WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Dec 19, 2023 – 06:16 PM EST

PDB ID : 1UKI

Title : Structural basis for the selective inhibition of JNK1 by the scaffolding protein JIP1 and SP600125

Authors : Heo, Y.-S.; Kim, Y.K.; Sung, B.-J.; Lee, H.S.; Lee, J.I.; Seo, C.I.; Park, S.-Y.; Kim, J.H.; Hyun, Y.-L.; Jeon, Y.H.; Ro, S.; Lee, T.G.; Cho, J.M.; Hwang, K.Y.; Yang, C.-H.

Deposited on : 2003-08-23

Resolution : 2.70 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
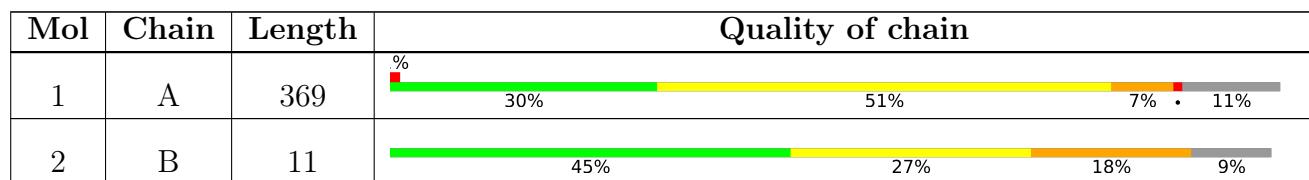
The reported resolution of this entry is 2.70 Å.

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		0.222
Clashscore		46
Ramachandran outliers		5.2%
Sidechain outliers		10.2%
RSRZ outliers		0.9%

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	369	% 30% 51% 7% · 11%
2	B	11	45% 27% 18% 9%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 2763 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 mitogen-activated protein kinase 8 isoform 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2647	1705	446	477	19			
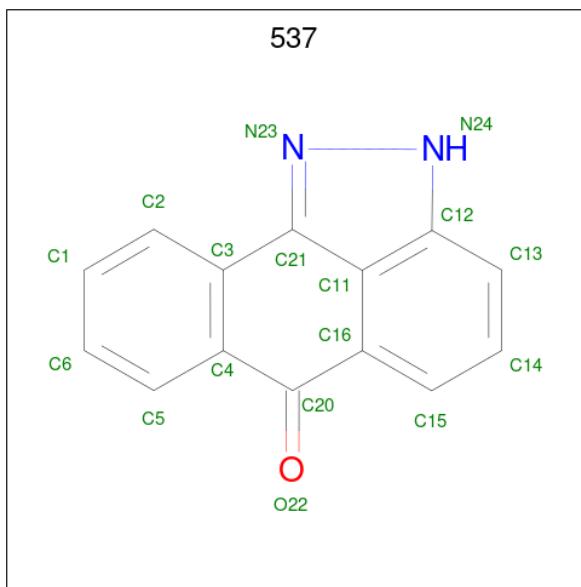
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	364	HIS	-	expression tag	UNP P45983
A	365	HIS	-	expression tag	UNP P45983
A	366	HIS	-	expression tag	UNP P45983
A	367	HIS	-	expression tag	UNP P45983
A	368	HIS	-	expression tag	UNP P45983
A	369	HIS	-	expression tag	UNP P45983

- Molecule 2 is a protein called 11-mer peptide from C-jun-amino-terminal kinase interacting protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	0	0	0
			84	55	15	14			

