Full wwPDB X-ray Structure Validation Report (i)

May 19, 2025 – 04:55 pm BST

PDB ID	:	9HJG / pdb_00009hjg
Title	:	Crystal structure of human CD73 (ecto-5'-nucleotidase) in complex with an N6-disubstituted acyclic ADP analog (compound 26 in publication) in the closed state
Authors	:	Strater, N.; Moschuetz, S.; Federico, S.; Renn, C.; Muller, C.E.
Deposited on	:	2024-11-29
Resolution	:	2.31 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:

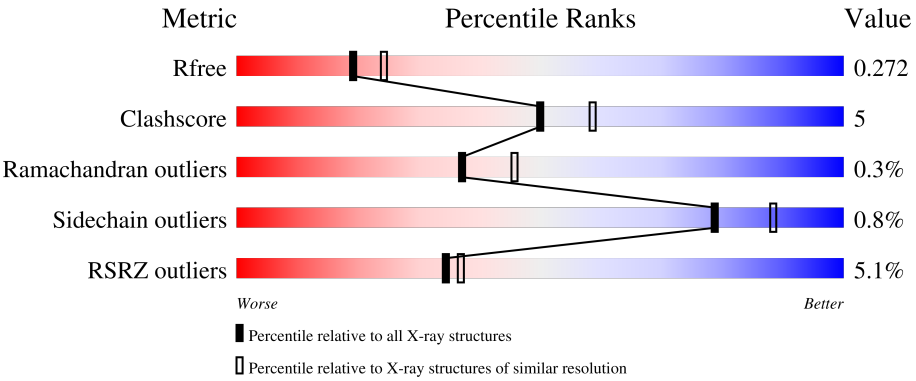
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.31 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}	164625	7250 (2.34-2.30)
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)
RSRZ outliers	164620	7250 (2.34-2.30)

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	547	6% 84% 11% 5%
1	B	547	3% 85% 10% 5%
1	C	547	5% 84% 11% .
1	D	547	5% 83% 11% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 32727 atoms, of which 16302 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 5'-nucleotidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	520	Total	C	H	N	O	S	0	0	0
			8110	2586	4047	691	767	19			
1	B	520	Total	C	H	N	O	S	0	0	0
			8099	2582	4041	692	766	18			
1	C	523	Total	C	H	N	O	S	0	1	0
			8168	2607	4071	697	774	19			
1	D	520	Total	C	H	N	O	S	0	1	0
			8115	2586	4051	691	768	19			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ASP	ASN	conflict	UNP P21589
A	311	ASP	ASN	conflict	UNP P21589
A	333	ASP	ASN	conflict	UNP P21589
A	403	ASP	ASN	conflict	UNP P21589
A	550	GLY	-	expression tag	UNP P21589
A	551	GLY	-	expression tag	UNP P21589
A	552	GLY	-	expression tag	UNP P21589
A	553	GLY	-	expression tag	UNP P21589
A	554	ALA	-	expression tag	UNP P21589
A	555	GLY	-	expression tag	UNP P21589
A	556	GLY	-	expression tag	UNP P21589
A	557	GLY	-	expression tag	UNP P21589
A	558	GLY	-	expression tag	UNP P21589
A	559	GLY	-	expression tag	UNP P21589
A	560	THR	-	expression tag	UNP P21589
A	561	ASP	-	expression tag	UNP P21589
A	562	ASP	-	expression tag	UNP P21589
A	563	ASP	-	expression tag	UNP P21589
A	564	ASP	-	expression tag	UNP P21589
A	565	LYS	-	expression tag	UNP P21589
A	566	TRP	-	expression tag	UNP P21589

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Chain	Residue	Modelled	Actual	Comment	Reference
A	567	SER	-	expression tag	UNP P21589
A	568	HIS	-	expression tag	UNP P21589
A	569	PRO	-	expression tag	UNP P21589
A	570	GLN	-	expression tag	UNP P21589
A	571	PHE	-	expression tag	UNP P21589
A	572	GLU	-	expression tag	UNP P21589
A	573	LYS	-	expression tag	UNP P21589
B	53	ASP	ASN	conflict	UNP P21589
B	311	ASP	ASN	conflict	UNP P21589
B	333	ASP	ASN	conflict	UNP P21589
B	403	ASP	ASN	conflict	UNP P21589
B	550	GLY	-	expression tag	UNP P21589
B	551	GLY	-	expression tag	UNP P21589
B	552	GLY	-	expression tag	UNP P21589
B	553	GLY	-	expression tag	UNP P21589
B	554	ALA	-	expression tag	UNP P21589
B	555	GLY	-	expression tag	UNP P21589
B	556	GLY	-	expression tag	UNP P21589
B	557	GLY	-	expression tag	UNP P21589
B	558	GLY	-	expression tag	UNP P21589
B	559	GLY	-	expression tag	UNP P21589
B	560	THR	-	expression tag	UNP P21589
B	561	ASP	-	expression tag	UNP P21589
B	562	ASP	-	expression tag	UNP P21589
B	563	ASP	-	expression tag	UNP P21589
B	564	ASP	-	expression tag	UNP P21589
B	565	LYS	-	expression tag	UNP P21589
B	566	TRP	-	expression tag	UNP P21589
B	567	SER	-	expression tag	UNP P21589
B	568	HIS	-	expression tag	UNP P21589
B	569	PRO	-	expression tag	UNP P21589
B	570	GLN	-	expression tag	UNP P21589
B	571	PHE	-	expression tag	UNP P21589
B	572	GLU	-	expression tag	UNP P21589
B	573	LYS	-	expression tag	UNP P21589
C	53	ASP	ASN	conflict	UNP P21589
C	311	ASP	ASN	conflict	UNP P21589
C	333	ASP	ASN	conflict	UNP P21589
C	403	ASP	ASN	conflict	UNP P21589
C	550	GLY	-	expression tag	UNP P21589
C	551	GLY	-	expression tag	UNP P21589
C	552	GLY	-	expression tag	UNP P21589

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Chain	Residue	Modelled	Actual	Comment	Reference
C	553	GLY	-	expression tag	UNP P21589
C	554	ALA	-	expression tag	UNP P21589
C	555	GLY	-	expression tag	UNP P21589
C	556	GLY	-	expression tag	UNP P21589
C	557	GLY	-	expression tag	UNP P21589
C	558	GLY	-	expression tag	UNP P21589
C	559	GLY	-	expression tag	UNP P21589
C	560	THR	-	expression tag	UNP P21589
C	561	ASP	-	expression tag	UNP P21589
C	562	ASP	-	expression tag	UNP P21589
C	563	ASP	-	expression tag	UNP P21589
C	564	ASP	-	expression tag	UNP P21589
C	565	LYS	-	expression tag	UNP P21589
C	566	TRP	-	expression tag	UNP P21589
C	567	SER	-	expression tag	UNP P21589
C	568	HIS	-	expression tag	UNP P21589
C	569	PRO	-	expression tag	UNP P21589
C	570	GLN	-	expression tag	UNP P21589
C	571	PHE	-	expression tag	UNP P21589
C	572	GLU	-	expression tag	UNP P21589
C	573	LYS	-	expression tag	UNP P21589
D	53	ASP	ASN	conflict	UNP P21589
D	311	ASP	ASN	conflict	UNP P21589
D	333	ASP	ASN	conflict	UNP P21589
D	403	ASP	ASN	conflict	UNP P21589
D	550	GLY	-	expression tag	UNP P21589
D	551	GLY	-	expression tag	UNP P21589
D	552	GLY	-	expression tag	UNP P21589
D	553	GLY	-	expression tag	UNP P21589
D	554	ALA	-	expression tag	UNP P21589
D	555	GLY	-	expression tag	UNP P21589
D	556	GLY	-	expression tag	UNP P21589
D	557	GLY	-	expression tag	UNP P21589
D	558	GLY	-	expression tag	UNP P21589
D	559	GLY	-	expression tag	UNP P21589
D	560	THR	-	expression tag	UNP P21589
D	561	ASP	-	expression tag	UNP P21589
D	562	ASP	-	expression tag	UNP P21589
D	563	ASP	-	expression tag	UNP P21589
D	564	ASP	-	expression tag	UNP P21589
D	565	LYS	-	expression tag	UNP P21589
D	566	TRP	-	expression tag	UNP P21589

