



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:37 AM UTC

PDB ID : 6H5O / pdb_00006h5o
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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

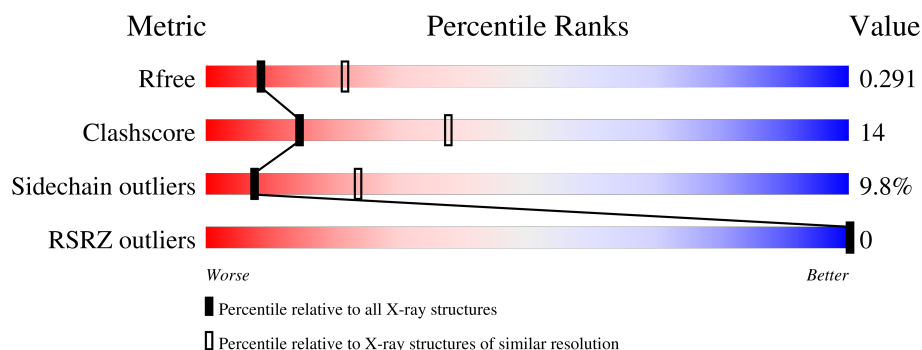
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (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 $\leq 5\%$. 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	642	
1	B	642	

2 Entry composition [i](#)

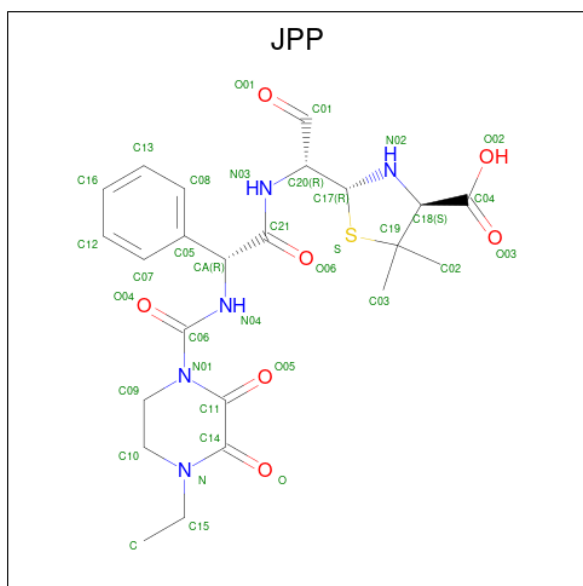
There are 4 unique types of molecules in this entry. The entry contains 10093 atoms, of which 0 are hydrogens and 0 are deuteriums.

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) (CCD ID: JPP) (formula: $C_{23}H_{29}N_5O_7S$).



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 (CCD ID: 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

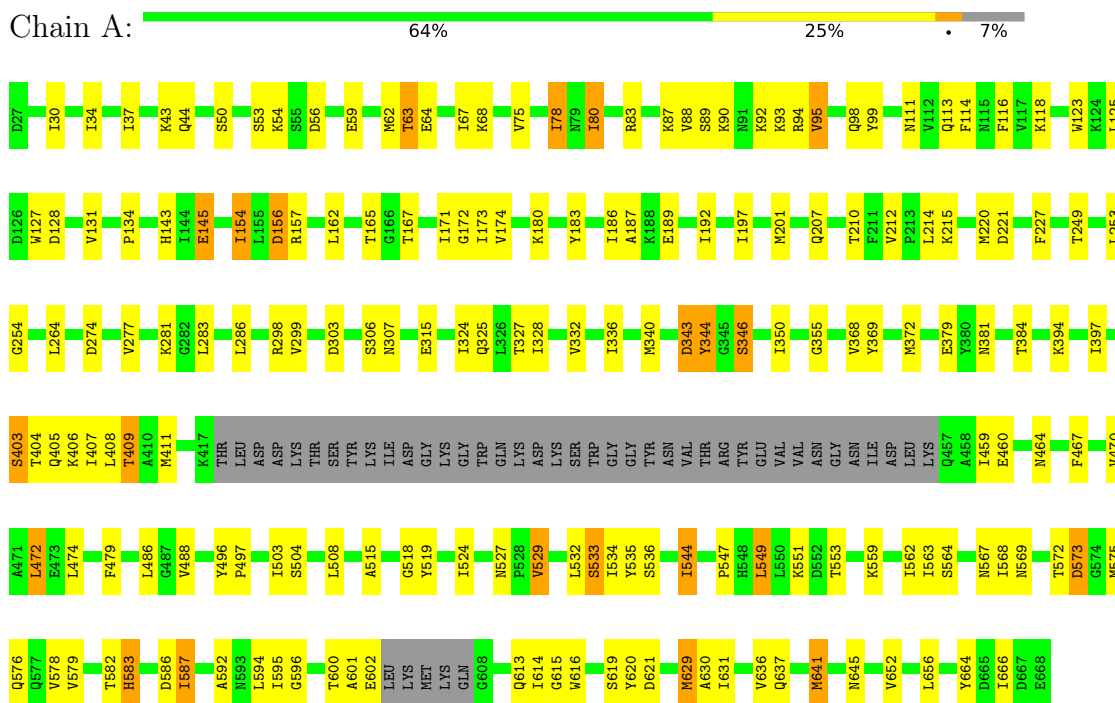
- Molecule 4 is water.