- Molecule 3 is 2,6-DIHYDROANTHRA/1,9-CD/PYRAZOL-6-ONE (three-letter code: 537) (formula: $C_{14}H_8N_2O$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	17	14	2	1	0	0
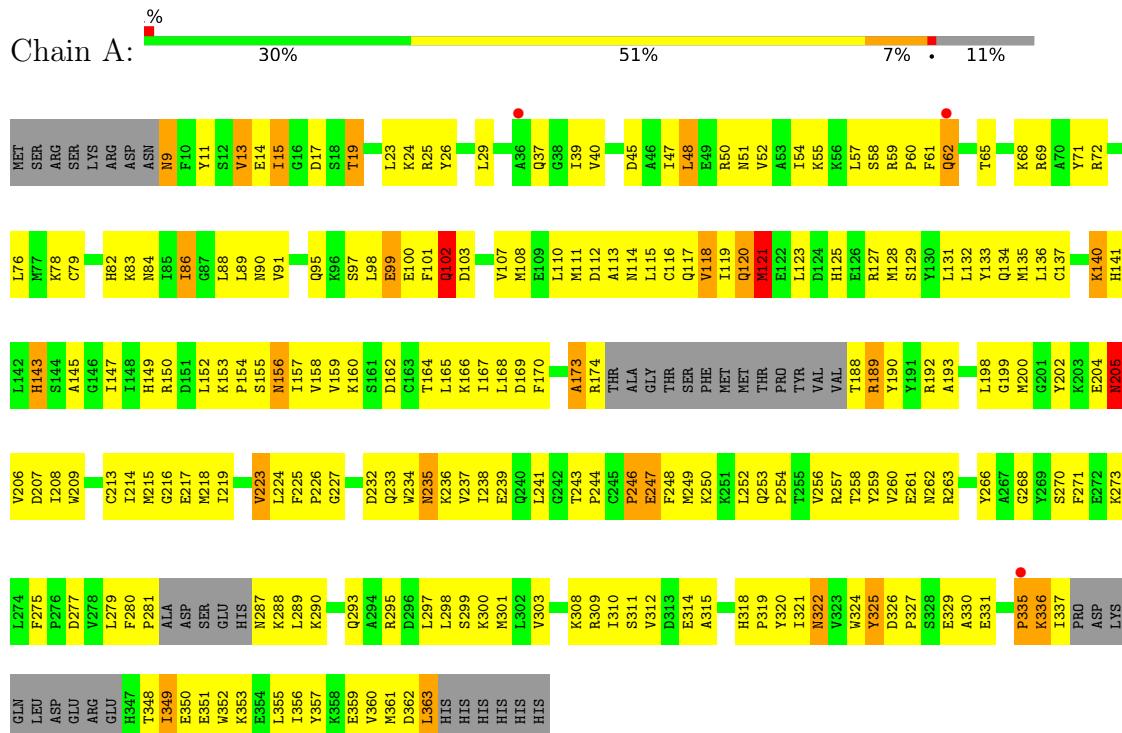
• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	15	15	15	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: mitogen-activated protein kinase 8 isoform 4

- Molecule 2: 11-mer peptide from C-jun-amino-terminal kinase interacting protein 1

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.70Å 79.46Å 82.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.70 19.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.96-2.70) 90.4 (19.96-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.241 0.219 , 0.222	Depositor DCC
R_{free} test set	552 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å^2)	48.0	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 54.7	EDS
L-test for twinning [2]	$< |L| > = 0.43, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.045 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	2763	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: 537

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	0.47	0/2704	0.65	0/3652
2	B	0.52	0/86	0.80	0/114
All	All	0.47	0/2790	0.66	0/3766

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2647	0	2683	252	0
2	B	84	0	91	7	0
3	A	17	0	8	1	0
4	A	15	0	0	1	0
All	All	2763	0	2782	255	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 46.

