



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 9, 2018 – 02:04 AM EST

PDB ID : 6B5I
Title : ALDH1A2 liganded with 1-(4-cyanophenyl)-N-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1H-pyrazole-4-carboxamide (compound CM121)
Authors : Chen, Y.; Zhu, J.-Y.; Schonbrunn, E.
Deposited on : 2017-09-29
Resolution : 2.60 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
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) : rb-20030736

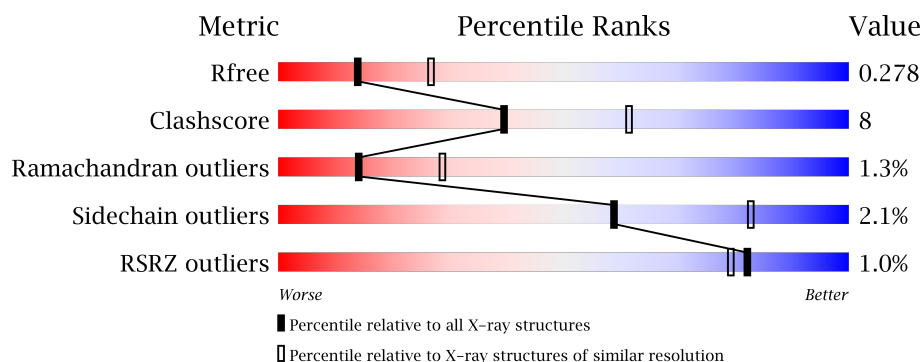
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	493	<div> <div>83%</div> <div>16%</div> </div>
1	B	493	<div> <div>2%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
1	C	493	<div> <div>%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
1	D	493	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CU4	B	601	-	-	-	X

2 Entry composition [i](#)

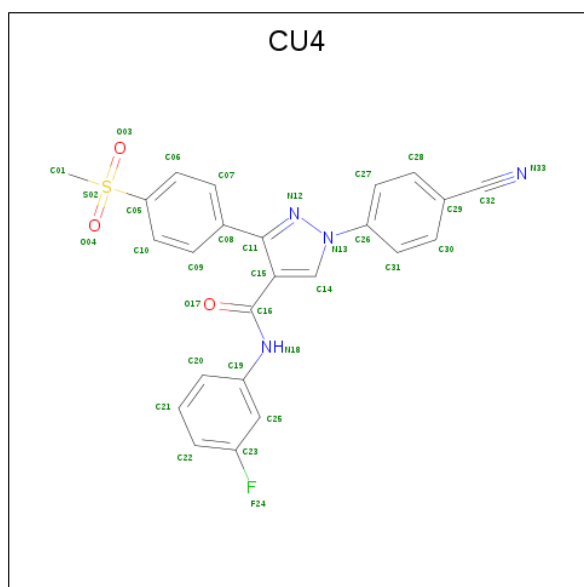
There are 3 unique types of molecules in this entry. The entry contains 15538 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Retinal dehydrogenase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3803	2420	651	714	18			
1	B	492	Total	C	N	O	S	0	0	0
			3803	2420	651	714	18			
1	C	492	Total	C	N	O	S	0	0	0
			3803	2420	651	714	18			
1	D	492	Total	C	N	O	S	0	0	0
			3803	2420	651	714	18			

- Molecule 2 is 1-(4-cyanophenyl)-N-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1H-pyrazole-4-carboxamide (three-letter code: CU4) (formula: $C_{24}H_{17}FN_4O_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			33	24	1	4	3	1		
2	B	1	Total	C	F	N	O	S	0	0
			33	24	1	4	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	F	N	O	S	0	0
			33	24	1	4	3	1		
2	D	1	Total	C	F	N	O	S	0	0
			33	24	1	4	3	1		

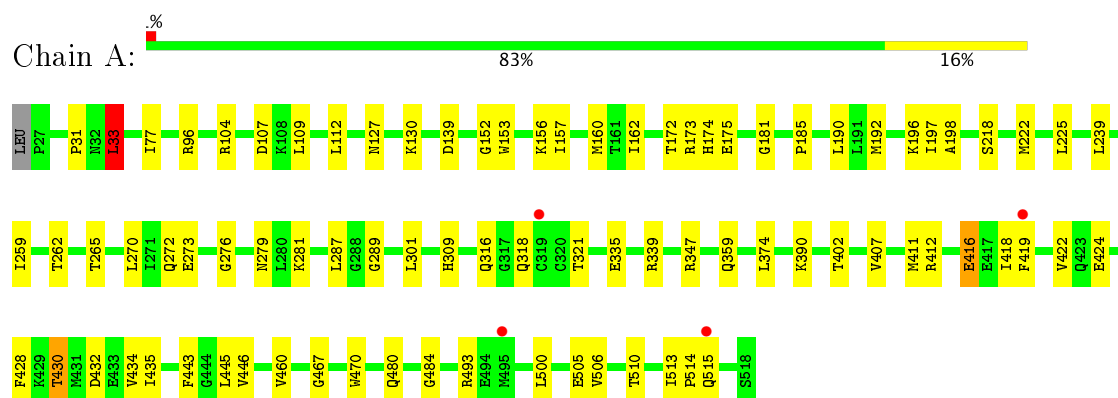
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total	O	0	0
			63	63		
3	B	39	Total	O	0	0
			39	39		
3	C	25	Total	O	0	0
			25	25		
3	D	67	Total	O	0	0
			67	67		

