720:SER:O	1:A:724:VAL:HG23	2.13	0.48
1:B:598:LEU:HG	1:B:631:TYR:OH	2.13	0.48
1:A:78:VAL:HG22	1:A:89:PHE:HB2	1.96	0.48
1:B:417:TYR:HE1	1:B:419:SER:HB3	1.78	0.48
1:B:519:LEU:O	1:B:520:ASN:C	2.57	0.48
1:A:351:THR:OG1	1:A:592:HIS:CD2	2.64	0.48
1:A:325:MET:HE3	1:A:327:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:THR:OG1	1:B:592:HIS:CD2	2.63	0.47
1:A:170:ASN:HD22	1:A:170:ASN:N	2.12	0.47
1:B:346:ILE:H	1:B:392:LYS:NZ	2.13	0.47
1:B:630:SER:OG	1:B:740:HIS:NE2	2.47	0.47
1:A:49:LEU:HD22	1:A:749:GLN:HA	1.97	0.47
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.95	0.47
1:A:655:PRO:HD2	1:A:716:SER:OG	2.15	0.47
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.96	0.47
1:A:658:ARG:HH21	1:A:687:THR:HG21	1.79	0.46
1:A:708:ASP:OD1	1:A:740:HIS:HA	2.15	0.46
1:A:59:SER:N	1:A:70:TYR:HE1	2.14	0.46
1:B:78:VAL:HG22	1:B:89:PHE:HB2	1.97	0.46
1:B:472:CYS:O	1:B:478:PRO:HA	2.15	0.46
1:B:626:ILE:HG23	1:B:636:THR:HG23	1.97	0.46
1:A:193:ILE:HG22	1:A:194:ILE:HG12	1.97	0.46
1:A:681:ASP:O	1:A:685:ASN:HB2	2.16	0.46
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.46	0.46
1:B:465:ALA:O	1:B:485:SER:OG	2.32	0.46
1:B:658:ARG:HH21	1:B:687:THR:HG21	1.81	0.46
1:A:346:ILE:H	1:A:392:LYS:NZ	2.15	0.45
1:B:720:SER:O	1:B:724:VAL:HG23	2.17	0.45
1:A:738:GLU:OE1	1:A:744:SER:OG	2.30	0.45
1:B:529:ILE:HB	1:B:575:VAL:HG22	1.98	0.45
1:A:293:MET:HG3	1:A:315:TRP:CB	2.47	0.45
1:A:529:ILE:HB	1:A:575:VAL:HG22	1.99	0.45
1:B:155:VAL:HG12	1:B:166:TYR:CB	2.47	0.45
1:B:578:PHE:CD2	1:B:609:ALA:HB2	2.52	0.45
1:B:106:SER:HB3	1:B:115:LEU:HB3	1.99	0.45
1:A:88:VAL:HG11	1:A:91:GLU:HG3	1.99	0.45
1:A:155:VAL:HG12	1:A:166:TYR:CB	2.48	0.44
1:A:658:ARG:HH12	1:A:684:ARG:NE	2.15	0.44
1:B:59:SER:N	1:B:70:TYR:HE1	2.15	0.44
1:B:293:MET:HG3	1:B:315:TRP:HB2	1.99	0.44
1:B:135:TYR:HD1	1:B:142:LEU:HD13	1.82	0.44
1:B:327:ILE:HD13	1:B:389:ILE:HD12	1.99	0.44
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.99	0.44
1:A:235:LEU:HD13	1:A:253:ARG:HB3	1.99	0.44
1:B:598:LEU:HD22	1:B:671:MET:HG2	2.00	0.44
1:B:129:THR:HG23	1:B:151:ASN:HA	1.99	0.44
1:A:293:MET:HG3	1:A:315:TRP:HB2	2.00	0.44
1:B:739:ASP:CG	1:B:740:HIS:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:TYR:OH	1:A:710:ASN:ND2	2.50	0.43
1:B:655:PRO:HD2	1:B:716:SER:OG	2.18	0.43
1:A:659:TRP:CD1	1:A:671:MET:HE2	2.54	0.43
1:B:734:TRP:CD1	1:B:734:TRP:C	2.96	0.43
1:A:744:SER:HB2	1:A:747:ALA:HB3	1.99	0.43
1:B:88:VAL:HG11	1:B:91:GLU:HG3	2.00	0.43
1:B:740:HIS:NE2	2:B:1000:CJP:CL2	2.89	0.43
1:A:414:TYR:CD2	1:A:433:LYS:HE2	2.54	0.43
