Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2026 – 10:14 AM EST

PDB ID	:	12LQ / pdb_000012lq
Title	:	LSD1-CoREST in complex with Alkyne probe and peptide PRCALVKSK
Authors	:	Caroli, J.; Mattevi, A.
Deposited on	:	2026-04-12
Resolution	:	2.67 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

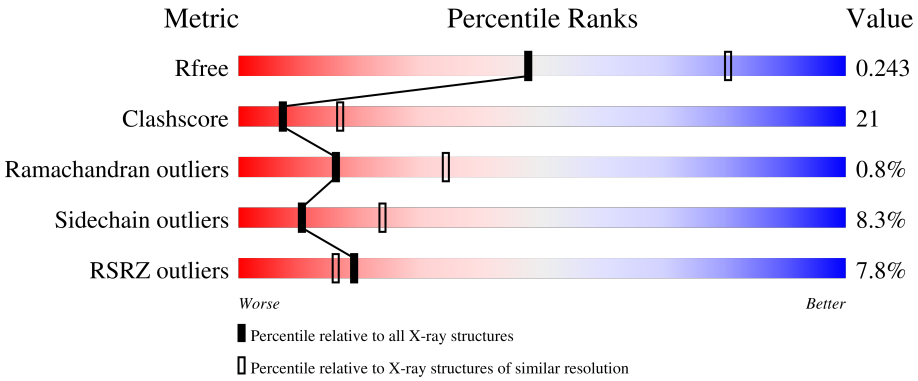
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.67 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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	871	4% 53% 20% · 24%
2	B	144	14% 53% 31% 9% 8%
3	C	7	86% 43% 43% 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6410 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 Lysine-specific histone demethylase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5217	3324	906	967	20			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP O60341
A	-17	SER	-	expression tag	UNP O60341
A	-16	SER	-	expression tag	UNP O60341
A	-15	HIS	-	expression tag	UNP O60341
A	-14	HIS	-	expression tag	UNP O60341
A	-13	HIS	-	expression tag	UNP O60341
A	-12	HIS	-	expression tag	UNP O60341
A	-11	HIS	-	expression tag	UNP O60341
A	-10	HIS	-	expression tag	UNP O60341
A	-9	SER	-	expression tag	UNP O60341
A	-8	SER	-	expression tag	UNP O60341
A	-7	GLY	-	expression tag	UNP O60341
A	-6	LEU	-	expression tag	UNP O60341
A	-5	VAL	-	expression tag	UNP O60341
A	-4	PRO	-	expression tag	UNP O60341
A	-3	ARG	-	expression tag	UNP O60341
A	-2	GLY	-	expression tag	UNP O60341
A	-1	SER	-	expression tag	UNP O60341
A	0	HIS	-	expression tag	UNP O60341

- Molecule 2 is a protein called REST corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

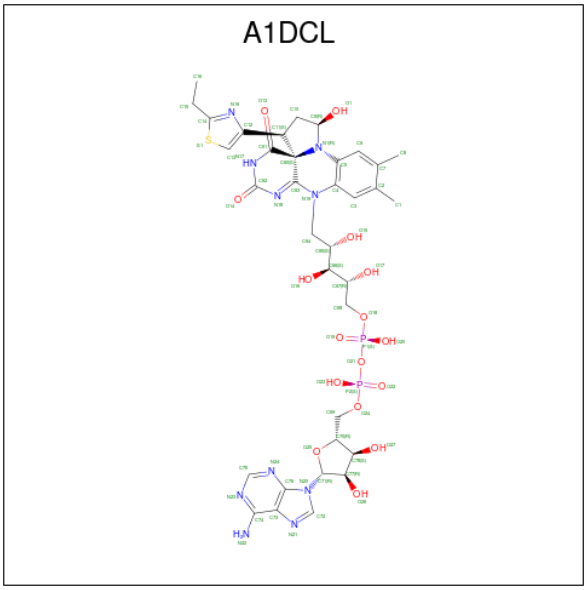
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	297	GLY	-	expression tag	UNP Q9UKL0
B	298	PRO	-	expression tag	UNP Q9UKL0
B	299	LEU	-	expression tag	UNP Q9UKL0
B	300	GLY	-	expression tag	UNP Q9UKL0
B	301	SER	-	expression tag	UNP Q9UKL0
B	302	PRO	-	expression tag	UNP Q9UKL0
B	303	GLU	-	expression tag	UNP Q9UKL0
B	304	PHE	-	expression tag	UNP Q9UKL0

- Molecule 3 is a protein called peptide PRCALVKSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	7	Total	C	N	O	S	0	0	0
			53	34	11	7	1			

- Molecule 4 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methyl (2R,3S,4S)-5-[(1R,3S,3aS,13R)-3-(2-ethyl-1,3-thiazol-4-yl)-1-hydroxy-10,11-dimethyl-4,6-dioxo-2,3,5,6-tetrahydro-1H-benzo[g]pyrrolo[2,1-e]pteridin-8(4H)-yl]-2,3,4-trihydroxypentyl dihydrogen diphosphate (non-preferred name) (CCD ID: A1DCL) (formula: $C_{35}H_{44}N_{10}O_{16}P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	S	0	0
			64	35	10	16	2	1		