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

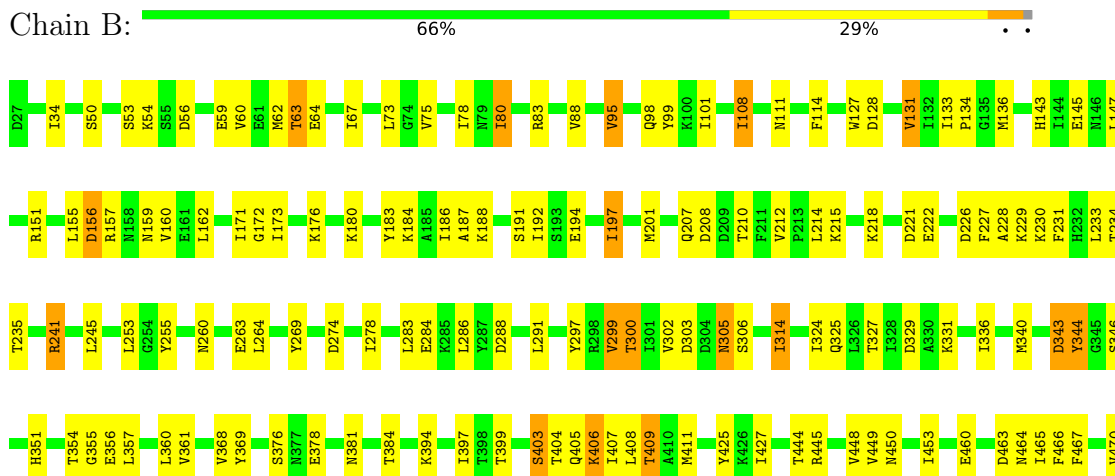
3 Residue-property plots

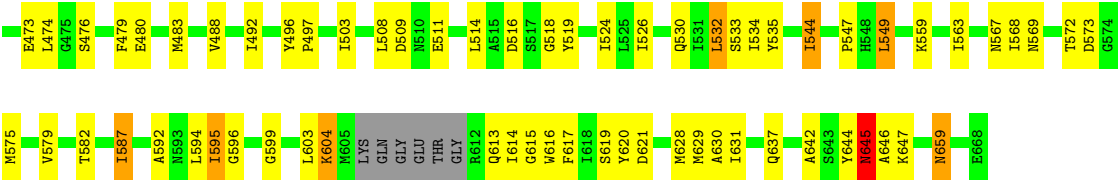
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Penicillin binding protein 2 prime





4 Data and refinement statistics

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 46.45 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.45-2.82) 99.6 (46.45-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.241 , 0.311 (Not available) , 0.291	Depositor DCC
R_{free} test set	1856 reflections (4.78%)	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)	0.30 , 77.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.59	0/4868	0.99	2/6543 (0.0%)
1	B	0.60	0/5194	0.99	3/6983 (0.0%)
All	All	0.60	0/10062	0.99	5/13526 (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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	403	SER	CA-CB-OG	7.72	126.53	111.10
1	B	645	ASN	CB-CA-C	7.13	124.71	110.17
1	B	403	SER	CA-CB-OG	6.37	123.85	111.10
1	A	403	SER	CB-CA-C	-5.95	100.91	110.79
1	B	645	ASN	CA-CB-CG	5.02	117.62	112.60

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	135	0
1	B	5109	0	5108	143	0
2	A	36	0	27	2	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	0	0
All	All	10093	0	9948	279	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 14.

