Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 02:44 AM EST

PDB ID	:	3KYC
Title	:	Human SUMO E1 complex with a SUMO1-AMP mimic
Authors	:	Lima, C.D.
Deposited on	:	2009-12-05
Resolution	:	2.45 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:

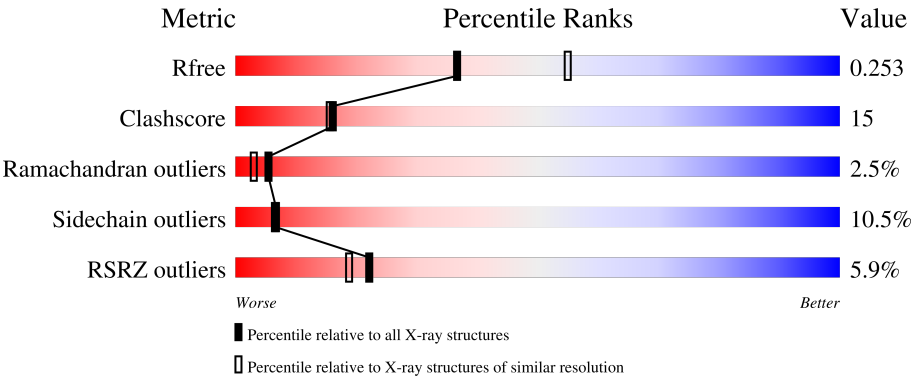
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	346	6% 60% 25% 5% 10%
2	B	660	5% 57% 23% • 17%
3	D	97	5% 39% 35% 5% • 19%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7681 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 SUMO-activating enzyme subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2445	1549	416	467	13			

- Molecule 2 is a protein called SUMO-activating enzyme subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	548	Total	C	N	O	S	0	0	0
			4320	2738	754	808	20			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP Q9UBT2
B	-18	GLY	-	expression tag	UNP Q9UBT2
B	-17	SER	-	expression tag	UNP Q9UBT2
B	-16	SER	-	expression tag	UNP Q9UBT2
B	-15	HIS	-	expression tag	UNP Q9UBT2
B	-14	HIS	-	expression tag	UNP Q9UBT2
B	-13	HIS	-	expression tag	UNP Q9UBT2
B	-12	HIS	-	expression tag	UNP Q9UBT2
B	-11	HIS	-	expression tag	UNP Q9UBT2
B	-10	HIS	-	expression tag	UNP Q9UBT2
B	-9	SER	-	expression tag	UNP Q9UBT2
B	-8	SER	-	expression tag	UNP Q9UBT2
B	-7	GLY	-	expression tag	UNP Q9UBT2
B	-6	LEU	-	expression tag	UNP Q9UBT2
B	-5	VAL	-	expression tag	UNP Q9UBT2
B	-4	PRO	-	expression tag	UNP Q9UBT2
B	-3	ARG	-	expression tag	UNP Q9UBT2
B	-2	GLY	-	expression tag	UNP Q9UBT2
B	-1	SER	-	expression tag	UNP Q9UBT2
B	0	HIS	-	expression tag	UNP Q9UBT2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	229	CYS	SER	variant	UNP Q9UBT2

- Molecule 3 is a protein called Small ubiquitin-related modifier 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	79	Total	C	N	O	S	0	0	0
			639	401	110	123	5			

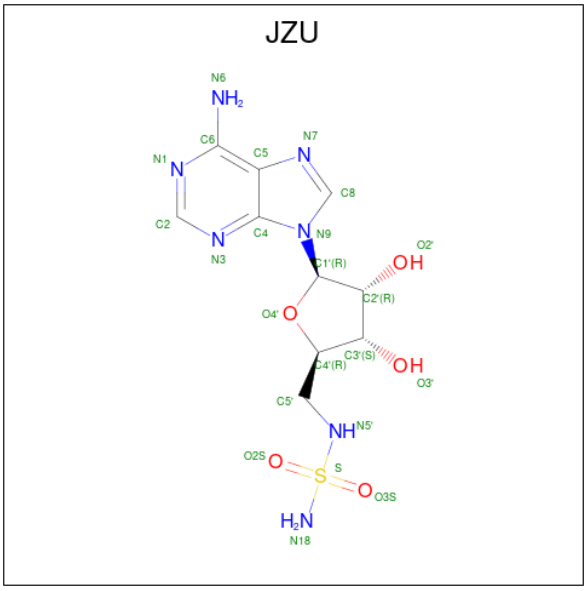
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	95	CYS	THR	engineered mutation	UNP P63165

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

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

- Molecule 5 is 5'-deoxy-5'-(sulfamoylamino)adenosine (three-letter code: JZU) (formula: $C_{10}H_{15}N_7O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	S	0	0
			23	10	7	5	1		

- Molecule 6 is water.

