W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2022 – 12:13 pm GMT

PDB ID	:	6H5O
Title	:	Crystal structure of PBP2a from MRSA in complex with piperacillin at active site.
Authors	:	Batuecas, M.T.; Martinez-Caballero, S.; Hermoso, J.A.
Deposited on	:	2018-07-25
Resolution	:	2.82 Å(reported)

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

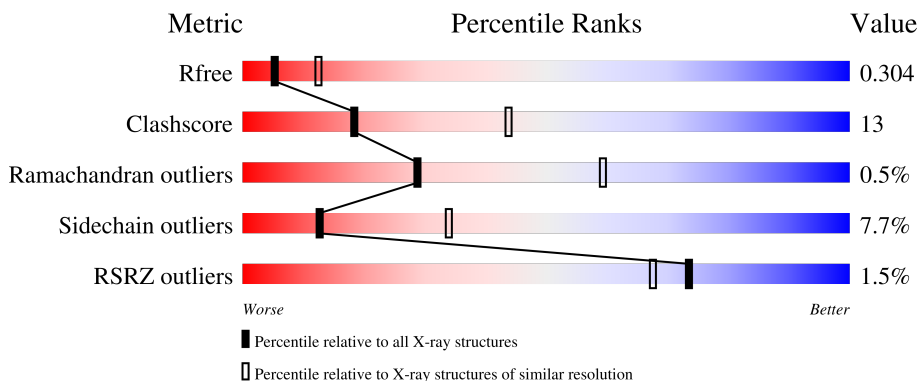|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.82 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		0.304
Clashscore		13
Ramachandran outliers		0.5%
Sidechain outliers		7.7%
RSRZ outliers		1.5%

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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	642	2% 67% 23% • 7%
1	B	642	% 68% 28% • •

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 10093 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 Penicillin binding protein 2 prime.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	0	0	0
			4791	3018	808	950	15			
1	B	636	Total	C	N	O	S	0	0	0
			5109	3222	862	1009	16			

- Molecule 2 is Piperacillin (Open Form) (three-letter code: JPP) (formula: $C_{23}H_{29}N_5O_7S$).
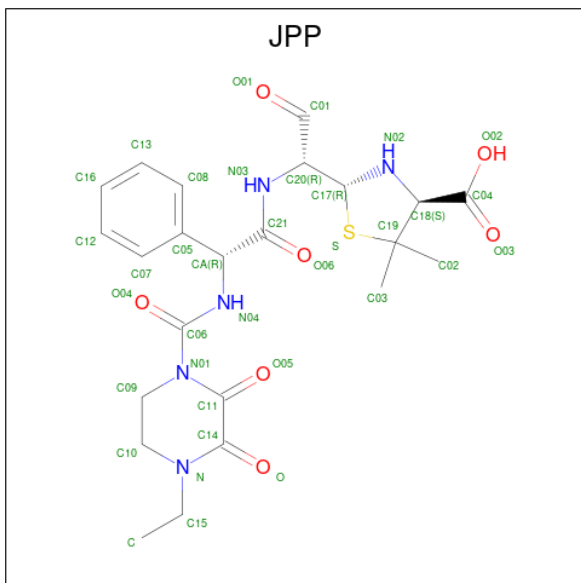
JPP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			36	23	5	7	1		
2	B	1	Total	C	N	O	S	0	0
			36	23	5	7	1		

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total 8	Cd 8	0	0
3	B	1	Total 1	Cd 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total 57	O 57	0	0
4	B	55	Total 55	O 55	0	0

3 Residue-property plots ⓘ

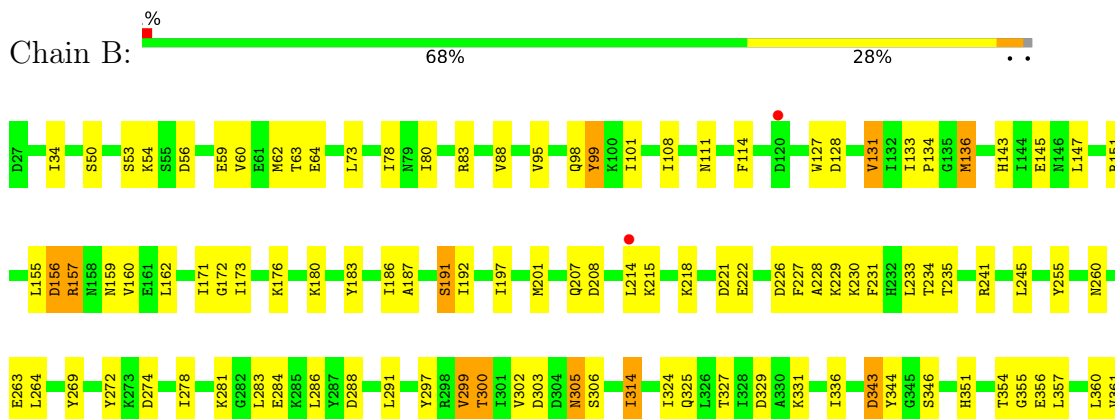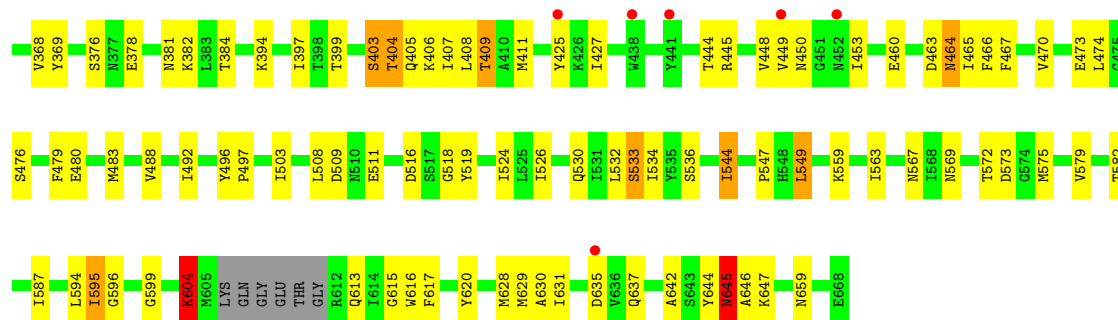These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A:

- Molecule 1: Penicillin binding protein 2 prime

Chain B:

V368 Y369 S376 N377 E378 N381 K382 L383 T384 K394 I397 T398 T399 S403 T404 Q405 K406 I407 L408 T409 A410 M411 Y425 K426 I427 W438 Y441 T444 R445 V448 V449 N450 G451 N452 I453 E460 D463 N464 I465 F466 F467 V470 E473 L474 G475