All (279) 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:B:340:MET:HE1	1:B:346:SER:C	2.15	0.70
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:B:156:ASP:CG	1:B:160:VAL:HG12	2.17	0.69
1:A:340:MET:HE1	1:A:346:SER:C	2.18	0.68
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:133:ILE:HB	1:B:136:MET:HE2	1.77	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:336:ILE:HG22	1:B:361:VAL:HG11	1.78	0.64
1:B:54:LYS:HA	1:B:62:MET:HE1	1.80	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:A:615:GLY:C	1:A:645:ASN:HD21	2.05	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:615:GLY:C	1:B:645:ASN:HD21	2.08	0.61
1:A:629:MET:HE2	1:A:631:ILE:HD11	1.83	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:336:ILE:HG22	1:A:629:MET:HE1	1.82	0.59
1:B:60:VAL:O	1:B:64:GLU:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:615:GLY:C	1:A:645:ASN:ND2	2.60	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
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:403:SER:O	1:B:404:THR:C	2.46	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
1:B:615:GLY:C	1:B:645:ASN:ND2	2.62	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:173:ILE:HD11	1:B:201:MET:HE1	1.87	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:403:SER:O	1:A:404:THR:C	2.48	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:54:LYS:HA	1:A:62:MET:HE1	1.92	0.51
1:B:343:ASP:OD1	1:B:343:ASP:N	2.43	0.51
1:B:228:ALA:HB1	1:B:233:LEU:HB2	1.93	0.51
1:B:186:ILE:HD11	1:B:231:PHE:CD2	2.45	0.51
1:A:629:MET:HE1	1:A:652:VAL:HG11	1.93	0.50
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:492:ILE:HD11	1:B:530:GLN:CD	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LYS:HA	1:A:397:ILE:HG22	1.95	0.49
1:B:340:MET:HE1	1:B:346:SER:O	2.13	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
1:A:227:PHE:C	1:A:227:PHE:CD1	2.91	0.49
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:535:TYR:CB	1:B:628:MET:HE1	2.43	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: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:A:403:SER:C	1:A:405:GLN:N	2.73	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:535:TYR:HB3	1:B:628:MET:HE1	1.99	0.45
1:B:544:ILE:CG2	1:B:559:LYS:HB2	2.46	0.45
1:A:340:MET:HE1	1:A:346:SER:O	2.16	0.45
1:A:460:GLU:C	1:A:460:GLU:CD	2.85	0.45
1:A:472:LEU:HD21	1:A:515:ALA:HB2	1.98	0.45
1:A:600:THR:OG1	1:A:641:MET:HE2	2.15	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:A:641:MET:HE1	2:A:701:JPP:H11	1.99	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: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: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: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:B:184:LYS:HG2	1:B:194:GLU:CD	2.43	0.43
1:B:403:SER:C	1:B:405:GLN:N	2.75	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:B:201:MET:HE3	1:B:201:MET:HA	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:220:MET:HE3	1:A:220:MET:HA	2.01	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:A:592:ALA:HB1	1:A:621:ASP:CG	2.45	0.42
1:B:579:VAL:HG22	1:B:587:ILE:HD11	2.01	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:344:TYR:CD1	1:B:344:TYR:C	2.98	0.41
1:A:171:ILE:HD12	1:A:171:ILE:O	2.20	0.41
1:A:369:TYR:HD1	1:A:372:MET:HE2	1.84	0.41
1:A:569:ASN:HA	1:A:572:THR:HG22	2.03	0.41
1:A:344:TYR:CD1	1:A:344:TYR:C	2.99	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:B:405:GLN:HE22	1:B:483:MET:HE1	1.86	0.41
1:A:641:MET:HE2	1:A:641:MET:HB2	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:592:ALA:HB1	1:B:621:ASP:CG	2.46	0.40
1:A:30:ILE:HD11	1:A:116:PHE:CD2	2.55	0.40
1:A:336:ILE:HG22	1:A:629:MET:CE	2.50	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:A:535:TYR:O	1:A:536:SER:C	2.64	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:B:409:THR:HG21	1:B:518:GLY:HA2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	533/572 (93%)	482 (90%)	51 (10%)	8	24
1	B	568/572 (99%)	511 (90%)	57 (10%)	7	23
All	All	1101/1144 (96%)	993 (90%)	108 (10%)	7	24