1:A:541:PRO:HG3	1:A:623:ARG:NH2	2.34	0.43
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.84	0.43
1:B:695:PHE:HB3	1:B:728:VAL:HG11	2.01	0.43
1:B:739:ASP:CG	1:B:740:HIS:H	2.27	0.42
1:B:545:ASP:OD2	1:B:545:ASP:C	2.62	0.42
1:A:237:GLU:HA	1:A:252:VAL:O	2.19	0.42
1:B:77:LEU:HD13	1:B:88:VAL:HA	2.01	0.42
1:B:325:MET:HE3	1:B:327:ILE:HD11	2.01	0.42
1:A:167:VAL:HG21	1:A:198:ILE:HG23	2.00	0.42
1:A:383:HIS:CE1	1:A:399:LYS:C	2.98	0.42
1:A:600:THR:CG2	1:A:682:HIS:HE1	2.33	0.42
1:A:129:THR:HG23	1:A:151:ASN:HA	2.02	0.42
1:A:765:LEU:HA	1:A:766:PRO:HD3	1.90	0.41
1:A:326:ASP:OD2	1:A:344:GLN:HG2	2.20	0.41
1:A:424:GLY:O	1:A:426:PRO:HD3	2.20	0.41
1:A:734:TRP:CD1	1:A:734:TRP:C	2.98	0.41
1:B:235:LEU:HD13	1:B:253:ARG:HB3	2.02	0.41
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.55	0.41
1:A:519:LEU:O	1:A:520:ASN:C	2.63	0.41
1:B:414:TYR:CD2	1:B:433:LYS:HE2	2.56	0.41
1:A:415:LEU:HB3	1:A:434:ILE:HG23	2.03	0.41
1:A:741:GLY:O	1:A:742:ILE:C	2.63	0.41
1:A:759:ILE:HD13	1:A:759:ILE:HA	1.97	0.41
1:B:765:LEU:HA	1:B:766:PRO:HD3	1.87	0.41
1:A:598:LEU:HD22	1:A:671:MET:HG2	2.03	0.41
1:A:739:ASP:CG	1:A:740:HIS:N	2.77	0.41
1:B:510:PRO:HD3	1:B:569:SER:HB2	2.03	0.41
1:A:135:TYR:HD1	1:A:142:LEU:HD13	1.86	0.41
1:A:417:TYR:CE1	1:A:419:SER:HB3	2.54	0.41
1:A:543:LEU:O	1:A:575:VAL:HA	2.21	0.41
1:B:651:ILE:HG12	1:B:701:LEU:HB3	2.03	0.41
1:A:541:PRO:HG3	1:A:623:ARG:CZ	2.50	0.41
1:A:745:SER:O	1:A:749:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:ALA:HB1	1:B:575:VAL:CG2	2.46	0.41
1:B:745:SER:O	1:B:749:GLN:HG3	2.21	0.41
1:A:598:LEU:HG	1:A:631:TYR:OH	2.21	0.40
1:A:710:ASN:HD22	1:A:710:ASN:C	2.30	0.40
1:B:164:LEU:HB3	1:B:175:LYS:HB2	2.03	0.40
1:B:167:VAL:HG21	1:B:198:ILE:HG23	2.03	0.40
1:B:293:MET:HG3	1:B:315:TRP:CB	2.51	0.40
1:A:201:TRP:CE3	1:A:202:VAL:HA	2.55	0.40
1:A:744:SER:O	1:A:745:SER:C	2.65	0.40
1:B:326:ASP:OD2	1:B:344:GLN:HG2	2.21	0.40
1:B:415:LEU:HB3	1:B:434:ILE:HG23	2.02	0.40
1:B:522:THR:HB	1:B:524:PHE:CE2	2.56	0.40
1:B:598:LEU:HB2	1:B:671:MET:SD	2.61	0.40
1:A:77:LEU:HD13	1:A:88:VAL:HA	2.02	0.40
1:A:477:LEU:HG	1:A:500:LEU:HD23	2.03	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	725/752 (96%)	672 (93%)	51 (7%)	2 (0%)	36	66
1	B	725/752 (96%)	672 (93%)	52 (7%)	1 (0%)	48	77
All	All	1450/1504 (96%)	1344 (93%)	103 (7%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	B	73	GLU
1	A	389	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	651/674 (97%)	599 (92%)	52 (8%)	11	37
1	B	651/674 (97%)	597 (92%)	54 (8%)	10	36
All	All	1302/1348 (97%)	1196 (92%)	106 (8%)	11	37