S476 F479 E480 M483 V488 I492 Y496 P497 I503 L508 D509 N510 E511 D516 S517 G518 Y519 I524 L525 I526 Q530 I531 L532 S533 I534 Y535 S536 I544 P547 H548 L549 K559 I563 N567 I568 N569 T572 D573 G574 M575 V579 T582

I587 L594 I595 G596 G599 K604 M605 LYS GLN GLY GLU THR GLY R612 Q613 I614 G615 W616 F617 Y620 M628 M629 A630 I631 D635 V636 Q637 A642 S643 Y644 N645 A646 K647 N659 E668

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.71Å 105.01Å 185.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.45 – 2.82 46.41 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.45-2.82) 99.7 (46.41-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.241 , 0.311 0.238 , 0.304	Depositor DCC
R_{free} test set	1856 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	94.7	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10093	wwPDB-VP
Average B, all atoms (Å^2)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: CD, JPP

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	1/4868 (0.0%)	0.62	1/6543 (0.0%)
1	B	0.37	1/5194 (0.0%)	0.63	1/6983 (0.0%)
All	All	0.37	2/10062 (0.0%)	0.62	2/13526 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	SER	CB-OG	6.56	1.50	1.42
1	B	403	SER	CB-OG	6.51	1.50	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	645	ASN	CB-CA-C	7.15	124.71	110.40
1	A	403	SER	CA-CB-OG	5.68	126.53	111.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	157	ARG	Sidechain

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	4791	0	4786	126	0
1	B	5109	0	5108	137	0
2	A	36	0	27	1	0
2	B	36	0	27	4	0
3	A	8	0	0	0	0
3	B	1	0	0	0	0
4	A	57	0	0	3	0
4	B	55	0	0	1	0
All	All	10093	0	9948	264	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 13.