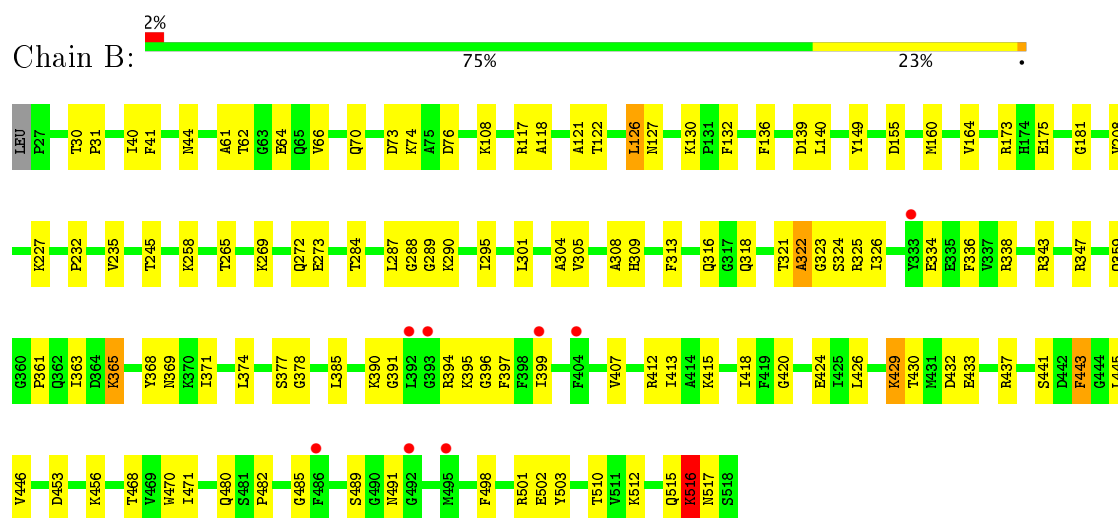
3 Residue-property plots

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.

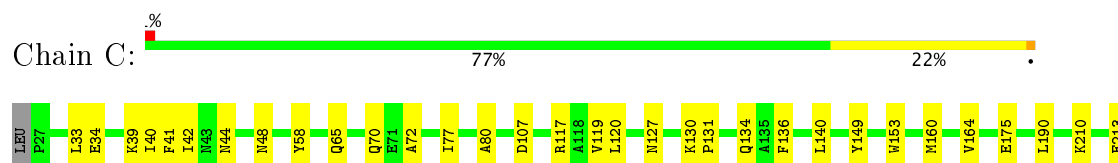
• Molecule 1: Retinal dehydrogenase 2

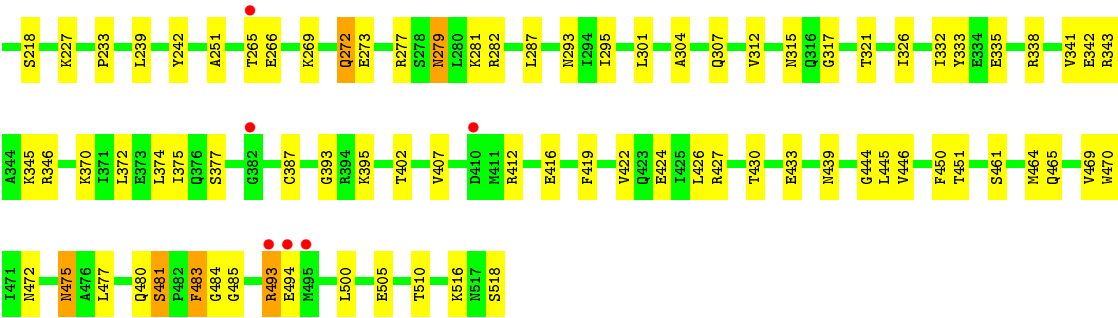


• Molecule 1: Retinal dehydrogenase 2

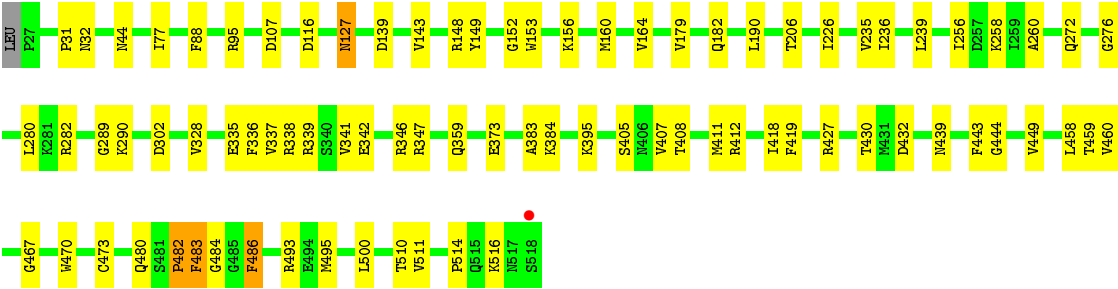
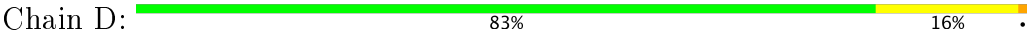


• Molecule 1: Retinal dehydrogenase 2





• Molecule 1: Retinal dehydrogenase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.83Å 139.47Å 163.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.53 – 2.60 81.53 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (81.53-2.60) 99.3 (81.53-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.05 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575_2575	Depositor
R, R_{free}	0.222 , 0.277 0.221 , 0.278	Depositor DCC
R_{free} test set	1076 reflections (1.80%)	DCC
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15538	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.15 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.7670e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU4