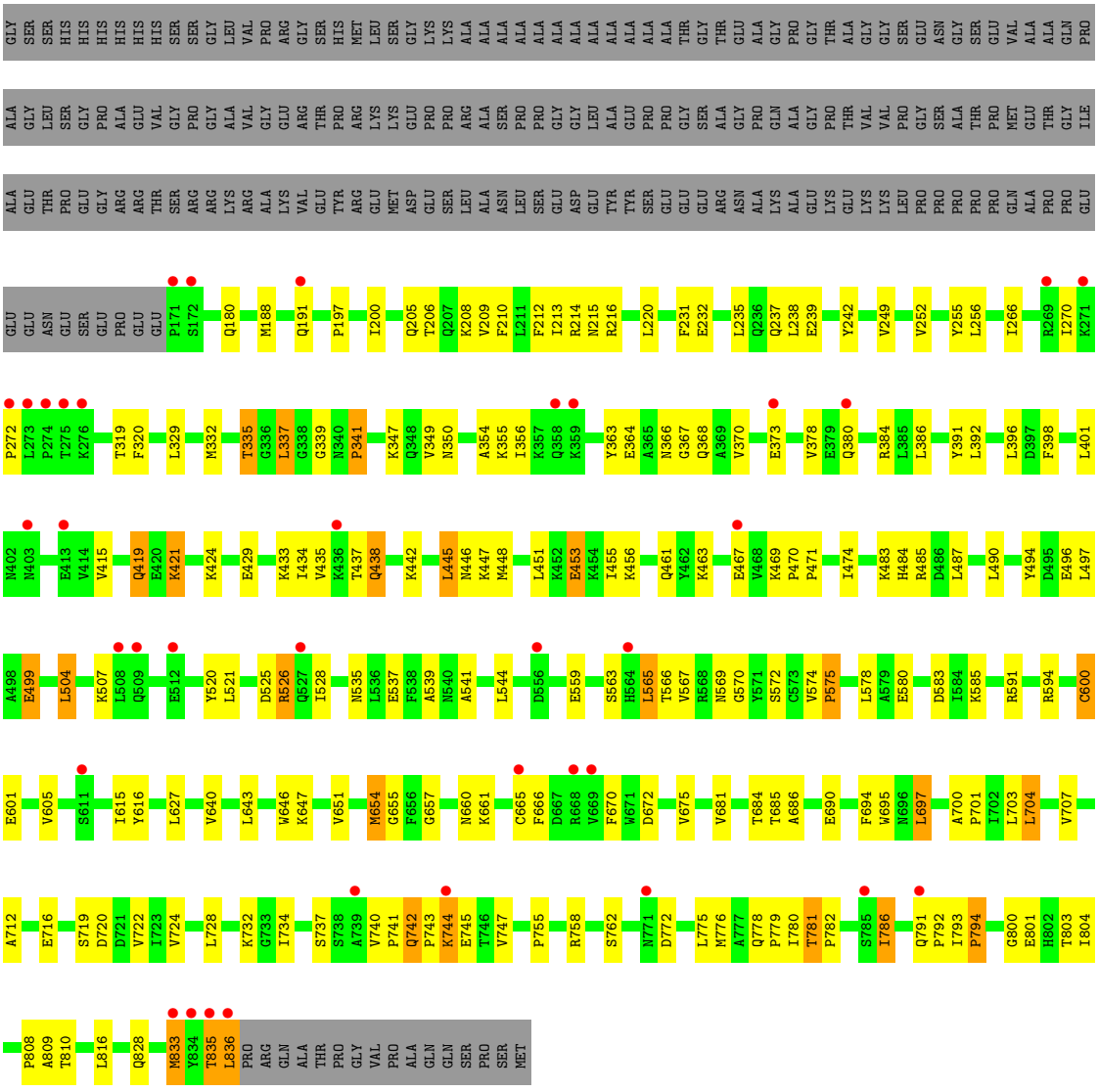
3 Residue-property plots (i)

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

• Molecule 1: Lysine-specific histone demethylase 1A

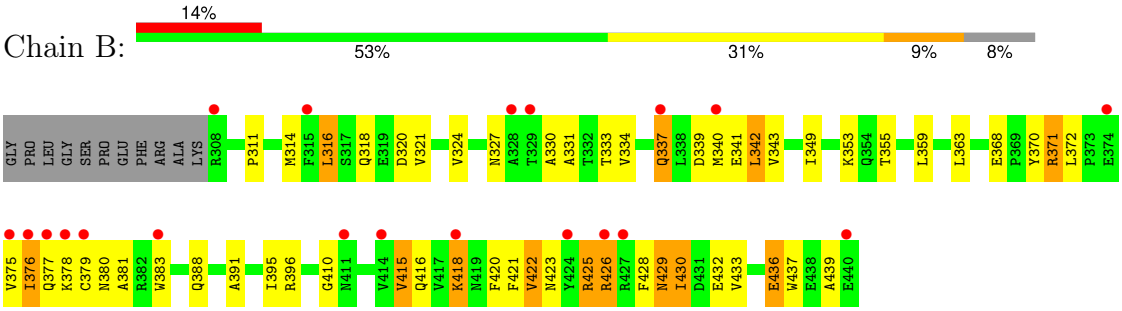
Chain A:





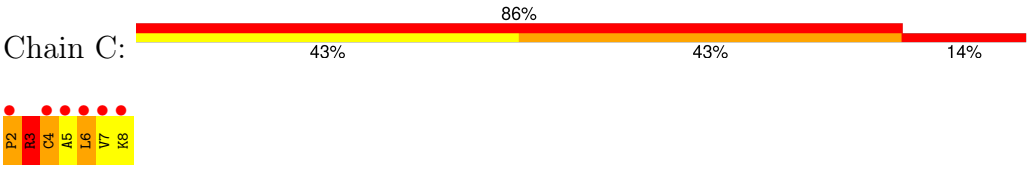
• Molecule 2: REST corepressor 1

Chain B:



• Molecule 3: peptide PRCALVKSK

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	118.87Å 180.49Å 234.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.81 – 2.67 48.81 – 2.67	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.81-2.67) 96.1 (48.81-2.67)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.220 , 0.248 0.225 , 0.243	Depositor DCC
R_{free} test set	2000 reflections (2.79%)	wwPDB-VP
Wilson B-factor (Å^2)	73.8	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6410	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1DCL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.91	8/5331 (0.2%)	1.01	4/7232 (0.1%)
2	B	0.68	0/1091	1.07	0/1471
3	C	0.73	0/53	1.50	0/69
All	All	0.88	8/6475 (0.1%)	1.03	4/8772 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	794	PRO	C-O	-5.78	1.17	1.23
1	A	575	PRO	C-O	-5.64	1.17	1.24
1	A	782	PRO	C-O	-5.54	1.17	1.23
1	A	779	PRO	C-O	-5.51	1.17	1.23
1	A	341	PRO	C-O	-5.43	1.16	1.24
1	A	804	ILE	C-O	-5.36	1.17	1.24
1	A	741	PRO	C-O	-5.07	1.17	1.23
1	A	349	VAL	C-O	-5.06	1.19	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	370	VAL	N-CA-C	-7.29	101.81	108.95
1	A	499	GLU	CB-CA-C	-6.44	101.05	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	335	THR	CA-CB-OG1	-5.51	101.34	109.60
1	A	800	GLY	CA-C-O	-5.21	118.57	122.37

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	3	ARG	Sidechain

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	5217	0	5252	194	0
2	B	1076	0	1091	79	0
3	C	53	0	63	19	0
4	C	64	0	0	0	0
All	All	6410	0	6406	264	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 21.