All (264) 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:411:MET:HG2	1:A:563:ILE:HD11	1.39	1.01
1:A:30:ILE:HD11	1:A:116:PHE:CZ	1.99	0.97
1:A:407:ILE:O	1:A:411:MET:HG3	1.69	0.92
1:B:464:ASN:ND2	2:B:701:JPP:O06	2.04	0.90
1:B:407:ILE:O	1:B:411:MET:HG3	1.76	0.86
1:B:575:MET:HG2	1:B:596:GLY:O	1.75	0.85
1:A:37:ILE:HD13	1:A:131:VAL:HG23	1.60	0.82
1:B:470:VAL:O	1:B:474:LEU:HG	1.80	0.82
1:B:151:ARG:NH2	1:B:288:ASP:OD1	2.14	0.80
1:A:30:ILE:HD11	1:A:116:PHE:CE2	2.16	0.80
1:A:411:MET:CG	1:A:563:ILE:HD11	2.11	0.80
1:A:532:LEU:HD11	1:A:630:ALA:CB	2.13	0.78
1:B:587:ILE:HG21	1:B:646:ALA:HB1	1.65	0.78
1:A:118:LYS:HG2	1:A:123:TRP:CZ3	2.20	0.77
1:A:575:MET:O	1:A:578:VAL:HG22	1.85	0.77
1:B:465:ILE:HD12	1:B:466:PHE:N	1.98	0.77
1:A:128:ASP:O	1:A:131:VAL:HG12	1.87	0.73
1:A:532:LEU:HD11	1:A:630:ALA:HB3	1.71	0.73
1:B:128:ASP:O	1:B:131:VAL:HG13	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:ILE:CG2	1:B:646:ALA:HB1	2.20	0.71
1:A:30:ILE:HD11	1:A:116:PHE:CE1	2.25	0.71
1:A:411:MET:HG2	1:A:563:ILE:CD1	2.17	0.71
1:B:351:HIS:HD2	1:B:354:THR:HG22	1.54	0.71
1:A:656:LEU:HD12	1:A:664:TYR:CD1	2.25	0.70
1:B:460:GLU:O	1:B:582:THR:HG21	1.91	0.69
1:A:156:ASP:HB3	1:A:162:LEU:HD11	1.75	0.67
1:B:616:TRP:N	1:B:645:ASN:HD21	1.93	0.67
1:B:34:ILE:HD11	1:B:83:ARG:CZ	2.25	0.66
1:B:173:ILE:HD11	1:B:201:MET:CE	2.25	0.66
1:B:406:LYS:HG2	1:B:467:PHE:CD2	2.30	0.66
1:B:351:HIS:CD2	1:B:354:THR:HG22	2.31	0.66
1:B:291:LEU:HD11	1:B:324:ILE:HG12	1.77	0.66
1:B:156:ASP:HB3	1:B:162:LEU:HD11	1.78	0.65
1:A:37:ILE:HD13	1:A:131:VAL:CG2	2.26	0.64
1:B:156:ASP:CG	1:B:160:VAL:HG12	2.17	0.64
1:B:336:ILE:HG22	1:B:361:VAL:HG11	1.78	0.64
1:A:30:ILE:CD1	1:A:116:PHE:CE1	2.80	0.64
1:A:587:ILE:O	1:A:594:LEU:HD12	1.99	0.63
1:B:50:SER:HG	1:B:53:SER:HG	1.45	0.63
1:A:127:TRP:CD1	1:A:131:VAL:HG11	2.33	0.63
1:B:595:ILE:HD11	1:B:620:TYR:CE1	2.32	0.63
1:B:218:LYS:HG3	1:B:369:TYR:CD2	2.33	0.63
1:B:516:ASP:HA	1:B:519:TYR:CE1	2.34	0.62
1:A:34:ILE:HD11	1:A:83:ARG:CZ	2.28	0.62
1:B:172:GLY:HA2	1:B:214:LEU:HD23	1.81	0.62
1:B:133:ILE:HB	1:B:136:MET:HE2	1.82	0.61
1:A:34:ILE:HD13	1:A:80:ILE:HD13	1.83	0.60
1:B:159:ASN:ND2	1:B:325:GLN:NE2	2.49	0.60
1:A:325:GLN:HE21	1:A:551:LYS:HE2	1.66	0.60
1:B:464:ASN:HB3	1:B:519:TYR:CD2	2.36	0.60
1:A:467:PHE:HA	1:A:470:VAL:HG12	1.82	0.60
1:B:503:ILE:HD11	1:B:524:ILE:HG23	1.84	0.60
1:A:615:GLY:C	1:A:645:ASN:HD21	2.05	0.60
1:B:60:VAL:O	1:B:64:GLU:HG2	2.02	0.59
1:B:563:ILE:HG23	1:B:567:ASN:HB2	1.84	0.59
1:A:113:GLN:HE22	1:B:176:LYS:HE2	1.66	0.59
1:A:325:GLN:HE21	1:A:551:LYS:CE	2.15	0.59
1:B:467:PHE:HA	1:B:470:VAL:HG12	1.84	0.59
1:B:269:TYR:CZ	1:B:278:ILE:HD11	2.37	0.59
1:B:183:TYR:CD2	1:B:197:ILE:CD1	2.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:SER:O	1:A:405:GLN:N	2.36	0.59
1:B:171:ILE:HG22	1:B:235:THR:HG22	1.86	0.58
1:B:54:LYS:HA	1:B:62:MET:HE1	1.85	0.58
1:B:305:ASN:H	1:B:305:ASN:HD22	1.50	0.58
1:B:143:HIS:HB2	1:B:300:THR:HG22	1.84	0.57
2:B:701:JPP:S	2:B:701:JPP:C07	2.93	0.57
1:A:563:ILE:HG23	1:A:567:ASN:HB2	1.86	0.57
1:B:305:ASN:HD22	1:B:305:ASN:N	2.02	0.57
1:B:615:GLY:C	1:B:645:ASN:HD21	2.08	0.57
1:A:157:ARG:HD3	1:A:666:ILE:O	2.03	0.57
1:B:403:SER:O	1:B:406:LYS:N	2.27	0.57
1:B:425:TYR:OH	1:B:473:GLU:OE1	2.22	0.57
1:A:403:SER:O	1:A:406:LYS:N	2.28	0.56
1:A:486:LEU:CD2	1:A:562:ILE:HG21	2.35	0.56
1:B:357:LEU:HD22	1:B:360:LEU:HD21	1.87	0.56
1:B:403:SER:O	1:B:405:GLN:N	2.38	0.56
1:A:143:HIS:HB3	1:A:145:GLU:OE1	2.05	0.56
1:A:64:GLU:O	1:A:67:ILE:HG22	2.04	0.56
1:B:617:PHE:CD2	1:B:646:ALA:HB2	2.41	0.56
1:A:43:LYS:HE2	1:A:63:THR:HG21	1.87	0.55
1:A:94:ARG:HH11	1:A:113:GLN:NE2	2.04	0.55
1:A:336:ILE:CG2	1:A:629:MET:HE3	2.36	0.55
1:A:54:LYS:HA	1:A:62:MET:HE1	1.88	0.55
1:B:183:TYR:CD2	1:B:197:ILE:HD11	2.41	0.55
1:A:186:ILE:HD11	1:A:197:ILE:HD13	1.89	0.55
1:A:249:THR:HB	1:A:253:LEU:HD13	1.88	0.55
1:B:255:TYR:HB3	1:B:368:VAL:CG1	2.36	0.55
1:A:615:GLY:C	1:A:645:ASN:ND2	2.60	0.54
1:A:636:VAL:HG22	1:A:641:MET:HA	1.89	0.54