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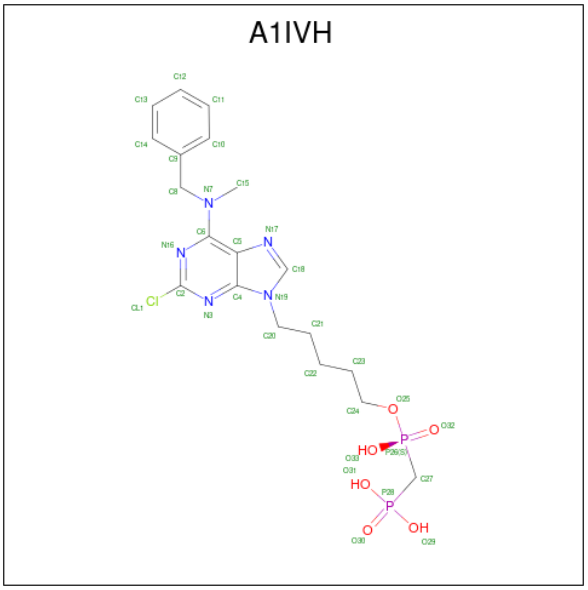
Chain	Residue	Modelled	Actual	Comment	Reference
D	567	SER	-	expression tag	UNP P21589
D	568	HIS	-	expression tag	UNP P21589
D	569	PRO	-	expression tag	UNP P21589
D	570	GLN	-	expression tag	UNP P21589
D	571	PHE	-	expression tag	UNP P21589
D	572	GLU	-	expression tag	UNP P21589
D	573	LYS	-	expression tag	UNP P21589

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0

- Molecule 3 is [5-[2-chloranyl-6-[methyl-(phenylmethyl)amino]purin-9-yl]pentoxy-oxidanyl-phosphoryl]methylphosphonic acid (CCD ID: A1IVH) (formula: $C_{19}H_{26}ClN_5O_6P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	H	N	O	P	0	0
			56	19	1	23	5	6	2		
3	B	1	Total	C	Cl	H	N	O	P	0	0
			56	19	1	23	5	6	2		
3	C	1	Total	C	Cl	H	N	O	P	0	0
			56	19	1	23	5	6	2		
3	D	1	Total	C	Cl	H	N	O	P	0	0
			56	19	1	23	5	6	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

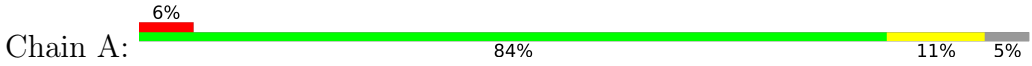
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Ca	0	0
			1	1		

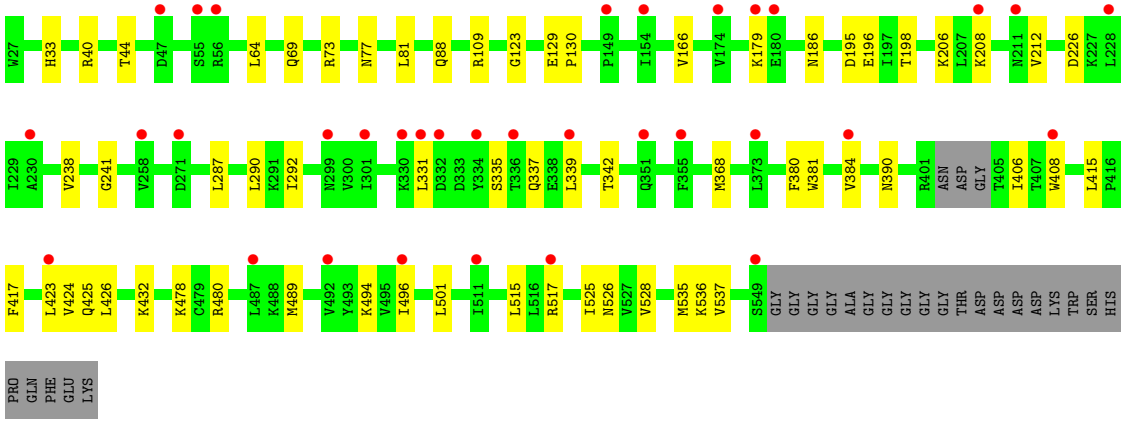
3 Residue-property plots (i)

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: 5'-nucleotidase

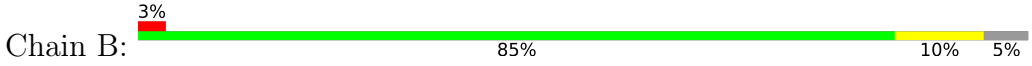
Chain A:

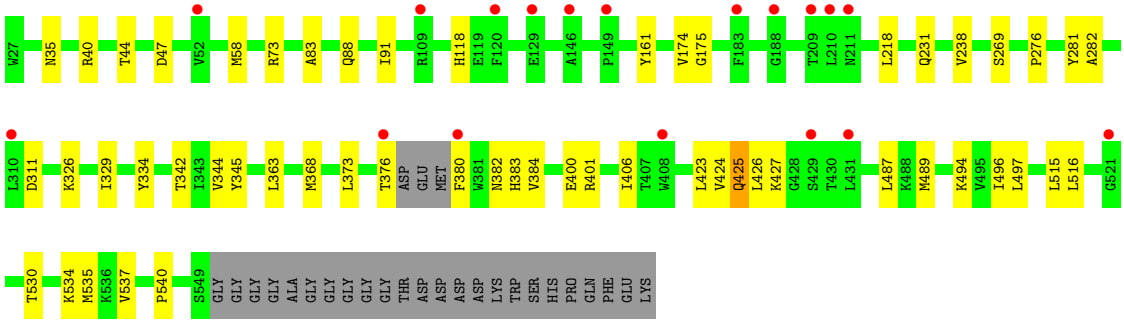




• Molecule 1: 5'-nucleotidase

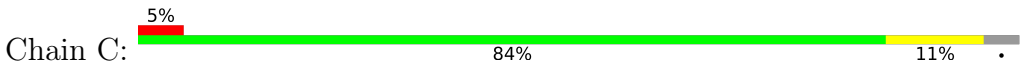
Chain B:

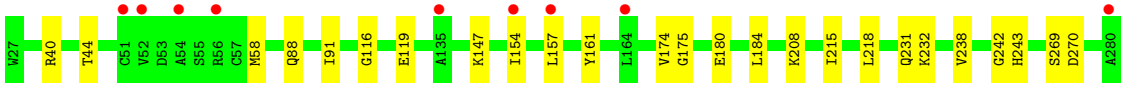


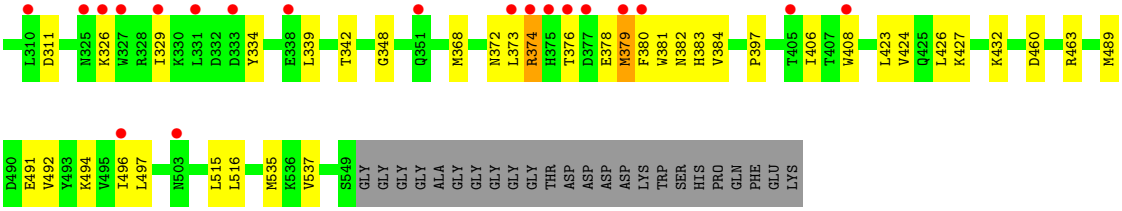


• Molecule 1: 5'-nucleotidase

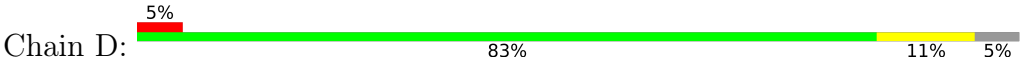
Chain C:

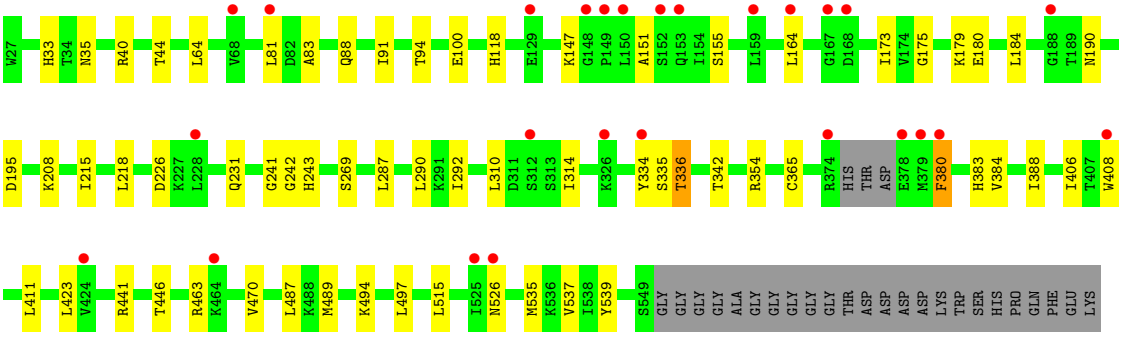






• Molecule 1: 5'-nucleotidase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.59Å 84.55Å 124.67Å 90.00° 102.62° 90.00°	Depositor
Resolution (Å)	121.66 – 2.31 121.66 – 2.31	Depositor EDS
% Data completeness (in resolution range)	44.1 (121.66-2.31) 44.1 (121.66-2.31)	Depositor EDS
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.32Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.237 , 0.271 0.237 , 0.272	Depositor DCC
R_{free} test set	4196 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 0.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	32727	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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 25.02 % 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 3.4297e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CA, A1IVH, ZN, CL

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	0/4148	0.46	1/5616 (0.0%)
1	B	0.27	0/4143	0.44	0/5610
1	C	0.27	0/4185	0.45	0/5669
1	D	0.27	0/4151	0.44	0/5619
All	All	0.27	0/16627	0.45	1/22514 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	206	LYS	CG-CD-CE	5.35	123.60	111.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4063	4047	4045	44	0
1	B	4058	4041	4039	34	1
1	C	4097	4071	4068	59	1
1	D	4064	4051	4048	44	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	33	23	0	2	0
3	B	33	23	0	2	0
3	C	33	23	0	1	0
3	D	33	23	0	4	0
4	A	1	0	0	1	0
4	C	1	0	0	0	0
5	C	1	0	0	0	0
All	All	16425	16302	16200	168	1

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 5.

