W O R L D W I D E

wwPDB

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

Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 02:55 am GMT

PDB ID	:	5EQY
Title	:	Crystal structure of choline kinase alpha-1 bound by 5-[(4-methyl-1,4-diazepan-1-yl)methyl]-2-[4-[(4-methyl-1,4-diazepan-1-yl)methyl]phenyl]benzenecarbonitrile (compound 65)
Authors	:	Zhou, T.; Zhu, X.; Dalgarno, D.C.
Deposited on	:	2015-11-13
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.50 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		0.273
Clashscore		14
Ramachandran outliers		0.1%
Sidechain outliers		5.5%
RSRZ outliers		3.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
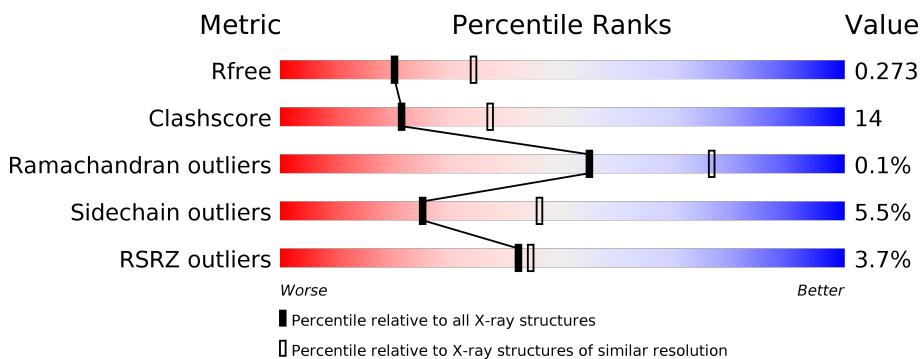
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	401	2% 60% 25% • 12%
1	B	401	4% 66% 20% • 12%
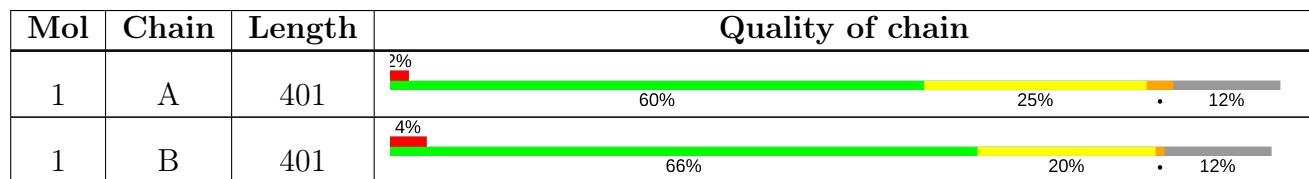
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	5RA	B	501	-	-	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 5980 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 Choline kinase alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total 2925	C 1892	N 492	O 525	S 16	0	0	0
1	B	351	Total 2916	C 1887	N 491	O 522	S 16	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	GLY	-	expression tag	UNP P35790
A	58	SER	-	expression tag	UNP P35790
A	59	SER	-	expression tag	UNP P35790
A	60	HIS	-	expression tag	UNP P35790
A	61	HIS	-	expression tag	UNP P35790
A	62	HIS	-	expression tag	UNP P35790
A	63	HIS	-	expression tag	UNP P35790
A	64	HIS	-	expression tag	UNP P35790
A	65	HIS	-	expression tag	UNP P35790
A	66	SER	-	expression tag	UNP P35790
A	67	SER	-	expression tag	UNP P35790
A	68	GLY	-	expression tag	UNP P35790
A	69	LEU	-	expression tag	UNP P35790
A	70	VAL	-	expression tag	UNP P35790
A	71	PRO	-	expression tag	UNP P35790
A	72	ARG	-	expression tag	UNP P35790
A	73	GLY	-	expression tag	UNP P35790
A	74	SER	-	expression tag	UNP P35790
B	57	GLY	-	expression tag	UNP P35790
B	58	SER	-	expression tag	UNP P35790
B	59	SER	-	expression tag	UNP P35790
B	60	HIS	-	expression tag	UNP P35790
B	61	HIS	-	expression tag	UNP P35790
B	62	HIS	-	expression tag	UNP P35790
B	63	HIS	-	expression tag	UNP P35790