1:B:159:ASN:HD21	1:B:325:GLN:HE22	1.55	0.54
1:B:354:THR:HG23	1:B:356:GLU:H	1.73	0.54
1:B:427:ILE:HG21	1:B:465:ILE:HD13	1.89	0.54
1:A:43:LYS:NZ	1:A:63:THR:HG21	2.22	0.54
1:A:464:ASN:ND2	2:A:701:JPP:O06	2.40	0.54
1:A:488:VAL:HG12	1:A:503:ILE:HD12	1.90	0.54
1:A:579:VAL:HG13	1:A:587:ILE:HD13	1.89	0.54
1:A:277:VAL:HG23	4:A:806:HOH:O	2.08	0.54
1:A:336:ILE:HG22	1:A:629:MET:HE3	1.90	0.54
1:B:409:THR:HG22	1:B:479:PHE:HE1	1.72	0.54
1:B:533:SER:O	1:B:544:ILE:HD13	2.08	0.54
1:A:527:ASN:OD1	1:A:529:VAL:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ILE:HD13	1:B:80:ILE:HD13	1.90	0.54
1:A:298:ARG:HD3	1:A:315:GLU:OE1	2.08	0.54
1:B:631:ILE:HD12	1:B:631:ILE:N	2.23	0.53
1:A:154:ILE:HD13	1:A:324:ILE:HD11	1.89	0.53
1:B:403:SER:O	1:B:404:THR:C	2.46	0.53
1:B:445:ARG:HD2	1:B:463:ASP:OD1	2.09	0.53
1:B:62:MET:HG2	1:B:127:TRP:CE2	2.43	0.53
1:A:59:GLU:O	1:A:63:THR:HB	2.08	0.53
1:B:381:ASN:HA	1:B:384:THR:HG22	1.90	0.53
1:B:405:GLN:HA	1:B:408:LEU:HD13	1.91	0.53
1:A:62:MET:HG2	1:A:127:TRP:CE2	2.44	0.53
1:A:343:ASP:N	1:A:343:ASP:OD1	2.42	0.53
1:B:615:GLY:C	1:B:645:ASN:ND2	2.62	0.53
1:A:172:GLY:HA2	1:A:214:LEU:HD13	1.89	0.52
1:A:381:ASN:HA	1:A:384:THR:HG22	1.91	0.52
1:A:125:LEU:HD23	1:A:127:TRP:N	2.23	0.52
1:A:180:LYS:HD3	1:A:183:TYR:CE2	2.44	0.52
1:B:59:GLU:O	1:B:63:THR:HB	2.08	0.52
1:B:226:ASP:O	1:B:230:LYS:HG3	2.10	0.52
1:B:241:ARG:HD3	1:B:284:GLU:OE2	2.10	0.52
1:A:578:VAL:HG21	1:A:596:GLY:O	2.10	0.52
1:B:406:LYS:HG2	1:B:467:PHE:CE2	2.45	0.52
1:A:403:SER:O	1:A:404:THR:C	2.48	0.51
1:B:343:ASP:OD1	1:B:343:ASP:N	2.43	0.51
1:B:536:SER:N	1:B:628:MET:HE1	2.25	0.51
1:B:228:ALA:HB1	1:B:233:LEU:HB2	1.93	0.51
1:B:173:ILE:HD11	1:B:201:MET:HE1	1.93	0.51
1:B:186:ILE:HD11	1:B:231:PHE:CD2	2.45	0.51
1:A:332:VAL:O	1:A:336:ILE:HG23	2.11	0.50
1:A:43:LYS:CE	1:A:63:THR:HG21	2.42	0.50
1:B:299:VAL:HG22	1:B:314:ILE:HG13	1.94	0.50
1:B:488:VAL:HG12	1:B:503:ILE:HD12	1.94	0.50
1:B:191:SER:HB2	1:B:376:SER:HB3	1.94	0.50
1:B:659:ASN:N	1:B:659:ASN:HD22	2.09	0.50
1:B:336:ILE:CG2	1:B:361:VAL:HG11	2.42	0.49
1:B:530:GLN:O	1:B:533:SER:HB2	2.12	0.49
1:B:159:ASN:ND2	1:B:325:GLN:HE22	2.10	0.49
1:A:165:THR:HG22	4:A:813:HOH:O	2.11	0.49
1:A:394:LYS:HA	1:A:397:ILE:HG22	1.95	0.49
1:A:118:LYS:HG2	1:A:123:TRP:CH2	2.47	0.49
1:A:411:MET:CB	1:A:563:ILE:HD11	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:HIS:HB3	1:A:586:ASP:OD2	2.13	0.49
2:B:701:JPP:S	2:B:701:JPP:H17	2.53	0.49
1:B:180:LYS:HA	1:B:183:TYR:CD1	2.48	0.48
1:B:616:TRP:CA	1:B:645:ASN:HD21	2.26	0.48
1:A:533:SER:O	1:A:544:ILE:HD13	2.12	0.48
1:B:405:GLN:O	1:B:408:LEU:HB2	2.14	0.48
1:A:180:LYS:HA	1:A:183:TYR:CD1	2.49	0.48
1:A:67:ILE:CD1	4:A:838:HOH:O	2.61	0.47
1:A:405:GLN:HA	1:A:408:LEU:HD13	1.96	0.47
1:B:503:ILE:HD11	1:B:526:ILE:HD11	1.95	0.47
1:A:89:SER:HB3	1:A:92:LYS:HB2	1.96	0.47
1:B:101:ILE:HB	1:B:108:ILE:HG13	1.95	0.47
1:B:327:THR:OG1	1:B:549:LEU:HA	2.14	0.47
2:B:701:JPP:O04	2:B:701:JPP:H18	2.13	0.47
1:A:50:SER:O	1:A:53:SER:OG	2.30	0.47
1:A:405:GLN:O	1:A:408:LEU:HB2	2.13	0.47
1:B:191:SER:O	1:B:191:SER:OG	2.31	0.47
1:B:218:LYS:HG3	1:B:369:TYR:CG	2.50	0.47
1:B:80:ILE:CD1	1:B:83:ARG:HH11	2.27	0.47
1:B:465:ILE:HD12	1:B:466:PHE:H	1.74	0.47
1:B:569:ASN:HA	1:B:572:THR:HG22	1.96	0.47
1:A:34:ILE:HD11	1:A:83:ARG:NH1	2.30	0.47
1:B:231:PHE:HB2	1:B:233:LEU:HD23	1.97	0.47
1:B:351:HIS:HD2	1:B:354:THR:CG2	2.26	0.46
1:A:43:LYS:HZ1	1:A:63:THR:HG21	1.80	0.46
1:A:464:ASN:HB3	1:A:519:TYR:CD1	2.51	0.46
1:B:151:ARG:NH1	1:B:284:GLU:OE1	2.49	0.46
1:A:532:LEU:HD11	1:A:630:ALA:HB2	1.95	0.46
1:A:579:VAL:HG13	1:A:587:ILE:CD1	2.46	0.46
1:A:325:GLN:HE22	1:B:325:GLN:HE22	1.63	0.46
1:B:599:GLY:O	1:B:642:ALA:HB2	2.15	0.46
1:A:125:LEU:CD2	1:A:127:TRP:HA	2.46	0.46
1:A:409:THR:HG22	1:A:479:PHE:HE1	1.81	0.45
1:B:480:GLU:HG3	1:B:508:LEU:HD13	1.99	0.45
1:A:254:GLY:HA3	1:A:281:LYS:O	2.16	0.45
1:A:327:THR:OG1	1:A:549:LEU:HA	2.15	0.45
1:A:89:SER:OG	1:A:90:LYS:N	2.50	0.45
1:B:476:SER:HB3	1:B:508:LEU:HG	1.97	0.45