All (264) 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:383:TRP:CZ3	2:B:420:PHE:CD2	2.33	1.16
1:A:378:VAL:HG21	1:A:528:ILE:CG2	1.82	1.09
1:A:378:VAL:HG21	1:A:528:ILE:HG21	1.37	1.03
2:B:383:TRP:CZ3	2:B:420:PHE:CE2	2.48	1.00
1:A:446:ASN:OD1	2:B:359:LEU:HD21	1.62	0.99
1:A:793:ILE:HD12	1:A:793:ILE:H	1.29	0.96
2:B:383:TRP:CE3	2:B:420:PHE:CE2	2.57	0.92
2:B:371:ARG:HG3	2:B:371:ARG:HH11	1.36	0.90
2:B:425:ARG:HH11	2:B:425:ARG:HG2	1.35	0.90
2:B:383:TRP:CH2	2:B:420:PHE:CD2	2.62	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:ALA:HB1	1:A:701:PRO:HD2	1.53	0.88
1:A:438:GLN:HE21	1:A:438:GLN:HA	1.39	0.85
1:A:654:MET:CE	1:A:776:MET:HE2	2.08	0.84
1:A:378:VAL:HG21	1:A:528:ILE:HG22	1.61	0.83
2:B:383:TRP:CE3	2:B:420:PHE:CD2	2.69	0.81
1:A:535:ASN:HD21	3:C:7:VAL:H	1.30	0.80
2:B:429:ASN:HB3	2:B:432:GLU:HG3	1.64	0.79
1:A:654:MET:HE1	1:A:776:MET:HE2	1.65	0.79
1:A:836:LEU:HD12	1:A:836:LEU:H	1.47	0.78
2:B:425:ARG:HA	2:B:430:ILE:HD13	1.64	0.78
2:B:311:PRO:HG2	2:B:314:MET:HG3	1.64	0.78
2:B:416:GLN:OE1	2:B:416:GLN:N	2.16	0.76
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.68	0.75
1:A:337:LEU:N	1:A:337:LEU:HD22	2.02	0.75
1:A:559:GLU:HG3	3:C:4:CYS:HB3	1.69	0.75
1:A:355:LYS:HA	1:A:565:LEU:CD1	2.16	0.74
1:A:445:LEU:N	1:A:445:LEU:HD23	2.01	0.74
3:C:6:LEU:HD23	3:C:6:LEU:O	1.86	0.74
1:A:801:GLU:HG2	1:A:809:ALA:H	1.53	0.74
1:A:332:MET:HE2	1:A:661:LYS:NZ	2.02	0.73
1:A:392:LEU:CD2	1:A:398:PHE:HB3	2.18	0.73
2:B:341:GLU:HG3	2:B:341:GLU:O	1.88	0.73
1:A:504:LEU:N	1:A:504:LEU:HD23	2.03	0.72
3:C:6:LEU:HD23	3:C:6:LEU:C	2.15	0.71
1:A:836:LEU:HD12	1:A:836:LEU:N	2.06	0.71
1:A:695:TRP:HE3	1:A:697:LEU:HD21	1.55	0.71
1:A:392:LEU:HD23	1:A:392:LEU:O	1.91	0.71
1:A:438:GLN:HE21	1:A:438:GLN:CA	2.00	0.69
1:A:435:VAL:HG12	2:B:349:ILE:CG1	2.21	0.69
1:A:384:ARG:HB3	2:B:314:MET:HE3	1.74	0.69
1:A:654:MET:HE2	1:A:772:ASP:HB3	1.74	0.69
2:B:430:ILE:N	2:B:430:ILE:HD12	2.08	0.68
1:A:793:ILE:HD12	1:A:793:ILE:N	2.06	0.67
2:B:425:ARG:HG2	2:B:425:ARG:NH1	1.96	0.67
1:A:435:VAL:HG12	2:B:349:ILE:HG13	1.77	0.67
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.77	0.67
2:B:383:TRP:CE3	2:B:420:PHE:HE2	2.08	0.66
1:A:438:GLN:HA	1:A:438:GLN:NE2	2.10	0.66
2:B:377:GLN:HG2	2:B:410:GLY:O	1.95	0.66
1:A:209:VAL:O	1:A:213:ILE:HD12	1.96	0.66
1:A:424:LYS:HD3	2:B:339:ASP:OD2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:TYR:HD2	1:A:256:LEU:HD22	1.61	0.65
2:B:377:GLN:OE1	2:B:377:GLN:HA	1.96	0.65
2:B:377:GLN:HG2	2:B:410:GLY:C	2.22	0.65
1:A:539:ALA:HB2	3:C:6:LEU:HB3	1.79	0.65
1:A:654:MET:HE3	1:A:776:MET:HE2	1.78	0.65
1:A:591:ARG:HH21	1:A:605:VAL:HG21	1.62	0.65
1:A:216:ARG:O	1:A:220:LEU:HD12	1.97	0.64
1:A:320:PHE:HB2	1:A:329:LEU:HD11	1.79	0.64
1:A:833:MET:HA	1:A:833:MET:HE3	1.80	0.64
1:A:793:ILE:HG23	1:A:828:GLN:NE2	2.12	0.63
1:A:356:ILE:HD11	1:A:566:THR:CG2	2.27	0.63
2:B:426:ARG:CG	2:B:426:ARG:HH11	2.11	0.63
2:B:380:ASN:OD1	2:B:381:ALA:N	2.31	0.62
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.81	0.62
1:A:337:LEU:HD22	1:A:337:LEU:H	1.62	0.62
2:B:421:PHE:O	2:B:425:ARG:HB2	1.99	0.62
1:A:521:LEU:HD22	1:A:525:ASP:HB3	1.81	0.62
1:A:594:ARG:O	1:A:600:CYS:HB3	2.00	0.62
2:B:375:VAL:O	2:B:375:VAL:HG13	2.01	0.61
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.30	0.61
1:A:455:ILE:HD11	1:A:490:LEU:O	2.00	0.61
1:A:740:VAL:HG12	1:A:740:VAL:O	2.00	0.61
2:B:426:ARG:HH11	2:B:426:ARG:HG2	1.65	0.61
1:A:567:VAL:HG11	1:A:570:GLY:O	2.00	0.61
1:A:355:LYS:HG2	1:A:565:LEU:HD11	1.83	0.61
1:A:526:ARG:HH11	1:A:526:ARG:HG3	1.66	0.61
1:A:720:ASP:O	1:A:724:VAL:HG23	2.01	0.60
1:A:421:LYS:NZ	2:B:320:ASP:OD1	2.35	0.60
1:A:666:PHE:O	1:A:701:PRO:CG	2.49	0.59
3:C:7:VAL:HG12	3:C:7:VAL:O	2.02	0.59
1:A:755:PRO:HA	1:A:758:ARG:HE	1.67	0.59
1:A:794:PRO:HD2	1:A:828:GLN:OE1	2.03	0.59
2:B:371:ARG:HG3	2:B:371:ARG:NH1	2.11	0.59
2:B:376:ILE:HG12	2:B:376:ILE:O	1.99	0.59
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.68	0.58
1:A:793:ILE:H	1:A:793:ILE:CD1	2.01	0.58
2:B:318:GLN:O	2:B:321:VAL:HG22	2.03	0.58
2:B:379:CYS:SG	2:B:416:GLN:NE2	2.76	0.58
1:A:188:MET:HE1	1:A:200:ILE:HA	1.85	0.58
2:B:324:VAL:HG13	2:B:331:ALA:HB2	1.84	0.58
1:A:463:LYS:O	1:A:467:GLU:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:ARG:C	3:C:5:ALA:H	2.11	0.58
1:A:332:MET:CE	1:A:661:LYS:NZ	2.67	0.58
1:A:559:GLU:HG3	3:C:4:CYS:CB	2.35	0.57
1:A:366:ASN:OD1	1:A:367:GLY:N	2.37	0.57
1:A:435:VAL:HG12	2:B:349:ILE:HG12	1.85	0.57
1:A:793:ILE:HG23	1:A:828:GLN:CD	2.30	0.57
1:A:355:LYS:HA	1:A:565:LEU:HD13	1.87	0.57
1:A:666:PHE:O	1:A:701:PRO:HG2	2.03	0.57
1:A:398:PHE:CZ	1:A:401:LEU:HD12	2.39	0.57
1:A:651:VAL:HA	1:A:776:MET:HE1	1.87	0.56
3:C:6:LEU:CD2	3:C:6:LEU:H	2.18	0.56
2:B:342:LEU:O	2:B:342:LEU:HG	2.05	0.56
1:A:341:PRO:HG3	1:A:816:LEU:CD1	2.36	0.56
1:A:335:THR:HG23	1:A:335:THR:O	2.05	0.56
1:A:801:GLU:CG	1:A:809:ALA:HA	2.35	0.56
1:A:654:MET:CE	1:A:776:MET:CE	2.83	0.56
2:B:415:VAL:HG23	2:B:418:LYS:HD3	1.88	0.55
1:A:835:THR:O	1:A:835:THR:OG1	2.21	0.55
3:C:6:LEU:H	3:C:6:LEU:HD22	1.70	0.55
2:B:377:GLN:CG	2:B:410:GLY:O	2.54	0.55
1:A:456:LYS:HG3	2:B:370:TYR:CZ	2.42	0.55
1:A:808:PRO:O	1:A:810:THR:HG23	2.07	0.54
2:B:371:ARG:HH11	2:B:371:ARG:CG	2.13	0.54
2:B:430:ILE:HD12	2:B:430:ILE:H	1.72	0.54
1:A:180:GLN:HA	1:A:339:GLY:HA2	1.89	0.54
1:A:445:LEU:HB2	2:B:359:LEU:HD23	1.89	0.54
1:A:209:VAL:HG12	1:A:213:ILE:HD11	1.89	0.54
2:B:327:ASN:OD1	2:B:330:ALA:N	2.41	0.53
1:A:732:LYS:HD3	1:A:740:VAL:HB	1.89	0.53
1:A:646:TRP:CZ3	1:A:647:LYS:HE2	2.44	0.53
1:A:794:PRO:CD	1:A:828:GLN:OE1	2.57	0.53
1:A:319:THR:HB	1:A:572:SER:HB3	1.91	0.53
1:A:654:MET:HE1	1:A:776:MET:HG2	1.90	0.52
2:B:430:ILE:H	2:B:430:ILE:CD1	2.22	0.52
2:B:430:ILE:N	2:B:430:ILE:CD1	2.72	0.52
3:C:6:LEU:CD2	3:C:6:LEU:N	2.73	0.52
1:A:776:MET:HB3	1:A:803:THR:HG22	1.91	0.52
1:A:197:PRO:HA	1:A:200:ILE:HG22	1.92	0.52
1:A:655:GLY:O	1:A:762:SER:HB2	2.10	0.51
1:A:337:LEU:N	1:A:337:LEU:CD2	2.72	0.51
3:C:3:ARG:O	3:C:6:LEU:HD22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:436:GLU:HA	2:B:436:GLU:OE2	2.11	0.51
2:B:429:ASN:HD22	2:B:429:ASN:N	2.09	0.51
1:A:569:ASN:OD1	1:A:569:ASN:N	2.38	0.50
1:A:574:VAL:HB	1:A:575:PRO:CD	2.42	0.50