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	56	ASP
1	A	63	THR
1	A	68	LYS
1	A	75	VAL
1	A	78	ILE
1	A	80	ILE
1	A	88	VAL
1	A	95	VAL
1	A	145	GLU
1	A	154	ILE
1	A	156	ASP
1	A	167	THR
1	A	174	VAL
1	A	207	GLN
1	A	210	THR
1	A	212	VAL
1	A	264	LEU
1	A	274	ASP
1	A	283	LEU
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	379	GLU
1	A	409	THR
1	A	459	ILE
1	A	472	LEU
1	A	474	LEU
1	A	504	SER
1	A	508	LEU
1	A	529	VAL
1	A	533	SER
1	A	544	ILE
1	A	549	LEU
1	A	553	THR
1	A	564	SER
1	A	568	ILE
1	A	573	ASP

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Mol	Chain	Res	Type
1	A	582	THR
1	A	583	HIS
1	A	587	ILE
1	A	614	ILE
1	A	619	SER
1	A	629	MET
1	A	637	GLN
1	A	641	MET
1	B	56	ASP
1	B	63	THR
1	B	67	ILE
1	B	73	LEU
1	B	75	VAL
1	B	78	ILE
1	B	80	ILE
1	B	88	VAL
1	B	95	VAL
1	B	108	ILE
1	B	131	VAL
1	B	155	LEU
1	B	156	ASP
1	B	188	LYS
1	B	197	ILE
1	B	207	GLN
1	B	210	THR
1	B	212	VAL
1	B	222	GLU
1	B	227	PHE
1	B	229	LYS
1	B	234	THR
1	B	241	ARG
1	B	245	LEU
1	B	253	LEU
1	B	264	LEU
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

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Mol	Chain	Res	Type
1	B	343	ASP
1	B	344	TYR
1	B	399	THR
1	B	406	LYS
1	B	409	THR
1	B	444	THR
1	B	450	ASN
1	B	514	LEU
1	B	532	LEU
1	B	544	ILE
1	B	549	LEU
1	B	568	ILE
1	B	573	ASP
1	B	587	ILE
1	B	594	LEU
1	B	595	ILE
1	B	603	LEU
1	B	604	LYS
1	B	614	ILE
1	B	619	SER
1	B	629	MET
1	B	645	ASN
1	B	659	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	113	GLN
1	A	207	GLN
1	A	236	ASN
1	A	307	ASN
1	A	325	GLN
1	A	342	ASN
1	A	393	ASN
1	A	405	GLN
1	A	415	ASN
1	A	530	GLN
1	A	540	ASN
1	A	567	ASN
1	A	576	GLN
1	A	580	ASN

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Mol	Chain	Res	Type
1	A	645	ASN
1	B	32	ASN
1	B	98	GLN
1	B	159	ASN
1	B	266	GLN
1	B	305	ASN
1	B	307	ASN
1	B	325	GLN
1	B	339	ASN
1	B	342	ASN
1	B	377	ASN
1	B	396	GLN
1	B	433	GLN
1	B	543	ASN
1	B	548	HIS
1	B	555	ASN
1	B	567	ASN
1	B	659	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	A	701	1	33,38,38	4.38	12 (36%)	41,55,55	2.35	13 (31%)
2	JPP	B	701	1	33,38,38	4.40	11 (33%)	41,55,55	2.46	13 (31%)