1:B:218:LYS:HE3	1:B:369:TYR:CE1	2.52	0.45
1:B:394:LYS:HA	1:B:397:ILE:HG22	1.97	0.45
1:B:544:ILE:CG2	1:B:559:LYS:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LEU:HD21	1:A:515:ALA:HB2	1.98	0.45
1:A:98:GLN:NE2	1:A:111:ASN:OD1	2.50	0.45
1:A:573:ASP:O	1:A:576:GLN:HB3	2.16	0.45
1:A:595:ILE:HD11	1:A:620:TYR:CZ	2.51	0.45
1:B:99:TYR:HB3	1:B:134:PRO:HG3	1.99	0.45
1:A:544:ILE:CG2	1:A:559:LYS:HB2	2.47	0.45
1:B:98:GLN:NE2	1:B:111:ASN:OD1	2.50	0.45
1:A:37:ILE:O	1:A:78:ILE:HD11	2.17	0.45
1:B:604:LYS:HE2	1:B:604:LYS:N	2.32	0.45
1:B:408:LEU:HG	1:B:534:ILE:HD13	1.99	0.45
1:B:492:ILE:HD11	1:B:530:GLN:CD	2.38	0.45
1:B:617:PHE:HB2	1:B:645:ASN:OD1	2.16	0.44
1:B:464:ASN:N	1:B:464:ASN:OD1	2.50	0.44
1:B:378:GLU:OE1	1:B:378:GLU:N	2.46	0.44
1:A:227:PHE:CD1	1:A:227:PHE:C	2.91	0.44
1:B:303:ASP:HB3	1:B:306:SER:OG	2.18	0.44
1:A:303:ASP:HB3	1:A:306:SER:HB3	1.99	0.44
1:B:281:LYS:NZ	4:B:801:HOH:O	2.47	0.44
1:A:601:ALA:O	1:A:613:GLN:HB2	2.18	0.44
1:A:503:ILE:HG12	1:A:524:ILE:HG22	2.00	0.43
1:A:631:ILE:HD12	1:A:631:ILE:N	2.33	0.43
1:A:350:ILE:HG22	1:A:532:LEU:HD23	2.01	0.43
1:B:171:ILE:O	1:B:171:ILE:HD12	2.19	0.43
1:A:87:LYS:HG2	1:A:93:LYS:HG3	2.00	0.43
1:B:532:LEU:HD12	1:B:532:LEU:HA	1.91	0.43
1:A:78:ILE:HD12	1:A:99:TYR:HE1	1.84	0.43
1:B:159:ASN:HD21	1:B:325:GLN:NE2	2.13	0.43
1:B:488:VAL:CG1	1:B:503:ILE:HD12	2.49	0.43
1:A:496:TYR:CG	1:A:497:PRO:HD2	2.53	0.43
1:A:171:ILE:HG13	1:A:215:LYS:O	2.19	0.43
1:A:464:ASN:OD1	1:A:464:ASN:N	2.51	0.42
1:B:187:ALA:O	1:B:192:ILE:O	2.37	0.42
1:A:173:ILE:HG12	1:A:201:MET:CE	2.48	0.42
1:A:629:MET:HE1	1:A:652:VAL:HG21	2.00	0.42
1:B:496:TYR:CG	1:B:497:PRO:HD2	2.54	0.42
1:B:509:ASP:O	1:B:511:GLU:OE2	2.37	0.42
1:A:30:ILE:CD1	1:A:116:PHE:CD1	3.02	0.42
1:A:616:TRP:N	1:A:645:ASN:ND2	2.68	0.42
1:B:532:LEU:HD13	1:B:630:ALA:HB2	2.01	0.42
1:A:156:ASP:CB	1:A:162:LEU:HD11	2.45	0.42
1:B:579:VAL:HG22	1:B:587:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:SER:C	1:A:405:GLN:N	2.73	0.42
1:A:409:THR:HG21	1:A:518:GLY:O	2.19	0.42
1:B:156:ASP:CB	1:B:162:LEU:HD11	2.47	0.42
1:B:260:ASN:HB3	1:B:263:GLU:HG3	2.02	0.42
1:A:95:VAL:HG13	1:A:114:PHE:HB2	2.02	0.42
1:B:171:ILE:HG13	1:B:215:LYS:O	2.20	0.42
1:A:30:ILE:CD1	1:A:116:PHE:CZ	2.86	0.42
1:A:189:GLU:HG2	1:A:227:PHE:CE1	2.55	0.42
1:A:656:LEU:CD1	1:A:664:TYR:CD1	3.00	0.42
1:A:601:ALA:O	1:A:602:GLU:HG3	2.19	0.42
1:B:480:GLU:CG	1:B:508:LEU:HD13	2.50	0.42
1:B:449:VAL:HG13	1:B:453:ILE:HD11	2.01	0.42
1:A:99:TYR:HB3	1:A:134:PRO:HG3	2.02	0.41
1:B:221:ASP:OD1	1:B:221:ASP:N	2.52	0.41
1:B:613:GLN:OE1	1:B:637:GLN:HG2	2.20	0.41
1:B:463:ASP:OD1	1:B:465:ILE:HG13	2.20	0.41
1:B:95:VAL:HG13	1:B:114:PHE:HB2	2.02	0.41
1:B:201:MET:HE3	1:B:201:MET:HA	2.01	0.41
1:A:171:ILE:HD12	1:A:171:ILE:O	2.20	0.41
1:A:569:ASN:HA	1:A:572:THR:HG22	2.03	0.41
1:A:355:GLY:O	1:A:547:PRO:HA	2.20	0.41
1:B:269:TYR:CE1	1:B:278:ILE:HD11	2.55	0.41
1:B:329:ASP:OD1	1:B:331:LYS:HG2	2.19	0.41
1:A:336:ILE:HG22	1:A:629:MET:CE	2.50	0.41
1:B:644:TYR:O	1:B:647:LYS:HB2	2.21	0.41
1:A:37:ILE:CD1	1:A:131:VAL:CG2	2.98	0.41
1:A:221:ASP:OD1	1:A:221:ASP:N	2.54	0.41
1:A:486:LEU:CD2	1:A:562:ILE:CG2	2.98	0.41
1:B:147:LEU:HD12	1:B:297:TYR:CA	2.50	0.40
1:A:488:VAL:HG23	1:A:534:ILE:HD11	2.03	0.40
1:B:355:GLY:O	1:B:547:PRO:HA	2.21	0.40
1:A:30:ILE:HD11	1:A:116:PHE:CD2	2.55	0.40
1:A:503:ILE:CD1	1:A:524:ILE:HG22	2.52	0.40
1:B:464:ASN:HB3	1:B:519:TYR:CG	2.57	0.40
1:A:187:ALA:O	1:A:192:ILE:O	2.38	0.40
1:B:143:HIS:HB3	1:B:145:GLU:OE2	2.21	0.40
1:B:176:LYS:HE3	1:B:208:ASP:HB3	2.03	0.40
1:B:445:ARG:NH2	1:B:448:VAL:HA	2.36	0.40
1:A:599:GLY:O	1:A:600:THR:OG1	2.39	0.40
1:B:409:THR:HG21	1:B:518:GLY:HA2	2.02	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	592/642 (92%)	553 (93%)	36 (6%)	3 (0%)	29	59
1	B	632/642 (98%)	586 (93%)	43 (7%)	3 (0%)	29	59
All	All	1224/1284 (95%)	1139 (93%)	79 (6%)	6 (0%)	29	59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	641	MET
1	B	404	THR
1	A	404	THR
1	A	533	SER
1	B	533	SER
1	B	604	LYS