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	0.28	0/3884	0.44	0/5254
1	B	0.28	0/3884	0.44	0/5254
1	C	0.29	0/3884	0.47	1/5254 (0.0%)
1	D	0.28	0/3884	0.44	0/5254
All	All	0.28	0/15536	0.45	1/21016 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	484	GLY	N-CA-C	-5.81	98.58	113.10

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	3803	0	3779	70	0
1	B	3803	0	3779	84	0
1	C	3803	0	3779	86	0
1	D	3803	0	3779	53	0
2	A	33	0	0	0	0
2	B	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	33	0	0	0	0
2	D	33	0	0	0	0
3	A	63	0	0	0	0
3	B	39	0	0	0	0
3	C	25	0	0	0	0
3	D	67	0	0	1	0
All	All	15538	0	15116	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 8.

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:335:GLU:OE1	1:A:339:ARG:HD2	1.54	1.07
1:A:301:LEU:HD21	1:A:335:GLU:OE2	1.56	1.03
1:A:276:GLY:HA3	1:C:272:GLN:HE21	1.37	0.89
1:A:273:GLU:OE1	1:C:277:ARG:HG3	1.72	0.87
1:A:301:LEU:CD2	1:A:335:GLU:OE2	2.22	0.86
1:A:272:GLN:HG2	1:C:272:GLN:OE1	1.81	0.81
1:B:371:ILE:HD11	1:B:399:ILE:HD13	1.65	0.79
1:C:342:GLU:O	1:C:346:ARG:HD2	1.80	0.79
1:B:30:THR:H	1:B:122:THR:HG21	1.46	0.79
1:C:375:ILE:HD11	1:C:402:THR:HG21	1.64	0.78
1:A:272:GLN:O	1:C:272:GLN:NE2	2.17	0.76
1:C:342:GLU:O	1:C:346:ARG:CD	2.36	0.74
1:B:288:GLY:HA2	1:B:445:LEU:HD22	1.71	0.72
1:D:77:ILE:HD13	1:D:239:LEU:HD22	1.72	0.71
1:B:62:THR:HG23	1:B:64:GLU:H	1.56	0.71
1:B:272:GLN:HE21	1:D:272:GLN:HG3	1.52	0.71
1:B:284:THR:HG21	1:B:502:GLU:HG3	1.73	0.70
1:A:196:LYS:NZ	1:A:262:THR:OG1	2.25	0.70
1:A:276:GLY:CA	1:C:272:GLN:HE21	2.05	0.70
1:C:213:GLU:HG2	1:C:242:TYR:HA	1.74	0.69
1:A:96:ARG:HH11	1:B:515:GLN:HG3	1.58	0.68
1:A:77:ILE:HD13	1:A:239:LEU:HD22	1.76	0.68
1:B:453:ASP:HB3	1:B:456:LYS:HB2	1.76	0.68
1:A:514:PRO:HD2	1:A:515:GLN:NE2	2.09	0.68
1:B:136:PHE:HA	1:B:140:LEU:HD12	1.77	0.67
1:B:374:LEU:HD13	1:B:418:ILE:HG13	1.77	0.67
1:D:335:GLU:HG3	1:D:338:ARG:HH11	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ARG:HE	1:B:359:GLN:HB2	1.61	0.66
1:C:120:LEU:HB2	1:C:140:LEU:HD21	1.78	0.66
1:B:498:PHE:HA	1:B:501:ARG:HD2	1.77	0.66
1:A:153:TRP:CE2	1:D:156:LYS:HD3	2.30	0.66
1:B:287:LEU:HD12	1:B:489:SER:HA	1.79	0.65
1:A:318:GLN:HA	1:A:419:PHE:HD1	1.61	0.65
1:B:44:ASN:HB3	1:B:227:LYS:HG3	1.77	0.65
1:A:470:TRP:HD1	1:C:510:THR:HB	1.63	0.63
1:A:109:LEU:HD21	1:A:222:MET:HE1	1.81	0.63
1:C:77:ILE:HD13	1:C:239:LEU:HD22	1.81	0.62
1:A:335:GLU:OE1	1:A:339:ARG:NH1	2.19	0.62
1:B:66:VAL:HG11	1:B:126:LEU:HD21	1.81	0.62
1:D:152:GLY:O	1:D:156:LYS:NZ	2.31	0.61
1:D:182:GLN:HG2	1:D:260:ALA:HB3	1.83	0.60
1:A:407:VAL:HG13	1:A:411:MET:HE2	1.83	0.60
1:A:335:GLU:OE1	1:A:339:ARG:CD	2.42	0.60
1:C:190:LEU:HD13	1:C:218:SER:HB2	1.84	0.59
1:B:480:GLN:HB2	1:D:164:VAL:HG12	1.85	0.59
1:B:173:ARG:NH1	1:B:175:GLU:OE2	2.37	0.58
1:C:251:ALA:O	1:C:281:LYS:NZ	2.26	0.57
1:C:446:VAL:HG13	1:C:470:TRP:CZ3	2.39	0.57
1:B:430:THR:HG22	1:B:432:ASP:H	1.70	0.57
1:D:484:GLY:HA3	1:D:493:ARG:HD3	1.87	0.57
1:B:510:THR:HB	1:D:470:TRP:HD1	1.69	0.57