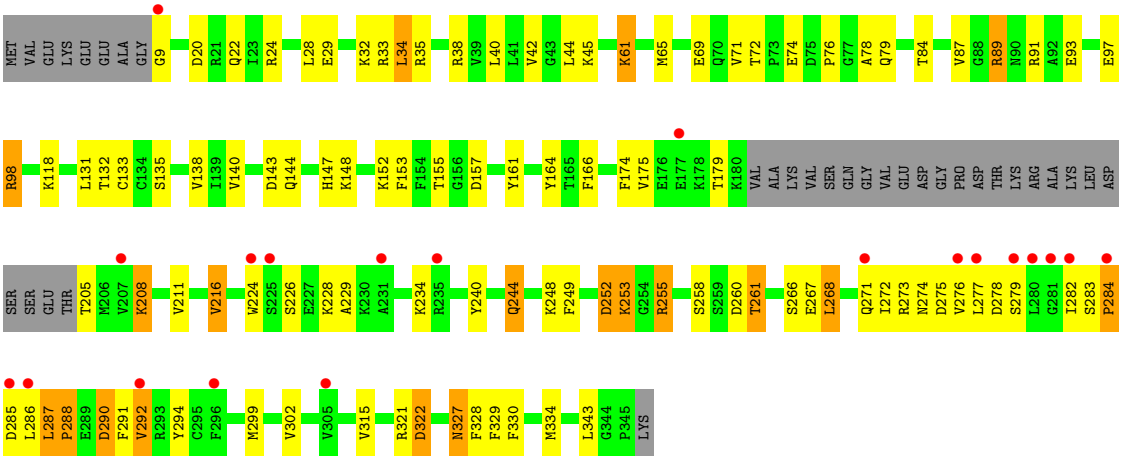
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	58	Total O 58 58	0	0
6	B	183	Total O 183 183	0	0
6	D	12	Total O 12 12	0	0

3 Residue-property plots (i)

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

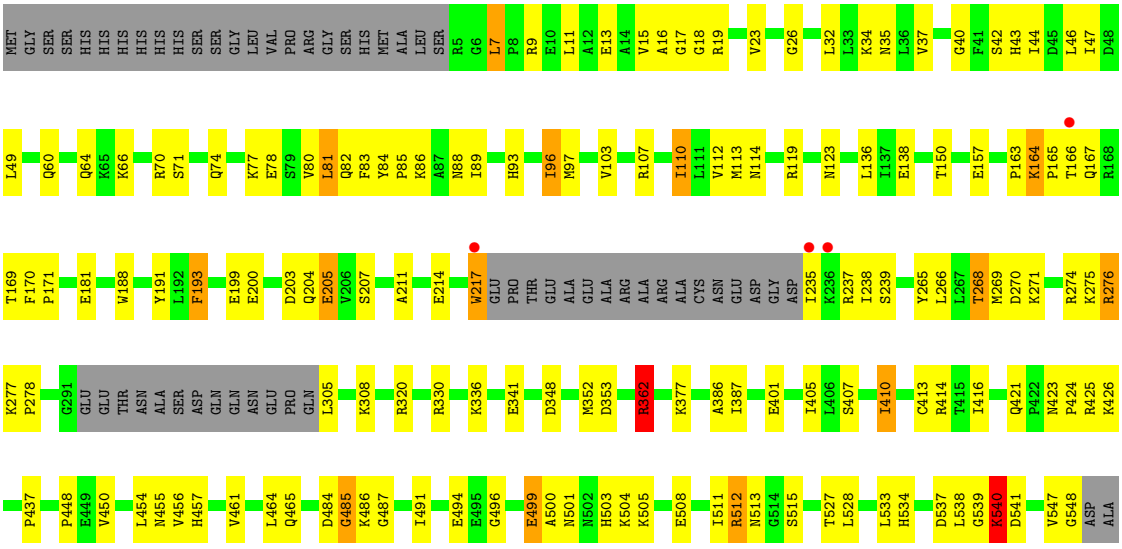
• Molecule 1: SUMO-activating enzyme subunit 1

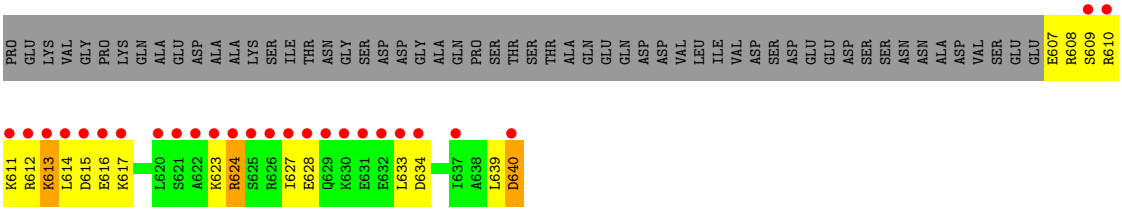
Chain A:



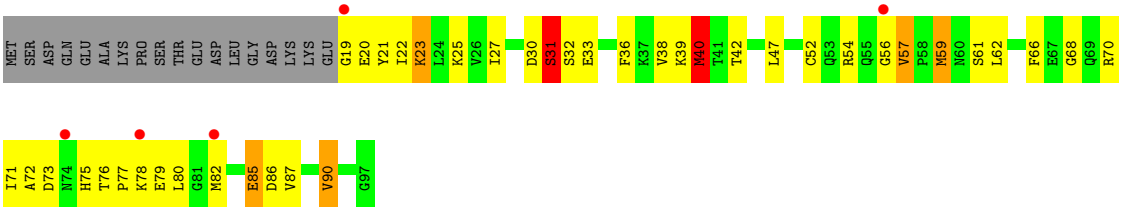
• Molecule 2: SUMO-activating enzyme subunit 2

Chain B:





• Molecule 3: Small ubiquitin-related modifier 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.17Å 133.37Å 159.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.45 44.26 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.2 (25.00-2.45) 99.2 (44.26-2.45)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.5.0093	Depositor
R, R_{free}	0.191 , 0.250 0.193 , 0.253	Depositor DCC
R_{free} test set	2378 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	53.0	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7681	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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