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Chain	Residue	Modelled	Actual	Comment	Reference
B	64	HIS	-	expression tag	UNP P35790
B	65	HIS	-	expression tag	UNP P35790
B	66	SER	-	expression tag	UNP P35790
B	67	SER	-	expression tag	UNP P35790
B	68	GLY	-	expression tag	UNP P35790
B	69	LEU	-	expression tag	UNP P35790
B	70	VAL	-	expression tag	UNP P35790
B	71	PRO	-	expression tag	UNP P35790
B	72	ARG	-	expression tag	UNP P35790
B	73	GLY	-	expression tag	UNP P35790
B	74	SER	-	expression tag	UNP P35790

- Molecule 2 is 5-[(4-methyl-1,4-diazepan-1-yl)methyl]-2-[4-[(4-methyl-1,4-diazepan-1-yl)meth yl]phenyl]benzenecarbonitrile (three-letter code: 5RA) (formula: $C_{27}H_{37}N_5$).
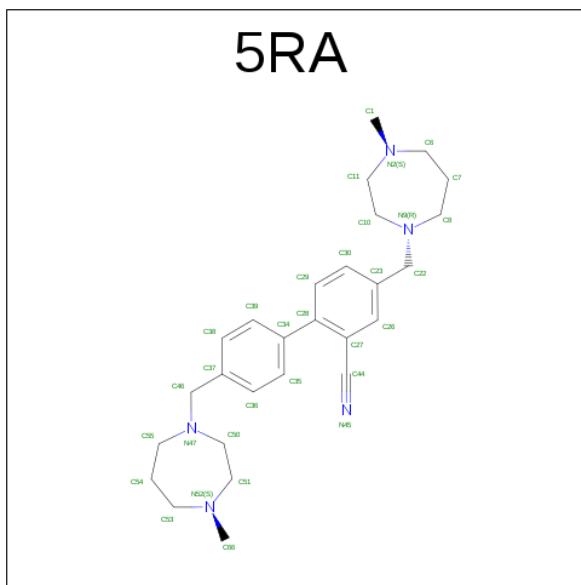
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total C N 32 27 5			0	0
2	B	1	Total C N 32 27 5			0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total O 33 33		0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	42	Total O 42 42		0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Choline kinase alpha
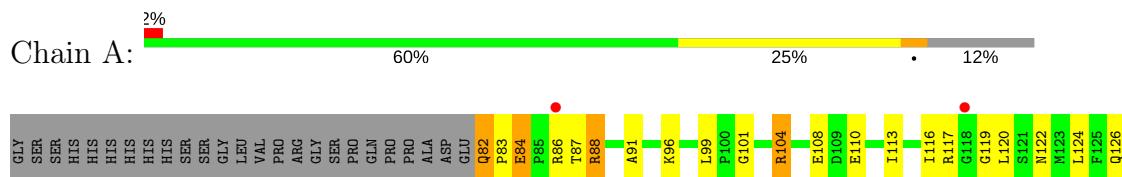
- Molecule 1: Choline kinase alpha
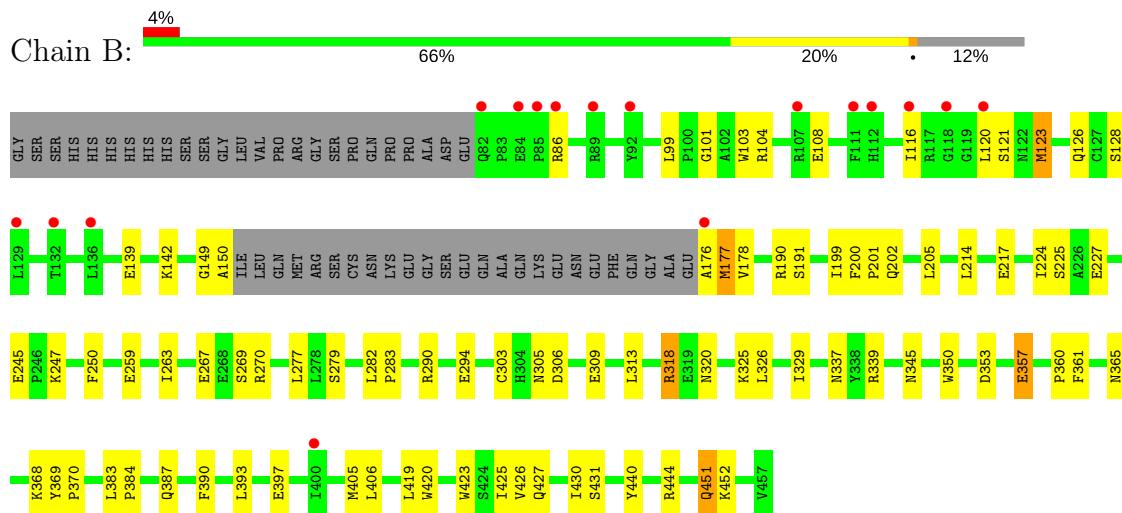
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.52Å 121.53Å 130.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 47.10 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.2 (50.00-2.50) 94.2 (47.10-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.51Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.223 , 0.277 0.222 , 0.273	Depositor DCC
R_{free} test set	1466 reflections (5.22%)	DCC
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5980	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: 5RA