All (255) 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:258:THR:HG22	1:A:262:ASN:HD21	1.15	1.06
1:A:128:MET:HG3	1:A:218:MET:HE3	1.41	1.02
1:A:190:TYR:HA	1:A:233:GLN:HE22	1.24	0.99
1:A:51:ASN:HB3	1:A:110:LEU:HD23	1.48	0.95
1:A:91:VAL:HG22	1:A:360:VAL:HG13	1.49	0.95
1:A:40:VAL:HG22	1:A:55:LYS:HB2	1.53	0.91
1:A:119:ILE:HG23	1:A:218:MET:HA	1.53	0.90
1:A:258:THR:HG22	1:A:262:ASN:ND2	1.87	0.88
1:A:238:ILE:HD12	1:A:244:PRO:HD3	1.56	0.86
1:A:253:GLN:HG2	1:A:254:PRO:HD2	1.58	0.84
1:A:11:TYR:HE2	1:A:13:VAL:HG13	1.43	0.83
1:A:336:LYS:HA	1:A:336:LYS:NZ	1.94	0.81
1:A:234:TRP:CZ2	1:A:238:ILE:HD11	2.16	0.80
1:A:72:ARG:HG2	1:A:76:LEU:HD11	1.62	0.79
2:B:162:LEU:H	2:B:162:LEU:HD22	1.47	0.79
1:A:120:GLN:HB2	1:A:121:MET:CE	2.12	0.78
1:A:233:GLN:O	1:A:237:VAL:HG23	1.84	0.78
1:A:351:GLU:O	1:A:355:LEU:HG	1.85	0.77
1:A:86:ILE:HG21	1:A:168:LEU:O	1.86	0.76
1:A:205:ASN:ND2	1:A:309:ARG:HB3	2.01	0.75
1:A:120:GLN:HB2	1:A:121:MET:HE3	1.67	0.75
1:A:9:ASN:O	1:A:24:LYS:HG3	1.88	0.74
1:A:55:LYS:HE2	1:A:57:LEU:HD21	1.70	0.74
1:A:205:ASN:HD21	1:A:309:ARG:HB3	1.52	0.73
1:A:150:ARG:HH12	1:A:174:ARG:HD2	1.53	0.72
1:A:208:ILE:HG23	1:A:301:MET:HG3	1.69	0.72
1:A:288:LYS:HD2	1:A:288:LYS:N	2.06	0.71
1:A:257:ARG:HG2	1:A:261:GLU:OE2	1.91	0.71
1:A:258:THR:CG2	1:A:262:ASN:HD21	1.97	0.70
1:A:13:VAL:HG21	1:A:29:LEU:HD22	1.74	0.70
1:A:244:PRO:HB3	1:A:248:PHE:HD2	1.56	0.70
1:A:145:ALA:O	1:A:147:ILE:HG13	1.93	0.69
1:A:114:ASN:HB2	1:A:154:PRO:O	1.92	0.69
1:A:310:ILE:HG12	1:A:311:SER:N	2.09	0.68
1:A:127:ARG:NH1	2:B:159:THR:HG23	2.09	0.68
1:A:115:LEU:HB3	1:A:119:ILE:HD13	1.75	0.67
1:A:127:ARG:HH12	2:B:159:THR:HG23	1.59	0.67
1:A:259:TYR:CE2	1:A:263:ARG:HD2	2.30	0.67
1:A:89:LEU:HB2	1:A:107:VAL:HG12	1.77	0.66
1:A:150:ARG:HH22	1:A:174:ARG:HG3	1.60	0.66
1:A:55:LYS:HE2	1:A:57:LEU:CD2	2.25	0.65
1:A:61:PHE:CZ	1:A:102:GLN:HA	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ILE:CG2	1:A:301:MET:HG3	2.25	0.65
1:A:114:ASN:OD1	1:A:116:CYS:HB2	1.97	0.65
1:A:198:LEU:HD22	1:A:256:VAL:HG11	1.78	0.65
2:B:162:LEU:HD22	2:B:162:LEU:N	2.10	0.65
1:A:214:ILE:O	1:A:218:MET:HB2	1.96	0.65
1:A:101:PHE:CE2	1:A:357:TYR:HB2	2.32	0.65
1:A:47:ILE:HG22	1:A:47:ILE:O	1.96	0.65
1:A:213:CYS:HA	1:A:224:LEU:HD12	1.80	0.63