All (168) 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:373:LEU:O	1:C:376:THR:HG23	1.07	1.24
1:C:376:THR:HG22	1:C:382:ASN:OD1	1.12	1.22
1:C:376:THR:CG2	1:C:382:ASN:OD1	1.92	1.16
1:C:373:LEU:O	1:C:376:THR:CG2	2.00	1.08
1:A:331:LEU:O	1:A:335:SER:OG	1.99	0.80
1:C:373:LEU:C	1:C:376:THR:HG23	2.07	0.77
1:A:109:ARG:NH2	4:A:604:CL:CL	2.56	0.76
1:B:373:LEU:HD23	1:B:382:ASN:ND2	2.00	0.75
1:A:408:TRP:NE1	1:C:329:ILE:HG22	2.02	0.73
1:D:118:HIS:NE2	3:D:603:A1IVH:O30	2.25	0.69
1:A:408:TRP:HE1	1:C:329:ILE:HG22	1.58	0.68
1:B:118:HIS:NE2	3:B:603:A1IVH:O31	2.28	0.67
1:D:40:ARG:HG3	1:D:44:THR:HG21	1.76	0.67
1:C:384:VAL:HG11	1:C:423:LEU:HD13	1.78	0.66
1:B:530:THR:HG22	1:B:534:LYS:HE3	1.79	0.65
1:C:382:ASN:ND2	1:C:384:VAL:O	2.30	0.65
1:C:384:VAL:HG12	1:C:494:LYS:HB3	1.78	0.65
1:D:384:VAL:HG11	1:D:423:LEU:HD13	1.78	0.65
1:D:354:ARG:NH1	3:D:603:A1IVH:O33	2.27	0.64
1:A:342:THR:HB	1:A:406:ILE:HD11	1.80	0.64
1:A:381:TRP:HB2	1:B:344:VAL:HG12	1.80	0.63
1:C:373:LEU:HD23	1:C:382:ASN:ND2	2.14	0.63
1:B:329:ILE:HG12	1:D:526:ASN:OD1	1.97	0.63
1:D:91:ILE:HD11	1:D:408:TRP:CZ3	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:THR:HB	1:B:406:ILE:HD11	1.80	0.62
1:D:118:HIS:CD2	3:D:603:A1IVH:O30	2.53	0.62
1:A:129:GLU:HB2	1:A:130:PRO:HD3	1.83	0.61
1:C:339:LEU:HD21	1:C:408[B]:TRP:NE1	2.16	0.61
1:D:342:THR:HB	1:D:406:ILE:HD11	1.83	0.60
1:C:535:MET:HE1	1:D:535:MET:HE1	1.84	0.59
1:B:384:VAL:HG12	1:B:494:LYS:HB3	1.84	0.59
1:D:487:LEU:HD23	1:D:489:MET:HE1	1.85	0.59
1:C:40:ARG:HG3	1:C:44:THR:HG21	1.83	0.58
1:B:384:VAL:HG11	1:B:423:LEU:HD13	1.85	0.58
1:C:342:THR:HB	1:C:406:ILE:HD11	1.85	0.58
1:A:69:GLN:O	1:A:73:ARG:HG2	2.03	0.58
1:D:179:LYS:NZ	1:D:195:ASP:OD1	2.28	0.58
1:D:64:LEU:HD11	1:D:287:LEU:HD13	1.87	0.56
1:C:232:LYS:HD3	1:C:270:ASP:OD2	2.05	0.56
1:C:380:PHE:O	1:C:382:ASN:N	2.31	0.56
1:D:35:ASN:HB3	1:D:83:ALA:HB3	1.89	0.55
1:B:427:LYS:HG3	1:B:516:LEU:HD11	1.90	0.54
1:B:487:LEU:HD23	1:B:489:MET:HE1	1.89	0.54
1:C:383:HIS:CD2	1:C:384:VAL:HG13	2.41	0.54
1:C:432:LYS:HB3	1:C:489:MET:HE1	1.89	0.54
1:C:208:LYS:HE3	1:C:215:ILE:HD12	1.89	0.54
1:B:175:GLY:HA2	1:B:218:LEU:O	2.08	0.54
1:D:384:VAL:HG12	1:D:494:LYS:HB3	1.89	0.53
1:B:424:VAL:HG12	1:B:426:LEU:HG	1.91	0.52
1:C:368:MET:HE2	1:C:496:ILE:HG22	1.90	0.52
1:A:186:ASN:HB2	3:A:603:A1IVH:C13	2.40	0.52
1:C:372:ASN:O	1:C:373:LEU:C	2.52	0.52
1:B:40:ARG:HG3	1:B:44:THR:HG21	1.92	0.52
1:B:91:ILE:HD11	1:B:334:TYR:CD2	2.45	0.52
1:B:161:TYR:HB3	1:B:174:VAL:HG12	1.91	0.52
1:C:339:LEU:HD21	1:C:408[B]:TRP:CE2	2.45	0.51
1:A:195:ASP:HB3	1:A:198:THR:HB	1.93	0.51
1:A:339:LEU:HD21	1:A:408:TRP:CZ3	2.46	0.51
3:C:603:A1IVH:O32	3:C:603:A1IVH:C23	2.59	0.51
1:D:208:LYS:HE3	1:D:215:ILE:HD12	1.93	0.51
1:C:373:LEU:HA	1:C:382:ASN:OD1	2.11	0.51
1:C:91:ILE:HD11	1:C:334:TYR:CD2	2.46	0.51
1:A:515:LEU:C	1:A:515:LEU:HD12	2.36	0.50
1:A:64:LEU:HD11	1:A:287:LEU:HD13	1.93	0.50
1:A:339:LEU:HD21	1:A:408:TRP:CH2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ALA:O	1:D:155:SER:HB2	2.11	0.50
1:A:417:PHE:HB3	3:A:603:A1IVH:C15	2.42	0.50
1:C:175:GLY:HA2	1:C:218:LEU:O	2.12	0.50
1:A:515:LEU:HD12	1:A:515:LEU:O	2.11	0.50
1:A:424:VAL:HG12	1:A:426:LEU:HG	1.94	0.49
1:A:526:ASN:OD1	1:C:329:ILE:HG12	2.13	0.49
1:C:373:LEU:O	1:C:374:ARG:C	2.56	0.49
1:A:480:ARG:NE	1:B:400:GLU:OE2	2.41	0.48
1:C:373:LEU:HD11	1:D:539:TYR:CE1	2.47	0.48
1:A:425:GLN:HB2	1:A:517:ARG:HB3	1.94	0.48
1:D:226:ASP:OD2	1:D:241:GLY:HA3	2.14	0.48
1:A:423:LEU:HD11	1:A:494:LYS:HB3	1.95	0.47
1:A:408:TRP:CE2	1:C:329:ILE:O	2.68	0.47
1:C:380:PHE:C	1:C:382:ASN:H	2.22	0.47
1:B:515:LEU:HD12	1:B:515:LEU:C	2.40	0.47
1:B:47:ASP:OD2	1:B:345:TYR:OH	2.32	0.47
1:D:388:ILE:HD11	1:D:497:LEU:HD23	1.97	0.46
1:A:33:HIS:HA	1:A:81:LEU:O	2.16	0.46
1:A:408:TRP:CD1	1:C:329:ILE:HG22	2.50	0.46
1:D:335:SER:O	1:D:336:THR:CB	2.63	0.46
1:C:424:VAL:HG12	1:C:426:LEU:HG	1.98	0.46
1:D:383:HIS:CD2	1:D:384:VAL:HG13	2.51	0.46
1:A:432:LYS:HB2	1:A:489:MET:HE1	1.97	0.46
1:C:535:MET:O	1:C:537:VAL:N	2.46	0.46
1:D:164:LEU:HD13	1:D:173:ILE:HD12	1.98	0.46
1:D:423:LEU:HD11	1:D:494:LYS:HB3	1.97	0.46
1:C:380:PHE:O	1:C:381:TRP:CD1	2.69	0.46
1:A:208:LYS:HD3	1:A:212:VAL:O	2.16	0.46
1:C:380:PHE:C	1:C:382:ASN:N	2.74	0.46
1:A:535:MET:HE1	1:B:535:MET:HE1	1.98	0.45
1:B:535:MET:O	1:B:537:VAL:N	2.44	0.45
1:D:100:GLU:OE1	1:D:100:GLU:N	2.44	0.45
1:C:491:GLU:HG2	1:C:492:VAL:H	1.82	0.45
1:D:231:GLN:HA	1:D:269:SER:HA	1.99	0.45
1:B:58:MET:HG2	1:B:311:ASP:HA	1.99	0.45
1:C:515:LEU:HD12	1:C:515:LEU:C	2.41	0.45
1:A:535:MET:O	1:A:537:VAL:N	2.44	0.45
1:A:77:ASN:HB3	1:A:166:VAL:HG12	1.98	0.44
1:A:368:MET:HE2	1:A:496:ILE:HG22	1.99	0.44
3:B:603:A1IVH:C23	3:B:603:A1IVH:O32	2.64	0.44
1:C:372:ASN:O	1:C:383:HIS:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ASP:OD2	1:A:241:GLY:HA3	2.18	0.44
1:A:179:LYS:CE	1:A:196:GLU:OE1	2.66	0.44
1:B:329:ILE:HG21	1:D:408:TRP:CD1	2.53	0.44
1:C:432:LYS:CB	1:C:489:MET:HE1	2.46	0.44
1:B:368:MET:HE2	1:B:496:ILE:HG22	1.99	0.44
1:C:242:GLY:O	1:C:243:HIS:HB3	2.17	0.44
1:C:326:LYS:O	1:C:329:ILE:CD1	2.66	0.44
1:D:441:ARG:NE	1:D:446:THR:HG21	2.32	0.44
1:A:40:ARG:HG3	1:A:44:THR:HG21	2.00	0.43
1:A:337:GLN:HB3	1:A:408:TRP:CZ3	2.53	0.43
1:B:530:THR:CG2	1:B:534:LYS:HE3	2.48	0.43
1:C:161:TYR:HB3	1:C:174:VAL:HG12	2.00	0.43
1:A:179:LYS:HE2	1:A:196:GLU:OE1	2.17	0.43
1:C:460:ASP:HB3	1:C:463:ARG:CD	2.48	0.43
1:C:373:LEU:HD11	1:D:539:TYR:CZ	2.54	0.43
1:D:175:GLY:HA2	1:D:218:LEU:O	2.19	0.43
1:D:335:SER:O	1:D:336:THR:OG1	2.26	0.43
1:B:35:ASN:HB3	1:B:83:ALA:HB3	2.00	0.42
1:C:378:GLU:HG3	1:C:379:MET:H	1.84	0.42
1:B:91:ILE:HD11	1:B:334:TYR:CE2	2.53	0.42
1:D:290:LEU:HD23	1:D:292:ILE:HD11	2.00	0.42
1:D:380:PHE:CD1	1:D:380:PHE:O	2.72	0.42
1:B:238:VAL:HG13	1:B:276:PRO:HG2	2.01	0.42
1:C:491:GLU:HG2	1:C:492:VAL:N	2.34	0.42
1:A:408:TRP:CZ2	1:C:329:ILE:O	2.72	0.42
1:B:231:GLN:HA	1:B:269:SER:HA	2.01	0.42
1:D:515:LEU:HD12	1:D:515:LEU:O	2.20	0.42
1:D:334:TYR:O	1:D:335:SER:HB2	2.20	0.42
1:B:382:ASN:OD1	1:B:383:HIS:N	2.53	0.42
1:A:339:LEU:HD21	1:A:408:TRP:CZ2	2.55	0.42
1:C:180:GLU:O	1:C:184:LEU:HG	2.20	0.42
1:C:116:GLY:N	1:C:119:GLU:OE1	2.49	0.41
1:C:427:LYS:HG3	1:C:516:LEU:HD11	2.03	0.41
1:A:123:GLY:HA2	1:A:186:ASN:O	2.20	0.41
1:C:154:ILE:HA	1:C:157:LEU:HD12	2.03	0.41
1:A:380:PHE:CE1	1:A:478:LYS:HG2	2.55	0.41
1:A:390:ASN:HB3	1:A:501:LEU:HD21	2.03	0.41
1:A:290:LEU:HD23	1:A:292:ILE:HD11	2.01	0.41
1:B:497:LEU:HD12	1:B:497:LEU:O	2.20	0.41
1:D:180:GLU:O	1:D:184:LEU:HG	2.20	0.41
3:D:603:A1IVH:C14	3:D:603:A1IVH:N17	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:LEU:HA	1:D:314:ILE:HD12	2.02	0.41
1:A:415:LEU:HD11	1:A:528:VAL:HG21	2.03	0.41
1:A:535:MET:O	1:A:536:LYS:HB2	2.21	0.41
1:B:363:LEU:HB2	1:B:540:PRO:HG3	2.01	0.41
1:D:242:GLY:O	1:D:243:HIS:HB3	2.21	0.41
1:D:515:LEU:HD12	1:D:515:LEU:C	2.45	0.41
1:B:281:TYR:CG	1:B:282:ALA:N	2.88	0.41
1:C:231:GLN:HA	1:C:269:SER:HA	2.03	0.41
1:C:379:MET:O	1:C:380:PHE:HD1	2.04	0.41
1:C:384:VAL:HG12	1:C:494:LYS:CB	2.48	0.41
1:C:58:MET:HG2	1:C:311:ASP:HA	2.03	0.41
1:C:348:GLY:H	1:C:397:PRO:HB3	1.86	0.41
1:D:463:ARG:HH11	1:D:470:VAL:HG12	1.86	0.41
1:B:326:LYS:HD3	1:D:94:THR:HG22	2.02	0.40
1:D:91:ILE:CD1	1:D:408:TRP:CZ3	3.03	0.40
1:D:535:MET:O	1:D:537:VAL:N	2.49	0.40
1:D:147:LYS:O	1:D:190:ASN:OD1	2.39	0.40
1:C:339:LEU:HD21	1:C:408[B]:TRP:CD1	2.56	0.40
1:B:425:GLN:HG3	1:B:494:LYS:HG2	2.03	0.40
1:D:33:HIS:HA	1:D:81:LEU:O	2.20	0.40
1:A:526:ASN:OD1	1:C:329:ILE:HG23	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:ARG:NH2	1:C:516:LEU:O[2_645]	2.14	0.06