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	533/572 (93%)	494 (93%)	39 (7%)	14	37
1	B	568/572 (99%)	522 (92%)	46 (8%)	11	32
All	All	1101/1144 (96%)	1016 (92%)	85 (8%)	13	34

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	56	ASP
1	A	68	LYS
1	A	78	ILE
1	A	99	TYR
1	A	145	GLU
1	A	156	ASP
1	A	157	ARG
1	A	167	THR
1	A	207	GLN
1	A	210	THR
1	A	264	LEU
1	A	272	TYR
1	A	274	ASP
1	A	286	LEU
1	A	299	VAL
1	A	307	ASN
1	A	328	ILE
1	A	343	ASP
1	A	344	TYR
1	A	346	SER
1	A	368	VAL
1	A	409	THR
1	A	415	ASN
1	A	464	ASN
1	A	474	LEU
1	A	504	SER
1	A	529	VAL
1	A	533	SER
1	A	544	ILE
1	A	549	LEU
1	A	564	SER
1	A	573	ASP
1	A	582	THR
1	A	583	HIS
1	A	614	ILE
1	A	629	MET
1	A	637	GLN
1	A	641	MET
1	B	56	ASP
1	B	73	LEU
1	B	78	ILE
1	B	88	VAL

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Mol	Chain	Res	Type
1	B	99	TYR
1	B	131	VAL
1	B	136	MET
1	B	155	LEU
1	B	156	ASP
1	B	157	ARG
1	B	191	SER
1	B	207	GLN
1	B	222	GLU
1	B	227	PHE
1	B	229	LYS
1	B	234	THR
1	B	245	LEU
1	B	264	LEU
1	B	272	TYR
1	B	274	ASP
1	B	283	LEU
1	B	286	LEU
1	B	299	VAL
1	B	300	THR
1	B	302	VAL
1	B	305	ASN
1	B	314	ILE
1	B	343	ASP
1	B	344	TYR
1	B	346	SER
1	B	382	LYS
1	B	399	THR
1	B	409	THR
1	B	444	THR
1	B	450	ASN
1	B	464	ASN
1	B	483	MET
1	B	544	ILE
1	B	549	LEU
1	B	573	ASP
1	B	594	LEU
1	B	595	ILE
1	B	604	LYS
1	B	629	MET
1	B	635	ASP
1	B	645	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	207	GLN
1	A	325	GLN
1	A	415	ASN
1	A	540	ASN
1	A	567	ASN
1	A	576	GLN
1	A	580	ASN
1	A	645	ASN
1	B	32	ASN
1	B	159	ASN
1	B	266	GLN
1	B	305	ASN
1	B	325	GLN
1	B	396	GLN
1	B	543	ASN
1	B	548	HIS
1	B	555	ASN
1	B	567	ASN
1	B	632	ASN
1	B	645	ASN
1	B	659	ASN

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 ⓘ

Of 11 ligands modelled in this entry, 9 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	#$|Z| > 2$
2	JPP	B	701	1	31,38,38	4.40	11 (35%)	39,55,55	2.73	14 (35%)
2	JPP	A	701	1	31,38,38	4.38	12 (38%)	39,55,55	2.54	13 (33%)

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	JPP	B	701	1	-	3/22/64/64	0/3/3/3
2	JPP	A	701	1	-	5/22/64/64	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	JPP	O04-C06	11.04	1.43	1.23
2	A	701	JPP	O04-C06	10.99	1.43	1.23
2	B	701	JPP	O06-C21	10.27	1.43	1.23
2	A	701	JPP	O06-C21	10.09	1.43	1.23
2	A	701	JPP	O-C14	9.70	1.43	1.23
2	B	701	JPP	O05-C11	9.56	1.43	1.23
2	A	701	JPP	O05-C11	9.41	1.43	1.23
2	B	701	JPP	O-C14	9.35	1.42	1.23
2	B	701	JPP	C14-C11	-8.06	1.40	1.53
2	A	701	JPP	C14-C11	-7.60	1.41	1.53
2	A	701	JPP	C10-N	-7.30	1.34	1.47
2	B	701	JPP	C10-N	-7.28	1.34	1.47
2	A	701	JPP	C09-N01	-5.38	1.39	1.48
2	B	701	JPP	C09-N01	-5.25	1.39	1.48
2	B	701	JPP	C10-C09	-2.87	1.40	1.51
2	A	701	JPP	C10-C09	-2.80	1.40	1.51
2	A	701	JPP	C18-N02	2.71	1.50	1.46
2	A	701	JPP	C19-S	-2.54	1.80	1.85
2	B	701	JPP	C21-N03	2.51	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	JPP	C19-S	-2.45	1.80	1.85
2	B	701	JPP	C18-N02	2.35	1.49	1.46
2	A	701	JPP	C08-C05	2.24	1.42	1.39
2	A	701	JPP	C06-N01	-2.06	1.38	1.42

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	JPP	N04-C06-N01	6.84	124.00	114.04
2	A	701	JPP	N04-C06-N01	6.27	123.16	114.04
2	B	701	JPP	C20-N03-C21	-5.71	116.88	123.12
2	A	701	JPP	C20-N03-C21	-5.27	117.36	123.12
2	B	701	JPP	C10-C09-N01	5.23	118.64	108.78
2	B	701	JPP	C10-N-C14	5.17	130.59	120.69
2	A	701	JPP	C10-C09-N01	5.05	118.30	108.78
2	A	701	JPP	C10-N-C14	4.96	130.17	120.69
2	B	701	JPP	C03-C19-S	-4.94	100.93	109.21
2	B	701	JPP	C19-S-C17	-4.79	83.74	93.99
2	A	701	JPP	C15-N-C14	-4.74	113.95	119.64
2	A	701	JPP	O-C14-N	4.71	128.55	123.66
2	B	701	JPP	O-C14-N	4.28	128.11	123.66
2	B	701	JPP	C18-C19-S	4.01	111.75	103.81
2	B	701	JPP	CA-N04-C06	-3.94	113.72	121.17
2	A	701	JPP	CA-N04-C06	-3.90	113.80	121.17
2	B	701	JPP	C15-N-C14	-3.84	115.03	119.64
2	A	701	JPP	C19-S-C17	-3.69	86.09	93.99
2	B	701	JPP	C03-C19-C02	3.52	116.51	110.78
2	A	701	JPP	C03-C19-S	-3.44	103.44	109.21
2	A	701	JPP	C02-C19-C18	-3.31	101.36	112.33
2	A	701	JPP	O04-C06-N04	-2.53	115.98	123.05
2	B	701	JPP	O04-C06-N04	-2.48	116.12	123.05
2	A	701	JPP	C03-C19-C18	2.35	120.12	112.33
2	B	701	JPP	O01-C01-C20	-2.21	118.67	124.83
2	A	701	JPP	C18-C19-S	2.21	108.18	103.81
2	B	701	JPP	C02-C19-C18	-2.03	105.61	112.33

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	JPP	C-C15-N-C10
2	A	701	JPP	C-C15-N-C14

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Mol	Chain	Res	Type	Atoms
2	B	701	JPP	C-C15-N-C10
2	B	701	JPP	O06-C21-CA-N04
2	B	701	JPP	C-C15-N-C14
2	A	701	JPP	C21-CA-N04-C06
2	A	701	JPP	C07-C05-CA-N04
2	A	701	JPP	C08-C05-CA-N04

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	JPP	4	0
2	A	701	JPP	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 JPP B 701