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	63	ILE
1	A	66	HIS
1	A	77	LEU
1	A	78	VAL
1	A	80	ASN
1	A	129	THR
1	A	142	LEU
1	A	145	GLU
1	A	170	ASN
1	A	179	ASN
1	A	182	SER
1	A	212	SER
1	A	246	LEU
1	A	276	LEU
1	A	283	THR
1	A	292	SER
1	A	313	LEU
1	A	316	LEU
1	A	339	CYS
1	A	354	VAL
1	A	370	SER
1	A	385	CYS
1	A	388	GLN
1	A	389	ILE
1	A	392	LYS
1	A	395	THR

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Mol	Chain	Res	Type
1	A	399	LYS
1	A	440	THR
1	A	443	THR
1	A	448	GLU
1	A	453	ARG
1	A	464	GLU
1	A	477	LEU
1	A	482	LEU
1	A	492	ARG
1	A	504	LEU
1	A	507	VAL
1	A	514	LEU
1	A	519	LEU
1	A	521	GLU
1	A	522	THR
1	A	538	LYS
1	A	575	VAL
1	A	615	LYS
1	A	627	TRP
1	A	658	ARG
1	A	663	ASP
1	A	677	GLU
1	A	684	ARG
1	A	688	VAL
1	A	731	GLN
1	B	61	ARG
1	B	63	ILE
1	B	66	HIS
1	B	77	LEU
1	B	78	VAL
1	B	80	ASN
1	B	129	THR
1	B	142	LEU
1	B	145	GLU
1	B	170	ASN
1	B	179	ASN
1	B	182	SER
1	B	212	SER
1	B	246	LEU
1	B	276	LEU
1	B	283	THR
1	B	292	SER

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Mol	Chain	Res	Type
1	B	313	LEU
1	B	316	LEU
1	B	339	CYS
1	B	354	VAL
1	B	370	SER
1	B	385	CYS
1	B	388	GLN
1	B	389	ILE
1	B	392	LYS
1	B	395	THR
1	B	399	LYS
1	B	440	THR
1	B	443	THR
1	B	448	GLU
1	B	453	ARG
1	B	464	GLU
1	B	477	LEU
1	B	482	LEU
1	B	492	ARG
1	B	504	LEU
1	B	507	VAL
1	B	514	LEU
1	B	519	LEU
1	B	521	GLU
1	B	522	THR
1	B	538	LYS
1	B	575	VAL
1	B	615	LYS
1	B	627	TRP
1	B	658	ARG
1	B	663	ASP
1	B	677	GLU
1	B	684	ARG
1	B	688	VAL
1	B	704	HIS
1	B	731	GLN
1	B	742	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN

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Mol	Chain	Res	Type
1	A	153	GLN
1	A	169	ASN
1	A	170	ASN
1	A	338	ASN
1	A	455	GLN
1	A	505	GLN
1	A	506	ASN
1	A	572	ASN
1	A	592	HIS
1	A	685	ASN
1	A	710	ASN
1	A	761	GLN
1	B	80	ASN
1	B	153	GLN
1	B	169	ASN
1	B	170	ASN
1	B	338	ASN
1	B	435	GLN
1	B	455	GLN
1	B	505	GLN
1	B	506	ASN
1	B	572	ASN
1	B	592	HIS
1	B	685	ASN
1	B	697	GLN
1	B	710	ASN
1	B	761	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 oligosaccharides in this entry.