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	0.37	0/3001	0.50	0/4040
1	B	0.38	0/2992	0.50	0/4028
All	All	0.37	0/5993	0.50	0/8068

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	2925	0	2898	87	0
1	B	2916	0	2892	59	0
2	A	32	0	37	11	0
2	B	32	0	37	11	0
3	A	33	0	0	1	0
3	B	42	0	0	0	0
All	All	5980	0	5864	159	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 (159) 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:501:5RA:C1	2:B:501:5RA:N2	1.72	1.52
2:A:501:5RA:C1	2:A:501:5RA:N2	1.72	1.49
2:B:501:5RA:C1	2:B:501:5RA:C11	2.06	1.34
2:B:501:5RA:C6	2:B:501:5RA:C1	2.04	1.34
2:A:501:5RA:C1	2:A:501:5RA:C11	2.06	1.33
2:A:501:5RA:C1	2:A:501:5RA:C6	2.06	1.31
2:B:501:5RA:H16	2:B:501:5RA:C1	1.78	1.13
2:A:501:5RA:C1	2:A:501:5RA:H6	1.79	1.12
2:A:501:5RA:C1	2:A:501:5RA:H16	1.79	1.07
2:B:501:5RA:C1	2:B:501:5RA:H6	1.83	1.06
1:A:270:ARG:HH11	1:A:270:ARG:HG3	1.20	1.03
1:A:104:ARG:HG2	1:A:104:ARG:HH11	1.29	0.95
2:B:501:5RA:H16	2:B:501:5RA:H3	1.51	0.90
2:A:501:5RA:H16	2:A:501:5RA:H3	1.53	0.89
2:A:501:5RA:H6	2:A:501:5RA:H3	1.53	0.89
2:B:501:5RA:H6	2:B:501:5RA:H3	1.55	0.88
1:A:126:GLN:HE21	1:A:142:LYS:HD3	1.40	0.86
1:B:176:ALA:O	1:B:177:MET:HB3	1.76	0.86
1:A:126:GLN:NE2	1:A:142:LYS:HD3	1.95	0.81
1:B:120:LEU:HG	1:B:150:ALA:HB2	1.62	0.81
1:A:88:ARG:HA	1:A:91:ALA:HB3	1.66	0.78
1:A:204:ARG:HD2	1:A:206:GLU:OE1	1.87	0.75
1:A:308:GLN:HE21	1:A:310:GLY:H	1.34	0.73
2:B:501:5RA:C6	2:B:501:5RA:H2	2.18	0.71
2:A:501:5RA:C11	2:A:501:5RA:H1	2.19	0.71
2:A:501:5RA:C6	2:A:501:5RA:H2	2.19	0.70
1:A:104:ARG:CG	1:A:104:ARG:HH11	2.04	0.69
1:A:259:GLU:O	1:A:263:ILE:HG23	1.93	0.68
1:B:121:SER:HB3	1:B:150:ALA:HB3	1.75	0.67
1:A:126:GLN:HE21	1:A:142:LYS:CD	2.08	0.67
1:A:270:ARG:NH1	1:A:270:ARG:HG3	1.95	0.66
1:B:430:ILE:HG13	1:B:431:SER:N	2.10	0.65
1:B:270:ARG:HG3	1:B:270:ARG:HH11	1.61	0.65
1:A:256:TYR:O	1:A:260:VAL:HG23	1.95	0.65
1:B:423:TRP:O	1:B:427:GLN:HG2	1.97	0.64
1:A:371:THR:O	1:A:375:GLN:HG3	1.97	0.63
1:A:195:LYS:H	1:A:207:GLN:HE21	1.45	0.63
1:B:357:GLU:CD	1:B:357:GLU:H	2.01	0.63
2:B:501:5RA:C11	2:B:501:5RA:H1	2.21	0.63
1:A:277:LEU:HD13	1:A:425:ILE:HD11	1.83	0.61
1:A:244:LYS:HB2	1:B:104:ARG:NH1	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:GLN:HE21	1:B:451:GLN:HA	1.66	0.60
1:B:101:GLY:HA3	1:B:139:GLU:OE2	2.02	0.59
1:A:405:MET:O	1:A:409:VAL:HG13	2.02	0.59
1:A:88:ARG:HB2	1:A:113:ILE:HG21	1.85	0.59
1:A:178:VAL:HG12	1:B:178:VAL:HG22	1.85	0.59
1:A:304:HIS:O	1:A:305:ASN:HB2	2.03	0.58
1:A:283:PRO:O	1:A:287:GLU:HG2	2.03	0.58