1:A:484:HIS:CD2	2:B:372:LEU:HD13	2.47	0.50
1:A:448:MET:CE	1:A:497:LEU:HB3	2.41	0.50
1:A:487:LEU:HD22	2:B:372:LEU:HG	1.94	0.50
1:A:341:PRO:HG3	1:A:816:LEU:HD13	1.93	0.50
1:A:684:THR:HG22	1:A:686:ALA:H	1.77	0.49
1:A:665:CYS:HB2	1:A:745:GLU:O	2.11	0.49
1:A:356:ILE:HD11	1:A:566:THR:HG22	1.92	0.49
1:A:319:THR:CB	1:A:572:SER:HB3	2.42	0.49
1:A:651:VAL:HG22	1:A:776:MET:HE1	1.93	0.49
2:B:371:ARG:NH1	2:B:371:ARG:CG	2.73	0.49
1:A:700:ALA:HB1	1:A:701:PRO:CD	2.34	0.49
1:A:661:LYS:HD3	1:A:704:LEU:CD2	2.42	0.48
3:C:3:ARG:C	3:C:5:ALA:N	2.71	0.48
1:A:526:ARG:HH11	1:A:526:ARG:CG	2.26	0.48
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.94	0.48
1:A:728:LEU:O	1:A:732:LYS:HG2	2.14	0.48
1:A:378:VAL:CG2	1:A:528:ILE:HG21	2.26	0.48
1:A:446:ASN:OD1	2:B:359:LEU:CD2	2.50	0.48
1:A:453:GLU:OE2	1:A:453:GLU:HA	2.12	0.48
1:A:742:GLN:OE1	1:A:742:GLN:HA	2.13	0.48
1:A:435:VAL:CG1	2:B:349:ILE:CG1	2.89	0.48
1:A:214:ARG:NH1	1:A:215:ASN:OD1	2.48	0.47
1:A:448:MET:HE2	1:A:497:LEU:HB3	1.96	0.47
1:A:496:GLU:O	1:A:499:GLU:HB2	2.15	0.47
1:A:732:LYS:HD2	1:A:737:SER:HA	1.96	0.47
1:A:188:MET:HE1	1:A:200:ILE:CA	2.43	0.47
1:A:448:MET:HB3	2:B:363:LEU:HD11	1.96	0.47
1:A:694:PHE:HA	1:A:704:LEU:O	2.15	0.47
1:A:438:GLN:OE1	2:B:353:LYS:HE3	2.14	0.47
1:A:205:GLN:O	1:A:208:LYS:N	2.47	0.47
1:A:469:LYS:HE2	1:A:469:LYS:HA	1.95	0.47
1:A:651:VAL:CG2	1:A:776:MET:HE1	2.45	0.47
1:A:654:MET:HE3	1:A:776:MET:CE	2.44	0.47
1:A:666:PHE:CE1	1:A:743:PRO:HB3	2.50	0.47
1:A:793:ILE:N	1:A:793:ILE:CD1	2.73	0.47
1:A:209:VAL:HG12	1:A:213:ILE:CD1	2.45	0.46
1:A:266:ILE:HD11	1:A:578:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:VAL:CG1	1:A:570:GLY:O	2.63	0.46
1:A:213:ILE:HG22	1:A:252:VAL:HG11	1.96	0.46
1:A:437:THR:HG21	1:A:507:LYS:HE2	1.97	0.46
2:B:337:GLN:N	2:B:337:GLN:OE1	2.49	0.46
2:B:383:TRP:CZ3	2:B:420:PHE:HD2	2.19	0.46
1:A:337:LEU:H	1:A:337:LEU:CD2	2.28	0.46
1:A:392:LEU:HD23	1:A:398:PHE:HB3	1.94	0.46
1:A:684:THR:HG22	1:A:685:THR:N	2.31	0.46
2:B:425:ARG:HH11	2:B:425:ARG:CG	2.15	0.45
1:A:354:ALA:C	1:A:565:LEU:HD12	2.41	0.45
1:A:535:ASN:ND2	3:C:6:LEU:HB2	2.31	0.45
1:A:627:LEU:HD21	1:A:654:MET:HB3	1.98	0.45
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.98	0.45
1:A:781:THR:O	1:A:781:THR:HG22	2.16	0.45
1:A:415:VAL:HG22	2:B:316:LEU:HD21	1.97	0.45
1:A:456:LYS:HG3	2:B:370:TYR:OH	2.17	0.45
1:A:583:ASP:OD1	1:A:585:LYS:NZ	2.47	0.45
2:B:383:TRP:CH2	2:B:420:PHE:HD2	2.27	0.45
2:B:426:ARG:CG	2:B:426:ARG:NH1	2.72	0.45
2:B:422:VAL:O	2:B:425:ARG:HB3	2.17	0.45
1:A:485:ARG:HD3	1:A:485:ARG:C	2.42	0.45
1:A:660:ASN:ND2	1:A:716:GLU:OE2	2.41	0.45
2:B:420:PHE:CD1	2:B:420:PHE:C	2.94	0.45
2:B:437:TRP:O	2:B:437:TRP:CG	2.70	0.45
3:C:2:PRO:O	3:C:2:PRO:HG2	2.17	0.45
1:A:801:GLU:HG3	1:A:809:ALA:CA	2.43	0.44
1:A:191:GLN:HG2	1:A:255:TYR:OH	2.18	0.44
1:A:332:MET:CE	1:A:661:LYS:HZ3	2.31	0.44
1:A:601:GLU:HA	1:A:616:TYR:O	2.17	0.44
1:A:363:TYR:HB3	1:A:734:ILE:HD12	2.00	0.44
2:B:368:GLU:OE2	2:B:371:ARG:NH1	2.42	0.44
1:A:438:GLN:OE1	2:B:353:LYS:HG2	2.17	0.44
1:A:419:GLN:HB3	1:A:520:TYR:CE1	2.53	0.43
1:A:707:VAL:HG12	1:A:712:ALA:HA	2.01	0.43
1:A:363:TYR:CD2	1:A:734:ILE:HG23	2.54	0.43
2:B:383:TRP:CE3	2:B:420:PHE:HD2	2.32	0.43
1:A:320:PHE:CD1	1:A:747:VAL:HG21	2.54	0.43
1:A:366:ASN:OD1	1:A:368:GLN:N	2.49	0.43
1:A:392:LEU:HD21	1:A:398:PHE:CD2	2.54	0.43
1:A:775:LEU:HD23	1:A:775:LEU:HA	1.71	0.43
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:PRO:HA	1:A:471:PRO:C	2.43	0.43
1:A:541:ALA:O	1:A:657:GLY:HA3	2.19	0.43
2:B:429:ASN:N	2:B:429:ASN:ND2	2.66	0.43
1:A:188:MET:HG2	1:A:210:PHE:HE2	1.83	0.43
1:A:232:GLU:CD	1:A:232:GLU:H	2.26	0.43
1:A:367:GLY:HA2	1:A:734:ILE:HD13	2.00	0.43
1:A:594:ARG:HA	1:A:640:VAL:O	2.19	0.43
1:A:445:LEU:CB	2:B:359:LEU:HD23	2.48	0.43
1:A:801:GLU:HG2	1:A:809:ALA:N	2.28	0.43
2:B:428:PHE:HB2	2:B:430:ILE:HD11	2.00	0.43
1:A:647:LYS:HE3	1:A:780:ILE:HD11	2.01	0.42
1:A:355:LYS:HA	1:A:565:LEU:HD12	1.99	0.42
1:A:535:ASN:HD21	3:C:7:VAL:N	2.07	0.42
1:A:672:ASP:O	1:A:675:VAL:HG22	2.18	0.42
1:A:786:ILE:H	1:A:786:ILE:HG13	1.67	0.42
1:A:474:ILE:HD12	1:A:474:ILE:HA	1.90	0.42
1:A:205:GLN:O	1:A:206:THR:C	2.63	0.42
1:A:419:GLN:NE2	2:B:314:MET:HA	2.35	0.42
1:A:654:MET:HE3	1:A:654:MET:HB2	1.68	0.42
2:B:395:ILE:HG22	2:B:433:VAL:CG1	2.49	0.42
1:A:654:MET:HE1	1:A:776:MET:CE	2.41	0.42
1:A:719:SER:OG	1:A:722:VAL:HG23	2.20	0.42
1:A:270:ILE:O	1:A:272:PRO:HD3	2.19	0.41
1:A:364:GLU:HA	1:A:681:VAL:HB	2.02	0.41
1:A:744:LYS:HA	1:A:744:LYS:HD2	1.94	0.41
1:A:670:PHE:CD1	1:A:670:PHE:C	2.98	0.41
2:B:426:ARG:HG2	2:B:426:ARG:H	1.58	0.41
1:A:666:PHE:O	1:A:701:PRO:HG3	2.21	0.41
2:B:368:GLU:CD	2:B:371:ARG:HH12	2.27	0.41
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.77	0.41
1:A:212:PHE:CE1	1:A:242:TYR:CD2	3.08	0.41
1:A:216:ARG:HG3	1:A:220:LEU:HD11	2.02	0.41
3:C:3:ARG:O	3:C:5:ALA:N	2.54	0.41
1:A:337:LEU:HD21	1:A:565:LEU:CD2	2.51	0.41
1:A:461:GLN:OE1	1:A:483:LYS:HE3	2.21	0.41
3:C:2:PRO:O	3:C:2:PRO:CG	2.69	0.41
1:A:329:LEU:HD21	1:A:747:VAL:CG1	2.51	0.40
1:A:497:LEU:N	1:A:497:LEU:CD1	2.84	0.40
1:A:537:GLU:CG	1:A:544:LEU:HG	2.51	0.40
1:A:643:LEU:HD23	1:A:643:LEU:HA	1.89	0.40
1:A:651:VAL:CA	1:A:776:MET:HE1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:GLN:O	2:B:391:ALA:HB3	2.22	0.40
3:C:2:PRO:O	3:C:3:ARG:CB	2.69	0.40
1:A:319:THR:OG1	1:A:572:SER:HB3	2.21	0.40
1:A:791:GLN:HA	1:A:792:PRO:HD3	1.91	0.40
1:A:188:MET:HG2	1:A:210:PHE:CE2	2.57	0.40
2:B:396:ARG:O	2:B:437:TRP:HD1	2.04	0.40
1:A:391:TYR:CE2	1:A:396:LEU:HD13	2.56	0.40
1:A:220:LEU:HD12	1:A:220:LEU:H	1.86	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	664/871 (76%)	628 (95%)	34 (5%)	2 (0%)	36 57
2	B	131/144 (91%)	121 (92%)	8 (6%)	2 (2%)	8 19
3	C	5/7 (71%)	2 (40%)	1 (20%)	2 (40%)	0 0
All	All	800/1022 (78%)	751 (94%)	43 (5%)	6 (1%)	16 34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	3	ARG
2	B	378	LYS
2	B	439	ALA
3	C	4	CYS
1	A	350	ASN
1	A	690	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	566/715 (79%)	530 (94%)	36 (6%)	16 35
2	B	117/125 (94%)	99 (85%)	18 (15%)	2 6
3	C	6/6 (100%)	3 (50%)	3 (50%)	0 0
All	All	689/846 (81%)	632 (92%)	57 (8%)	10 24