5.6 Ligand geometry

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	CJP	A	1000	-	25,25,25	2.79	8 (32%)	33,38,38	3.56	13 (39%)
2	CJP	B	1000	-	25,25,25	3.00	9 (36%)	33,38,38	3.56	13 (39%)

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	CJP	A	1000	-	-	4/10/12/12	0/3/3/3
2	CJP	B	1000	-	-	4/10/12/12	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	CJP	C8-C7	6.94	1.48	1.37
2	B	1000	CJP	C10-C11	6.81	1.49	1.39
2	A	1000	CJP	C8-C7	6.40	1.47	1.37
2	B	1000	CJP	C3-C4	5.95	1.48	1.41
2	A	1000	CJP	C3-C4	5.86	1.48	1.41
2	A	1000	CJP	C10-C11	5.62	1.47	1.39
2	B	1000	CJP	C4-N9	-5.45	1.35	1.42
2	A	1000	CJP	C4-N9	-5.18	1.36	1.42
2	B	1000	CJP	C8-N9	-5.14	1.35	1.43
2	A	1000	CJP	C8-N9	-4.85	1.36	1.43
2	A	1000	CJP	C21-S20	-3.59	1.68	1.75
2	B	1000	CJP	C21-S20	-3.50	1.68	1.75
2	B	1000	CJP	C11-CL2	3.10	1.80	1.73
2	A	1000	CJP	C11-CL2	2.49	1.79	1.73
2	B	1000	CJP	S20-N9	-2.45	1.62	1.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	CJP	C3-C7	2.40	1.48	1.44
2	A	1000	CJP	C3-C7	2.33	1.48	1.44

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	CJP	C4-N9-C8	9.99	115.12	107.22
2	A	1000	CJP	C4-N9-C8	9.51	114.74	107.22
2	A	1000	CJP	C10-C8-C7	-8.46	119.54	128.34
2	B	1000	CJP	C10-C8-C7	-8.26	119.75	128.34
2	A	1000	CJP	O22-S20-O23	-8.01	106.48	118.46
2	B	1000	CJP	O22-S20-O23	-7.61	107.08	118.46
2	A	1000	CJP	C10-C8-N9	6.80	132.98	123.36
2	B	1000	CJP	C10-C8-N9	6.74	132.90	123.36
2	A	1000	CJP	O23-S20-N9	5.30	112.50	106.79
2	A	1000	CJP	C21-S20-N9	5.04	112.03	104.83
2	B	1000	CJP	O23-S20-N9	4.71	111.86	106.79
2	B	1000	CJP	C21-S20-N9	4.52	111.28	104.83
2	A	1000	CJP	C5-C4-N9	4.44	136.73	130.48
2	B	1000	CJP	C5-C4-N9	4.41	136.68	130.48
2	A	1000	CJP	C5-C4-C3	-4.32	117.12	121.95
2	B	1000	CJP	C5-C4-C3	-4.28	117.17	121.95
2	B	1000	CJP	C12-C11-C10	-3.48	118.74	121.59
2	B	1000	CJP	O22-S20-N9	3.40	110.45	106.79
2	B	1000	CJP	C3-C7-C8	-2.71	104.88	107.12
2	A	1000	CJP	O22-S20-N9	2.49	109.47	106.79
2	A	1000	CJP	C3-C7-C8	-2.37	105.17	107.12
2	B	1000	CJP	C2-C3-C4	2.28	121.87	119.24
2	A	1000	CJP	C12-C11-C10	-2.25	119.74	121.59
2	B	1000	CJP	C15-C10-C11	2.24	120.41	117.79
2	A	1000	CJP	C16-C7-C3	2.06	129.34	126.15
2	A	1000	CJP	C2-C3-C4	2.02	121.57	119.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	CJP	C4-N9-S20-O22
2	A	1000	CJP	C8-N9-S20-O22
2	B	1000	CJP	C4-N9-S20-O22
2	B	1000	CJP	C8-N9-S20-O22
2	B	1000	CJP	C4-N9-S20-C21

