



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:35 PM GMT

PDB ID : 4FEX
Title : Crystal structure of the aminoglycoside phosphotransferase APH(3')-Ia, with substrate kanamycin and small molecule inhibitor tyrphostin AG1478
Authors : Stogios, P.J.; Evdokimova, E.; Wawrzak, Z.; Minasov, G.; Egorova, O.; Di Leo, R.; Shakya, T.; Spanogiannopoulos, P.; Wright, G.D.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2012-05-30
Resolution : 2.71 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

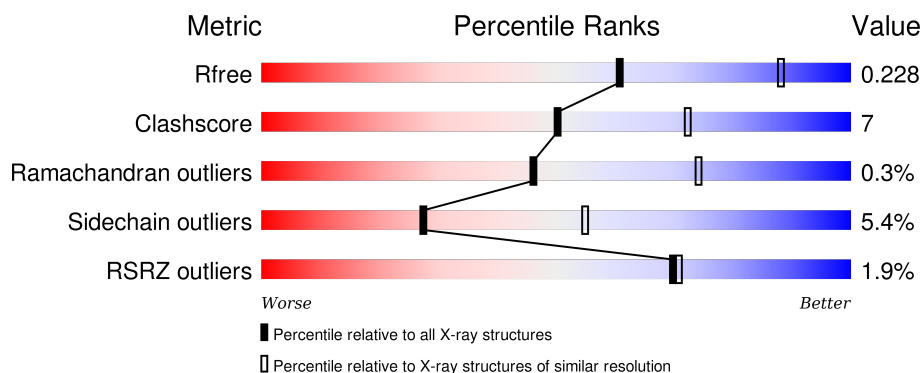
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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}	91344	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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 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 $\leq 5\%$. 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	272	
1	B	272	
1	C	272	
1	D	272	
1	E	272	

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
3	OTO	A	302	-	-	-	X
3	OTO	C	302	-	-	X	X
3	OTO	D	302	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10846 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.

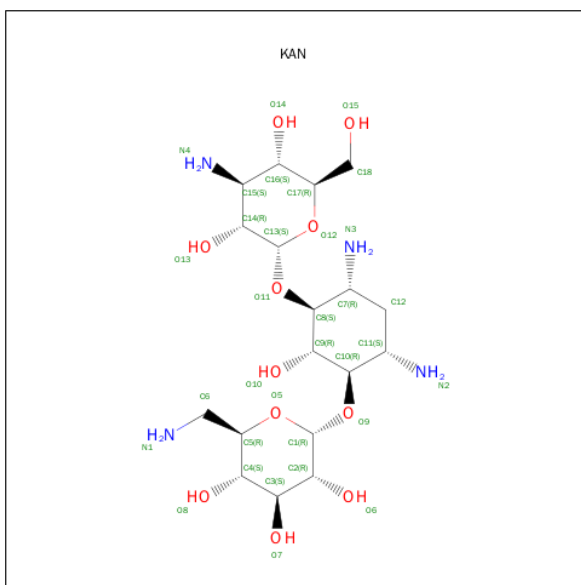
- Molecule 1 is a protein called Aminoglycoside 3'-phosphotransferase AphA1-IAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	1	0
			2048	1312	349	377	10			
1	B	261	Total	C	N	O	S	0	2	0
			2120	1350	368	391	11			
1	C	261	Total	C	N	O	S	0	4	0
			2131	1361	368	391	11			
1	D	253	Total	C	N	O	S	0	3	0
			2051	1314	348	379	10			
1	E	254	Total	C	N	O	S	0	2	0
			2059	1318	353	378	10			

There are 5 discrepancies between the modelled and reference sequences:

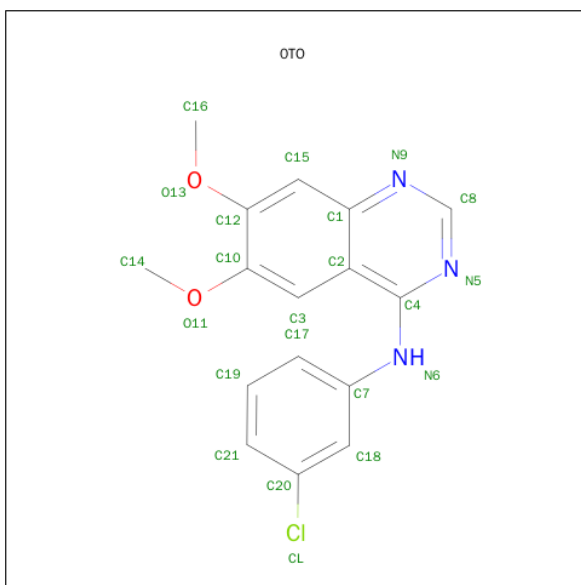
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP B0VD92
B	0	GLY	-	EXPRESSION TAG	UNP B0VD92
C	0	GLY	-	EXPRESSION TAG	UNP B0VD92
D	0	GLY	-	EXPRESSION TAG	UNP B0VD92
E	0	GLY	-	EXPRESSION TAG	UNP B0VD92