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	0.91	0/2488	0.88	2/3357 (0.1%)
2	B	1.03	4/4396 (0.1%)	1.04	17/5936 (0.3%)
3	D	0.85	0/649	0.87	0/866
All	All	0.98	4/7533 (0.1%)	0.98	19/10159 (0.2%)

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
2	B	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	193	PHE	CE2-CZ	5.33	1.47	1.37
2	B	205	GLU	CG-CD	5.15	1.59	1.51
2	B	607	GLU	CB-CG	-5.13	1.42	1.52
2	B	341	GLU	CD-OE2	5.08	1.31	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	362	ARG	NE-CZ-NH2	-11.96	114.32	120.30
2	B	362	ARG	NE-CZ-NH1	8.23	124.41	120.30
2	B	362	ARG	CG-CD-NE	-8.02	94.96	111.80
1	A	327	ASN	N-CA-C	7.64	131.64	111.00
2	B	7	LEU	CA-CB-CG	7.34	132.19	115.30
2	B	276	ARG	NE-CZ-NH1	6.89	123.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	276	ARG	NE-CZ-NH2	-6.52	117.04	120.30
2	B	348	ASP	CB-CG-OD1	6.30	123.97	118.30
2	B	119	ARG	NE-CZ-NH1	6.13	123.37	120.30
2	B	353	ASP	CB-CG-OD1	6.04	123.73	118.30
2	B	270	ASP	CB-CG-OD1	5.91	123.62	118.30
2	B	330	ARG	NE-CZ-NH1	5.87	123.24	120.30
2	B	203	ASP	CB-CG-OD2	5.86	123.57	118.30
2	B	107	ARG	NE-CZ-NH2	-5.59	117.51	120.30
2	B	207	SER	N-CA-CB	-5.56	102.16	110.50
1	A	216	VAL	CB-CA-C	-5.52	100.91	111.40
2	B	540	LYS	N-CA-C	5.46	125.74	111.00
2	B	353	ASP	CB-CG-OD2	-5.38	113.46	118.30
2	B	362	ARG	CD-NE-CZ	5.03	130.64	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	485	GLY	Peptide
2	B	93	HIS	Peptide

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	2445	0	2424	74	0
2	B	4320	0	4378	116	1
3	D	639	0	633	33	0
4	B	1	0	0	0	0
5	D	23	0	14	1	0
6	A	58	0	0	6	0
6	B	183	0	0	17	0
6	D	12	0	0	0	0
All	All	7681	0	7449	216	1

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 15.