1:A:120:GLN:HE21	1:A:120:GLN:HA	1.62	0.63
1:A:150:ARG:HH21	1:A:173:ALA:N	1.97	0.63
1:A:11:TYR:CE2	1:A:13:VAL:HG13	2.30	0.63
1:A:140:LYS:HB2	1:A:312:VAL:HG11	1.79	0.63
1:A:57:LEU:HB2	1:A:60:PRO:HG3	1.81	0.63
1:A:336:LYS:HA	1:A:336:LYS:HZ2	1.63	0.63
1:A:348:THR:HG22	1:A:351:GLU:HG3	1.80	0.63
1:A:219:ILE:HD13	1:A:280:PHE:CE1	2.34	0.62
1:A:157:ILE:HG22	1:A:165:LEU:HD21	1.81	0.62
1:A:336:LYS:HA	1:A:336:LYS:HZ3	1.62	0.62
1:A:79:CYS:O	1:A:335:PRO:HB3	1.99	0.61
1:A:95:GLN:CB	1:A:101:PHE:HA	2.30	0.61
1:A:91:VAL:CG2	1:A:360:VAL:HG13	2.27	0.61
1:A:117:GLN:O	1:A:121:MET:HE3	2.00	0.61
1:A:78:LYS:NZ	1:A:362:ASP:HB2	2.16	0.61
1:A:190:TYR:HB3	1:A:225:PHE:O	2.00	0.61
1:A:249:MET:O	1:A:252:LEU:HD13	2.01	0.60
1:A:153:LYS:O	1:A:156:ASN:ND2	2.35	0.60
1:A:14:GLU:OE2	1:A:19:THR:HG23	2.01	0.60
1:A:153:LYS:HG3	1:A:155:SER:HB3	1.82	0.60
1:A:159:VAL:CG1	1:A:165:LEU:HD23	2.32	0.59
1:A:135:MET:HG2	1:A:165:LEU:HD11	1.85	0.59
1:A:356:ILE:O	1:A:359:GLU:HB2	2.01	0.59
1:A:318:HIS:CG	1:A:319:PRO:HD2	2.38	0.59
1:A:289:LEU:HD23	1:A:289:LEU:H	1.68	0.58
1:A:114:ASN:HA	1:A:158:VAL:HA	1.85	0.58
1:A:88:LEU:HD12	1:A:107:VAL:O	2.04	0.58
1:A:143:HIS:HE1	1:A:207:ASP:OD2	1.85	0.58
1:A:336:LYS:HG3	1:A:337:ILE:H	1.69	0.57
1:A:120:GLN:HB2	1:A:121:MET:HE2	1.86	0.57
1:A:199:GLY:C	1:A:200:MET:HG3	2.24	0.56
1:A:37:GLN:HG3	1:A:69:ARG:HD2	1.87	0.56
1:A:249:MET:HA	1:A:252:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:TRP:CE3	2:B:156:ARG:HG2	2.40	0.56
1:A:311:SER:HB2	1:A:314:GLU:OE1	2.04	0.56
1:A:215:MET:O	1:A:218:MET:HB3	2.05	0.56
1:A:247:GLU:HG3	1:A:248:PHE:N	2.21	0.55
1:A:25:ARG:NH2	1:A:47:ILE:HB	2.20	0.55
1:A:11:TYR:HD1	1:A:24:LYS:HA	1.72	0.55
1:A:189:ARG:HE	1:A:192:ARG:HH11	1.54	0.55
2:B:162:LEU:H	2:B:162:LEU:CD2	2.17	0.55
1:A:287:ASN:HD22	1:A:288:LYS:NZ	2.05	0.55
1:A:157:ILE:CG2	1:A:165:LEU:HD21	2.36	0.54
1:A:61:PHE:HZ	1:A:102:GLN:HA	1.70	0.54
1:A:111:MET:O	3:A:0:537:HC2	2.06	0.54
1:A:61:PHE:O	1:A:62:GLN:HB2	2.06	0.54
1:A:209:TRP:HH2	1:A:241:LEU:CD1	2.21	0.54
1:A:232:ASP:OD2	1:A:236:LYS:HE2	2.07	0.54
1:A:115:LEU:HA	1:A:118:VAL:HG12	1.90	0.54
1:A:244:PRO:HB3	1:A:248:PHE:CD2	2.41	0.54
1:A:349:ILE:HD13	1:A:349:ILE:C	2.28	0.54
1:A:86:ILE:HG22	1:A:167:ILE:O	2.08	0.54