- Molecule 2 is KANAMYCIN A (three-letter code: KAN) (formula: C₁₈H₃₆N₄O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 33	C 18	N 4	O 11	0	0
2	B	1	Total 33	C 18	N 4	O 11	0	0
2	C	1	Total 33	C 18	N 4	O 11	0	0
2	D	1	Total 33	C 18	N 4	O 11	0	0
2	E	1	Total 33	C 18	N 4	O 11	0	0

- Molecule 3 is N-(3-CHLOROPHENYL)-6,7-DIMETHOXYQUINAZOLIN-4-AMINE (three-letter code: 0TO) (formula: C₁₆H₁₄ClN₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			22	16	1	3	2		
3	C	1	Total	C	Cl	N	O	0	0
			22	16	1	3	2		
3	D	1	Total	C	Cl	N	O	0	0
			22	16	1	3	2		
3	E	1	Total	C	Cl	N	O	0	0
			22	16	1	3	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		

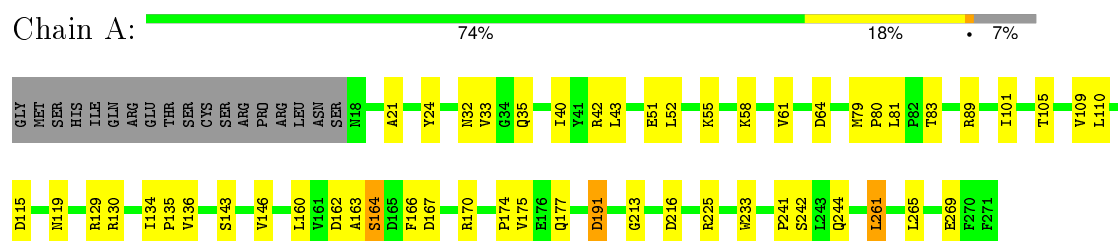
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	34	Total	O	0	3
			37	37		
6	B	41	Total	O	0	1
			42	42		
6	C	40	Total	O	0	0
			40	40		
6	D	25	Total	O	0	0
			25	25		
6	E	34	Total	O	0	0
			34	34		

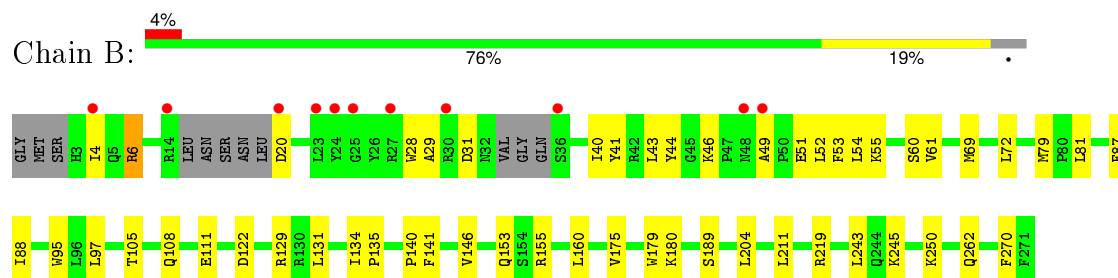
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

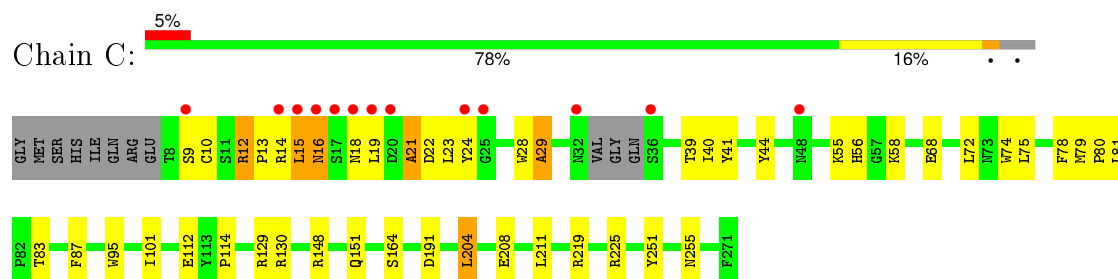
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



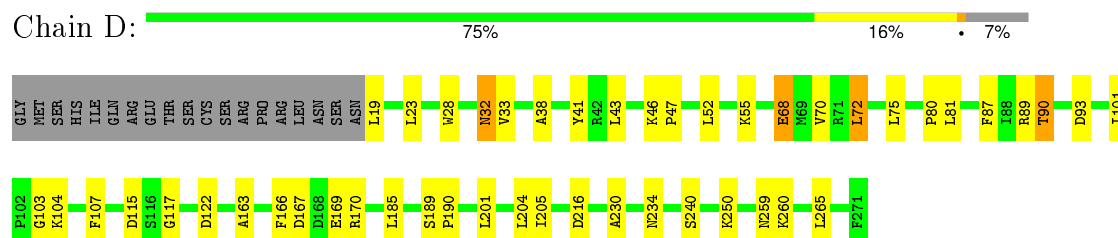
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



Chain E:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.67Å 93.69Å 96.32Å 118.84° 103.56° 93.44°	Depositor
Resolution (Å)	19.90 – 2.71 19.90 – 2.69	Depositor EDS
% Data completeness (in resolution range)	97.9 (19.90-2.71) 76.1 (19.90-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.71Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.184 , 0.240 0.178 , 0.228	Depositor DCC
R_{free} test set	2012 reflections (4.87%)	DCC
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.0	EDS
Estimated twinning fraction	0.000 for -h,-k,h+k+l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 44887 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10846	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 0TO, NA, KAN, ACT