1:B:269:LYS:HA	1:D:280:LEU:HD21	1.87	0.57
1:A:160:MET:HA	1:B:160:MET:HA	1.87	0.56
1:D:335:GLU:HG3	1:D:338:ARG:NH1	2.20	0.56
1:C:445:LEU:HD12	1:C:485:GLY:H	1.68	0.56
1:D:206:THR:HG22	1:D:235:VAL:HA	1.87	0.56
1:C:131:PRO:HB2	1:C:134:GLN:HG3	1.88	0.56
1:C:377:SER:HB2	1:C:412:ARG:HH21	1.69	0.56
1:A:265:THR:HA	1:A:287:LEU:HD13	1.88	0.56
1:D:302:ASP:OD1	1:D:339:ARG:NH1	2.38	0.55
1:B:118:ALA:O	1:B:122:THR:HG23	2.06	0.55
1:A:493:ARG:NH1	1:C:505:GLU:OE1	2.39	0.55
1:D:373:GLU:OE1	1:D:412:ARG:NH2	2.40	0.55
1:B:321:THR:HA	1:B:322:ALA:O	2.07	0.55
1:D:258:LYS:HG3	1:D:282:ARG:HB2	1.89	0.55
1:A:173:ARG:NH2	1:A:175:GLU:OE1	2.39	0.55
1:B:30:THR:N	1:B:122:THR:HG21	2.21	0.55
1:B:371:ILE:HD13	1:B:420:GLY:HA3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LEU:HD13	1:A:418:ILE:HG12	1.89	0.54
1:C:470:TRP:CZ2	1:C:475:ASN:HA	2.42	0.54
1:B:40:ILE:HG13	1:B:70:GLN:HB2	1.89	0.54
1:B:61:ALA:HB2	1:B:361:PRO:HG3	1.89	0.54
1:D:449:VAL:HG21	1:D:460:VAL:HG21	1.88	0.54
1:A:321:THR:HG22	1:A:446:VAL:HG21	1.88	0.54
1:A:506:VAL:HB	1:C:493:ARG:CD	2.37	0.54
1:C:335:GLU:HG2	1:C:338:ARG:HH12	1.74	0.53
1:A:467:GLY:HA3	1:A:484:GLY:O	2.08	0.53
1:B:325:ARG:HH12	1:B:441:SER:HB2	1.73	0.53
1:C:439:ASN:ND2	1:C:465:GLN:H	2.07	0.53
1:A:279:ASN:OD1	1:A:281:LYS:NZ	2.40	0.53
1:A:480:GLN:HB2	1:C:164:VAL:HG23	1.91	0.53
1:D:430:THR:HG22	1:D:432:ASP:H	1.74	0.53
1:C:293:ASN:HB3	1:C:326:ILE:HG13	1.92	0.53
1:D:482:PRO:O	1:D:483:PHE:HB3	2.08	0.53
1:B:73:ASP:O	1:B:76:ASP:N	2.41	0.52
1:A:318:GLN:HA	1:A:419:PHE:CD1	2.44	0.52
1:A:112:LEU:HB3	1:A:225:LEU:HD22	1.93	0.51
1:A:273:GLU:OE1	1:C:277:ARG:CG	2.51	0.51
1:B:269:LYS:HE2	1:D:276:GLY:O	2.11	0.51
1:D:347:ARG:HE	1:D:359:GLN:HB2	1.76	0.51
1:B:512:LYS:HB2	1:D:473:CYS:HB3	1.93	0.51
1:C:451:THR:H	1:C:472:ASN:HD21	1.59	0.51
1:D:383:ALA:HB2	1:D:411:MET:HE1	1.92	0.51
1:A:513:ILE:HD13	1:D:458:LEU:HD13	1.93	0.51
1:C:301:LEU:HD21	1:C:332:ILE:HD12	1.91	0.51
1:B:365:LYS:O	1:B:369:ASN:N	2.44	0.51
1:A:162:ILE:HD13	1:C:481:SER:HA	1.92	0.51
1:C:407:VAL:HB	1:C:426:LEU:HD23	1.92	0.50
1:C:279:ASN:HB3	1:C:281:LYS:HG2	1.93	0.50
1:C:265:THR:HG23	1:C:287:LEU:HD13	1.92	0.50
1:A:270:LEU:HA	1:A:273:GLU:HB3	1.94	0.50
1:C:117:ARG:HG3	1:C:140:LEU:HD22	1.92	0.50
1:C:342:GLU:HG3	1:C:346:ARG:NH2	2.26	0.50
1:C:483:PHE:O	1:C:494:GLU:N	2.41	0.50
1:B:446:VAL:HG22	1:B:468:THR:HB	1.93	0.49
1:D:153:TRP:CG	1:D:500:LEU:HD11	2.46	0.49
1:A:430:THR:HG22	1:A:432:ASP:H	1.77	0.49
1:B:269:LYS:O	1:B:273:GLU:HG3	2.12	0.49
1:B:308:ALA:HB1	1:B:326:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:SER:OG	1:B:412:ARG:NH1	2.46	0.49
1:B:321:THR:HG21	1:B:446:VAL:HG21	1.93	0.49
1:A:96:ARG:NH1	1:B:515:GLN:HG3	2.28	0.49
1:C:153:TRP:CG	1:C:500:LEU:HD11	2.47	0.49
1:B:471:ILE:HD12	1:D:511:VAL:HG22	1.95	0.49
1:B:130:LYS:HA	1:B:316:GLN:HE22	1.78	0.49
1:B:122:THR:HG22	1:B:132:PHE:CE1	2.47	0.49
1:C:130:LYS:HD3	1:C:315:ASN:HA	1.94	0.49
1:A:506:VAL:HB	1:C:493:ARG:NE	2.28	0.49