1:A:59:ARG:HG3	1:A:102:GLN:O	2.08	0.54
1:A:227:GLY:HA2	1:A:236:LYS:HE2	1.90	0.53
1:A:310:ILE:HG12	1:A:311:SER:H	1.74	0.53
1:A:357:TYR:O	1:A:361:MET:HG2	2.07	0.53
1:A:23:LEU:HB3	1:A:25:ARG:HG2	1.91	0.52
1:A:215:MET:O	1:A:219:ILE:HG13	2.09	0.52
1:A:348:THR:HG22	1:A:351:GLU:CG	2.40	0.52
1:A:131:LEU:HD23	1:A:134:GLN:NE2	2.24	0.52
1:A:297:LEU:HG	1:A:301:MET:HE3	1.92	0.52
1:A:72:ARG:HG2	1:A:76:LEU:CD1	2.34	0.51
1:A:98:LEU:HD23	1:A:357:TYR:CD1	2.45	0.51
1:A:40:VAL:HG22	1:A:55:LYS:CB	2.32	0.51
1:A:61:PHE:CZ	1:A:353:LYS:HG3	2.46	0.51
1:A:101:PHE:O	1:A:353:LYS:HE3	2.10	0.51
1:A:25:ARG:HH21	1:A:47:ILE:HB	1.76	0.51
1:A:128:MET:HG3	1:A:218:MET:CE	2.28	0.51
1:A:318:HIS:CD2	1:A:320:TYR:H	2.29	0.51
1:A:76:LEU:HD22	1:A:147:ILE:HD11	1.92	0.50
1:A:238:ILE:HG23	1:A:243:THR:HA	1.93	0.50
1:A:86:ILE:HG23	1:A:86:ILE:O	2.12	0.50
1:A:227:GLY:HA2	1:A:232:ASP:OD2	2.11	0.50
1:A:99:GLU:HA	1:A:99:GLU:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ASP:O	1:A:113:ALA:HB2	2.11	0.50
1:A:287:ASN:HD22	1:A:288:LYS:HZ1	1.59	0.50
1:A:159:VAL:HG12	1:A:165:LEU:HD23	1.94	0.49
1:A:204:GLU:C	1:A:206:VAL:H	2.15	0.49
1:A:216:GLY:C	1:A:218:MET:H	2.15	0.49
1:A:98:LEU:O	1:A:353:LYS:HE2	2.12	0.49
1:A:348:THR:HG23	1:A:351:GLU:H	1.75	0.49
1:A:128:MET:CG	1:A:218:MET:HE3	2.29	0.49
1:A:113:ALA:O	1:A:159:VAL:HG22	2.11	0.49
1:A:249:MET:SD	1:A:260:VAL:HG11	2.53	0.49
1:A:15:ILE:C	1:A:15:ILE:HD12	2.33	0.49
1:A:209:TRP:HZ3	1:A:303:VAL:N	2.10	0.49
1:A:219:ILE:O	1:A:279:LEU:HD22	2.13	0.48
1:A:206:VAL:HG13	1:A:207:ASP:N	2.28	0.48
1:A:318:HIS:HD2	1:A:320:TYR:H	1.59	0.48
1:A:141:HIS:NE2	1:A:335:PRO:HG3	2.29	0.48
1:A:216:GLY:HA3	1:A:224:LEU:HD11	1.95	0.48
1:A:234:TRP:CH2	1:A:238:ILE:HD11	2.49	0.48
1:A:120:GLN:HA	1:A:120:GLN:NE2	2.29	0.48
1:A:129:SER:HB3	1:A:320:TYR:CZ	2.49	0.48
1:A:150:ARG:NH2	1:A:173:ALA:C	2.67	0.48
1:A:247:GLU:HG3	1:A:248:PHE:H	1.77	0.48
1:A:216:GLY:O	1:A:219:ILE:N	2.45	0.47
1:A:361:MET:O	1:A:363:LEU:HD22	2.14	0.47
1:A:11:TYR:CD1	1:A:24:LYS:HA	2.49	0.47
1:A:136:LEU:HD21	1:A:315:ALA:HB1	1.97	0.47
1:A:150:ARG:HD3	1:A:202:TYR:CE1	2.50	0.47
1:A:217:GLU:HG2	1:A:223:VAL:HA	1.96	0.47
1:A:235:ASN:HD21	1:A:263:ARG:HE	1.62	0.47
1:A:15:ILE:HD11	1:A:39:ILE:HG21	1.96	0.47
1:A:149:HIS:O	1:A:150:ARG:HB2	2.14	0.47