All (216) 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)
2:B:512:ARG:HH11	2:B:512:ARG:HG2	1.07	1.15
2:B:11:LEU:HD13	2:B:407:SER:HB3	1.40	1.01
2:B:217:TRP:HZ3	2:B:274:ARG:NH2	1.58	1.01
2:B:512:ARG:HH11	2:B:512:ARG:CG	1.75	1.00
2:B:150:THR:CG2	2:B:405:ILE:HD11	1.92	1.00
2:B:512:ARG:HG2	2:B:512:ARG:NH1	1.68	0.97
1:A:9:GLY:N	1:A:32:LYS:HZ3	1.64	0.96
3:D:72:ALA:H	3:D:75:HIS:HD2	1.21	0.89
2:B:150:THR:HG23	2:B:405:ILE:HD11	1.52	0.88
2:B:265:TYR:O	2:B:268:THR:HB	1.73	0.88
2:B:114:ASN:ND2	2:B:138:GLU:OE1	2.07	0.88
2:B:640:ASP:HB2	3:D:54:ARG:HH12	1.37	0.87
1:A:273:ARG:HG2	1:A:277:LEU:HD11	1.59	0.83
1:A:252:ASP:O	1:A:253:LYS:HB2	1.77	0.82
2:B:624:ARG:HB2	2:B:624:ARG:NH1	1.94	0.81
1:A:33:ARG:HD3	6:A:355:HOH:O	1.80	0.80
1:A:143:ASP:OD1	1:A:216:VAL:HG23	1.81	0.80
1:A:157:ASP:HB2	1:A:164:TYR:HE2	1.44	0.80
2:B:11:LEU:CD1	2:B:407:SER:HB3	2.12	0.80
1:A:89:ARG:HH11	1:A:89:ARG:CG	1.95	0.79
2:B:512:ARG:HG3	2:B:513:ASN:N	2.00	0.76
2:B:150:THR:HG21	2:B:405:ILE:HD11	1.69	0.75
1:A:274:ASN:HA	1:A:277:LEU:HD12	1.69	0.74
2:B:74:GLN:HG2	6:B:797:HOH:O	1.88	0.74
1:A:9:GLY:N	1:A:32:LYS:NZ	2.36	0.74
1:A:34:LEU:HD11	1:A:315:VAL:HG13	1.68	0.73
1:A:143:ASP:CG	1:A:216:VAL:HG23	2.08	0.73
2:B:496:GLY:HA2	2:B:499:GLU:OE2	1.88	0.73
2:B:217:TRP:CZ3	2:B:274:ARG:NH2	2.50	0.72
1:A:89:ARG:HH11	1:A:89:ARG:HG3	1.54	0.71
1:A:98:ARG:HH21	2:B:82:GLN:HB2	1.55	0.70
1:A:132:THR:HG21	6:A:363:HOH:O	1.91	0.69
2:B:277:LYS:HE3	6:B:715:HOH:O	1.91	0.69
2:B:268:THR:HG23	6:B:721:HOH:O	1.92	0.68
2:B:16:ALA:HA	2:B:42:SER:OG	1.94	0.68
1:A:244:GLN:HE21	1:A:244:GLN:HA	1.59	0.67
2:B:266:LEU:HD23	2:B:269:MET:CE	2.24	0.67
2:B:188:TRP:CE3	2:B:362:ARG:HG3	2.30	0.66
2:B:64:GLN:HG2	6:B:761:HOH:O	1.95	0.66
2:B:34:LYS:HE3	2:B:35:ASN:OD1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:THR:CG2	6:B:721:HOH:O	2.44	0.65
2:B:457:HIS:O	2:B:505:LYS:HG2	1.96	0.65
1:A:288:PRO:HB3	1:A:290:ASP:OD1	1.96	0.65
2:B:123:ASN:HD21	2:B:164:LYS:HE2	1.62	0.65
2:B:217:TRP:CH2	2:B:271:LYS:HB2	2.32	0.64
1:A:249:PHE:O	1:A:249:PHE:CD2	2.50	0.64
2:B:484:ASP:O	2:B:486:LYS:N	2.29	0.64
2:B:70:ARG:NH2	2:B:78:GLU:OE2	2.29	0.64
1:A:157:ASP:HB2	1:A:164:TYR:CE2	2.30	0.64
2:B:266:LEU:HD23	2:B:269:MET:HE3	1.79	0.63
3:D:72:ALA:N	3:D:75:HIS:HD2	1.95	0.62
2:B:624:ARG:HB2	2:B:624:ARG:CZ	2.27	0.62
2:B:43:HIS:CD2	2:B:88:ASN:HD22	2.18	0.62
2:B:547:VAL:HG12	2:B:548:GLY:N	2.15	0.62
3:D:66:PHE:HB2	3:D:71:ILE:HD11	1.82	0.62
3:D:78:LYS:HG2	3:D:79:GLU:N	2.14	0.61
1:A:147:HIS:CE1	6:A:382:HOH:O	2.53	0.61
2:B:64:GLN:CG	6:B:761:HOH:O	2.48	0.60
3:D:76:THR:HG23	3:D:77:PRO:HD2	1.83	0.60
2:B:15:VAL:HG12	2:B:40:GLY:O	2.02	0.60
3:D:19:GLY:CA	3:D:39:LYS:HE3	2.31	0.60
6:A:383:HOH:O	2:B:421:GLN:HG2	2.00	0.59
3:D:19:GLY:HA3	3:D:39:LYS:HE3	1.82	0.59
2:B:103:VAL:HG23	6:B:720:HOH:O	2.01	0.59
1:A:35:ARG:O	1:A:61:LYS:HB2	2.02	0.59
3:D:59:MET:O	3:D:61:SER:N	2.31	0.58
3:D:72:ALA:H	3:D:75:HIS:CD2	2.10	0.58
3:D:78:LYS:HG2	3:D:79:GLU:H	1.68	0.58
1:A:273:ARG:O	1:A:277:LEU:HG	2.03	0.58
2:B:77:LYS:HG3	2:B:89:ILE:HB	1.86	0.58
2:B:171:PRO:HA	2:B:541:ASP:OD2	2.03	0.57
1:A:155:THR:HG22	1:A:166:PHE:HB3	1.87	0.57
3:D:76:THR:HB	3:D:79:GLU:HG3	1.84	0.57
1:A:277:LEU:HD13	1:A:284:PRO:HA	1.87	0.57