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	0.43	0/2105	0.61	0/2858
1	B	0.45	0/2177	0.59	0/2950
1	C	0.46	0/2193	0.61	1/2976 (0.0%)
1	D	0.44	0/2111	0.59	1/2866 (0.0%)
1	E	0.45	0/2116	0.59	1/2872 (0.0%)
All	All	0.45	0/10702	0.60	3/14522 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	204	LEU	CA-CB-CG	-5.92	101.68	115.30
1	E	204	LEU	CA-CB-CG	-5.50	102.65	115.30
1	C	204	LEU	CA-CB-CG	-5.10	103.56	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2048	0	1989	29	0
1	B	2120	0	2050	29	0
1	C	2131	0	2069	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2051	0	1991	28	0
1	E	2059	0	2001	28	0
2	A	33	0	36	0	0
2	B	33	0	36	0	0
2	C	33	0	36	1	0
2	D	33	0	36	1	0
2	E	33	0	36	0	0
3	A	22	0	14	3	0
3	C	22	0	14	7	0
3	D	22	0	14	7	0
3	E	22	0	14	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	C	4	0	3	0	0
6	A	37	0	0	2	0
6	B	42	0	0	3	0
6	C	40	0	0	1	0
6	D	25	0	0	0	0
6	E	34	0	0	1	0
All	All	10846	0	10339	147	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 7.