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	516/547 (94%)	491 (95%)	24 (5%)	1 (0%)	44	54
1	B	516/547 (94%)	490 (95%)	25 (5%)	1 (0%)	44	54
1	C	522/547 (95%)	492 (94%)	28 (5%)	2 (0%)	30	37
1	D	517/547 (94%)	489 (95%)	26 (5%)	2 (0%)	30	37
All	All	2071/2188 (95%)	1962 (95%)	103 (5%)	6 (0%)	37	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	336	THR
1	C	374	ARG
1	C	88	GLN
1	A	88	GLN
1	B	88	GLN
1	D	88	GLN

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	449/465 (97%)	446 (99%)	3 (1%)	81	90
1	B	448/465 (96%)	444 (99%)	4 (1%)	75	86
1	C	452/465 (97%)	448 (99%)	4 (1%)	75	86
1	D	449/465 (97%)	446 (99%)	3 (1%)	81	90
All	All	1798/1860 (97%)	1784 (99%)	14 (1%)	79	88

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	VAL
1	A	384	VAL
1	A	525	ILE
1	B	73	ARG
1	B	376	THR

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Mol	Chain	Res	Type
1	B	380	PHE
1	B	425	GLN
1	C	147	LYS
1	C	238	VAL
1	C	379	MET
1	C	497	LEU
1	D	365	CYS
1	D	380	PHE
1	D	411	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	279	GLN
1	B	69	GLN
1	B	370	ASN
1	C	279	GLN
1	C	370	ASN
1	C	383	HIS
1	C	503	ASN
1	D	77	ASN
1	D	279	GLN
1	D	299	ASN
1	D	370	ASN
1	D	371	ASN
1	D	382	ASN
1	D	383	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	A1IVH	D	603	2	30,35,35	1.12	2 (6%)	35,50,50	1.27	6 (17%)
3	A1IVH	B	603	2	30,35,35	1.64	3 (10%)	35,50,50	1.21	5 (14%)
3	A1IVH	C	603	2	30,35,35	1.52	4 (13%)	35,50,50	1.08	4 (11%)
3	A1IVH	A	603	2	30,35,35	1.17	4 (13%)	35,50,50	1.21	4 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1IVH	D	603	2	-	7/23/24/24	0/3/3/3
3	A1IVH	B	603	2	-	8/23/24/24	0/3/3/3
3	A1IVH	C	603	2	-	7/23/24/24	0/3/3/3
3	A1IVH	A	603	2	-	8/23/24/24	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	A1IVH	P26-O25	6.89	1.67	1.57
3	C	603	A1IVH	P26-O25	6.32	1.66	1.57
3	D	603	A1IVH	C2-N3	3.33	1.32	1.30
3	B	603	A1IVH	C2-N3	3.22	1.32	1.30
3	A	603	A1IVH	P26-O25	3.15	1.62	1.57
3	B	603	A1IVH	P26-O33	-2.97	1.49	1.56
3	C	603	A1IVH	C2-N3	2.94	1.32	1.30
3	D	603	A1IVH	P26-O33	-2.91	1.49	1.56
3	A	603	A1IVH	C2-N3	2.91	1.32	1.30
3	C	603	A1IVH	P26-O33	-2.62	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	A1IVH	P26-O33	-2.59	1.50	1.56
3	C	603	A1IVH	C18-N17	-2.05	1.31	1.34
3	A	603	A1IVH	C6-N16	2.04	1.35	1.32

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	603	A1IVH	C2-N3-C4	-4.16	110.81	114.09
3	D	603	A1IVH	C2-N3-C4	-3.84	111.06	114.09
3	A	603	A1IVH	C5-C6-N16	-3.64	117.79	120.81
3	A	603	A1IVH	C2-N3-C4	-3.51	111.31	114.09
3	C	603	A1IVH	C2-N3-C4	-3.20	111.56	114.09
3	A	603	A1IVH	O33-P26-O32	2.93	119.86	110.07
3	D	603	A1IVH	O30-P28-C27	-2.84	105.12	111.24
3	D	603	A1IVH	P26-O25-C24	-2.62	114.13	122.28
3	D	603	A1IVH	C5-C6-N16	-2.61	118.64	120.81
3	C	603	A1IVH	O30-P28-C27	-2.51	105.83	111.24
3	B	603	A1IVH	O33-P26-O32	2.47	118.31	110.07
3	C	603	A1IVH	O33-P26-O32	2.47	118.31	110.07
3	D	603	A1IVH	O33-P26-O32	2.47	118.30	110.07
3	A	603	A1IVH	C2-N16-C6	2.37	118.08	111.04
3	D	603	A1IVH	C2-N16-C6	2.32	117.94	111.04
3	C	603	A1IVH	C2-N16-C6	2.16	117.46	111.04
3	B	603	A1IVH	C2-N16-C6	2.15	117.43	111.04
3	B	603	A1IVH	O30-P28-C27	-2.12	106.68	111.24
3	B	603	A1IVH	P26-O25-C24	2.10	128.82	122.28

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	A1IVH	C5-C6-N7-C15
3	A	603	A1IVH	N16-C6-N7-C8
3	A	603	A1IVH	P28-C27-P26-O32
3	A	603	A1IVH	P28-C27-P26-O33
3	B	603	A1IVH	N16-C6-N7-C8
3	B	603	A1IVH	C23-C24-O25-P26
3	B	603	A1IVH	P26-C27-P28-O29
3	B	603	A1IVH	P26-C27-P28-O30
3	B	603	A1IVH	P26-C27-P28-O31
3	C	603	A1IVH	C23-C24-O25-P26
3	C	603	A1IVH	P26-C27-P28-O29

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Mol	Chain	Res	Type	Atoms
3	C	603	A1IVH	P26-C27-P28-O30
3	C	603	A1IVH	P26-C27-P28-O31
3	D	603	A1IVH	C5-C6-N7-C15
3	D	603	A1IVH	N16-C6-N7-C15
3	D	603	A1IVH	P26-C27-P28-O29
3	D	603	A1IVH	P26-C27-P28-O30
3	D	603	A1IVH	P26-C27-P28-O31
3	C	603	A1IVH	C20-C21-C22-C23
3	D	603	A1IVH	C20-C21-C22-C23
3	A	603	A1IVH	C9-C8-N7-C15
3	B	603	A1IVH	C9-C8-N7-C15
3	C	603	A1IVH	C9-C8-N7-C15
3	B	603	A1IVH	C20-C21-C22-C23
3	A	603	A1IVH	N16-C6-N7-C15
3	A	603	A1IVH	P28-C27-P26-O25
3	A	603	A1IVH	C23-C24-O25-P26
3	C	603	A1IVH	C24-O25-P26-O33
3	D	603	A1IVH	C9-C8-N7-C15
3	B	603	A1IVH	N19-C20-C21-C22

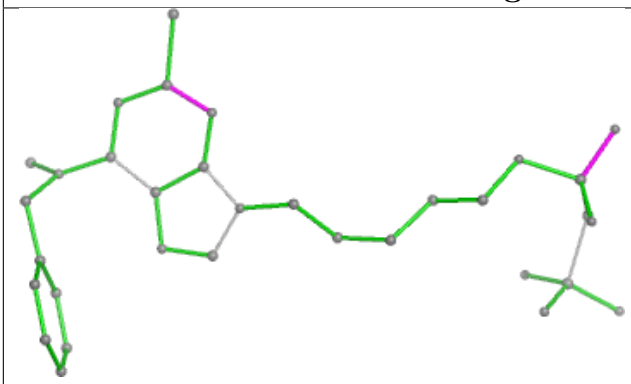
There are no ring outliers.