Bond lengths

Bond angles

Torsions

Rings

Ligand JPP A 701

Bond lengths

Bond angles

Torsions

Rings
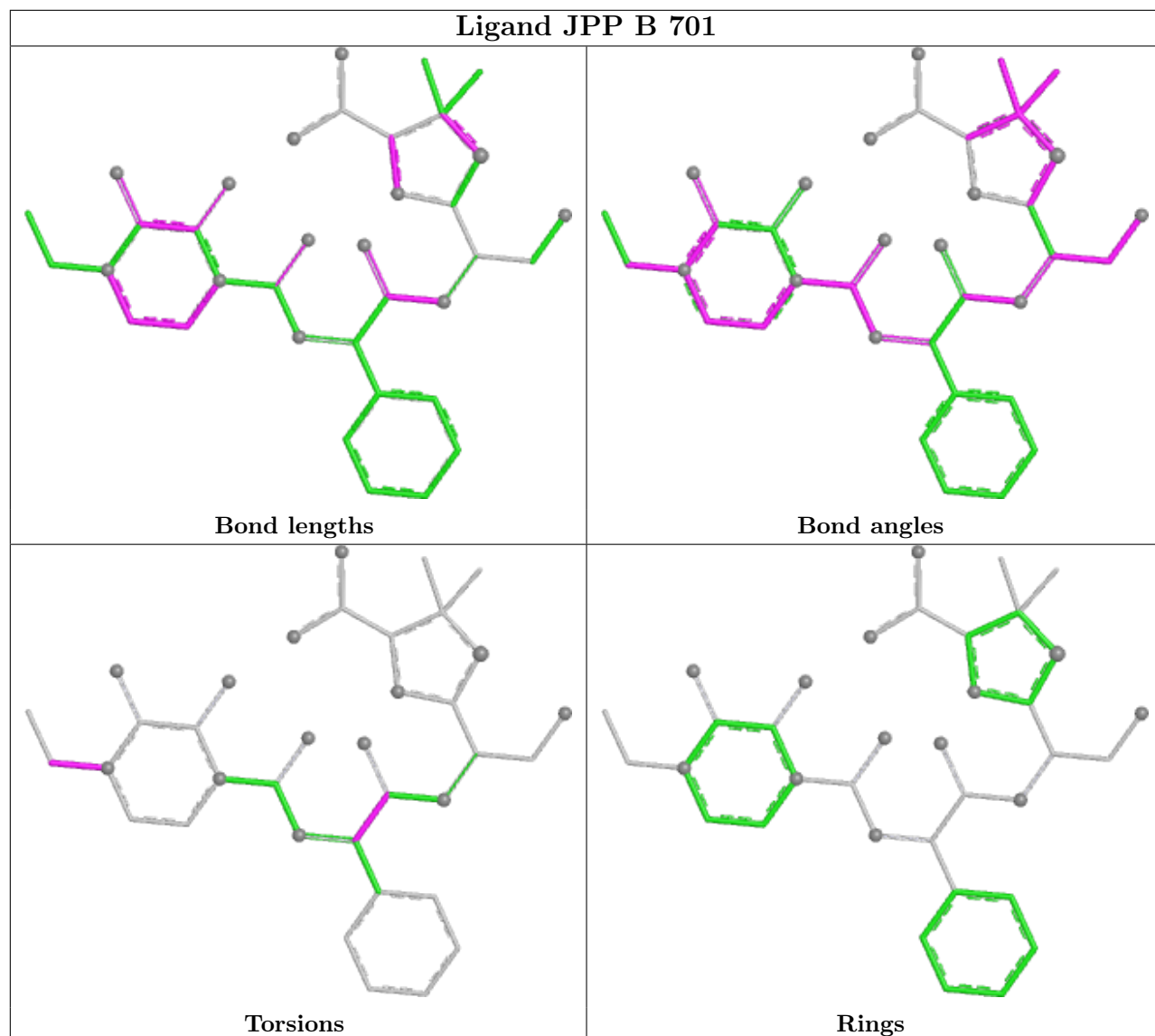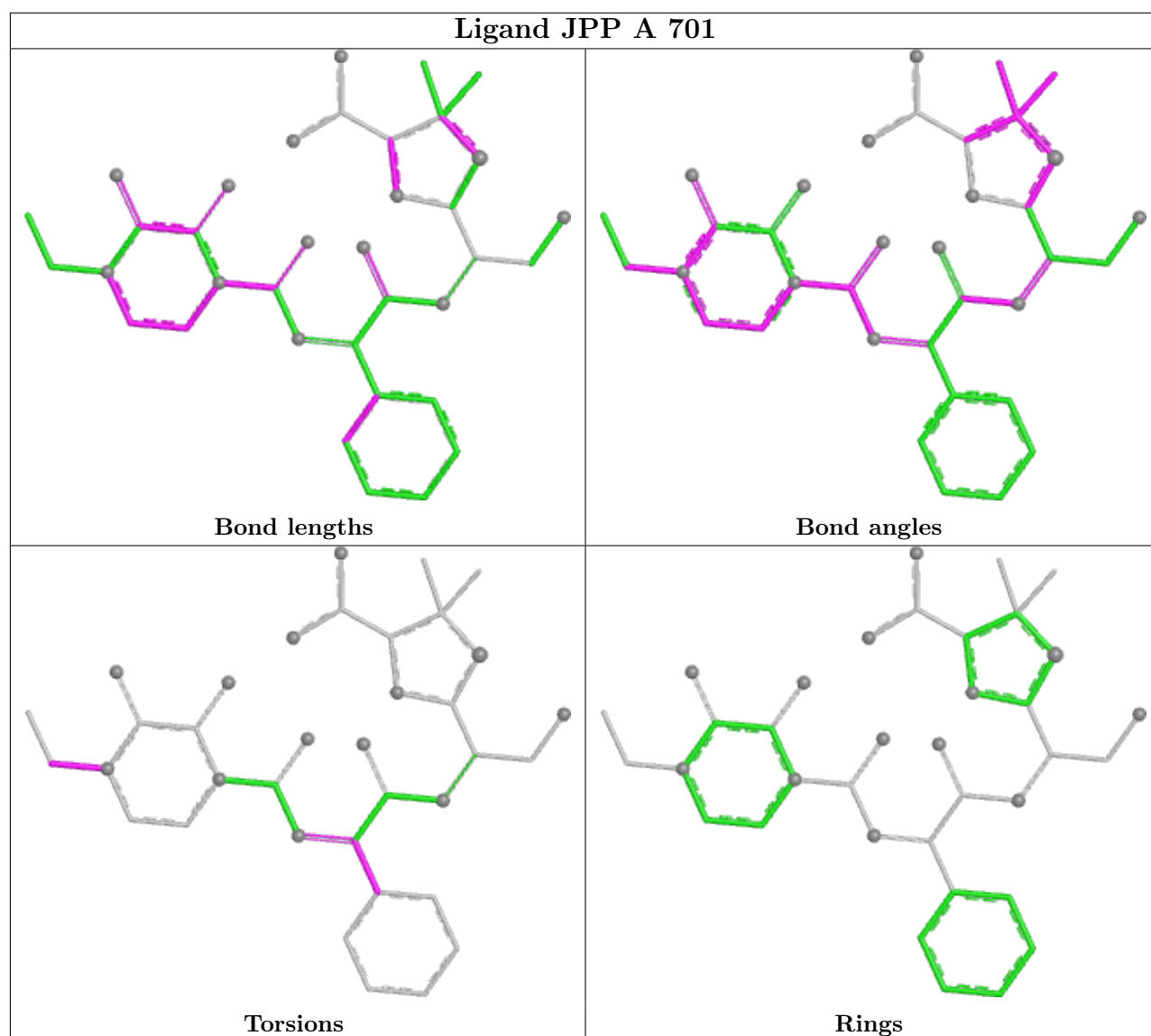
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	598/642 (93%)	0.02	10 (1%)	70	63	79, 119, 169, 247	0
1	B	636/642 (99%)	-0.01	8 (1%)	77	72	75, 124, 175, 211	2 (0%)
All	All	1234/1284 (96%)	0.00	18 (1%)	73	67	75, 122, 172, 247	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	441	TYR	4.8
1	B	635	ASP	4.3
1	A	205	TRP	3.1
1	A	459	ILE	3.0
1	A	233	LEU	2.9
1	A	183	TYR	2.7
1	B	438	TRP	2.5
1	B	120	ASP	2.5
1	A	460	GLU	2.5
1	A	101	ILE	2.4
1	A	611	GLY	2.3
1	B	425	TYR	2.3
1	B	449	VAL	2.3
1	A	226	ASP	2.3
1	B	214	LEU	2.2
1	B	452	ASN	2.2
1	A	83	ARG	2.0
1	A	610	THR	2.0