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	A	701	1	-	4/26/64/64	0/3/3/3
2	JPP	B	701	1	-	6/26/64/64	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	11.38	1.43	1.23
2	A	701	JPP	O04-C06	11.33	1.43	1.23
2	B	701	JPP	O06-C21	10.63	1.43	1.23
2	A	701	JPP	O06-C21	10.45	1.43	1.23
2	A	701	JPP	O-C14	10.06	1.43	1.23
2	B	701	JPP	O05-C11	9.91	1.43	1.23
2	A	701	JPP	O05-C11	9.75	1.43	1.23
2	B	701	JPP	O-C14	9.69	1.42	1.23
2	B	701	JPP	C14-C11	-8.03	1.40	1.53
2	A	701	JPP	C14-C11	-7.57	1.41	1.53
2	A	701	JPP	C10-N	-7.25	1.34	1.47
2	B	701	JPP	C10-N	-7.23	1.34	1.47
2	A	701	JPP	C09-N01	-5.61	1.39	1.47
2	B	701	JPP	C09-N01	-5.48	1.39	1.47
2	A	701	JPP	O02-C04	-3.21	1.20	1.30
2	B	701	JPP	C10-C09	-2.98	1.40	1.51
2	A	701	JPP	C10-C09	-2.90	1.40	1.51
2	A	701	JPP	C19-S	-2.65	1.80	1.85
2	B	701	JPP	C21-N03	2.57	1.39	1.34
2	B	701	JPP	C19-S	-2.55	1.80	1.85
2	B	701	JPP	O02-C04	-2.51	1.22	1.30
2	A	701	JPP	C08-C05	2.24	1.42	1.39
2	A	701	JPP	C06-N01	-2.16	1.38	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	JPP	C10-C09-N01	6.18	118.64	109.06
2	A	701	JPP	C10-C09-N01	5.97	118.30	109.06
2	B	701	JPP	C20-N03-C21	-5.41	116.88	123.08
2	B	701	JPP	C03-C19-S	-5.13	100.93	109.18
2	A	701	JPP	C20-N03-C21	-4.99	117.36	123.08
2	B	701	JPP	C10-N-C14	4.88	130.59	120.82
2	A	701	JPP	C15-N-C14	-4.71	113.95	119.59
2	A	701	JPP	C10-N-C14	4.67	130.17	120.82
2	A	701	JPP	O-C14-N	4.42	128.55	123.55
2	B	701	JPP	C18-C19-S	4.15	111.75	103.86
2	B	701	JPP	O-C14-N	4.02	128.11	123.55
2	B	701	JPP	CA-N04-C06	-3.92	113.72	121.22
2	A	701	JPP	CA-N04-C06	-3.88	113.80	121.22
2	B	701	JPP	C19-S-C17	-3.81	83.74	93.41
2	B	701	JPP	C15-N-C14	-3.81	115.03	119.59
2	B	701	JPP	C03-C19-C02	3.57	116.51	110.70
2	A	701	JPP	C03-C19-S	-3.57	103.44	109.18
2	A	701	JPP	C02-C19-C18	-3.31	101.36	112.33
2	A	701	JPP	C19-S-C17	-2.89	86.09	93.41
2	A	701	JPP	C19-C18-C04	2.76	117.58	112.37
2	A	701	JPP	O04-C06-N04	-2.52	115.98	122.96
2	B	701	JPP	O04-C06-N04	-2.47	116.12	122.96
2	A	701	JPP	C03-C19-C18	2.35	120.12	112.33
2	B	701	JPP	O01-C01-C20	-2.34	118.67	124.86
2	A	701	JPP	C18-C19-S	2.27	108.18	103.86
2	B	701	JPP	C02-C19-C18	-2.03	105.61	112.33

There are no chirality outliers.