All (147) 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:C:55:LYS:HZ1	3:C:302:0TO:H1	1.42	0.85
3:E:302:0TO:N5	3:E:302:0TO:H2	1.99	0.76
1:C:101:ILE:O	3:C:302:0TO:H11	1.90	0.72
1:B:79:MET:HE3	1:B:131:LEU:HA	1.72	0.71
1:E:33:VAL:HG13	1:E:37:GLY:HA2	1.75	0.69
1:C:219:ARG:NH2	6:C:425:HOH:O	2.26	0.68
1:C:39:THR:HG22	1:C:41:TYR:HE1	1.60	0.66
3:C:302:0TO:N5	3:C:302:0TO:H2	2.09	0.66
1:B:40:ILE:HD13	1:B:55:LYS:HG2	1.77	0.65
1:E:19:LEU:HD11	1:E:88:ILE:HD11	1.78	0.65
1:A:32:ASN:HD22	1:B:6:ARG:HG3	1.62	0.64
3:D:302:0TO:H2	3:D:302:0TO:N5	2.12	0.64
1:C:55:LYS:NZ	3:C:302:0TO:H1	2.12	0.64
1:C:87:PHE:HB3	1:D:89:ARG:HB3	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ARG:HH22	1:C:15:LEU:HD22	1.61	0.63
1:A:174:PRO:HG2	1:A:177:GLN:HB2	1.79	0.63
1:C:21:ALA:O	1:C:23:LEU:N	2.32	0.63
1:B:43:LEU:HB2	1:B:52:LEU:HB2	1.81	0.61
1:D:205:ILE:HD12	3:D:302:0TO:H13	1.82	0.60
1:C:79:MET:HA	1:C:79:MET:HE2	1.83	0.60
1:E:124:LEU:HD22	1:E:204:LEU:HD13	1.85	0.59
1:C:79:MET:HE1	1:C:130[B]:ARG:HG2	1.84	0.59
1:A:191:ASP:OD2	1:A:225:ARG:NH1	2.36	0.59
1:D:68:GLU:OE1	3:D:302:0TO:H1	2.03	0.58
1:D:55:LYS:HD2	3:D:302:0TO:H3	1.84	0.58
3:A:302:0TO:N5	3:A:302:0TO:H2	2.19	0.57
1:E:173:TRP:CZ3	1:E:181:GLU:HG3	2.40	0.56
1:C:29:ALA:HB2	1:C:44:TYR:HE2	1.70	0.56
1:B:122:ASP:OD1	1:B:250:LYS:HG3	2.06	0.55
1:E:41:TYR:HB2	1:E:54:LEU:HB3	1.89	0.55
1:A:42:ARG:NH2	1:A:51:GLU:OE1	2.39	0.55
1:B:155:ARG:NH2	1:B:270:PHE:O	2.38	0.55
1:A:170:ARG:NH1	1:A:269:GLU:OE2	2.39	0.55
1:B:219:ARG:NH2	6:B:421:HOH:O	2.39	0.54
1:D:43[A]:LEU:HB2	1:D:52:LEU:HB2	1.89	0.54
1:D:90:THR:HG22	1:D:93:ASP:H	1.72	0.54
1:E:130:ARG:O	1:E:133:SER:OG	2.24	0.54
1:B:105:THR:OG1	1:B:108:GLN:HG3	2.08	0.54
1:D:101:ILE:O	3:D:302:0TO:H11	2.07	0.53
1:A:21:ALA:HA	1:A:24:TYR:CE2	2.43	0.53
1:E:148:ARG:HB3	1:E:267:LEU:HD21	1.90	0.53
1:D:80:PRO:O	1:D:81:LEU:HD23	2.09	0.52
1:C:101:ILE:H	3:C:302:0TO:C8	2.22	0.52
1:A:101:ILE:H	3:A:302:0TO:H6	1.75	0.52
1:E:27:ARG:HG2	1:E:44:TYR:CZ	2.43	0.52
1:D:75:LEU:HD23	1:D:81:LEU:HD11	1.92	0.51
1:C:129:ARG:HD2	1:C:251:TYR:O	2.09	0.51
1:D:185:LEU:HB3	1:D:259:ASN:OD1	2.10	0.51
1:A:43[B]:LEU:HB2	1:A:52:LEU:HB2	1.93	0.51
1:A:43[A]:LEU:HB2	1:A:52:LEU:HB2	1.94	0.50
1:A:162:ASP:OD1	1:A:164:SER:HB3	2.12	0.50
1:C:56:HIS:HB2	1:C:95:TRP:CE3	2.47	0.49
1:E:173:TRP:HZ3	1:E:181:GLU:HG3	1.76	0.49
1:A:80:PRO:O	1:A:81:LEU:HD23	2.13	0.49
1:E:103:GLY:O	3:E:302:0TO:H12	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:PHE:CZ	1:E:211:LEU:HB2	2.47	0.49
1:E:75:LEU:HD23	1:E:81:LEU:HD21	1.94	0.49
1:C:74:TRP:CZ3	1:C:75:LEU:HD13	2.47	0.49
1:B:175:VAL:HG23	6:B:404:HOH:O	2.13	0.49
1:B:262[A]:GLN:NE2	6:B:435:HOH:O	2.42	0.48
1:A:80:PRO:HG2	1:A:213:GLY:HA2	1.95	0.48
1:D:122:ASP:OD1	1:D:250:LYS:HG3	2.13	0.48
1:A:79:MET:HE1	1:A:130:ARG:HG2	1.96	0.48
1:B:31:ASP:HA	1:E:210:LYS:NZ	2.29	0.48
1:B:29:ALA:HB2	1:B:44:TYR:HE1	1.79	0.48
1:B:4:ILE:HB	1:B:6:ARG:HD3	1.96	0.48
1:C:148:ARG:NH1	1:C:151:GLN:OE1	2.46	0.48
1:A:166:PHE:HZ	1:A:175:VAL:HG22	1.78	0.48
1:C:40:ILE:C	1:C:41:TYR:HD1	2.18	0.47
1:A:101:ILE:H	3:A:302:OTO:C8	2.27	0.47
1:D:90:THR:HG22	1:D:93:ASP:N	2.30	0.47
1:A:241:PRO:HA	1:A:244:GLN:OE1	2.15	0.47
1:D:32:ASN:HA	1:D:33:VAL:HA	1.76	0.47
3:E:302:OTO:N5	3:E:302:OTO:C18	2.67	0.46
1:D:234:ASN:HB2	1:D:265:LEU:HD21	1.96	0.46
1:C:204:LEU:HB3	1:C:211:LEU:HD11	1.98	0.46
1:E:240:SER:O	1:E:244:GLN:HG3	2.16	0.46
1:B:72:LEU:HD23	1:B:81:LEU:HD23	1.96	0.46