3:D:20:GLU:HG2	3:D:21:TYR:H	1.70	0.57
1:A:72:THR:HG22	1:A:74:GLU:H	1.71	0.56
3:D:22:ILE:HG23	3:D:40:MET:HE1	1.88	0.55
1:A:268:LEU:O	1:A:272:ILE:HG13	2.07	0.55
3:D:25:LYS:HE2	3:D:33:GLU:OE2	2.07	0.55
2:B:496:GLY:CA	2:B:499:GLU:OE2	2.55	0.55
1:A:44:LEU:HD21	1:A:65:MET:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:CG	1:A:89:ARG:NH1	2.62	0.54
2:B:540:LYS:HD2	6:B:702:HOH:O	2.07	0.54
1:A:283:SER:O	1:A:285:ASP:N	2.40	0.54
1:A:131:LEU:HD22	1:A:153:PHE:CE1	2.42	0.54
2:B:456:VAL:HG21	2:B:511:ILE:O	2.08	0.54
1:A:282:ILE:O	1:A:284:PRO:HD3	2.08	0.53
1:A:282:ILE:HG23	1:A:286:LEU:HD12	1.91	0.53
2:B:214:GLU:OE1	2:B:276:ARG:NH2	2.37	0.53
2:B:624:ARG:HA	2:B:627:ILE:HB	1.89	0.52
3:D:77:PRO:HA	3:D:82:MET:HG3	1.92	0.52
2:B:504:LYS:HB3	2:B:508:GLU:OE1	2.10	0.52
2:B:634:ASP:HA	3:D:42:THR:HG23	1.92	0.52
1:A:164:TYR:HA	1:A:329:PHE:O	2.09	0.52
1:A:299:MET:HE3	1:A:299:MET:HA	1.91	0.52
3:D:62:LEU:HD13	3:D:90:VAL:HG11	1.92	0.52
3:D:85:GLU:OE2	3:D:85:GLU:HA	2.10	0.52
1:A:143:ASP:CB	1:A:216:VAL:HG23	2.39	0.51
3:D:59:MET:C	3:D:61:SER:H	2.13	0.51
2:B:624:ARG:HB2	2:B:624:ARG:HH11	1.73	0.51
1:A:174:PHE:HE2	1:A:211:VAL:HG12	1.74	0.51
1:A:42:VAL:O	1:A:132:THR:HB	2.11	0.51
2:B:44:ILE:O	2:B:89:ILE:HA	2.11	0.50
3:D:25:LYS:HG3	3:D:87:VAL:HG22	1.93	0.50
1:A:261:THR:O	1:A:261:THR:OG1	2.27	0.50
2:B:191:TYR:CD2	2:B:204:GLN:HG2	2.46	0.50
2:B:217:TRP:N	2:B:217:TRP:CD1	2.80	0.50
2:B:157:GLU:HA	2:B:437:PRO:HA	1.94	0.50
2:B:448:PRO:HG2	2:B:527:THR:O	2.12	0.49
2:B:47:ILE:HG21	2:B:96:ILE:HG23	1.94	0.49
1:A:299:MET:HA	1:A:299:MET:CE	2.43	0.49
2:B:614:LEU:HA	2:B:617:LYS:HD2	1.94	0.49
2:B:450:VAL:HG22	2:B:528:LEU:HD11	1.94	0.49
2:B:217:TRP:HZ3	2:B:274:ARG:HH22	1.51	0.49
1:A:20:ASP:O	1:A:24:ARG:HG3	2.13	0.49
1:A:22:GLN:HB3	2:B:387:ILE:HG22	1.95	0.49
2:B:613:LYS:HG3	2:B:616:GLU:OE2	2.13	0.49
2:B:70:ARG:HH22	2:B:78:GLU:CD	2.16	0.48
3:D:47:LEU:C	3:D:47:LEU:HD23	2.34	0.48
2:B:386:ALA:HA	6:B:657:HOH:O	2.13	0.48
2:B:80:VAL:HA	2:B:83:PHE:CE2	2.49	0.48
1:A:97:GLU:HA	1:A:97:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ASP:CB	1:A:216:VAL:CG2	2.93	0.47
2:B:199:GLU:O	2:B:200:GLU:C	2.50	0.47
1:A:224:TRP:HA	1:A:229:ALA:HB1	1.97	0.47
1:A:135:SER:OG	1:A:138:VAL:HG23	2.15	0.47
2:B:211:ALA:HB1	2:B:540:LYS:NZ	2.30	0.47
2:B:457:HIS:O	2:B:505:LYS:CG	2.63	0.46
2:B:504:LYS:NZ	6:B:703:HOH:O	2.47	0.46
2:B:23:VAL:CG1	2:B:96:ILE:HG12	2.46	0.46
1:A:226:SER:HB3	1:A:229:ALA:HB3	1.96	0.46
2:B:539:GLY:O	2:B:541:ASP:N	2.47	0.46
2:B:465:GLN:HB2	2:B:491:ILE:HD13	1.97	0.46
2:B:421:GLN:HB2	3:D:31:SER:HB2	1.96	0.46
1:A:155:THR:CG2	1:A:166:PHE:HB3	2.44	0.46
2:B:165:PRO:HG3	3:D:61:SER:HA	1.98	0.46
1:A:45:LYS:HD2	1:A:133:CYS:SG	2.56	0.46
2:B:537:ASP:HA	6:B:789:HOH:O	2.16	0.46
2:B:77:LYS:HE3	2:B:89:ILE:O	2.15	0.45
2:B:193:PHE:C	2:B:193:PHE:CD2	2.90	0.45
2:B:494:GLU:HG3	6:B:808:HOH:O	2.16	0.45
1:A:69:GLU:OE2	1:A:91:ARG:NH2	2.49	0.45
2:B:455:ASN:HA	2:B:534:HIS:CE1	2.52	0.45
3:D:19:GLY:HA3	3:D:39:LYS:CE	2.45	0.45
1:A:140:VAL:HG12	1:A:144:GLN:NE2	2.31	0.45
1:A:244:GLN:HA	1:A:244:GLN:NE2	2.29	0.45
1:A:321:ARG:O	1:A:322:ASP:HB2	2.17	0.45
2:B:624:ARG:HG2	2:B:627:ILE:HD12	1.98	0.45
3:D:19:GLY:N	3:D:39:LYS:HE3	2.32	0.45