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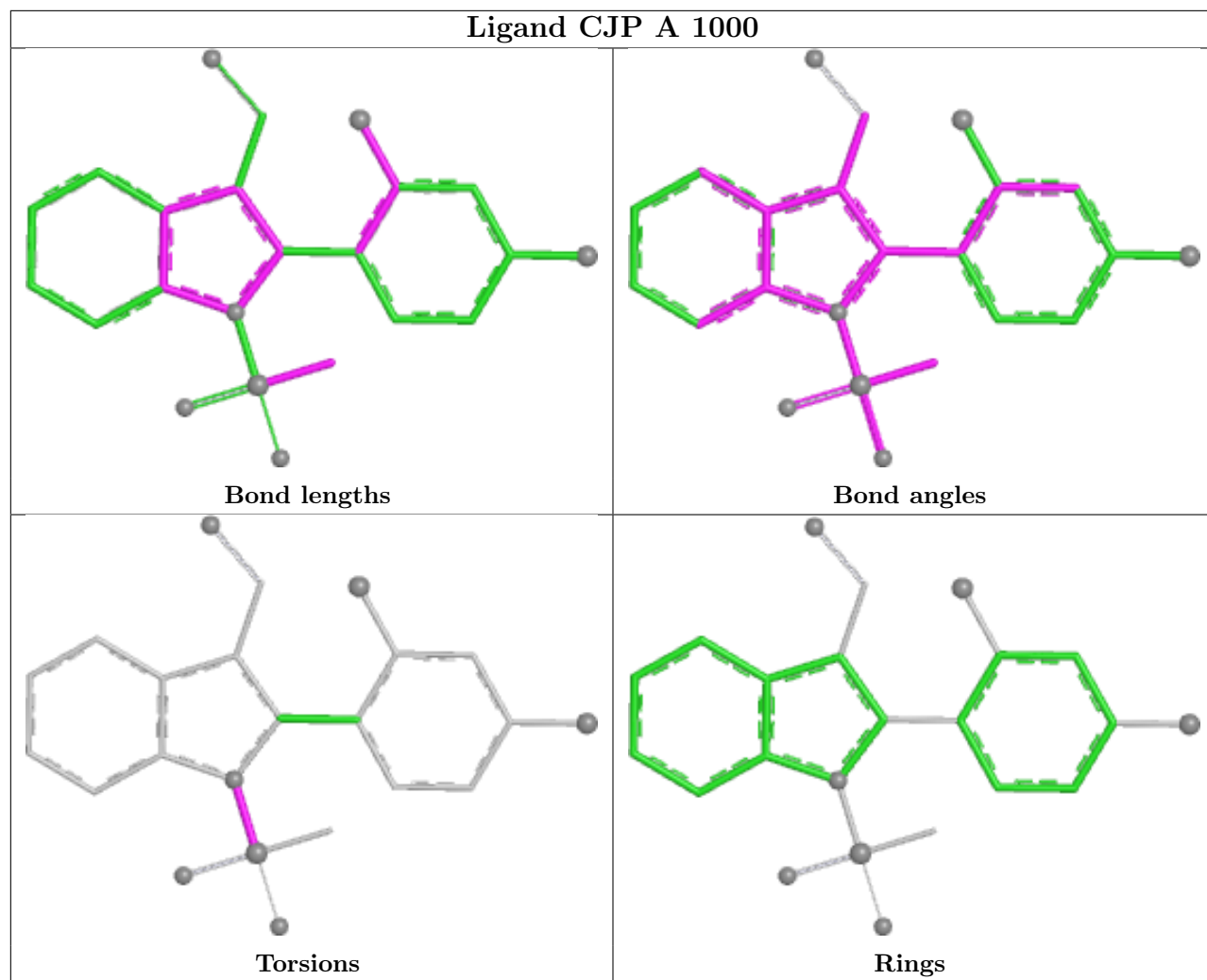
Mol	Chain	Res	Type	Atoms
2	A	1000	CJP	C4-N9-S20-C21
2	A	1000	CJP	C8-N9-S20-C21
2	B	1000	CJP	C8-N9-S20-C21