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

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

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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
2	JPP	A	701	36/36	0.89	0.24	115,137,153,156	0
3	CD	A	707	1/1	0.91	0.12	176,176,176,176	0
2	JPP	B	701	36/36	0.94	0.13	87,109,143,144	0
3	CD	A	705	1/1	0.99	0.14	153,153,153,153	0
3	CD	A	706	1/1	0.99	0.09	202,202,202,202	0
3	CD	A	703	1/1	0.99	0.10	128,128,128,128	0
3	CD	A	709	1/1	0.99	0.16	92,92,92,92	1
3	CD	A	702	1/1	1.00	0.14	102,102,102,102	0
3	CD	A	708	1/1	1.00	0.16	94,94,94,94	0
3	CD	A	704	1/1	1.00	0.18	99,99,99,99	0
3	CD	B	702	1/1	1.00	0.15	122,122,122,122	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.

WORLDWIDE PDB
PROTEIN DATA BANK

Electron density around JPP A 701:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
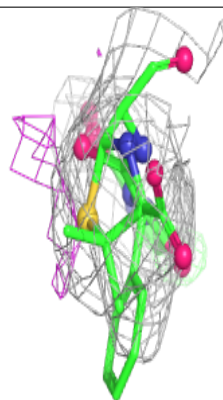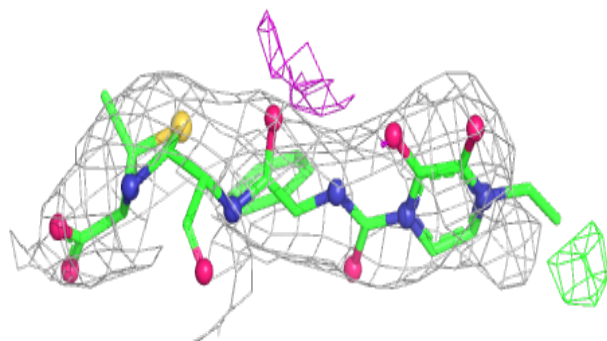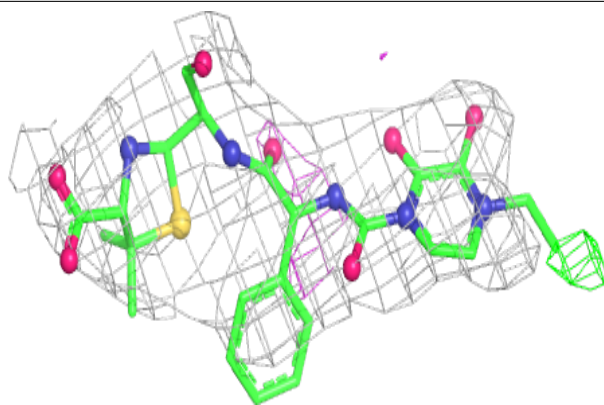
Electron density around JPP B 701:

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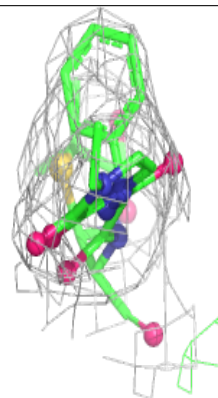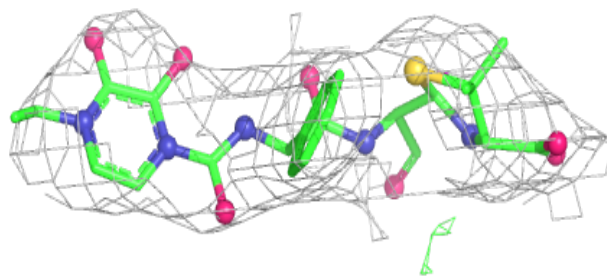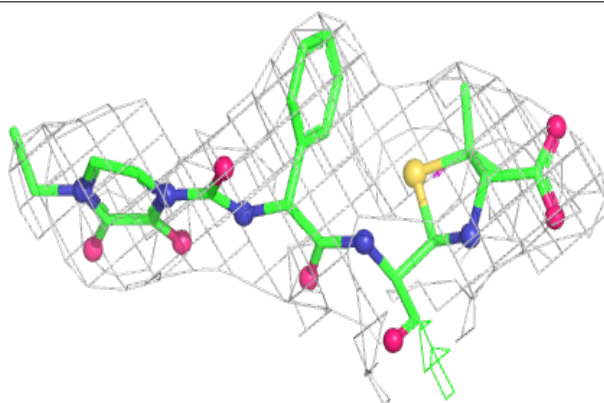
6.5 Other polymers (i)

There are no such residues in this entry.