4 monomers are involved in 9 short contacts:

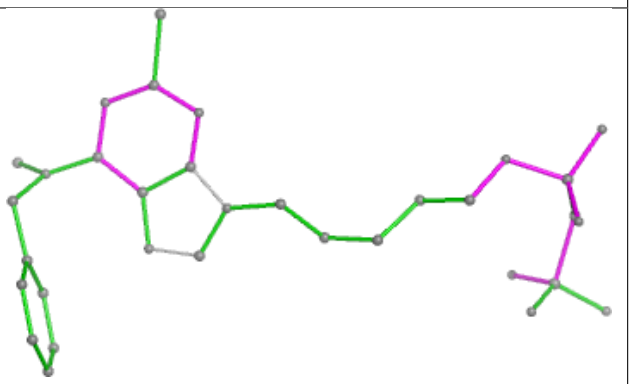
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	603	A1IVH	4	0
3	B	603	A1IVH	2	0
3	C	603	A1IVH	1	0
3	A	603	A1IVH	2	0

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.

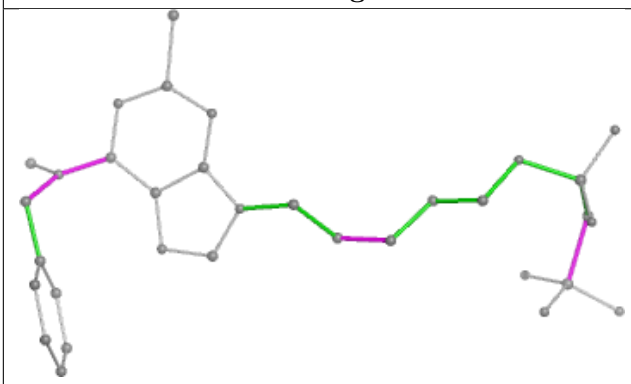
Ligand A1IVH D 603



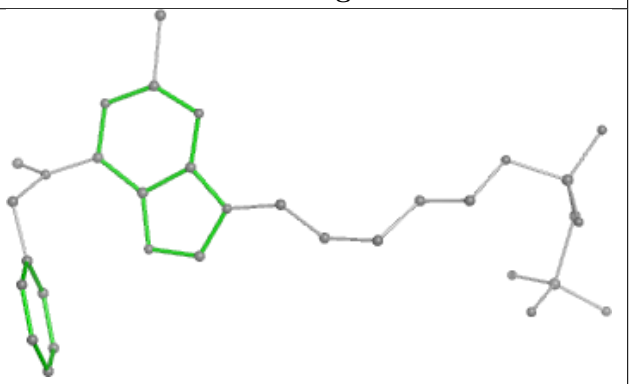
Bond lengths



Bond angles

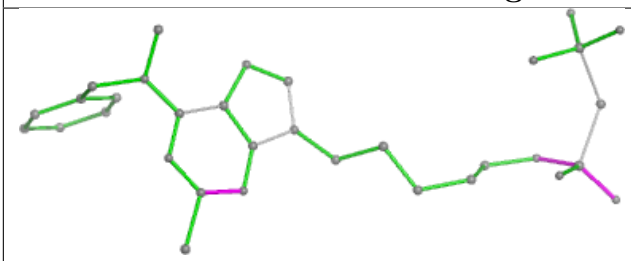


Torsions

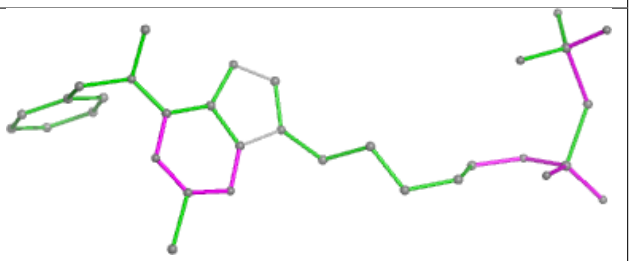


Rings

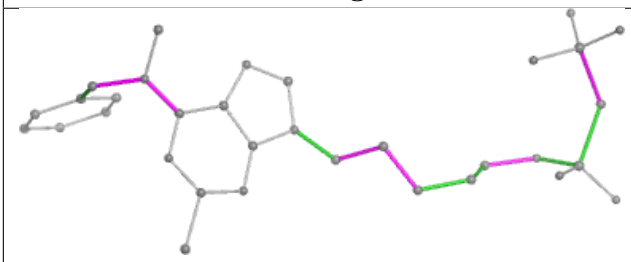
Ligand A1IVH B 603



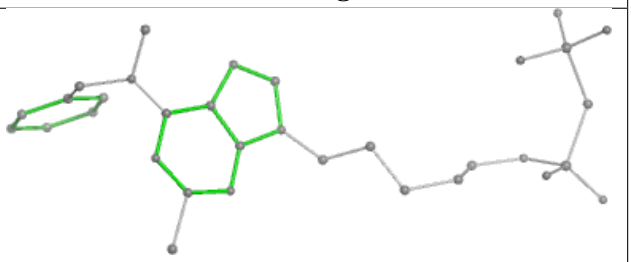
Bond lengths



Bond angles

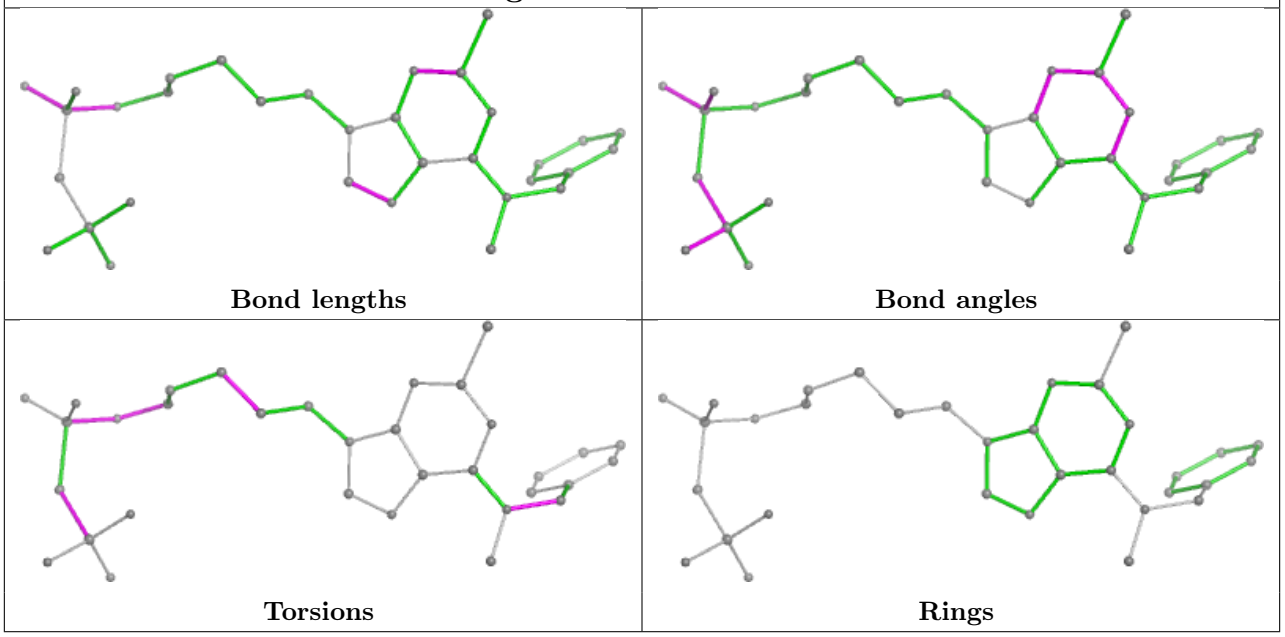


Torsions

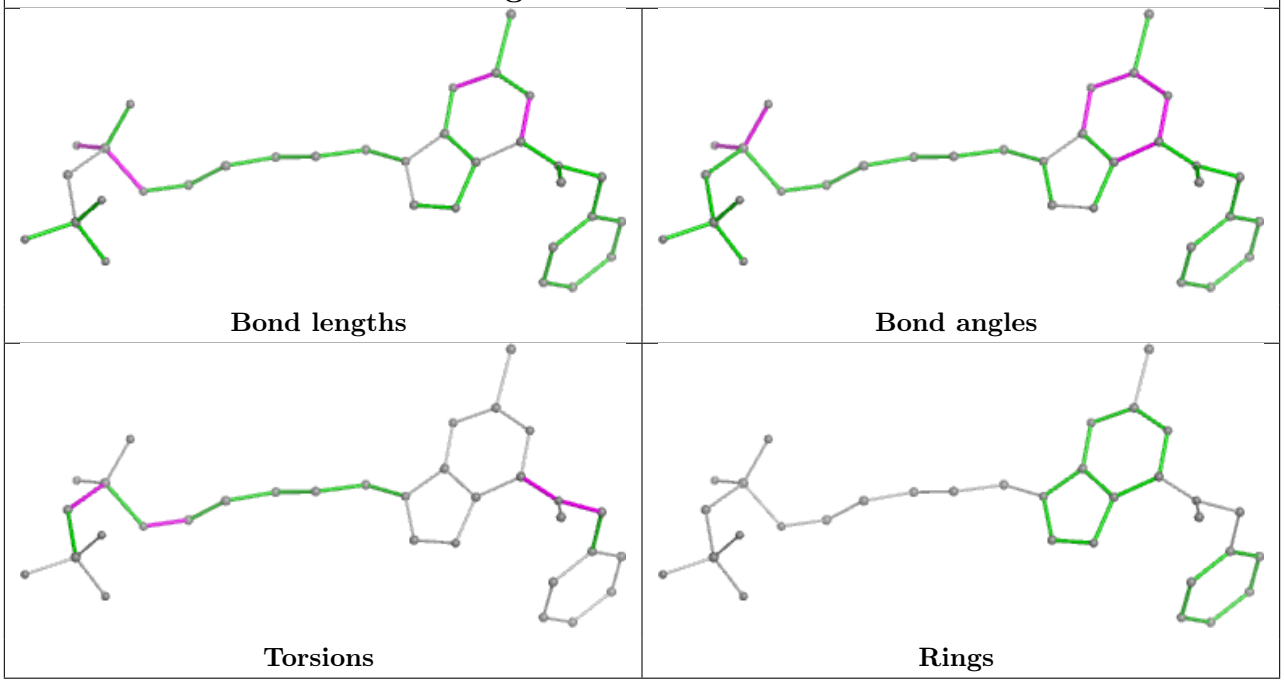


Rings

Ligand A1IVH C 603



Ligand A1IVH A 603



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	520/547 (95%)	0.72	34 (6%)	26	29	22, 29, 39, 51	0
1	B	520/547 (95%)	0.59	18 (3%)	47	50	20, 28, 39, 54	0
1	C	523/547 (95%)	0.72	29 (5%)	32	34	16, 30, 42, 63	1 (0%)
1	D	520/547 (95%)	0.60	26 (5%)	35	37	19, 25, 38, 51	1 (0%)
All	All	2083/2188 (95%)	0.66	107 (5%)	34	37	16, 28, 40, 63	2 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	408	TRP	5.6
1	C	380	PHE	4.9
1	A	351	GLN	4.2
1	B	209	THR	3.8
1	D	464	LYS	3.6
1	C	373	LEU	3.6
1	C	374	ARG	3.6
1	A	331	LEU	3.6
1	A	334	TYR	3.5
1	C	408[A]	TRP	3.4
1	A	174	VAL	3.4
1	A	149	PRO	3.4
1	C	375	HIS	3.4
1	D	408	TRP	3.4
1	C	333	ASP	3.3
1	B	129	GLU	3.3
1	D	380	PHE	3.3
1	B	52	VAL	3.2
1	D	168	ASP	3.2
1	A	154	ILE	3.2
1	C	157	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	492	VAL	3.1