All (10) 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
2	B	701	JPP	C-C15-N-C10
2	B	701	JPP	O03-C04-C18-C19
2	B	701	JPP	O02-C04-C18-C19
2	B	701	JPP	C-C15-N-C14
2	A	701	JPP	C07-C05-CA-N04
2	B	701	JPP	O06-C21-CA-N04
2	A	701	JPP	C08-C05-CA-N04
2	B	701	JPP	C07-C05-CA-C21

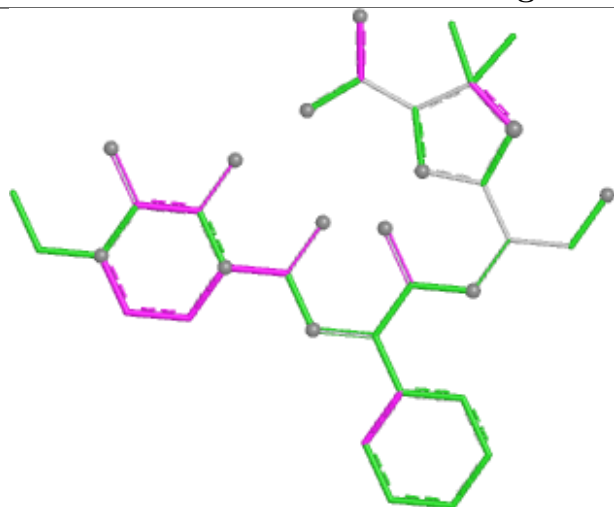
There are no ring outliers.

2 monomers are involved in 6 short contacts:

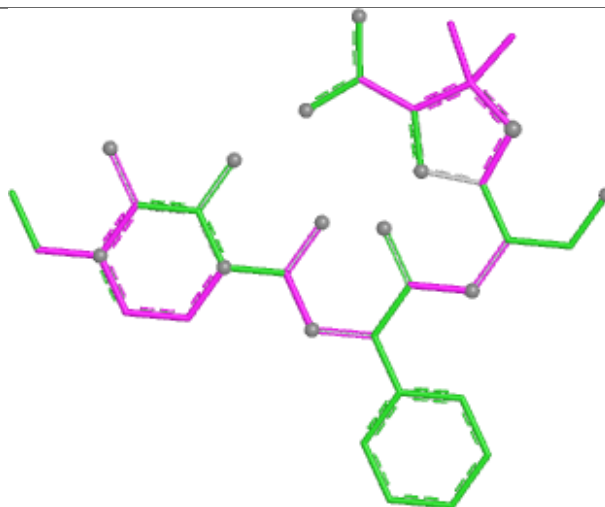
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	JPP	2	0
2	B	701	JPP	4	0