1:A:104:ARG:HD3	1:D:148:ARG:HD2	1.95	0.49
1:C:341:VAL:O	1:C:345:LYS:HG3	2.12	0.49
1:D:179:VAL:HG23	1:D:256:ILE:HA	1.94	0.49
1:A:156:LYS:HD3	1:D:153:TRP:CE2	2.48	0.48
1:B:321:THR:HA	1:B:322:ALA:C	2.34	0.48
1:B:301:LEU:O	1:B:305:VAL:HG22	2.14	0.48
1:B:365:LYS:HA	1:B:368:TYR:HB3	1.96	0.48
1:B:394:ARG:O	1:B:394:ARG:HG3	2.13	0.48
1:B:318:GLN:HE22	1:B:363:ILE:H	1.61	0.48
1:C:44:ASN:HB2	1:C:233:PRO:HB3	1.95	0.48
1:B:41:PHE:CZ	1:B:44:ASN:HA	2.49	0.48
1:C:342:GLU:HG2	1:C:346:ARG:CZ	2.43	0.48
1:C:439:ASN:HD21	1:C:464:MET:HA	1.78	0.48
1:D:407:VAL:O	1:D:407:VAL:HG23	2.14	0.48
1:B:385:LEU:HA	1:B:385:LEU:HD12	1.73	0.48
1:C:295:ILE:HD12	1:C:304:ALA:HB1	1.96	0.48
1:D:335:GLU:OE1	1:D:338:ARG:HD3	2.13	0.48
1:B:164:VAL:HG12	1:D:480:GLN:HB2	1.94	0.48
1:C:333:TYR:CG	1:C:427:ARG:HG2	2.48	0.47
1:D:342:GLU:O	1:D:346:ARG:HG2	2.14	0.47
1:C:269:LYS:O	1:C:273:GLU:HG3	2.14	0.47
1:A:153:TRP:CG	1:A:500:LEU:HD11	2.49	0.47
1:A:172:THR:HG23	1:A:506:VAL:HG13	1.97	0.47
1:B:413:ILE:HG12	1:B:424:GLU:OE2	2.14	0.47
1:C:58:TYR:CE1	1:C:65:GLN:HG2	2.49	0.47
1:B:485:GLY:HA3	1:B:489:SER:O	2.14	0.47
1:C:80:ALA:HB2	1:C:239:LEU:HD21	1.95	0.47
1:D:127:ASN:ND2	1:D:127:ASN:O	2.46	0.47
1:D:467:GLY:HA3	1:D:484:GLY:O	2.15	0.47
1:A:289:GLY:HA2	1:A:443:PHE:HB3	1.97	0.47
1:A:109:LEU:HD21	1:A:222:MET:CE	2.44	0.46
1:C:470:TRP:HZ2	1:C:477:LEU:HD21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:HA	1:A:104:ARG:HD2	1.73	0.46
1:B:295:ILE:HD13	1:B:304:ALA:HB1	1.96	0.46
1:A:190:LEU:HD13	1:A:218:SER:HB2	1.97	0.46
1:A:505:GLU:OE2	1:C:493:ARG:NH2	2.37	0.46
1:B:365:LYS:HE2	1:B:365:LYS:HB3	1.70	0.46
1:A:412:ARG:NE	1:A:416:GLU:OE2	2.49	0.46
1:B:265:THR:HA	1:B:287:LEU:HD22	1.97	0.46
1:B:347:ARG:NE	1:B:359:GLN:HB2	2.27	0.46
1:C:175:GLU:O	1:C:505:GLU:N	2.50	0.45
1:C:321:THR:HB	1:C:446:VAL:HG21	1.97	0.45
1:A:510:THR:HB	1:C:470:TRP:CD1	2.52	0.45
1:C:312:VAL:O	1:C:317:GLY:HA2	2.16	0.45
1:A:515:GLN:CD	1:D:459:THR:HA	2.37	0.45
1:C:33:LEU:HD21	1:C:119:VAL:HG13	1.97	0.45
1:C:40:ILE:HG22	1:C:42:ILE:HD13	1.99	0.45
1:B:426:LEU:HD23	1:B:437:ARG:NH2	2.31	0.45
1:C:445:LEU:HD12	1:C:485:GLY:N	2.31	0.45
1:A:31:PRO:O	1:A:33:LEU:N	2.49	0.45
1:B:290:LYS:HE2	1:B:415:LYS:N	2.31	0.45
1:B:258:LYS:HE2	1:B:503:TYR:CE1	2.51	0.45
1:A:185:PRO:HD2	1:A:192:MET:HG3	1.99	0.45
1:B:117:ARG:HG3	1:B:140:LEU:HD13	1.99	0.45
1:C:518:SER:HA	1:D:95:ARG:HH21	1.82	0.45
1:A:445:LEU:HG	1:A:446:VAL:HG23	1.99	0.44
1:B:62:THR:HG23	1:B:64:GLU:HG3	1.98	0.44
1:C:117:ARG:HG2	1:C:136:PHE:CE1	2.52	0.44
1:C:44:ASN:HB3	1:C:227:LYS:HD3	1.98	0.44
1:C:470:TRP:CH2	1:C:475:ASN:HA	2.51	0.44
1:A:514:PRO:HD2	1:A:515:GLN:HE22	1.82	0.44
1:C:160:MET:HA	1:D:160:MET:HA	1.98	0.44
1:A:316:GLN:HG3	1:A:359:GLN:HG3	1.98	0.44
1:B:309:HIS:CD2	1:B:343:ARG:HE	2.35	0.44
1:A:276:GLY:N	1:C:272:GLN:NE2	2.66	0.44
1:C:39:LYS:HE2	1:C:48:ASN:OD1	2.18	0.44
1:B:108:LYS:HA	1:B:108:LYS:HD2	1.81	0.44
1:A:484:GLY:HA3	1:A:493:ARG:HD3	2.00	0.44
1:B:407:VAL:HG12	1:B:426:LEU:HD11	1.99	0.44