1	D	129	GLU	3.1
1	D	334	TYR	3.1
1	C	329	ILE	3.0
1	A	496	ILE	2.9
1	B	149	PRO	2.9
1	D	150	LEU	2.9
1	B	376	THR	2.9
1	A	373	LEU	2.9
1	C	325	ASN	2.9
1	D	152	SER	2.8
1	A	56	ARG	2.8
1	C	377	ASP	2.8
1	A	211	ASN	2.7
1	A	299	ASN	2.7
1	A	384	VAL	2.7
1	A	336	THR	2.7
1	B	211	ASN	2.7
1	A	228	LEU	2.6
1	D	312	SER	2.6
1	A	517	ARG	2.6
1	B	380	PHE	2.6
1	D	374	ARG	2.6
1	D	68	VAL	2.6
1	C	496	ILE	2.5
1	D	188	GLY	2.5
1	C	154	ILE	2.5
1	D	526	ASN	2.5
1	C	52	VAL	2.4
1	A	208	LYS	2.4
1	B	521	GLY	2.4
1	A	423	LEU	2.4
1	C	280	ALA	2.4
1	A	179	LYS	2.4
1	B	109	ARG	2.4
1	C	54	ALA	2.4
1	C	379	MET	2.4
1	D	149	PRO	2.4
1	A	47	ASP	2.4
1	C	51	CYS	2.4
1	B	408	TRP	2.3
1	D	326	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	258	VAL	2.3
1	C	338	GLU	2.3
1	D	525	ILE	2.3
1	A	330	LYS	2.3
1	B	431	LEU	2.3
1	C	331	LEU	2.3
1	A	301	ILE	2.3
1	A	339	LEU	2.2
1	A	487	LEU	2.2
1	C	164	LEU	2.2
1	B	120	PHE	2.2
1	C	326	LYS	2.2
1	B	210	LEU	2.2
1	B	146	ALA	2.2
1	C	405	THR	2.2
1	C	56	ARG	2.2
1	C	503	ASN	2.2
1	C	351	GLN	2.2
1	A	549	SER	2.2
1	B	188	GLY	2.2
1	C	327	TRP	2.2
1	C	135	ALA	2.2
1	D	164	LEU	2.1
1	D	228	LEU	2.1
1	C	376	THR	2.1
1	A	355	PHE	2.1
1	D	378	GLU	2.1
1	B	429	SER	2.1
1	B	310	LEU	2.1
1	C	310	LEU	2.1
1	D	159	LEU	2.1
1	A	230	ALA	2.1
1	A	55	SER	2.1
1	D	148	GLY	2.1
1	A	180	GLU	2.1
1	B	183	PHE	2.1
1	A	332	ASP	2.1
1	D	167	GLY	2.1
1	D	153	GLN	2.1
1	D	379	MET	2.1
1	D	424	VAL	2.0
1	A	271	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	511	ILE	2.0
1	D	81	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

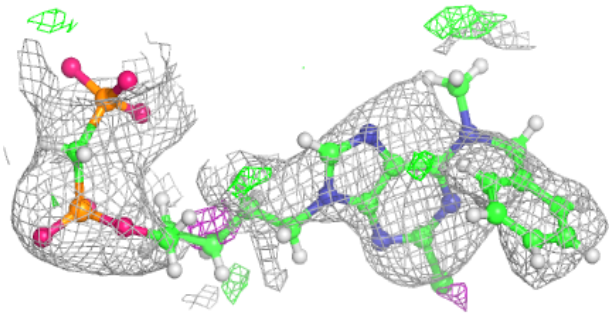
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