1:A:124:LEU:HG	1:A:144:LEU:HD21	1.87	0.57
1:A:451:GLN:HA	1:A:451:GLN:HE21	1.70	0.57
1:A:82:GLN:N	1:A:83:PRO:HD3	2.20	0.57
1:B:123:MET:H	1:B:123:MET:CE	2.17	0.57
1:A:411:ARG:O	1:A:414:LEU:HB2	2.05	0.56
1:B:387:GLN:HG3	1:B:390:PHE:HB2	1.87	0.56
1:A:87:THR:O	1:A:88:ARG:HG3	2.05	0.56
1:B:267:GLU:OE1	1:B:269:SER:HB3	2.05	0.56
1:B:123:MET:HE1	1:B:149:GLY:HA3	1.89	0.55
1:B:270:ARG:HG3	1:B:270:ARG:NH1	2.22	0.54
1:A:145:LEU:HD22	1:A:147:LEU:HD12	1.89	0.54
1:B:277:LEU:HD13	1:B:425:ILE:HD11	1.90	0.54
1:A:178:VAL:HG23	1:A:179:LEU:HD13	1.89	0.54
1:A:178:VAL:HG23	1:A:179:LEU:CD1	2.38	0.54
1:B:200:PHE:HB2	1:B:201:PRO:CD	2.38	0.54
1:A:318:ARG:O	1:A:325:LYS:HB3	2.08	0.54
1:A:434:GLU:HB3	2:A:501:5RA:H41	1.91	0.53
1:A:258:LYS:O	1:A:262:ARG:HG2	2.09	0.52
1:B:393:LEU:HD13	1:B:397:GLU:HG2	1.91	0.52
1:B:282:LEU:N	1:B:283:PRO:CD	2.73	0.52
1:A:246:PRO:HG3	1:A:300:VAL:HG21	1.92	0.51
1:B:224:ILE:HD13	1:B:325:LYS:HE2	1.92	0.51
1:A:321:SER:OG	1:A:324:GLN:HB2	2.11	0.51
1:A:117:ARG:NH1	1:A:122:ASN:O	2.43	0.51
1:B:227:GLU:HB3	1:B:326:LEU:HD12	1.92	0.51
1:A:360:PRO:O	1:A:361:PHE:HB2	2.11	0.51
2:B:501:5RA:H7	2:B:501:5RA:C1	2.27	0.50
1:A:270:ARG:HH11	1:A:270:ARG:CG	2.06	0.50
1:B:305:ASN:HD21	1:B:337:ASN:HD22	1.60	0.50
1:A:175:GLU:HG2	1:A:175:GLU:O	2.11	0.50
2:A:501:5RA:C44	2:A:501:5RA:H23	2.42	0.50
1:A:351:MET:SD	1:A:366:ILE:HA	2.51	0.50
1:A:104:ARG:HG2	1:A:104:ARG:NH1	2.10	0.49
1:A:104:ARG:CG	1:A:104:ARG:NH1	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:HH22	1:B:245:GLU:CD	2.16	0.49
1:A:257:LEU:HD22	1:A:261:LEU:HG	1.94	0.49
1:A:276:LYS:O	1:A:279:SER:HB2	2.12	0.49
1:A:350:TRP:CZ3	1:A:370:PRO:HB3	2.48	0.49
1:B:339:ARG:NH2	1:B:405:MET:HE2	2.27	0.49
1:B:123:MET:H	1:B:123:MET:HE3	1.77	0.48
1:A:104:ARG:NH2	1:B:245:GLU:OE2	2.44	0.48
1:B:303:CYS:SG	1:B:337:ASN:HB3	2.53	0.48
1:A:126:GLN:HE21	1:A:142:LYS:CE	2.26	0.48
1:A:308:GLN:HB3	1:A:349:GLU:HG3	1.95	0.48
1:A:88:ARG:CA	1:A:91:ALA:HB3	2.40	0.48
1:B:263:ILE:HD11	1:B:426:VAL:HA	1.96	0.48
1:B:318:ARG:C	1:B:320:ASN:N	2.66	0.47
1:A:387:GLN:HG3	1:A:390:PHE:HB2	1.95	0.47
1:A:101:GLY:HA3	1:A:139:GLU:OE1	2.14	0.47
1:A:178:VAL:HG23	1:A:179:LEU:N	2.29	0.47
1:B:200:PHE:HB2	1:B:201:PRO:HD2	1.96	0.47
1:B:99:LEU:HD21	1:B:205:LEU:HD13	1.96	0.47
1:B:177:MET:HG2	1:B:178:VAL:HG23	1.97	0.47
1:A:277:LEU:HD13	1:A:425:ILE:CD1	2.45	0.47
1:B:99:LEU:HD12	1:B:103:TRP:CD2	2.50	0.47
1:B:419:LEU:C	1:B:419:LEU:HD23	2.35	0.46
1:B:357:GLU:CD	1:B:357:GLU:N	2.68	0.46
1:A:427:GLN:O	1:A:431:SER:HB3	2.15	0.45