1:C:412:ARG:HG2	1:C:416:GLU:HG3	1.99	0.44
1:A:152:GLY:HA3	1:D:156:LYS:HZ3	1.83	0.44
1:B:149:TYR:CE1	1:B:480:GLN:HG3	2.53	0.43
1:B:394:ARG:C	1:B:396:GLY:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:PHE:CD2	1:A:434:VAL:HB	2.52	0.43
1:D:143:VAL:HG21	1:D:190:LEU:HG	1.99	0.43
1:D:444:GLY:O	1:D:486:PHE:HB2	2.18	0.43
1:B:295:ILE:HD12	1:B:336:PHE:CE2	2.53	0.43
1:C:342:GLU:CG	1:C:346:ARG:CZ	2.96	0.43
1:C:372:LEU:HA	1:C:375:ILE:HG22	2.01	0.43
1:A:402:THR:OG1	1:A:422:VAL:HG13	2.18	0.43
1:A:276:GLY:H	1:C:272:GLN:NE2	2.16	0.43
1:D:384:LYS:HB3	1:D:405:SER:HB2	1.99	0.43
1:C:370:LYS:O	1:C:374:LEU:HD13	2.19	0.43
1:B:390:LYS:HB2	1:B:391:GLY:H	1.64	0.43
1:B:73:ASP:CG	1:B:245:THR:HG22	2.40	0.43
1:B:470:TRP:CD1	1:D:510:THR:HB	2.54	0.42
1:D:328:VAL:HG21	1:D:336:PHE:CD1	2.55	0.42
1:D:289:GLY:HA3	1:D:443:PHE:HB3	2.00	0.42
1:C:343:ARG:HA	1:C:346:ARG:HD3	2.01	0.42
1:C:446:VAL:CG1	1:C:470:TRP:HZ3	2.32	0.42
1:A:407:VAL:HG21	1:A:424:GLU:HB3	2.02	0.42
1:C:41:PHE:CZ	1:C:44:ASN:HA	2.54	0.42
1:C:402:THR:HB	1:C:422:VAL:HG12	2.01	0.42
1:C:461:SER:HA	1:C:469:VAL:HG11	2.02	0.42
1:D:44:ASN:N	3:D:703:HOH:O	2.51	0.42
1:D:328:VAL:O	1:D:427:ARG:HA	2.19	0.42
1:A:130:LYS:HB2	1:A:130:LYS:HE2	1.71	0.42
1:A:181:GLY:O	1:A:259:ILE:HA	2.20	0.42
1:B:334:GLU:O	1:B:338:ARG:HG2	2.19	0.42
1:C:446:VAL:CG1	1:C:470:TRP:CZ3	3.03	0.42
1:D:337:VAL:O	1:D:341:VAL:HG23	2.19	0.42
1:D:88:PHE:O	1:D:95:ARG:NH1	2.46	0.42
1:B:313:PHE:HB3	1:B:347:ARG:NH1	2.35	0.42
1:B:429:LYS:HD2	1:B:433:GLU:OE2	2.19	0.42
1:B:181:GLY:HA2	1:B:208:VAL:O	2.20	0.42
1:C:321:THR:HG22	1:C:445:LEU:HD23	2.02	0.42
1:A:435:ILE:HD11	1:A:460:VAL:HG22	2.02	0.41
1:B:301:LEU:HA	1:B:301:LEU:HD23	1.82	0.41
1:B:365:LYS:HB2	1:B:397:PHE:CE2	2.55	0.41
1:B:374:LEU:HD22	1:B:418:ILE:HD11	2.02	0.41
1:C:40:ILE:HG13	1:C:70:GLN:HB2	2.02	0.41
1:A:197:ILE:HG13	1:A:198:ALA:N	2.35	0.41
1:C:372:LEU:O	1:C:375:ILE:HG22	2.20	0.41
1:C:430:THR:HG23	1:C:433:GLU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ILE:HD13	1:C:72:ALA:HB2	2.03	0.41
1:D:149:TYR:CE1	1:D:480:GLN:HG3	2.55	0.41
1:C:307:GLN:HG2	1:C:450:PHE:HZ	1.85	0.41
1:C:483:PHE:O	1:C:494:GLU:HG2	2.21	0.41
1:B:269:LYS:HG2	1:D:280:LEU:HG	2.03	0.41
1:B:232:PRO:HD2	1:B:235:VAL:HG21	2.03	0.41
1:B:121:ALA:HB2	1:B:140:LEU:HD11	2.01	0.41
1:B:516:LYS:H	1:B:516:LYS:HG3	1.48	0.41
1:A:276:GLY:N	1:C:272:GLN:HE21	2.18	0.41
1:C:342:GLU:O	1:C:346:ARG:NE	2.54	0.41
1:D:116:ASP:N	1:D:116:ASP:OD1	2.54	0.41
1:A:153:TRP:O	1:A:157:ILE:HG13	2.21	0.40
1:A:185:PRO:HG3	1:A:262:THR:HG22	2.04	0.40
1:A:309:HIS:CE1	1:A:347:ARG:HD2	2.56	0.40
1:B:289:GLY:HA3	1:B:443:PHE:CG	2.56	0.40
1:B:322:ALA:HA	1:B:323:GLY:HA3	1.74	0.40
1:B:482:PRO:HG3	1:B:498:PHE:CD2	2.56	0.40
1:D:290:LYS:NZ	1:D:418:ILE:HD12	2.36	0.40
1:C:149:TYR:CE1	1:C:480:GLN:HG3	2.56	0.40
1:D:226:ILE:HD13	1:D:236:ILE:HG21	2.03	0.40
1:B:130:LYS:NZ	1:B:139:ASP:OD2	2.52	0.40
1:C:346:ARG:HD2	1:C:346:ARG:N	2.36	0.40
1:C:407:VAL:HG21	1:C:424:GLU:HB3	2.04	0.40