3:D:27:ILE:CD1	3:D:87:VAL:HG13	2.46	0.45
2:B:456:VAL:H	2:B:534:HIS:CE1	2.35	0.45
2:B:611:LYS:O	2:B:615:ASP:HB2	2.16	0.45
2:B:18:GLY:HA3	2:B:110:ILE:HD11	1.99	0.45
2:B:112:VAL:O	2:B:136:LEU:HA	2.17	0.45
1:A:174:PHE:HE2	1:A:211:VAL:CG1	2.30	0.44
1:A:208:LYS:HE3	1:A:208:LYS:HB2	1.79	0.44
2:B:352:MET:SD	2:B:377:LYS:HG3	2.58	0.44
3:D:23:LYS:HA	3:D:36:PHE:O	2.17	0.44
2:B:401:GLU:OE1	2:B:413:CYS:HA	2.17	0.44
1:A:249:PHE:CD2	1:A:249:PHE:C	2.90	0.44
1:A:255:ARG:HH22	1:A:261:THR:HG21	1.81	0.44
2:B:23:VAL:HG11	2:B:96:ILE:HG12	2.00	0.44
2:B:484:ASP:OD1	2:B:487:GLY:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:52:CYS:HB3	3:D:57:VAL:O	2.18	0.44
2:B:43:HIS:CD2	2:B:88:ASN:ND2	2.84	0.44
2:B:47:ILE:HD13	2:B:96:ILE:HG23	1.98	0.44
2:B:547:VAL:CG1	2:B:548:GLY:N	2.80	0.44
2:B:49:LEU:HD23	5:D:98:JZU:C6	2.47	0.43
1:A:291:PHE:CD1	1:A:292:VAL:N	2.87	0.43
2:B:170:PHE:HA	2:B:171:PRO:HD2	1.84	0.43
3:D:76:THR:HG21	3:D:78:LYS:HD3	2.01	0.43
1:A:131:LEU:HD22	1:A:153:PHE:HE1	1.83	0.43
1:A:226:SER:HB3	1:A:229:ALA:CB	2.49	0.43
2:B:405:ILE:HD13	2:B:405:ILE:HG21	1.73	0.43
1:A:252:ASP:O	1:A:253:LYS:CB	2.56	0.43
1:A:71:VAL:O	1:A:87:VAL:HG13	2.18	0.43
2:B:624:ARG:HH11	2:B:624:ARG:CB	2.32	0.43
2:B:501:ASN:HA	2:B:504:LYS:HD2	2.00	0.43
2:B:512:ARG:HH11	2:B:512:ARG:CB	2.28	0.43
2:B:608:ARG:CG	2:B:612:ARG:NH2	2.82	0.43
2:B:77:LYS:NZ	6:B:762:HOH:O	2.52	0.42
2:B:18:GLY:HA3	2:B:110:ILE:CD1	2.48	0.42
2:B:533:LEU:HD23	2:B:533:LEU:HA	1.85	0.42
1:A:272:ILE:O	1:A:276:VAL:HG23	2.18	0.42
2:B:461:VAL:O	2:B:464:LEU:HB3	2.19	0.42
2:B:496:GLY:N	2:B:499:GLU:OE2	2.53	0.42
1:A:89:ARG:NH1	1:A:89:ARG:HG2	2.35	0.42
1:A:161:TYR:HA	1:A:302:VAL:HG21	2.00	0.42
1:A:78:ALA:O	1:A:79:GLN:HG3	2.19	0.42
1:A:148:LYS:HD3	6:A:350:HOH:O	2.20	0.42
1:A:78:ALA:HB2	2:B:84:TYR:CD1	2.55	0.41
2:B:26:GLY:HA2	2:B:60:GLN:OE1	2.20	0.41
2:B:163:PRO:HA	6:B:758:HOH:O	2.20	0.41
2:B:278:PRO:HD2	6:B:715:HOH:O	2.20	0.41
1:A:328:PHE:HB3	1:A:330:PHE:CE1	2.55	0.41
2:B:410:ILE:H	2:B:410:ILE:HG13	1.40	0.41
1:A:240:TYR:CD1	1:A:343:LEU:CD1	3.04	0.41
1:A:143:ASP:HB2	1:A:216:VAL:CG2	2.50	0.41
1:A:258:SER:HB3	1:A:261:THR:HG23	2.03	0.41
2:B:164:LYS:H	2:B:164:LYS:HG2	1.37	0.41
3:D:27:ILE:HD12	3:D:87:VAL:HG13	2.02	0.41
2:B:277:LYS:HG3	6:B:715:HOH:O	2.21	0.41
3:D:75:HIS:CE1	3:D:80:LEU:HD21	2.54	0.41
1:A:174:PHE:CE2	1:A:211:VAL:HG12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LEU:HA	1:A:288:PRO:HD2	1.90	0.41
2:B:43:HIS:HD2	2:B:88:ASN:HD22	1.65	0.41
2:B:81:LEU:HD12	2:B:81:LEU:HA	1.95	0.41
2:B:623:LYS:HE3	2:B:627:ILE:HD11	2.03	0.41
3:D:76:THR:HG23	3:D:77:PRO:CD	2.50	0.41
1:A:272:ILE:O	1:A:273:ARG:C	2.57	0.40
2:B:423:ASN:HB2	2:B:424:PRO:CD	2.51	0.40
2:B:13:GLU:O	2:B:17:GLY:N	2.54	0.40
2:B:500:ALA:O	2:B:503:HIS:CE1	2.75	0.40
2:B:81:LEU:HD12	2:B:85:PRO:HA	2.03	0.40
1:A:229:ALA:HB2	6:A:390:HOH:O	2.21	0.40
2:B:166:THR:HG23	6:B:745:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:ARG:NH1	2:B:639:LEU:O[1_455]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	309/346 (89%)	272 (88%)	28 (9%)	9 (3%)	4 2
2	B	540/660 (82%)	502 (93%)	32 (6%)	6 (1%)	14 14
3	D	77/97 (79%)	62 (80%)	7 (9%)	8 (10%)	0 0
All	All	926/1103 (84%)	836 (90%)	67 (7%)	23 (2%)	5 3