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	LEU
1	A	237	GLN
1	A	238	LEU
1	A	239	GLU
1	A	337	LEU
1	A	347	LYS
1	A	373	GLU
1	A	380	GLN
1	A	419	GLN
1	A	421	LYS
1	A	429	GLU
1	A	433	LYS
1	A	434	ILE
1	A	438	GLN
1	A	445	LEU
1	A	447	LYS
1	A	453	GLU
1	A	504	LEU
1	A	526	ARG
1	A	563	SER
1	A	565	LEU
1	A	580	GLU
1	A	600	CYS
1	A	615	ILE
1	A	654	MET
1	A	697	LEU

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Mol	Chain	Res	Type
1	A	703	LEU
1	A	704	LEU
1	A	742	GLN
1	A	744	LYS
1	A	778	GLN
1	A	781	THR
1	A	786	ILE
1	A	833	MET
1	A	835	THR
1	A	836	LEU
2	B	316	LEU
2	B	333	THR
2	B	334	VAL
2	B	337	GLN
2	B	340	MET
2	B	342	LEU
2	B	343	VAL
2	B	371	ARG
2	B	376	ILE
2	B	415	VAL
2	B	418	LYS
2	B	422	VAL
2	B	423	ASN
2	B	425	ARG
2	B	426	ARG
2	B	429	ASN
2	B	430	ILE
2	B	436	GLU
3	C	2	PRO
3	C	6	LEU
3	C	8	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	GLN
1	A	298	GLN
1	A	324	ASN
1	A	399	ASN
1	A	438	GLN
1	A	484	HIS
1	A	535	ASN