There are no symmetry-related clashes.

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	490/493 (99%)	460 (94%)	27 (6%)	3 (1%)	28 53
1	B	490/493 (99%)	446 (91%)	35 (7%)	9 (2%)	10 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	490/493 (99%)	451 (92%)	32 (6%)	7 (1%)	13	26
1	D	490/493 (99%)	464 (95%)	20 (4%)	6 (1%)	15	32
All	All	1960/1972 (99%)	1821 (93%)	114 (6%)	25 (1%)	14	29

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	516	LYS
1	C	475	ASN
1	D	31	PRO
1	B	443	PHE
1	C	483	PHE
1	D	482	PRO
1	D	514	PRO
1	A	416	GLU
1	B	31	PRO
1	C	395	LYS
1	C	516	LYS
1	A	33	LEU
1	A	430	THR
1	B	324	SER
1	B	491	ASN
1	B	517	ASN
1	C	444	GLY
1	D	516	LYS
1	B	74	LYS
1	B	322	ALA
1	C	481	SER
1	D	483	PHE
1	D	495	MET
1	C	393	GLY
1	B	378	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	401/402 (100%)	395 (98%)	6 (2%)	70	88
1	B	401/402 (100%)	394 (98%)	7 (2%)	66	86
1	C	401/402 (100%)	390 (97%)	11 (3%)	50	77
1	D	401/402 (100%)	392 (98%)	9 (2%)	57	81
All	All	1604/1608 (100%)	1571 (98%)	33 (2%)	59	83

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	107	ASP
1	A	127	ASN
1	A	139	ASP
1	A	174	HIS
1	A	390	LYS
1	B	126	LEU
1	B	127	ASN
1	B	155	ASP
1	B	365	LYS
1	B	395	LYS
1	B	429	LYS
1	B	516	LYS
1	C	34	GLU
1	C	107	ASP
1	C	127	ASN
1	C	210	LYS
1	C	266	GLU
1	C	272	GLN
1	C	279	ASN
1	C	282	ARG
1	C	387	CYS
1	C	419	PHE
1	C	493	ARG
1	D	32	ASN
1	D	107	ASP
1	D	127	ASN
1	D	139	ASP
1	D	395	LYS
1	D	408	THR
1	D	419	PHE
1	D	439	ASN
1	D	486	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	515	GLN
1	B	272	GLN
1	B	316	GLN
1	B	318	GLN
1	C	272	GLN
1	C	439	ASN
1	C	472	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	CU4	A	601	-	34,36,36	2.73	10 (29%)	43,52,52	2.06	8 (18%)
2	CU4	B	601	-	34,36,36	2.78	11 (32%)	43,52,52	1.96	8 (18%)
2	CU4	C	601	-	34,36,36	2.75	10 (29%)	43,52,52	1.95	7 (16%)
2	CU4	D	601	-	34,36,36	2.70	10 (29%)	43,52,52	1.93	7 (16%)

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	CU4	A	601	-	-	0/22/24/24	0/4/4/4
2	CU4	B	601	-	-	0/22/24/24	0/4/4/4
2	CU4	C	601	-	-	0/22/24/24	0/4/4/4
2	CU4	D	601	-	-	0/22/24/24	0/4/4/4