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	LYS
1	A	284	PRO
1	A	327	ASN
2	B	9	ARG
2	B	540	LYS
3	D	31	SER
3	D	59	MET
1	A	179	THR
3	D	68	GLY
3	D	86	ASP
1	A	76	PRO
3	D	30	ASP
3	D	40	MET
1	A	260	ASP
1	A	271	GLN
2	B	239	SER
2	B	613	LYS
2	B	633	LEU
1	A	288	PRO
3	D	56	GLY
3	D	73	ASP
2	B	485	GLY
1	A	322	ASP

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	266/296 (90%)	233 (88%)	33 (12%)	4 4
2	B	475/569 (84%)	432 (91%)	43 (9%)	9 10
3	D	71/87 (82%)	62 (87%)	9 (13%)	4 3
All	All	812/952 (85%)	727 (90%)	85 (10%)	7 6

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

Mol	Chain	Res	Type
1	A	28	LEU
1	A	29	GLU
1	A	34	LEU
1	A	38	ARG
1	A	40	LEU
1	A	61	LYS
1	A	84	THR
1	A	89	ARG
1	A	93	GLU
1	A	98	ARG
1	A	118	LYS
1	A	152	LYS
1	A	175	VAL
1	A	205	THR
1	A	208	LYS
1	A	228	LYS
1	A	234	LYS
1	A	244	GLN
1	A	248	LYS
1	A	252	ASP
1	A	255	ARG
1	A	261	THR
1	A	266	SER
1	A	267	GLU
1	A	268	LEU
1	A	275	ASP
1	A	278	ASP
1	A	279	SER
1	A	287	LEU
1	A	290	ASP
1	A	292	VAL
1	A	294	TYR
1	A	334	MET
2	B	7	LEU
2	B	32	LEU
2	B	37	VAL
2	B	46	LEU
2	B	66	LYS
2	B	71	SER
2	B	81	LEU
2	B	86	LYS
2	B	96	ILE
2	B	97	MET

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Mol	Chain	Res	Type
2	B	110	ILE
2	B	113	MET
2	B	164	LYS
2	B	167	GLN
2	B	169	THR
2	B	181	GLU
2	B	205	GLU
2	B	217	TRP
2	B	235	ILE
2	B	237	ARG
2	B	238	ILE
2	B	268	THR
2	B	275	LYS
2	B	305	LEU
2	B	308	LYS
2	B	320	ARG
2	B	336	LYS
2	B	362	ARG
2	B	410	ILE
2	B	414	ARG
2	B	416	ILE
2	B	425	ARG
2	B	426	LYS
2	B	454	LEU
2	B	499	GLU
2	B	512	ARG
2	B	515	SER
2	B	538	LEU
2	B	609	SER
2	B	610	ARG
2	B	624	ARG
2	B	628	GLU
2	B	640	ASP
3	D	23	LYS
3	D	31	SER
3	D	32	SER
3	D	38	VAL
3	D	40	MET
3	D	57	VAL
3	D	70	ARG
3	D	85	GLU
3	D	90	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	144	GLN
1	A	162	HIS
1	A	172	HIS
1	A	244	GLN
2	B	43	HIS
2	B	123	ASN
2	B	195	GLN
2	B	204	GLN
2	B	619	ASN
3	D	75	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
5	JZU	D	98	3	22,25,25	1.21	4 (18%)	22,38,38	2.13	7 (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
5	JZU	D	98	3	-	2/5/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	98	JZU	C2-N3	2.67	1.36	1.32
5	D	98	JZU	C5'-N5'	-2.26	1.43	1.47
5	D	98	JZU	O4'-C1'	2.21	1.44	1.41
5	D	98	JZU	S-N5'	-2.16	1.54	1.62

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	98	JZU	C4'-C5'-N5'	-4.83	102.83	112.51
5	D	98	JZU	O3S-S-O2S	-3.74	111.39	119.96
5	D	98	JZU	O2S-S-N5'	3.71	114.17	106.88
5	D	98	JZU	C3'-C2'-C1'	3.37	106.05	100.98
5	D	98	JZU	N3-C2-N1	-3.28	123.55	128.68
5	D	98	JZU	O4'-C1'-C2'	-2.31	103.55	106.93
5	D	98	JZU	N6-C6-N1	2.19	123.11	118.57

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	98	JZU	O4'-C4'-C5'-N5'
5	D	98	JZU	C3'-C4'-C5'-N5'

There are no ring outliers.

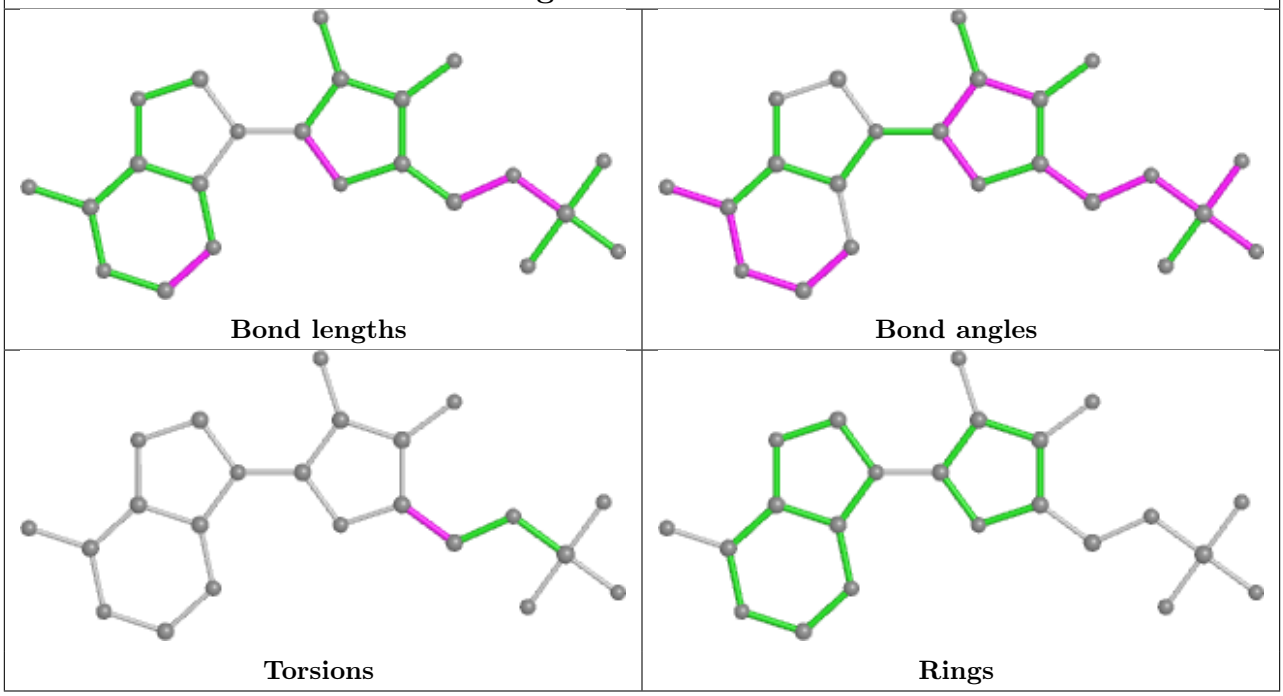
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	98	JZU	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 JZU D 98