1:B:250:PHE:CZ	1:B:290:ARG:HA	2.50	0.45
1:B:116:ILE:HD11	1:B:126:GLN:HE21	1.81	0.45
1:A:202:GLN:OE1	1:A:202:GLN:N	2.49	0.45
1:A:332:GLU:H	1:A:332:GLU:HG2	1.26	0.45
1:A:282:LEU:N	1:A:283:PRO:CD	2.79	0.45
1:A:135:THR:HG23	1:A:141:ARG:NH1	2.32	0.45
1:A:393:LEU:O	1:A:398:LYS:HE3	2.17	0.44
1:A:254:GLU:OE1	1:A:290:ARG:NH2	2.43	0.44
1:A:245:GLU:OE1	1:B:104:ARG:NH2	2.51	0.44
1:B:440:TYR:O	1:B:444:ARG:HG2	2.18	0.44
1:B:360:PRO:O	1:B:361:PHE:HB2	2.18	0.44
1:A:241:PRO:O	1:B:199:ILE:HG22	2.18	0.44
1:A:421:GLY:O	1:A:425:ILE:HG13	2.18	0.43
1:B:224:ILE:CD1	1:B:325:LYS:HE2	2.48	0.43
1:B:306:ASP:OD1	2:B:501:5RA:N2	2.51	0.43
1:B:190:ARG:O	1:B:191:SER:HB2	2.19	0.43
1:B:313:LEU:HG	1:B:329:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:H	1:A:207:GLN:NE2	2.13	0.43
1:B:318:ARG:C	1:B:320:ASN:H	2.21	0.43
1:A:269:SER:O	1:A:273:LYS:HG3	2.18	0.43
1:A:120:LEU:N	1:A:120:LEU:HD12	2.34	0.43
1:A:308:GLN:NE2	1:A:310:GLY:H	2.10	0.43
1:A:225:SER:HA	3:A:608:HOH:O	2.18	0.43
1:B:345:ASN:ND2	1:B:420:TRP:HE1	2.17	0.43
1:B:383:LEU:HB2	1:B:384:PRO:HD3	1.99	0.43
1:A:190:ARG:O	1:A:191:SER:HB2	2.19	0.42
1:B:214:LEU:O	1:B:309:GLU:HB2	2.19	0.42
1:A:119:GLY:C	1:A:120:LEU:HD12	2.40	0.42
1:A:420:TRP:CE3	1:A:420:TRP:HA	2.53	0.42
1:A:419:LEU:HD23	1:A:419:LEU:C	2.39	0.42
1:A:175:GLU:OE2	1:B:201:PRO:HB3	2.20	0.42
1:A:99:LEU:O	1:A:104:ARG:HG3	2.20	0.42
1:A:82:GLN:HA	1:A:82:GLN:HE21	1.84	0.41
1:A:221:LEU:HA	1:A:222:PRO:HD3	1.87	0.41
1:B:365:ASN:ND2	1:B:368:LYS:HG2	2.35	0.41
1:B:350:TRP:CZ3	1:B:370:PRO:HB3	2.55	0.41
1:A:116:ILE:HB	1:A:124:LEU:HB3	2.02	0.41
1:B:452:LYS:HB3	1:B:452:LYS:HE2	1.93	0.41
1:B:126:GLN:OE1	1:B:142:LYS:HD3	2.21	0.41
1:B:353:ASP:C	1:B:353:ASP:OD1	2.58	0.41
1:A:146:ARG:O	1:A:203:GLY:HA3	2.20	0.41
1:A:396:GLU:HG3	1:A:397:GLU:N	2.34	0.41
1:A:353:ASP:O	1:A:362:PHE:HA	2.21	0.41
1:A:406:LEU:HA	1:A:406:LEU:HD23	1.89	0.41
1:B:305:ASN:ND2	1:B:337:ASN:HD22	2.18	0.41
1:A:101:GLY:HA3	1:A:139:GLU:CD	2.42	0.40
1:A:282:LEU:HA	1:A:282:LEU:HD23	1.92	0.40
1:A:303:CYS:SG	1:A:337:ASN:HB3	2.61	0.40
1:A:383:LEU:HD13	1:A:390:PHE:CZ	2.56	0.40
1:B:369:TYR:CG	1:B:370:PRO:HD2	2.56	0.40
1:B:387:GLN:O	1:B:387:GLN:HG3	2.21	0.40
1:A:84:GLU:H	1:A:84:GLU:HG3	1.58	0.40
1:A:88:ARG:C	1:A:88:ARG:HD3	2.42	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	348/401 (87%)	322 (92%)	26 (8%)	0	100	100
1	B	347/401 (86%)	328 (94%)	18 (5%)	1 (0%)	44	66
All	All	695/802 (87%)	650 (94%)	44 (6%)	1 (0%)	55	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	177	MET