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

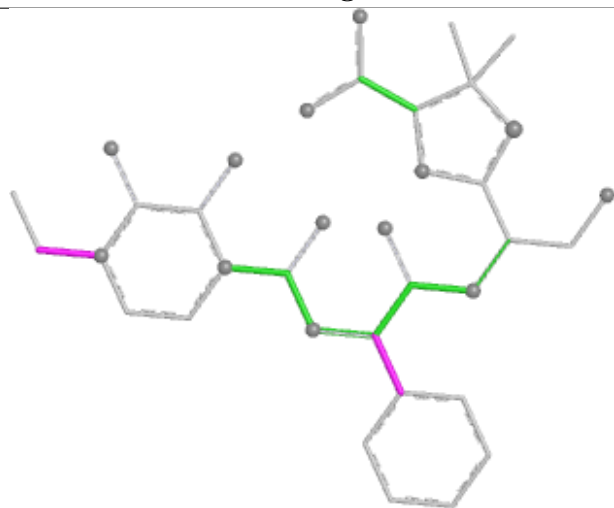
Ligand JPP A 701



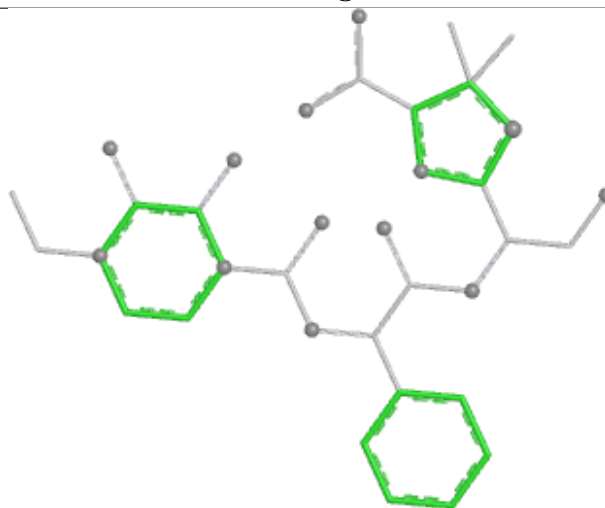
Bond lengths



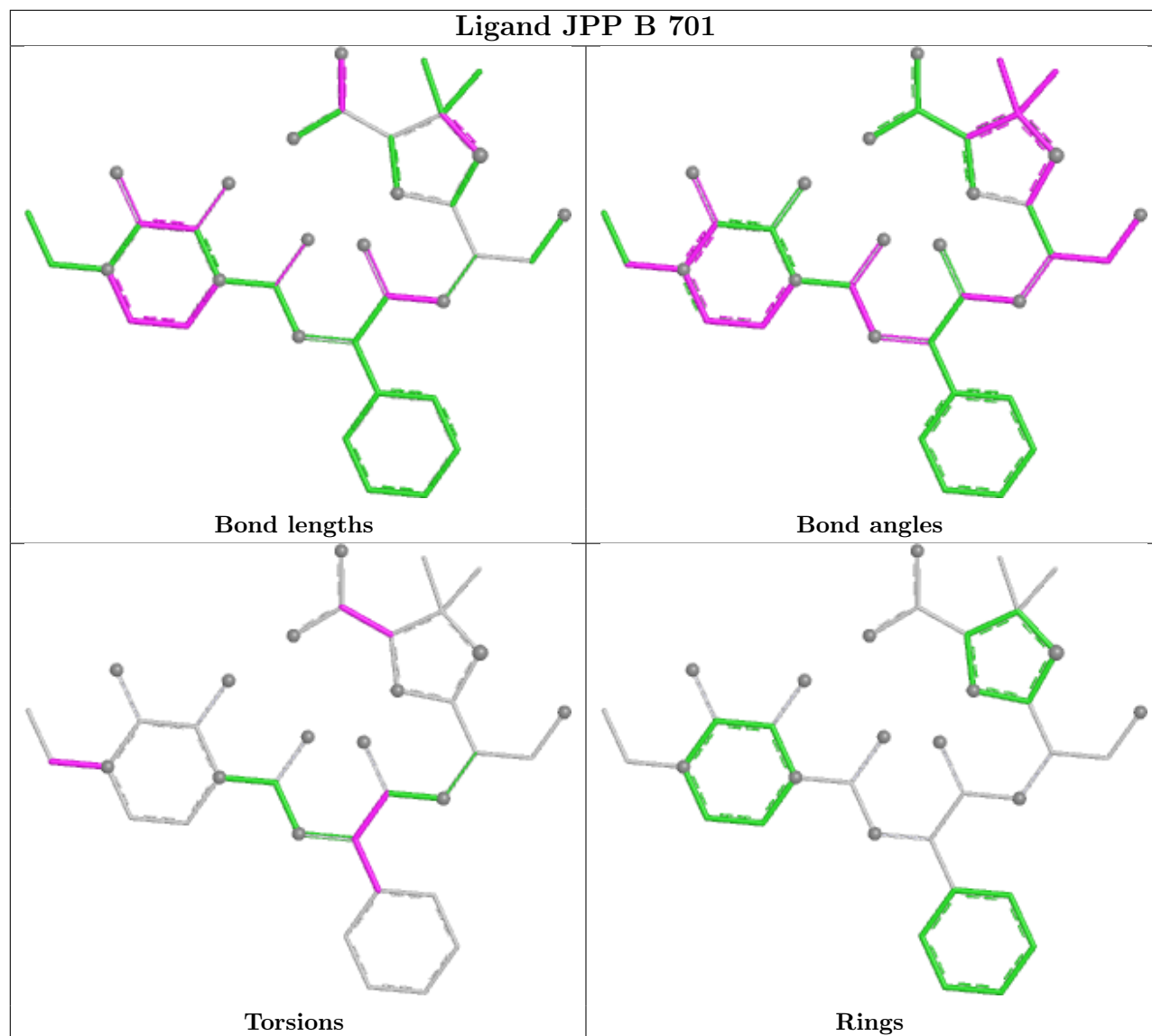
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	598/642 (93%)	-0.58	0 100 100	79, 119, 169, 247	0
1	B	636/642 (99%)	-0.49	0 100 100	75, 124, 175, 211	2 (0%)
All	All	1234/1284 (96%)	-0.54	0 100 100	75, 122, 172, 247	2 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	JPP	A	701	36/36	0.77	0.08	115,137,153,156	0
2	JPP	B	701	36/36	0.86	0.09	87,109,143,144	0
3	CD	A	706	1/1	0.93	0.11	202,202,202,202	0
3	CD	A	707	1/1	0.95	0.06	176,176,176,176	0
3	CD	A	705	1/1	0.97	0.08	153,153,153,153	0
3	CD	A	703	1/1	0.99	0.10	128,128,128,128	0
3	CD	A	709	1/1	0.99	0.03	92,92,92,92	1