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	313/346 (90%)	0.34	20 (6%)	19	16	47, 75, 115, 128	0
2	B	548/660 (83%)	0.09	30 (5%)	25	22	33, 63, 117, 147	0
3	D	79/97 (81%)	0.38	5 (6%)	20	16	50, 89, 102, 108	0
All	All	940/1103 (85%)	0.20	55 (5%)	22	19	33, 67, 114, 147	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	627	ILE	7.6
2	B	628	GLU	6.7
2	B	624	ARG	5.5
2	B	629	GLN	5.4
2	B	614	LEU	5.3
2	B	609	SER	5.0
2	B	612	ARG	5.0
2	B	630	LYS	4.9
2	B	610	ARG	4.7
1	A	224	TRP	4.6
2	B	620	LEU	4.5
1	A	284	PRO	4.2
2	B	633	LEU	4.2
3	D	19	GLY	4.2
2	B	625	SER	4.2
2	B	217	TRP	4.1
2	B	631	GLU	3.9
1	A	9	GLY	3.8
1	A	277	LEU	3.8
1	A	225	SER	3.7
1	A	281	GLY	3.7
2	B	235	ILE	3.5
2	B	640	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	632	GLU	3.3
1	A	231	ALA	3.3
1	A	285	ASP	3.2
1	A	276	VAL	3.2
1	A	280	LEU	3.1
1	A	279	SER	3.1
1	A	286	LEU	3.1
2	B	615	ASP	2.8
2	B	613	LYS	2.8
1	A	207	VAL	2.7
3	D	82	MET	2.7
1	A	296	PHE	2.6
3	D	56	GLY	2.6
1	A	177	GLU	2.5
2	B	236	LYS	2.5
2	B	637	ILE	2.5
2	B	611	LYS	2.5
2	B	623	LYS	2.5
2	B	622	ALA	2.4
2	B	626	ARG	2.4
2	B	621	SER	2.4
2	B	617	LYS	2.4
1	A	305	VAL	2.3
2	B	616	GLU	2.3
1	A	282	ILE	2.3
2	B	166	THR	2.2
2	B	634	ASP	2.2
3	D	78	LYS	2.1
1	A	292	VAL	2.1
3	D	74	ASN	2.1
1	A	235	ARG	2.1
1	A	271	GLN	2.0

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 monosaccharides in this entry.

6.4 Ligands

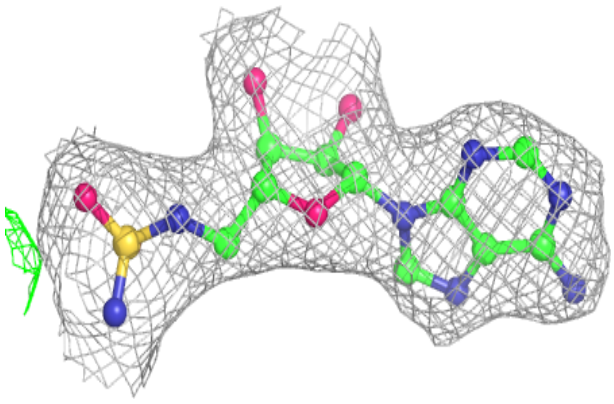
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

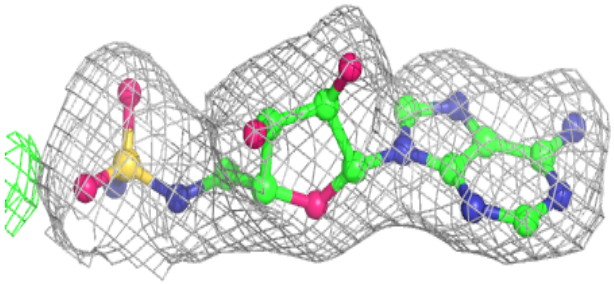
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	JZU	D	98	23/23	0.99	0.14	46,53,60,62	0
4	ZN	B	641	1/1	1.00	0.16	62,62,62,62	0

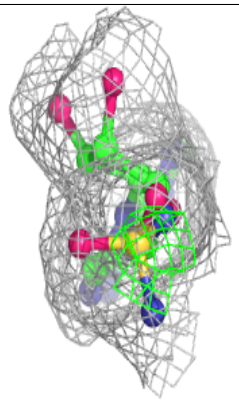
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JZU D 98:

$2mF_o$-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

There are no such residues in this entry.