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	CU4	C08-C11	-6.57	1.42	1.49
2	C	601	CU4	C08-C11	-6.55	1.42	1.49
2	A	601	CU4	C08-C11	-6.13	1.42	1.49
2	D	601	CU4	C08-C11	-6.00	1.42	1.49
2	A	601	CU4	C29-C32	-5.78	1.30	1.44
2	D	601	CU4	C29-C32	-5.78	1.30	1.44
2	C	601	CU4	C29-C32	-5.75	1.30	1.44
2	B	601	CU4	C29-C32	-5.73	1.30	1.44
2	B	601	CU4	N12-N13	-5.49	1.29	1.39
2	A	601	CU4	N12-N13	-5.31	1.30	1.39
2	C	601	CU4	N12-N13	-5.28	1.30	1.39
2	D	601	CU4	N12-N13	-5.27	1.30	1.39
2	B	601	CU4	C26-N13	-3.80	1.36	1.44
2	A	601	CU4	C26-N13	-3.70	1.36	1.44
2	C	601	CU4	C26-N13	-3.63	1.36	1.44
2	D	601	CU4	C26-N13	-3.61	1.36	1.44
2	B	601	CU4	C15-C16	-3.58	1.42	1.50
2	C	601	CU4	C15-C16	-3.56	1.42	1.50
2	A	601	CU4	C15-C16	-3.50	1.42	1.50
2	D	601	CU4	C15-C16	-3.46	1.42	1.50
2	C	601	CU4	F24-C23	-2.27	1.31	1.36
2	D	601	CU4	F24-C23	-2.27	1.31	1.36
2	B	601	CU4	F24-C23	-2.21	1.31	1.36
2	A	601	CU4	F24-C23	-2.13	1.31	1.36
2	D	601	CU4	C22-C23	2.05	1.41	1.37
2	B	601	CU4	C25-C19	2.09	1.43	1.39
2	D	601	CU4	C01-S02	2.11	1.83	1.75
2	C	601	CU4	C01-S02	2.12	1.83	1.75
2	B	601	CU4	C01-S02	2.13	1.83	1.75
2	A	601	CU4	C01-S02	2.15	1.83	1.75
2	A	601	CU4	C22-C23	2.18	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	CU4	C25-C23	2.32	1.41	1.37
2	B	601	CU4	C25-C23	2.38	1.41	1.37
2	D	601	CU4	O04-S02	5.71	1.60	1.43
2	C	601	CU4	O04-S02	5.74	1.60	1.43
2	C	601	CU4	O03-S02	5.76	1.61	1.43
2	A	601	CU4	O04-S02	5.78	1.61	1.43
2	A	601	CU4	O03-S02	5.78	1.61	1.43
2	D	601	CU4	O03-S02	5.80	1.61	1.43
2	B	601	CU4	O04-S02	5.81	1.61	1.43
2	B	601	CU4	O03-S02	5.81	1.61	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	CU4	O04-S02-O03	-5.79	107.19	117.84
2	A	601	CU4	O04-S02-O03	-5.72	107.32	117.84
2	B	601	CU4	O04-S02-O03	-5.72	107.32	117.84
2	D	601	CU4	O04-S02-O03	-5.36	107.98	117.84
2	A	601	CU4	C22-C23-C25	-3.20	119.09	123.29
2	B	601	CU4	C22-C23-C25	-2.79	119.63	123.29
2	D	601	CU4	C22-C23-C25	-2.79	119.63	123.29
2	C	601	CU4	C22-C23-C25	-2.57	119.91	123.29
2	B	601	CU4	C10-C05-S02	2.15	121.69	119.60
2	C	601	CU4	C15-C16-N18	2.22	120.49	116.11
2	B	601	CU4	C19-N18-C16	2.23	132.36	126.61
2	D	601	CU4	C15-C16-N18	2.33	120.72	116.11
2	A	601	CU4	C15-C16-N18	2.49	121.03	116.11
2	C	601	CU4	O03-S02-C05	2.84	110.61	108.30
2	A	601	CU4	O03-S02-C05	3.21	110.91	108.30
2	C	601	CU4	C19-C25-C23	3.85	121.35	117.96
2	B	601	CU4	O03-S02-C05	3.92	111.49	108.30
2	B	601	CU4	C19-C25-C23	4.00	121.49	117.96
2	D	601	CU4	C19-C25-C23	4.08	121.56	117.96
2	A	601	CU4	O04-S02-C05	4.16	111.69	108.30
2	C	601	CU4	C11-N12-N13	4.27	109.75	105.43
2	B	601	CU4	C11-N12-N13	4.28	109.76	105.43
2	D	601	CU4	C01-S02-C05	4.58	110.03	104.58
2	A	601	CU4	C11-N12-N13	4.70	110.18	105.43
2	A	601	CU4	C19-C25-C23	4.71	122.11	117.96
2	D	601	CU4	C11-N12-N13	4.75	110.24	105.43
2	D	601	CU4	O03-S02-C05	5.05	112.41	108.30
2	B	601	CU4	C01-S02-C05	5.12	110.68	104.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	CU4	C01-S02-C05	5.14	110.70	104.58
2	C	601	CU4	C01-S02-C05	6.09	111.84	104.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	492/493 (99%)	-0.23	4 (0%) 86 83	20, 38, 54, 63	0
1	B	492/493 (99%)	0.02	8 (1%) 72 67	27, 50, 76, 81	0
1	C	492/493 (99%)	0.05	6 (1%) 79 75	25, 52, 71, 82	0
1	D	492/493 (99%)	-0.21	1 (0%) 94 95	20, 37, 54, 67	0
All	All	1968/1972 (99%)	-0.09	19 (0%) 82 79	20, 43, 71, 82	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	392	LEU	3.1
1	C	493	ARG	3.0
1	C	382	GLY	2.9
1	A	515	GLN	2.8
1	A	319	CYS	2.8
1	D	518	SER	2.8
1	C	495	MET	2.7
1	C	410	ASP	2.6
1	B	492	GLY	2.6
1	C	265	THR	2.5
1	B	495	MET	2.5
1	C	494	GLU	2.4
1	B	404	PHE	2.3
1	B	399	ILE	2.3
1	B	393	GLY	2.2
1	A	495	MET	2.2
1	B	333	TYR	2.1
1	B	486	PHE	2.1
1	A	419	PHE	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(\AA^2)	Q<0.9
2	CU4	B	601	33/33	0.89	0.28	2.05	48,65,77,81	0
2	CU4	C	601	33/33	0.90	0.27	1.38	51,63,71,82	0
2	CU4	A	601	33/33	0.93	0.22	0.76	38,48,57,71	0
2	CU4	D	601	33/33	0.93	0.17	-0.06	39,49,54,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.