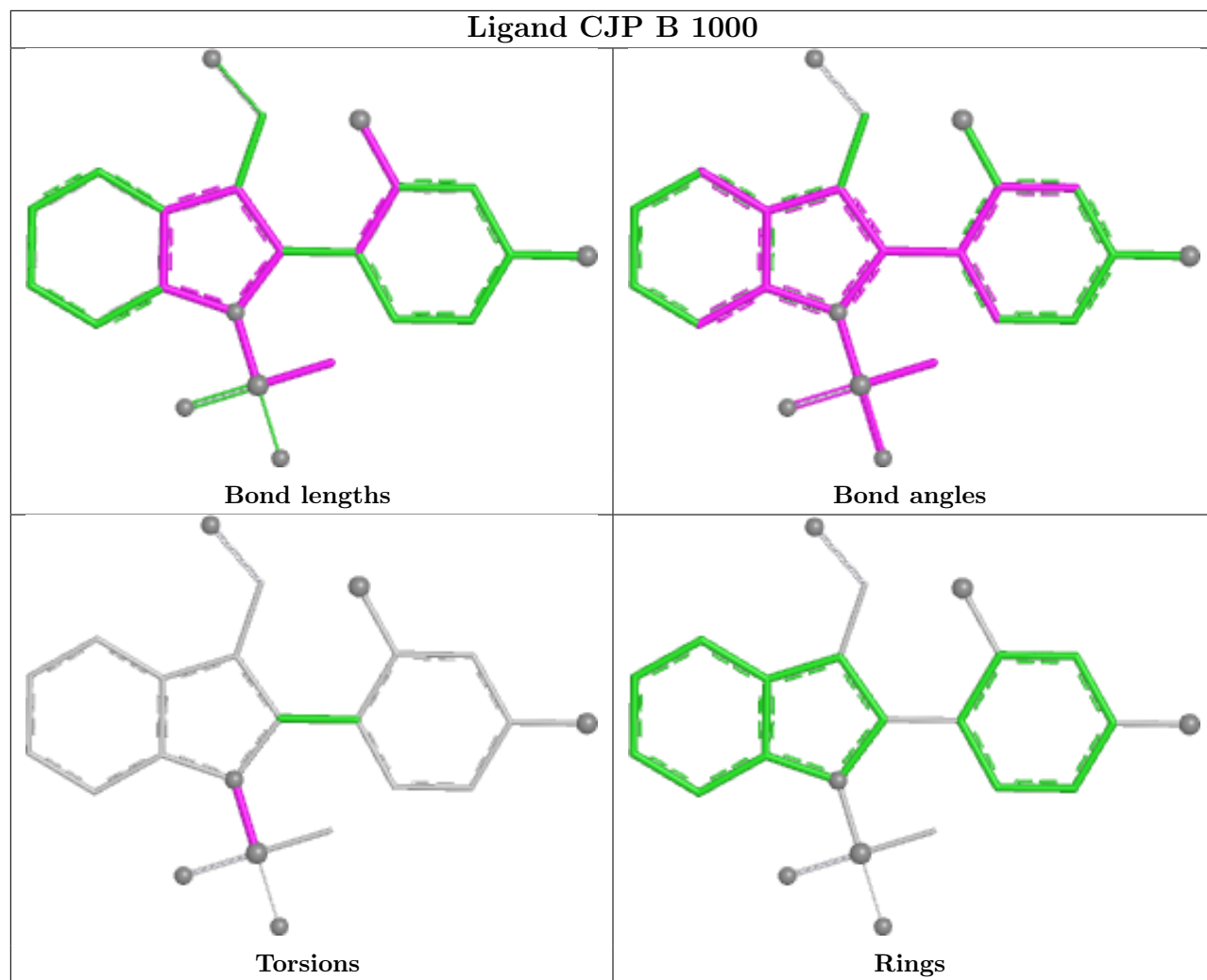
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	CJP	1	0
2	B	1000	CJP	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 [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 [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	727/752 (96%)	-0.54	3 (0%)	88 79	92, 140, 193, 226	0
1	B	727/752 (96%)	-0.53	2 (0%)	90 81	96, 150, 199, 235	0
All	All	1454/1504 (96%)	-0.53	5 (0%)	90 81	92, 145, 198, 235	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	695	PHE	3.1
1	A	300	LEU	2.4
1	A	188	THR	2.3
1	B	223	LEU	2.2
1	A	469	GLN	2.2

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](#)