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	316/357 (88%)	296 (94%)	20 (6%)	21	38
1	B	315/357 (88%)	300 (95%)	15 (5%)	30	53
All	All	631/714 (88%)	596 (94%)	35 (6%)	25	46

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	84	GLU
1	A	86	ARG
1	A	88	ARG
1	A	96	LYS

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Mol	Chain	Res	Type
1	A	104	ARG
1	A	108	GLU
1	A	110	GLU
1	A	145	LEU
1	A	180	GLU
1	A	192	LEU
1	A	257	LEU
1	A	262	ARG
1	A	270	ARG
1	A	291	SER
1	A	308	GLN
1	A	332	GLU
1	A	396	GLU
1	A	451	GLN
1	A	454	LYS
1	B	86	ARG
1	B	108	GLU
1	B	123	MET
1	B	128	SER
1	B	202	GLN
1	B	217	GLU
1	B	225	SER
1	B	247	LYS
1	B	259	GLU
1	B	279	SER
1	B	294	GLU
1	B	318	ARG
1	B	357	GLU
1	B	406	LEU
1	B	451	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	126	GLN
1	A	207	GLN
1	A	308	GLN
1	A	377	HIS
1	A	451	GLN
1	B	202	GLN
1	B	305	ASN

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Mol	Chain	Res	Type
1	B	345	ASN
1	B	392	ASN
1	B	410	ASN
1	B	450	HIS
1	B	451	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6   Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	5RA	A	501	-	35,35,35	2.35	9 (25%)	45,47,47	3.39	14 (31%)
2	5RA	B	501	-	35,35,35	2.22	4 (11%)	45,47,47	3.15	9 (20%)