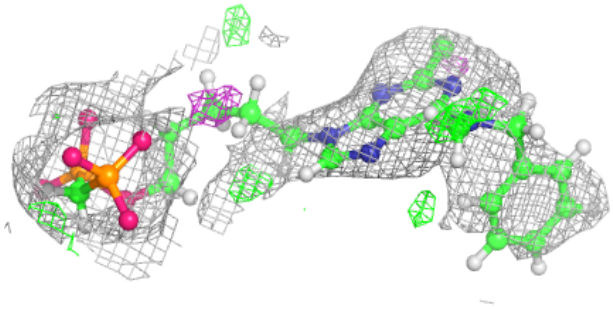
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	C	604	1/1	0.78	0.16	34,34,34,34	1
3	A1IVH	C	603	33/33	0.87	0.14	20,28,35,45	0
3	A1IVH	A	603	33/33	0.88	0.12	20,26,32,35	0
3	A1IVH	D	603	33/33	0.90	0.11	17,22,29,33	0
3	A1IVH	B	603	33/33	0.91	0.11	21,32,42,42	0
4	CL	C	605	1/1	0.92	0.13	33,33,33,33	0
4	CL	A	604	1/1	0.92	0.18	31,31,31,31	0
2	ZN	D	602	1/1	0.95	0.09	24,24,24,24	0
2	ZN	D	601	1/1	0.96	0.08	20,20,20,20	0
2	ZN	A	601	1/1	0.96	0.08	22,22,22,22	0
2	ZN	A	602	1/1	0.96	0.09	21,21,21,21	0
2	ZN	B	602	1/1	0.97	0.08	21,21,21,21	0
2	ZN	B	601	1/1	0.97	0.08	23,23,23,23	0
2	ZN	C	602	1/1	0.98	0.09	23,23,23,23	0
2	ZN	C	601	1/1	0.99	0.05	22,22,22,22	0

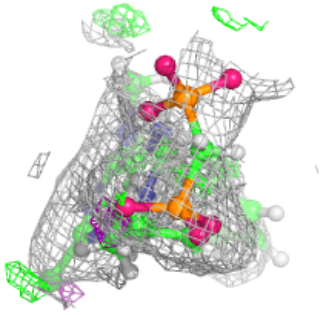
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1IVH C 603:

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

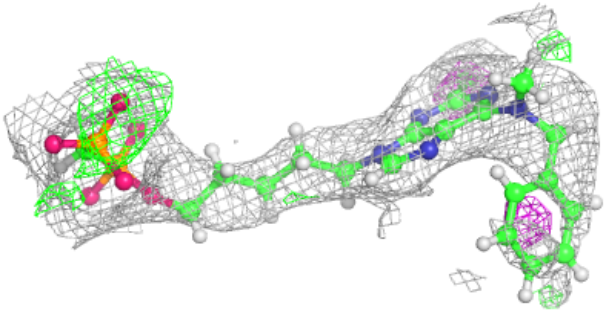


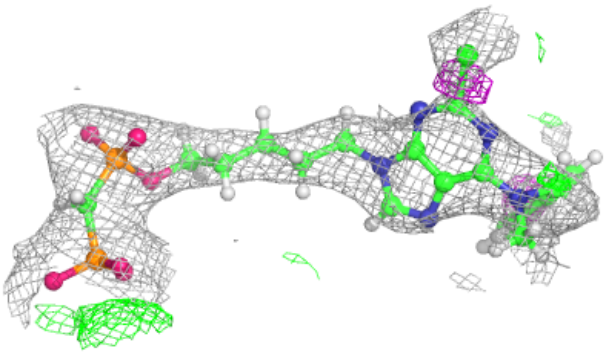


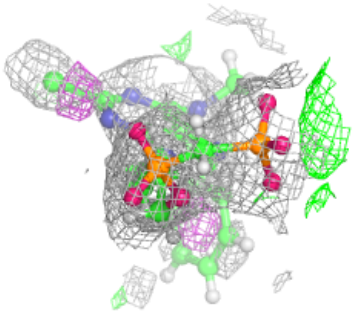


Electron density around A1IVH A 603:

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

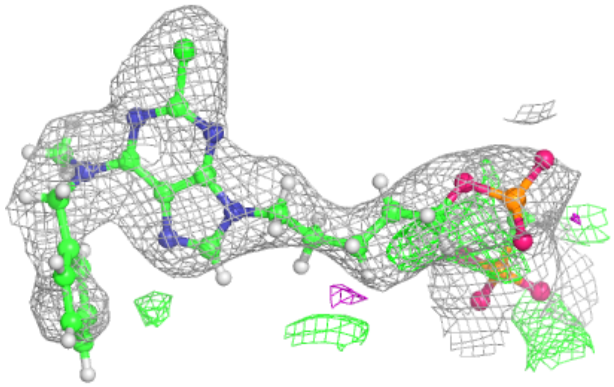


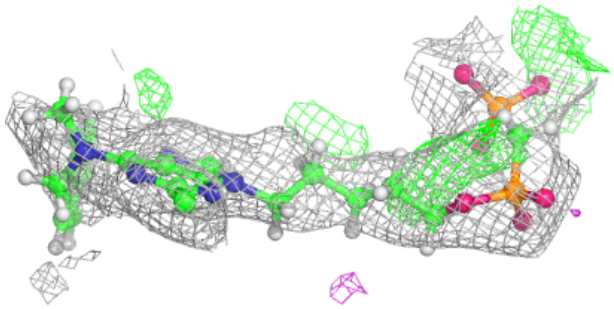


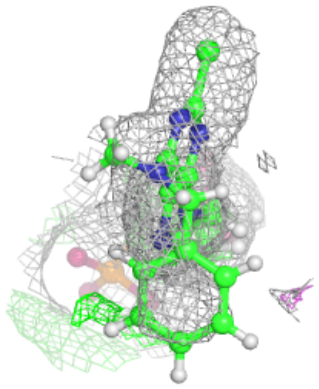


Electron density around A1IVH D 603:

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

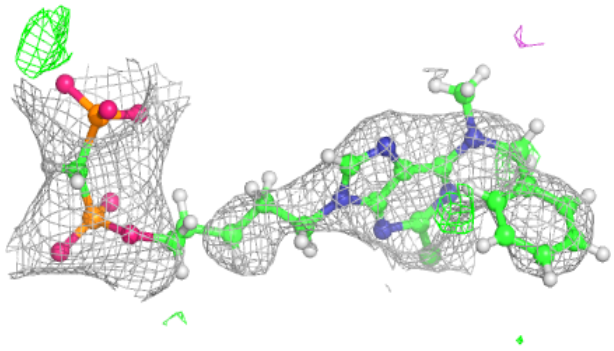


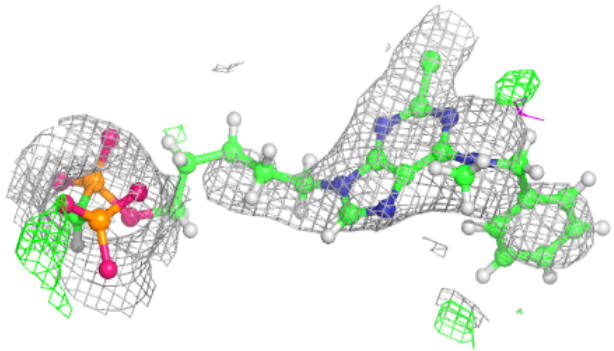


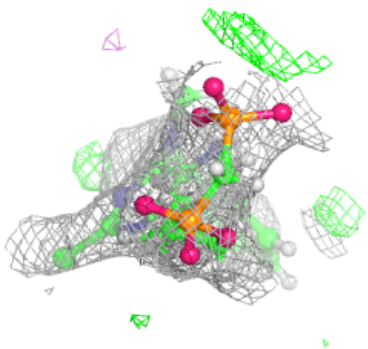


Electron density around A1IVH B 603:

$2mF_o$-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.