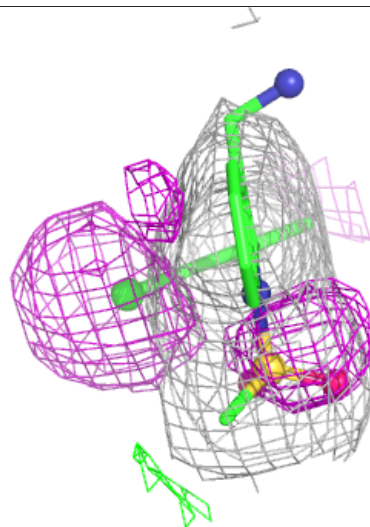
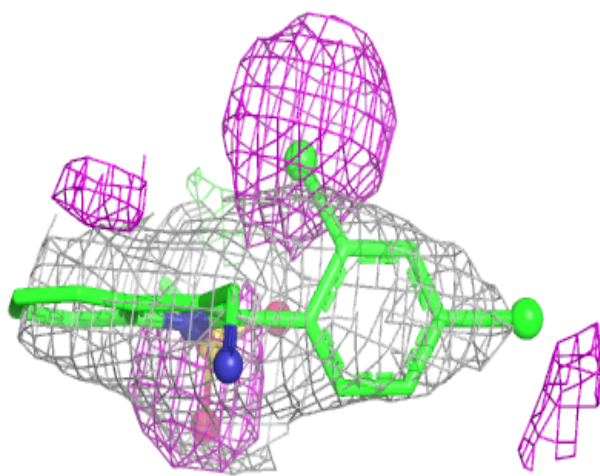
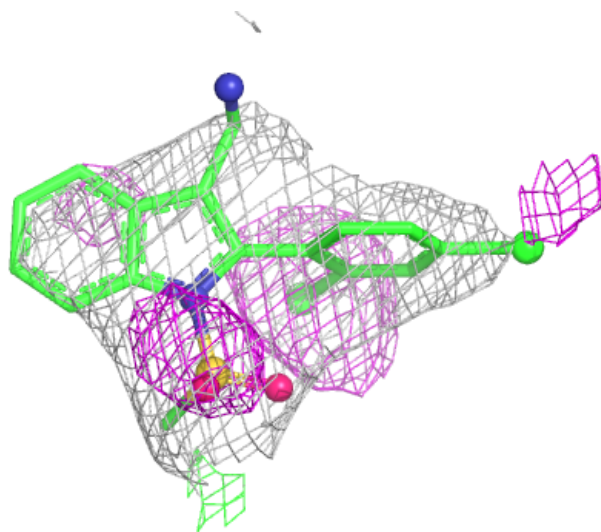
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	CJP	A	1000	23/23	0.82	0.12	139,139,142,142	0
2	CJP	B	1000	23/23	0.86	0.10	139,139,142,142	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.

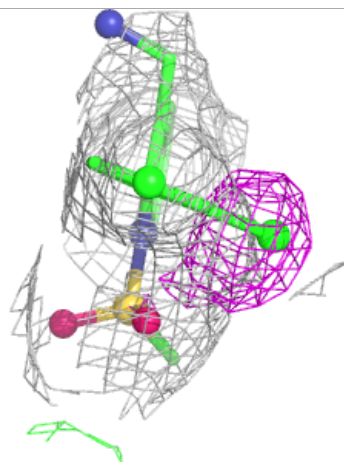
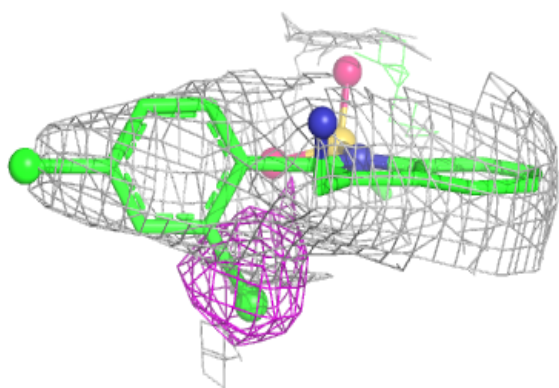
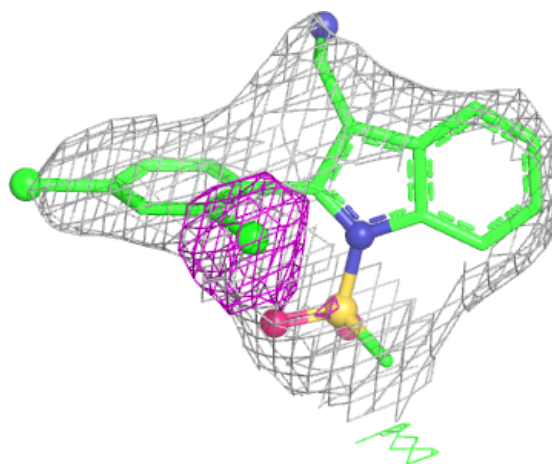
Electron density around CJP A 1000:

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 CJP B 1000:

$2mF_o-DF_c$ (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.