1:A:160:LYS:HB3	1:A:162:ASP:OD1	2.14	0.47
1:A:165:LEU:HD13	1:A:166:LYS:N	2.30	0.47
1:A:232:ASP:O	1:A:236:LYS:HG3	2.14	0.47
1:A:101:PHE:CD2	1:A:357:TYR:HB2	2.50	0.47
1:A:239:GLU:O	1:A:268:GLY:HA2	2.14	0.47
1:A:143:HIS:CE1	1:A:207:ASP:OD2	2.67	0.47
1:A:275:PHE:CE2	1:A:298:LEU:HD13	2.50	0.47
1:A:121:MET:HB2	4:A:384:HOH:O	2.15	0.46
1:A:143:HIS:C	1:A:145:ALA:H	2.18	0.46
1:A:152:LEU:HD12	1:A:207:ASP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ALA:HB2	1:A:209:TRP:HB3	1.98	0.46
1:A:356:ILE:N	1:A:356:ILE:HD13	2.29	0.46
1:A:57:LEU:CB	1:A:60:PRO:HG3	2.45	0.46
1:A:97:SER:O	1:A:101:PHE:HB2	2.16	0.46
1:A:45:ASP:HB2	1:A:52:VAL:HG11	1.98	0.46
1:A:48:LEU:HB3	1:A:50:ARG:HG2	1.96	0.46
1:A:58:SER:HA	1:A:103:ASP:OD2	2.16	0.46
1:A:83:LYS:O	1:A:166:LYS:NZ	2.39	0.46
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.76	0.46
1:A:216:GLY:C	1:A:218:MET:N	2.68	0.46
1:A:11:TYR:HE1	1:A:26:TYR:O	1.99	0.45
1:A:82:HIS:CD2	1:A:84:ASN:H	2.34	0.45
1:A:95:GLN:HG2	1:A:101:PHE:HA	1.98	0.45
1:A:290:LYS:HD3	1:A:293:GLN:OE1	2.16	0.45
1:A:303:VAL:HG11	1:A:308:LYS:HB2	1.97	0.45
1:A:170:PHE:N	1:A:170:PHE:CD1	2.84	0.45
1:A:160:LYS:HB3	1:A:164:THR:OG1	2.15	0.45
1:A:263:ARG:HG2	1:A:263:ARG:HH11	1.82	0.45
1:A:326:ASP:HB3	1:A:329:GLU:OE1	2.15	0.45
1:A:259:TYR:O	1:A:263:ARG:HG3	2.16	0.45
1:A:326:ASP:HA	1:A:327:PRO:HD2	1.79	0.45
1:A:129:SER:HA	1:A:132:LEU:HD12	1.98	0.45
1:A:352:TRP:O	1:A:355:LEU:N	2.50	0.45
1:A:271:PHE:CZ	1:A:299:SER:HA	2.52	0.45
1:A:324:TRP:CZ3	2:B:156:ARG:HG2	2.52	0.45
1:A:82:HIS:HD2	1:A:84:ASN:HB2	1.82	0.44
1:A:337:ILE:HG23	1:A:337:ILE:O	2.17	0.44
1:A:54:ILE:HG12	1:A:107:VAL:HG22	1.99	0.44
1:A:89:LEU:O	1:A:90:ASN:HB2	2.17	0.44
1:A:58:SER:O	1:A:59:ARG:C	2.56	0.44
1:A:95:GLN:HB3	1:A:101:PHE:HA	1.98	0.44
1:A:117:GLN:O	1:A:118:VAL:C	2.55	0.44
1:A:119:ILE:HG13	1:A:218:MET:HG3	1.99	0.44
1:A:71:TYR:HB2	1:A:356:ILE:HD11	2.00	0.44
1:A:133:TYR:CE1	1:A:325:TYR:HA	2.52	0.44
1:A:48:LEU:CB	1:A:50:ARG:HG2	2.48	0.44
1:A:125:HIS:CD2	1:A:290:LYS:HB3	2.53	0.44
1:A:190:TYR:HA	1:A:233:GLN:NE2	2.09	0.44
1:A:9:ASN:C	1:A:9:ASN:HD22	2.19	0.44
1:A:280:PHE:HB3	1:A:281:PRO:HD2	2.00	0.44
1:A:219:ILE:HD13	1:A:280:PHE:HE1	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:MET:HA	1:A:310:ILE:HG22	2.00	0.43