1:A:167:ASP:HB2	1:A:170:ARG:NH1	2.31	0.46
1:D:103:GLY:O	3:D:302:OTO:H12	2.16	0.46
1:A:163:ALA:HA	1:A:166:PHE:CE1	2.51	0.46
1:A:166:PHE:HA	1:A:269:GLU:OE1	2.15	0.46
1:A:136:VAL:HG13	6:A:427:HOH:O	2.16	0.45
1:E:101:ILE:O	3:E:302:OTO:H11	2.16	0.45
1:D:46:LYS:HA	1:D:47:PRO:HD3	1.74	0.45
1:E:136:VAL:HB	1:E:222:ILE:HD13	1.99	0.45
1:C:78:PHE:O	1:C:79:MET:HE2	2.17	0.45
3:D:302:OTO:C18	3:D:302:OTO:N5	2.79	0.45
1:C:72:LEU:HD23	1:C:81:LEU:HD13	1.98	0.44
1:C:112:GLU:C	1:C:114:PRO:HD3	2.37	0.44
1:B:54:LEU:HD13	1:B:97:LEU:HD13	1.99	0.44
1:B:6:ARG:H	1:B:6:ARG:HG2	1.55	0.44
1:C:16:ASN:OD1	1:C:16:ASN:N	2.46	0.44
1:B:140:PRO:HG2	1:B:141:PHE:CE2	2.52	0.44
1:D:38:ALA:HB3	1:D:55:LYS:HE3	1.98	0.44
1:C:75:LEU:HB3	1:C:81:LEU:HD11	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:301:KAN:HN21	2:C:301:KAN:H5	1.82	0.44
1:B:204:LEU:HB3	1:B:211:LEU:HD11	1.99	0.43
1:D:189:SER:HA	1:D:190:PRO:HD3	1.76	0.43
1:A:40:ILE:HG12	1:A:55:LYS:HG2	1.99	0.43
1:B:88:ILE:HG23	1:B:95:TRP:HB2	2.00	0.43
1:A:33:VAL:N	1:A:35:GLN:OE1	2.51	0.43
1:E:20:ASP:O	1:E:24:TYR:N	2.51	0.43
1:E:51:GLU:O	1:E:52:LEU:HD23	2.18	0.43
1:E:27:ARG:HG2	1:E:44:TYR:OH	2.18	0.43
1:E:175:VAL:HG23	6:E:418:HOH:O	2.18	0.43
1:C:68:GLU:OE2	3:C:302:OTO:H1	2.18	0.43
1:A:58:LYS:HE2	1:A:58:LYS:HB3	1.75	0.43
1:D:72:LEU:HA	1:D:72:LEU:HD23	1.89	0.43
1:B:153:GLN:HB2	1:B:179:TRP:CH2	2.53	0.43
1:D:72:LEU:HD23	1:D:81:LEU:HD13	2.01	0.43
1:C:191:ASP:OD2	1:C:225:ARG:NE	2.39	0.43
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.71	0.43
1:C:80:PRO:O	1:C:81:LEU:HD23	2.19	0.42
1:E:139:CYS:HA	1:E:140:PRO:HD2	1.78	0.42
1:A:61:VAL:HA	1:A:64:ASP:OD2	2.19	0.42
1:C:13:PRO:HG3	1:D:41:TYR:CZ	2.55	0.42
1:A:80:PRO:HA	6:A:433:HOH:O	2.20	0.42
1:D:107:PHE:HB2	1:D:201:LEU:HB3	2.02	0.42
1:E:47:PRO:O	1:E:48:ASN:HB2	2.20	0.42
1:A:105:THR:O	1:A:109:VAL:HG23	2.20	0.42
1:C:9:SER:O	1:C:10:CYS:HB3	2.20	0.42
1:E:90:THR:OG1	1:E:93:ASP:HB2	2.20	0.42
1:A:134:ILE:HA	1:A:135:PRO:HD3	1.92	0.41
1:B:243:LEU:HA	1:B:243:LEU:HD23	1.82	0.41
3:C:302:OTO:N5	3:C:302:OTO:C18	2.77	0.41
1:D:163:ALA:HA	1:D:166:PHE:CE1	2.54	0.41
1:B:160:LEU:HD23	1:B:160:LEU:HA	1.83	0.41
1:C:148:ARG:HD3	1:C:148:ARG:HA	1.87	0.41
1:B:88:ILE:CG2	1:B:95:TRP:HB2	2.50	0.41
1:E:186:LEU:HD21	1:E:263:PHE:CE1	2.56	0.41
1:B:134:ILE:HA	1:B:135:PRO:HD3	1.78	0.41
1:B:69:MET:HG3	1:B:87:PHE:CG	2.55	0.41
1:A:233:TRP:CE3	1:A:261:LEU:HD11	2.55	0.41
1:B:46:LYS:HB3	1:B:49:ALA:HB3	2.02	0.41
1:D:87:PHE:CE1	1:D:89:ARG:HB2	2.56	0.41
1:D:167:ASP:HB2	1:D:170:ARG:NH1	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:ALA:HB1	1:D:265:LEU:HG	2.03	0.41
2:D:301:KAN:H5	2:D:301:KAN:HN21	1.85	0.41
1:E:129:ARG:HA	1:E:129:ARG:HD3	1.74	0.41
1:E:174:PRO:HD2	1:E:177:GLN:OE1	2.21	0.41
1:B:111:GLU:HG2	1:E:246:ARG:CZ	2.50	0.41
1:E:224:ASP:OD1	1:E:226:TYR:HB2	2.20	0.41
1:B:245:LYS:HA	1:B:245:LYS:HD3	1.91	0.41
1:D:19:LEU:O	1:D:23:LEU:HG	2.21	0.40
1:C:13:PRO:HD2	1:D:28:TRP:CZ3	2.56	0.40
1:B:41:TYR:O	1:B:53:PHE:HA	2.22	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	253/272 (93%)	235 (93%)	18 (7%)	0	100	100
1	B	257/272 (94%)	238 (93%)	19 (7%)	0	100	100
1	C	261/272 (96%)	248 (95%)	10 (4%)	3 (1%)	17	41
1	D	254/272 (93%)	242 (95%)	11 (4%)	1 (0%)	39	68
1	E	254/272 (93%)	242 (95%)	12 (5%)	0	100	100
All	All	1279/1360 (94%)	1205 (94%)	70 (6%)	4 (0%)	46	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	22	ASP
1	C	21	ALA
1	C	29	ALA
1	D	117	GLY