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Mol	Chain	Res	Type
1	A	564	HIS
1	A	638	GLN
1	A	778	GLN
2	B	429	ASN
2	B	435	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 oligosaccharides 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	$\#\|Z\| > 2$
4	A1DCL	C	101	3	68,71,71	1.71	14 (20%)	89,111,111	1.25	5 (5%)

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
4	A1DCL	C	101	3	-	4/37/108/108	0/7/8/8

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	101	A1DCL	C12-N16	-6.75	1.27	1.38
4	C	101	A1DCL	C16-C15	-3.70	1.35	1.51
4	C	101	A1DCL	P2-O21	-3.37	1.55	1.59
4	C	101	A1DCL	C61-N17	-3.36	1.32	1.37
4	C	101	A1DCL	P1-O21	-3.29	1.55	1.59
4	C	101	A1DCL	C62-N18	-3.21	1.29	1.36
4	C	101	A1DCL	O15-C65	-2.88	1.37	1.43
4	C	101	A1DCL	C5-N1	-2.48	1.36	1.41
4	C	101	A1DCL	O16-C66	-2.31	1.37	1.43
4	C	101	A1DCL	O14-C62	-2.27	1.19	1.24
4	C	101	A1DCL	C15-C14	-2.21	1.44	1.51
4	C	101	A1DCL	C63-N19	-2.19	1.33	1.38
4	C	101	A1DCL	P1-O20	-2.18	1.45	1.55
4	C	101	A1DCL	P2-O23	-2.17	1.45	1.55

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	101	A1DCL	C12-C13-S1	-5.75	107.48	111.32
4	C	101	A1DCL	C5-N1-C9	-5.21	111.97	123.92
4	C	101	A1DCL	C61-C60-C63	-3.50	107.18	113.40
4	C	101	A1DCL	C61-N17-C62	-3.10	120.74	125.42
4	C	101	A1DCL	C13-S1-C14	-2.86	86.48	89.59

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	101	A1DCL	C69-O24-P2-O23
4	C	101	A1DCL	C69-O24-P2-O21
4	C	101	A1DCL	C69-O24-P2-O22
4	C	101	A1DCL	C10-C11-C12-C13