1:A:156:ASN:C	1:A:156:ASN:HD22	2.22	0.43
1:A:234:TRP:HE1	1:A:260:VAL:HG22	1.82	0.43
1:A:270:SER:OG	1:A:273:LYS:HG3	2.18	0.43
1:A:300:LYS:O	1:A:310:ILE:HG22	2.19	0.43
1:A:219:ILE:HD13	1:A:280:PHE:CZ	2.54	0.43
1:A:219:ILE:HG22	1:A:279:LEU:HB3	2.00	0.43
1:A:298:LEU:C	1:A:300:LYS:H	2.22	0.43
1:A:15:ILE:HG13	1:A:15:ILE:O	2.18	0.43
1:A:143:HIS:HA	1:A:147:ILE:O	2.18	0.42
1:A:266:TYR:C	1:A:268:GLY:H	2.23	0.42
1:A:145:ALA:HB2	1:A:335:PRO:HD2	2.00	0.42
1:A:47:ILE:O	1:A:48:LEU:HG	2.20	0.42
1:A:119:ILE:HG21	1:A:217:GLU:OE1	2.19	0.42
1:A:336:LYS:HG3	1:A:337:ILE:N	2.32	0.42
1:A:349:ILE:HG23	1:A:350:GLU:N	2.34	0.42
1:A:90:ASN:O	1:A:107:VAL:N	2.40	0.42
1:A:115:LEU:HB3	1:A:119:ILE:CD1	2.46	0.42
1:A:253:GLN:CG	1:A:254:PRO:HD2	2.41	0.42
1:A:29:LEU:HD12	1:A:29:LEU:N	2.35	0.41
1:A:131:LEU:O	1:A:135:MET:HG3	2.19	0.41
1:A:71:TYR:HD1	1:A:356:ILE:HD13	1.85	0.41
1:A:143:HIS:C	1:A:145:ALA:N	2.73	0.41
1:A:335:PRO:O	1:A:336:LYS:HB2	2.20	0.41
1:A:117:GLN:O	1:A:119:ILE:N	2.52	0.41
1:A:97:SER:HA	1:A:357:TYR:OH	2.20	0.41
1:A:271:PHE:O	1:A:295:ARG:HD2	2.20	0.41
1:A:48:LEU:HD13	1:A:50:ARG:HD3	2.02	0.41
1:A:310:ILE:CG1	1:A:311:SER:N	2.83	0.41
1:A:348:THR:CG2	1:A:351:GLU:HG3	2.49	0.41
1:A:97:SER:O	1:A:101:PHE:N	2.52	0.41
1:A:136:LEU:O	1:A:140:LYS:HB2	2.20	0.41
1:A:263:ARG:HG2	1:A:263:ARG:NH1	2.35	0.41
1:A:209:TRP:CZ3	1:A:303:VAL:N	2.89	0.41
1:A:72:ARG:O	1:A:76:LEU:HG	2.19	0.41
1:A:84:ASN:HD22	1:A:137:CYS:HB3	1.85	0.41
1:A:117:GLN:O	1:A:120:GLN:N	2.53	0.41
1:A:275:PHE:CD2	1:A:298:LEU:HD13	2.55	0.41
1:A:188:THR:O	1:A:189:ARG:HB2	2.21	0.41
1:A:15:ILE:O	1:A:15:ILE:CG1	2.69	0.40
1:A:133:TYR:HB2	1:A:321:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:TRP:O	1:A:353:LYS:C	2.60	0.40
1:A:83:LYS:C	1:A:166:LYS:HZ3	2.21	0.40
1:A:318:HIS:O	1:A:322:ASN:HB2	2.20	0.40
1:A:61:PHE:CE2	1:A:353:LYS:HG3	2.56	0.40
1:A:243:THR:HG23	1:A:266:TYR:O	2.21	0.40
1:A:209:TRP:HZ3	1:A:303:VAL:C	2.25	0.40
1:A:318:HIS:HD2	1:A:320:TYR:HB3	1.87	0.40
1:A:348:THR:HG22	1:A:351:GLU:OE2	2.21	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	320/369 (87%)	245 (77%)	58 (18%)	17 (5%)	2	3
2	B	8/11 (73%)	8 (100%)	0	0	100	100
All	All	328/380 (86%)	253 (77%)	58 (18%)	17 (5%)	2	3