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	222/238 (93%)	208 (94%)	14 (6%)	22	47
1	B	231/238 (97%)	221 (96%)	10 (4%)	35	65
1	C	233/238 (98%)	219 (94%)	14 (6%)	24	49
1	D	223/238 (94%)	211 (95%)	12 (5%)	27	55
1	E	223/238 (94%)	211 (95%)	12 (5%)	27	55
All	All	1132/1190 (95%)	1070 (94%)	62 (6%)	27	54

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	THR
1	A	89	ARG
1	A	110	LEU
1	A	115	ASP
1	A	119	ASN
1	A	129	ARG
1	A	143	SER
1	A	146	VAL
1	A	160	LEU
1	A	164	SER
1	A	191	ASP
1	A	216	ASP
1	A	242	SER
1	A	261	LEU
1	B	6	ARG
1	B	20	ASP
1	B	28	TRP
1	B	51	GLU
1	B	60	SER
1	B	61	VAL
1	B	129	ARG
1	B	146	VAL
1	B	180	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	189	SER
1	C	12	ARG
1	C	14	ARG
1	C	15	LEU
1	C	16	ASN
1	C	18	ASN
1	C	19	LEU
1	C	24	TYR
1	C	28[A]	TRP
1	C	28[B]	TRP
1	C	58	LYS
1	C	83	THR
1	C	164	SER
1	C	208	GLU
1	C	255	ASN
1	D	32	ASN
1	D	68	GLU
1	D	70	VAL
1	D	72	LEU
1	D	90	THR
1	D	104	LYS
1	D	115[A]	ASP
1	D	115[B]	ASP
1	D	169	GLU
1	D	216	ASP
1	D	240	SER
1	D	260	LYS
1	E	19	LEU
1	E	20	ASP
1	E	23	LEU
1	E	33	VAL
1	E	35	GLN
1	E	42	ARG
1	E	81	LEU
1	E	86	HIS
1	E	99	THR
1	E	129	ARG
1	E	144	ASP
1	E	188	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	234	ASN
1	B	86	HIS
1	B	227	GLN
1	C	119	ASN
1	D	227	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	KAN	A	301	-	35,35,35	0.83	1 (2%)	44,52,52	1.57	6 (13%)
3	OTO	A	302	-	24,24,24	1.57	4 (16%)	33,33,33	4.39	16 (48%)
2	KAN	B	301	-	35,35,35	0.74	0	44,52,52	1.93	5 (11%)
2	KAN	C	301	-	35,35,35	0.89	2 (5%)	44,52,52	1.44	7 (15%)
3	OTO	C	302	-	24,24,24	1.58	3 (12%)	33,33,33	4.19	18 (54%)
5	ACT	C	303	-	1,3,3	1.57	0	0,3,3	0.00	-
2	KAN	D	301	-	35,35,35	0.84	1 (2%)	44,52,52	1.76	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	0TO	D	302	-	24,24,24	1.84	6 (25%)	33,33,33	4.94	18 (54%)
2	KAN	E	301	-	35,35,35	0.95	1 (2%)	44,52,52	1.74	10 (22%)
3	0TO	E	302	-	24,24,24	1.42	5 (20%)	33,33,33	3.85	16 (48%)

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	KAN	A	301	-	-	0/12/72/72	0/3/3/3
3	0TO	A	302	-	-	0/8/8/8	0/3/3/3
2	KAN	B	301	-	-	0/12/72/72	0/3/3/3
2	KAN	C	301	-	-	0/12/72/72	0/3/3/3
3	0TO	C	302	-	-	0/8/8/8	0/3/3/3
5	ACT	C	303	-	-	0/0/0/0	0/0/0/0
2	KAN	D	301	-	-	0/12/72/72	0/3/3/3
3	0TO	D	302	-	-	0/8/8/8	0/3/3/3
2	KAN	E	301	-	-	0/12/72/72	0/3/3/3
3	0TO	E	302	-	-	0/8/8/8	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	0TO	C4-C2	-6.05	1.37	1.44
3	C	302	0TO	C4-C2	-4.85	1.39	1.44
3	A	302	0TO	C4-C2	-4.78	1.39	1.44
3	E	302	0TO	C4-C2	-3.68	1.40	1.44
3	D	302	0TO	C7-N6	-3.49	1.33	1.40
3	C	302	0TO	C7-N6	-3.22	1.33	1.40
3	D	302	0TO	C2-C1	-2.93	1.38	1.42
3	E	302	0TO	C7-N6	-2.89	1.34	1.40
3	A	302	0TO	C7-N6	-2.87	1.34	1.40
3	C	302	0TO	C2-C1	-2.84	1.38	1.42
2	A	301	KAN	C14-C15	-2.68	1.50	1.53
2	C	301	KAN	C14-C15	-2.56	1.50	1.53
3	D	302	0TO	C15-C1	-2.39	1.38	1.41
3	E	302	0TO	C15-C1	-2.36	1.38	1.41
3	E	302	0TO	C1-N9	-2.12	1.33	1.37
3	A	302	0TO	C1-N9	-2.12	1.33	1.37
3	D	302	0TO	C1-N9	-2.02	1.33	1.37
3	D	302	0TO	C3-C2	-2.02	1.38	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	302	0TO	C3-C10	2.04	1.40	1.36
2	D	301	KAN	O11-C13	2.11	1.47	1.41
2	E	301	KAN	O5-C1	2.18	1.47	1.41
3	A	302	0TO	C15-C12	2.19	1.40	1.36
2	C	301	KAN	O11-C13	2.42	1.48	1.41