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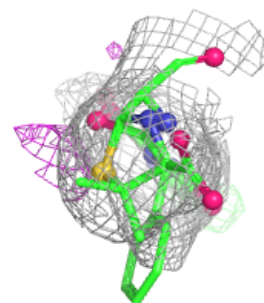
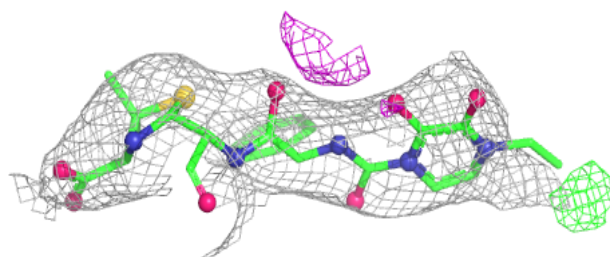
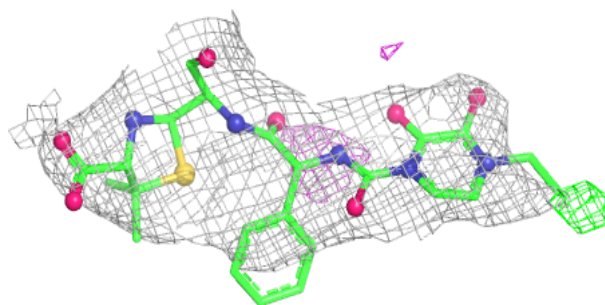
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CD	B	702	1/1	0.99	0.02	122,122,122,122	1
3	CD	A	708	1/1	1.00	0.02	94,94,94,94	0
3	CD	A	704	1/1	1.00	0.02	99,99,99,99	0
3	CD	A	702	1/1	1.00	0.05	102,102,102,102	0

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.

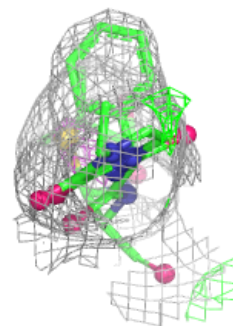
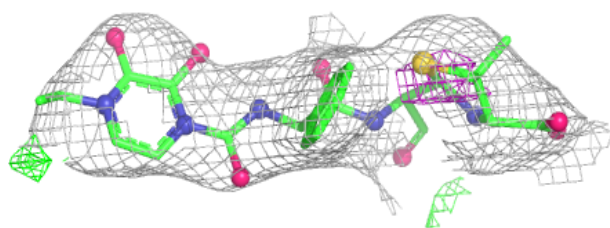
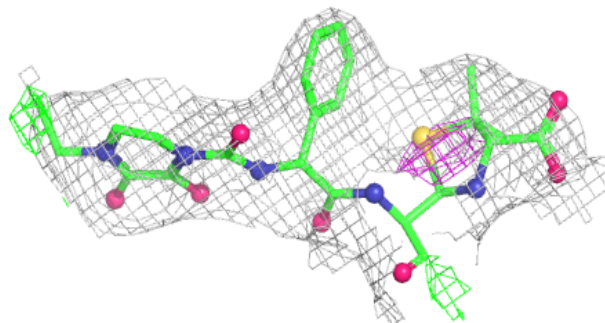
Electron density around JPP A 701:

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.