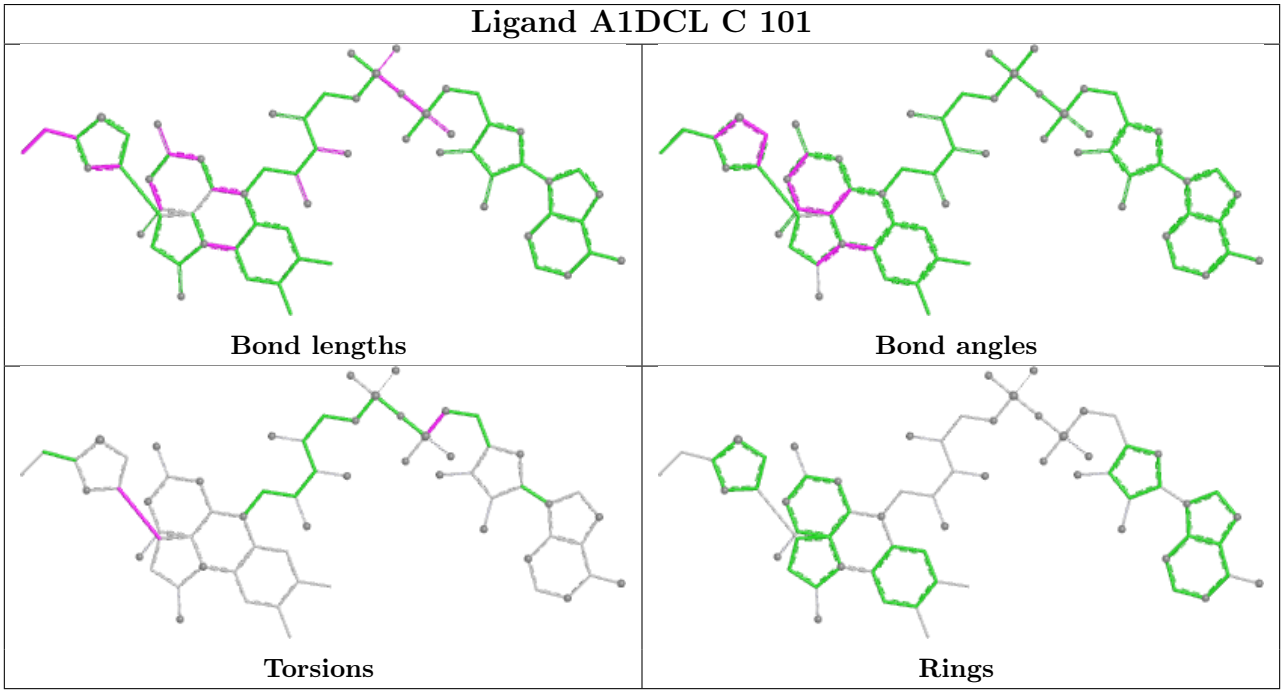
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand A1DCL C 101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	666/871 (76%)	0.42	37 (5%) 30 26	30, 79, 112, 135	0
2	B	133/144 (92%)	1.08	20 (15%) 5 4	75, 110, 133, 146	0
3	C	7/7 (100%)	3.08	6 (85%) 0 0	91, 94, 104, 108	0
All	All	806/1022 (78%)	0.55	63 (7%) 19 16	30, 86, 121, 146	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	836	LEU	8.5
3	C	8	LYS	6.8
1	A	171	PRO	6.0
1	A	835	THR	5.1
2	B	375	VAL	4.2
1	A	509	GLN	4.2
1	A	275	THR	4.1
2	B	376	ILE	4.0
1	A	508	LEU	3.3
2	B	308	ARG	3.3
1	A	833	MET	3.2
1	A	669	VAL	3.2
1	A	172	SER	3.2
3	C	4	CYS	3.1
1	A	564	HIS	3.1
1	A	358	GLN	3.0
2	B	328	ALA	3.0
1	A	611	SER	2.9
1	A	771	ASN	2.9
1	A	191	GLN	2.9
1	A	269	ARG	2.8
2	B	378	LYS	2.8
3	C	7	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	340	MET	2.7
1	A	739	ALA	2.7
2	B	426	ARG	2.7
1	A	512	GLU	2.7
2	B	379	CYS	2.6
1	A	668	ARG	2.6
2	B	414	VAL	2.6
3	C	5	ALA	2.5
1	A	276	LYS	2.5
3	C	2	PRO	2.5
1	A	834	TYR	2.5
1	A	744	LYS	2.4
2	B	383	TRP	2.4
1	A	791	GLN	2.4
1	A	665	CYS	2.3
2	B	329	THR	2.3
1	A	436	LYS	2.3
1	A	271	LYS	2.3
1	A	380	GLN	2.3
1	A	403	ASN	2.3
1	A	273	LEU	2.3
2	B	440	GLU	2.2
1	A	527	GLN	2.2
1	A	556	ASP	2.2
3	C	6	LEU	2.2
2	B	374	GLU	2.2
2	B	337	GLN	2.2
1	A	359	LYS	2.2
2	B	418	LYS	2.1
2	B	424	TYR	2.1
1	A	785	SER	2.1
2	B	377	GLN	2.1
1	A	413	GLU	2.1
1	A	272	PRO	2.1
1	A	274	PRO	2.1
2	B	315	PHE	2.1
2	B	411	ASN	2.0
2	B	427	ARG	2.0
1	A	373	GLU	2.0
1	A	467	GLU	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 oligosaccharides in this entry.

6.4 Ligands (i)

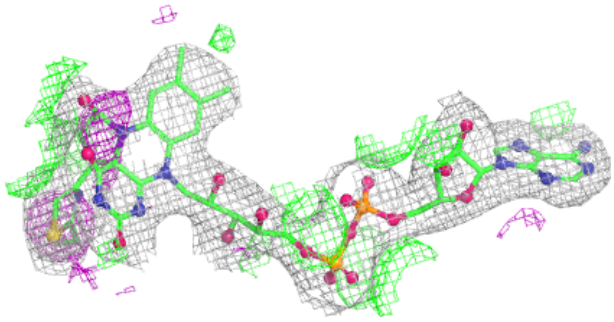
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

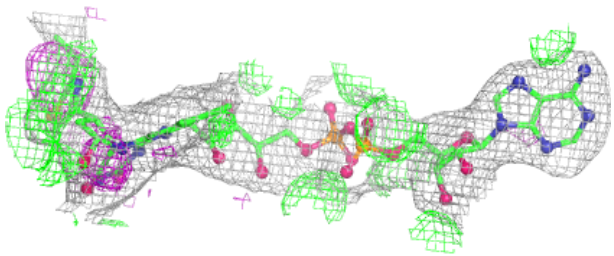
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	A1DCL	C	101	64/64	0.95	0.09	48,61,86,98	0

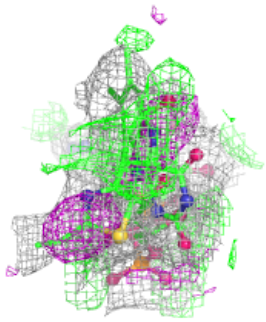
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1DCL C 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.