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	0TO	C3-C2-C4	-12.54	118.20	124.89
3	A	302	0TO	C3-C2-C4	-11.88	118.56	124.89
3	C	302	0TO	N9-C8-N5	-10.51	120.85	128.89
3	D	302	0TO	N9-C8-N5	-9.54	121.59	128.89
3	C	302	0TO	C3-C2-C4	-9.33	119.92	124.89
3	E	302	0TO	N9-C8-N5	-9.17	121.87	128.89
3	A	302	0TO	N9-C8-N5	-8.58	122.32	128.89
3	D	302	0TO	O11-C10-C3	-8.29	114.14	125.25
3	A	302	0TO	C2-C4-N5	-8.23	115.59	121.46
3	D	302	0TO	C2-C4-N5	-7.62	116.03	121.46
2	B	301	KAN	C6-C5-C4	-7.48	99.04	113.17
2	D	301	KAN	C6-C5-C4	-7.47	99.05	113.17
3	E	302	0TO	C16-O13-C12	-7.38	106.34	117.54
3	E	302	0TO	C2-C4-N5	-7.23	116.30	121.46
3	D	302	0TO	O13-C12-C15	-6.17	116.98	125.25
3	E	302	0TO	C3-C2-C4	-5.66	121.87	124.89
2	B	301	KAN	C18-C17-C16	-5.51	99.43	113.02
3	A	302	0TO	C14-O11-C10	-5.50	109.20	117.54
3	C	302	0TO	C16-O13-C12	-5.42	109.32	117.54
3	A	302	0TO	C16-O13-C12	-5.39	109.37	117.54
3	C	302	0TO	O13-C12-C15	-5.09	118.42	125.25
3	C	302	0TO	C2-C4-N5	-4.82	118.02	121.46
3	A	302	0TO	O11-C10-C3	-4.75	118.88	125.25
3	E	302	0TO	O13-C12-C15	-4.74	118.90	125.25
3	C	302	0TO	O11-C10-C3	-4.17	119.66	125.25
3	D	302	0TO	C16-O13-C12	-3.98	111.50	117.54
2	C	301	KAN	C18-C17-C16	-3.85	103.52	113.02
3	E	302	0TO	C14-O11-C10	-3.84	111.72	117.54
3	E	302	0TO	O11-C10-C3	-3.70	120.29	125.25
3	C	302	0TO	C2-C1-N9	-3.58	119.07	122.88
2	E	301	KAN	C18-C17-C16	-3.46	104.48	113.02
3	C	302	0TO	C2-C4-N6	-3.41	116.67	119.63
3	A	302	0TO	O13-C12-C15	-3.35	120.76	125.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	0TO	C21-C20-C18	-3.25	117.18	121.53
3	C	302	0TO	C14-O11-C10	-3.18	112.72	117.54
2	A	301	KAN	C18-C17-C16	-3.14	105.27	113.02
3	A	302	0TO	C2-C1-N9	-3.04	119.65	122.88
3	A	302	0TO	C17-C7-C18	-2.94	116.18	119.69
3	D	302	0TO	C2-C1-N9	-2.93	119.76	122.88
3	D	302	0TO	C2-C4-N6	-2.93	117.08	119.63
2	C	301	KAN	C6-C5-C4	-2.85	107.78	113.17
2	A	301	KAN	O9-C1-O5	-2.80	103.59	110.68
2	E	301	KAN	O13-C14-C13	-2.69	104.13	110.02
3	E	302	0TO	C2-C1-N9	-2.54	120.18	122.88
2	C	301	KAN	O9-C1-O5	-2.37	104.67	110.68
2	E	301	KAN	O9-C1-O5	-2.34	104.75	110.68
2	E	301	KAN	O12-C13-C14	-2.17	105.82	110.28
2	D	301	KAN	O13-C14-C13	-2.16	105.28	110.02
2	B	301	KAN	O9-C1-O5	-2.14	105.26	110.68
2	A	301	KAN	C6-C5-C4	-2.05	109.29	113.17
3	E	302	0TO	C21-C20-C18	-2.05	118.79	121.53
3	D	302	0TO	C17-C7-C18	-2.04	117.25	119.69
3	D	302	0TO	C21-C20-CL	2.08	122.77	119.35
2	D	301	KAN	O12-C17-C18	2.09	111.64	106.36
2	C	301	KAN	C10-C9-C8	2.17	113.44	109.06
2	D	301	KAN	C10-C9-C8	2.19	113.48	109.06
2	A	301	KAN	O9-C10-C9	2.21	112.86	107.17
2	E	301	KAN	C13-C14-C15	2.37	113.58	110.40
2	E	301	KAN	O9-C10-C9	2.53	113.69	107.17
2	E	301	KAN	C10-C9-C8	2.59	114.29	109.06
3	D	302	0TO	C15-C1-N9	2.66	120.89	117.95
2	E	301	KAN	O5-C5-C6	2.72	111.42	106.10
3	A	302	0TO	O13-C12-C10	2.87	119.48	115.40
2	C	301	KAN	O11-C8-C9	2.88	114.59	107.17
3	E	302	0TO	O11-C10-C12	2.92	119.57	115.40
3	E	302	0TO	N6-C4-N5	3.04	121.73	118.85
2	A	301	KAN	O11-C8-C9	3.15	115.31	107.17
3	C	302	0TO	C15-C1-N9	3.31	121.60	117.95
2	C	301	KAN	O12-C17-C18	3.43	115.03	106.36
2	B	301	KAN	O11-C8-C9	3.55	116.34	107.17
2	C	301	KAN	O5-C5-C6	3.61	113.15	106.10