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	121	MET
1	A	189	ARG
1	A	226	PRO
1	A	173	ALA
1	A	335	PRO
1	A	48	LEU
1	A	246	PRO
1	A	65	THR
1	A	86	ILE

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Mol	Chain	Res	Type
1	A	99	GLU
1	A	102	GLN
1	A	205	ASN
1	A	223	VAL
1	A	325	TYR
1	A	330	ALA
1	A	118	VAL

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	293/331 (88%)	266 (91%)	27 (9%)	9	21
2	B	10/11 (91%)	6 (60%)	4 (40%)	0	0
All	All	303/342 (89%)	272 (90%)	31 (10%)	7	17

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	13	VAL
1	A	15	ILE
1	A	17	ASP
1	A	19	THR
1	A	68	LYS
1	A	100	GLU
1	A	102	GLN
1	A	108	MET
1	A	120	GLN
1	A	121	MET
1	A	123	LEU
1	A	140	LYS
1	A	143	HIS
1	A	156	ASN
1	A	169	ASP

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Mol	Chain	Res	Type
1	A	205	ASN
1	A	235	ASN
1	A	246	PRO
1	A	247	GLU
1	A	250	LYS
1	A	277	ASP
1	A	322	ASN
1	A	331	GLU
1	A	336	LYS
1	A	349	ILE
1	A	363	LEU
2	B	158	THR
2	B	159	THR
2	B	161	ASN
2	B	162	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	27	GLN
1	A	28	ASN
1	A	51	ASN
1	A	62	GLN
1	A	82	HIS
1	A	84	ASN
1	A	90	ASN
1	A	120	GLN
1	A	143	HIS
1	A	156	ASN
1	A	205	ASN
1	A	233	GLN
1	A	235	ASN
1	A	262	ASN
1	A	287	ASN
1	A	318	HIS
1	A	322	ASN
2	B	161	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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	537	A	0	-	16,20,20	2.59	9 (56%)	23,30,30	2.08	5 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	537	A	0	-	-	-	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	0	537	O22-C20	4.18	1.30	1.22
3	A	0	537	C14-C13	4.08	1.46	1.36
3	A	0	537	C15-C16	3.54	1.44	1.38
3	A	0	537	C5-C4	3.45	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	0	537	C14-C15	3.37	1.46	1.38
3	A	0	537	C16-C20	-3.23	1.43	1.48
3	A	0	537	C1-C2	3.11	1.43	1.36
3	A	0	537	C4-C3	2.29	1.47	1.43
3	A	0	537	C6-C5	2.14	1.43	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	0	537	C15-C16-C20	7.39	125.91	119.61
3	A	0	537	C11-C16-C20	-3.48	117.05	119.92
3	A	0	537	C3-C21-C11	-2.42	120.15	121.92
3	A	0	537	C16-C11-C12	2.25	125.40	120.00
3	A	0	537	C5-C4-C20	2.05	121.36	119.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	0	537	1	0

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	328/369 (88%)	-0.27	3 (0%)	84	85	26, 47, 71, 83	0
2	B	10/11 (90%)	-0.26	0	100	100	42, 47, 55, 57	0
All	All	338/380 (88%)	-0.27	3 (0%)	84	85	26, 47, 71, 83	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	ALA	2.9
1	A	335	PRO	2.3
1	A	62	GLN	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
3	537	A	0	17/17	0.94	0.14	37,41,43,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.