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	5RA	A	501	-	-	0/14/36/36	1/4/4/4
2	5RA	B	501	-	-	0/14/36/36	1/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	5RA	C36-C35	2.02	1.42	1.38
2	A	501	5RA	C10-N9	2.04	1.52	1.46
2	A	501	5RA	C26-C27	2.04	1.42	1.39
2	B	501	5RA	C22-N9	2.13	1.51	1.47
2	A	501	5RA	C22-N9	2.17	1.51	1.47
2	A	501	5RA	C30-C29	2.22	1.42	1.38
2	B	501	5RA	C30-C29	2.27	1.42	1.38
2	B	501	5RA	C36-C35	2.38	1.43	1.38
2	A	501	5RA	C29-C28	2.39	1.43	1.39
2	A	501	5RA	C28-C27	2.79	1.47	1.40
2	A	501	5RA	C28-C34	3.35	1.55	1.49
2	B	501	5RA	C1-N2	10.67	1.72	1.46
2	A	501	5RA	C1-N2	10.79	1.72	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	5RA	C1-N2-C6	-13.25	79.35	110.52
2	B	501	5RA	C1-N2-C6	-13.14	79.62	110.52
2	A	501	5RA	C1-N2-C11	-13.07	79.77	110.52
2	B	501	5RA	C1-N2-C11	-12.88	80.21	110.52
2	A	501	5RA	C26-C27-C44	-4.09	113.33	119.70
2	B	501	5RA	C26-C27-C44	-2.91	115.17	119.70
2	A	501	5RA	C29-C28-C27	-2.35	115.29	117.89
2	A	501	5RA	C50-C51-N52	-2.27	109.38	116.12
2	A	501	5RA	C66-N52-C53	2.04	115.32	110.52
2	A	501	5RA	C37-C46-N47	2.10	117.21	113.17
2	A	501	5RA	C55-N47-C50	2.18	119.18	113.24
2	B	501	5RA	C66-N52-C51	2.23	115.76	110.52
2	A	501	5RA	C66-N52-C51	2.34	116.04	110.52
2	B	501	5RA	C23-C22-N9	2.51	118.01	113.17
2	B	501	5RA	C55-N47-C50	2.70	120.60	113.24
2	A	501	5RA	C23-C22-N9	2.74	118.44	113.17
2	A	501	5RA	C22-N9-C10	3.24	116.70	111.15
2	B	501	5RA	C22-N9-C10	3.40	116.97	111.15
2	A	501	5RA	C46-N47-C50	3.66	117.42	111.15
2	B	501	5RA	C46-N47-C50	4.16	118.27	111.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	5RA	C34-C28-C27	4.59	128.00	122.46
2	B	501	5RA	C46-N47-C55	5.67	120.86	111.15
2	A	501	5RA	C46-N47-C55	6.51	122.30	111.15

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	5RA	C50-C51-C53-C54-C55-N47-N52
2	A	501	5RA	C50-C51-C53-C54-C55-N47-N52

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	5RA	11	0
2	B	501	5RA	11	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(Å^2)	Q<0.9
1	A	352/401 (87%)	0.07	9 (2%)	56	59	28, 48, 80, 102	0
1	B	351/401 (87%)	0.22	17 (4%)	31	32	23, 44, 84, 114	0
All	All	703/802 (87%)	0.14	26 (3%)	42	44	23, 46, 83, 114	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	LEU	4.8
1	B	89	ARG	4.6
1	A	318	ARG	4.4
1	A	320	ASN	4.2
1	A	322	GLU	4.1
1	A	118	GLY	3.9
1	B	129	LEU	3.9
1	A	323	LYS	3.9
1	B	86	ARG	3.5
1	A	175	GLU	3.4
1	A	319	GLU	3.2
1	B	132	THR	3.0
1	B	176	ALA	2.9
1	B	84	GLU	2.8
1	B	107	ARG	2.7
1	B	116	ILE	2.6
1	B	111	PHE	2.6
1	B	85	PRO	2.6
1	B	82	GLN	2.4
1	B	118	GLY	2.4
1	A	86	ARG	2.4
1	B	92	TYR	2.3
1	A	317	GLY	2.2
1	B	400	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	136	LEU	2.1
1	B	112	HIS	2.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	5RA	B	501	32/32	0.91	0.20	2.12	32,48,74,75	0
2	5RA	A	501	32/32	0.88	0.23	1.37	47,63,83,84	0

6.5 Other polymers ⓘ

There are no such residues in this entry.