3	A	302	0TO	O11-C10-C12	3.87	120.92	115.40
2	D	301	KAN	O11-C8-C9	3.87	117.16	107.17
2	E	301	KAN	O11-C8-C9	3.88	117.19	107.17
2	D	301	KAN	O5-C5-C6	3.89	113.70	106.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	302	OTO	O13-C12-C10	4.27	121.49	115.40
3	A	302	OTO	C8-N9-C1	4.27	119.13	115.19
3	C	302	OTO	O11-C10-C12	4.39	121.67	115.40
3	C	302	OTO	O13-C12-C10	4.53	121.86	115.40
3	D	302	OTO	C8-N9-C1	4.59	119.42	115.19
3	C	302	OTO	C7-C18-C20	4.70	122.47	118.65
3	A	302	OTO	C7-C18-C20	4.72	122.48	118.65
3	E	302	OTO	C8-N9-C1	4.78	119.60	115.19
3	E	302	OTO	C7-C18-C20	4.82	122.56	118.65
2	B	301	KAN	O5-C5-C6	4.99	115.85	106.10
2	E	301	KAN	O12-C17-C18	5.09	119.22	106.36
3	D	302	OTO	C7-C18-C20	5.17	122.85	118.65
2	A	301	KAN	O5-C5-C6	5.18	116.21	106.10
3	E	302	OTO	C4-C2-C1	5.60	118.96	115.77
3	C	302	OTO	C4-C2-C1	5.62	118.97	115.77
3	D	302	OTO	O13-C12-C10	5.84	123.73	115.40
3	A	302	OTO	N6-C4-N5	6.04	124.56	118.85
3	C	302	OTO	N6-C4-N5	6.10	124.63	118.85
3	C	302	OTO	C8-N9-C1	6.37	121.08	115.19
3	C	302	OTO	C8-N5-C4	6.83	121.40	116.48
3	D	302	OTO	N6-C4-N5	7.23	125.69	118.85
3	A	302	OTO	C8-N5-C4	7.69	122.02	116.48
3	D	302	OTO	C8-N5-C4	7.79	122.09	116.48
3	D	302	OTO	C4-C2-C1	7.96	120.30	115.77
3	D	302	OTO	O11-C10-C12	8.46	127.47	115.40
3	A	302	OTO	C4-C2-C1	8.51	120.62	115.77
3	E	302	OTO	C8-N5-C4	8.75	122.78	116.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	OTO	3	0
2	C	301	KAN	1	0
3	C	302	OTO	7	0
2	D	301	KAN	1	0
3	D	302	OTO	7	0
3	E	302	OTO	4	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	254/272 (93%)	-0.43	0 100 100	28, 50, 79, 97	0
1	B	261/272 (95%)	-0.21	11 (4%) 40 40	32, 48, 108, 144	0
1	C	261/272 (95%)	-0.19	13 (4%) 32 32	28, 46, 109, 150	0
1	D	253/272 (93%)	-0.45	0 100 100	34, 50, 77, 101	0
1	E	254/272 (93%)	-0.39	1 (0%) 93 94	29, 49, 83, 111	0
All	All	1283/1360 (94%)	-0.33	25 (1%) 70 71	28, 49, 91, 150	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	17	SER	5.6
1	C	14	ARG	5.5
1	B	24	TYR	5.5
1	B	48	ASN	5.3
1	B	4	ILE	4.3
1	B	36	SER	4.0
1	B	25	GLY	3.8
1	C	24	TYR	3.6
1	B	27	ARG	3.6
1	C	48	ASN	3.5
1	C	25	GLY	3.5
1	C	18	ASN	3.2
1	B	14	ARG	3.1
1	B	30	ARG	3.1
1	B	23	LEU	3.0
1	C	15	LEU	3.0
1	C	20	ASP	2.7
1	C	19	LEU	2.7
1	E	33	VAL	2.6
1	C	36	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	16	ASN	2.4
1	B	20	ASP	2.3
1	C	9	SER	2.2
1	B	49	ALA	2.0
1	C	32	ASN	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 carbohydrates 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. 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
3	OTO	C	302	22/22	0.81	0.39	8.30	62,73,78,86	22
3	OTO	D	302	22/22	0.88	0.28	3.80	51,64,82,89	22
3	OTO	A	302	22/22	0.83	0.29	2.36	46,62,76,82	22
4	NA	A	303	1/1	0.89	0.17	1.98	57,57,57,57	0
4	NA	B	302	1/1	0.83	0.18	1.79	76,76,76,76	0
3	OTO	E	302	22/22	0.90	0.19	1.62	50,61,78,85	22
2	KAN	D	301	33/33	0.93	0.17	0.50	28,45,58,72	0
2	KAN	C	301	33/33	0.96	0.12	0.16	27,39,45,57	0
5	ACT	C	303	4/4	0.93	0.12	-0.12	49,63,69,73	0
2	KAN	E	301	33/33	0.95	0.12	-0.49	24,39,50,61	0
2	KAN	B	301	33/33	0.97	0.10	-0.71	27,37,47,62	0
2	KAN	A	301	33/33	0.94	0.12	-1.01	45,50,60,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.