Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 02:54 AM EDT

PDB ID	:	1PZG
Title	:	T.gondii LDH1 complexed with APAD and sulfate at 1.6 Angstroms
Authors	:	Kavanagh, K.L.; Elling, R.A.; Wilson, D.K.
Deposited on	:	2003-07-10
Resolution	:	1.60 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
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:

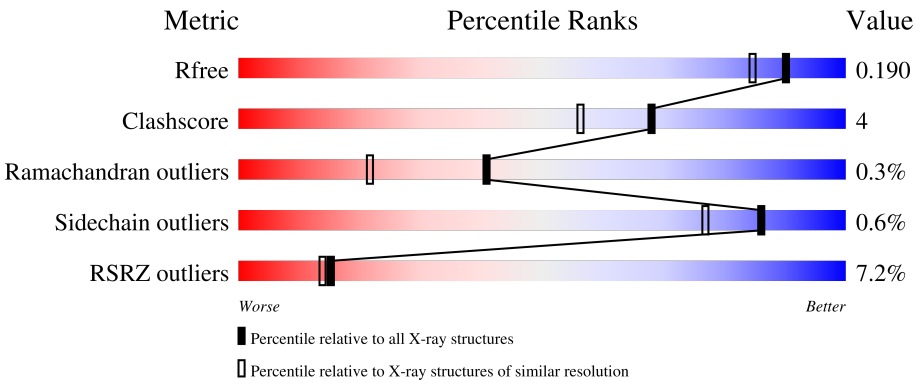
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.60 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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 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	331	5% 93% 6% •
1	B	331	4% 89% 10% •
1	C	331	10% 86% 12% • •
1	D	331	9% 87% 11% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10639 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.

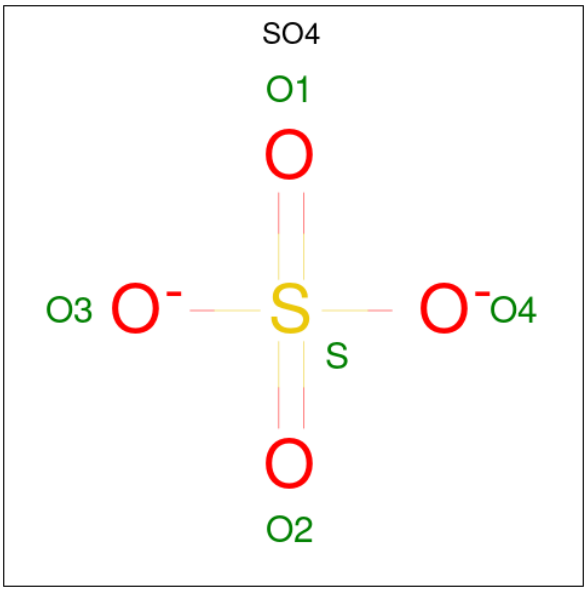
- Molecule 1 is a protein called lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	328	2478	1568	418	468	24	0	0	0
1	B	328	2478	1568	418	468	24	0	0	0
1	C	325	2459	1555	415	465	24	0	0	0
1	D	326	2466	1560	416	466	24	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

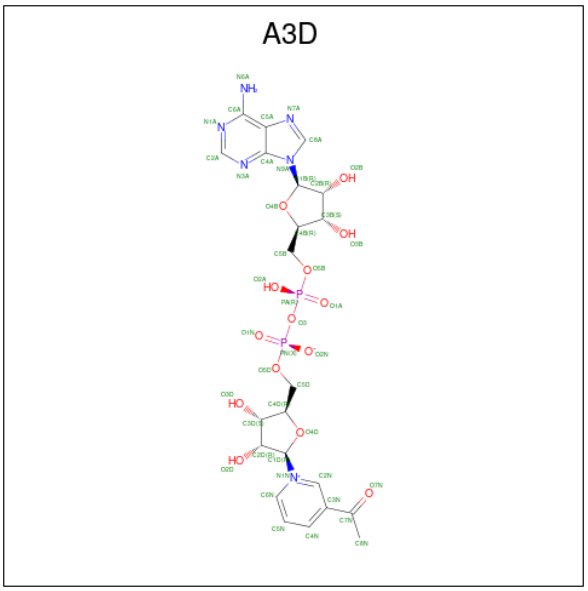
Chain	Residue	Modelled	Actual	Comment	Reference
A	150	CME	CYS	modified residue	UNP P90613
A	334	PRO	-	cloning artifact	UNP P90613
A	335	GLY	-	cloning artifact	UNP P90613
B	150	CME	CYS	modified residue	UNP P90613
B	334	PRO	-	cloning artifact	UNP P90613
B	335	GLY	-	cloning artifact	UNP P90613
C	150	CME	CYS	modified residue	UNP P90613
C	334	PRO	-	cloning artifact	UNP P90613
C	335	GLY	-	cloning artifact	UNP P90613
D	150	CME	CYS	modified residue	UNP P90613
D	334	PRO	-	cloning artifact	UNP P90613
D	335	GLY	-	cloning artifact	UNP P90613

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is 3-ACETYLPYRIDINE ADENINE DINUCLEOTIDE (three-letter code: A3D) (formula: $C_{22}H_{28}N_6O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	44	22	6	14	2	0	0
3	B	1	44	22	6	14	2	0	0
3	C	1	44	22	6	14	2	0	0
3	D	1	44	22	6	14	2	0	0

- Molecule 4 is water.

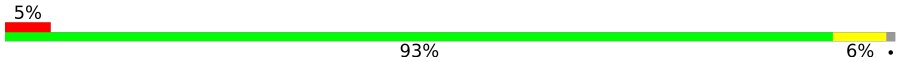
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	160	160	160	0	0
4	B	149	149	149	0	0
4	C	121	121	121	0	0
4	D	132	132	132	0	0

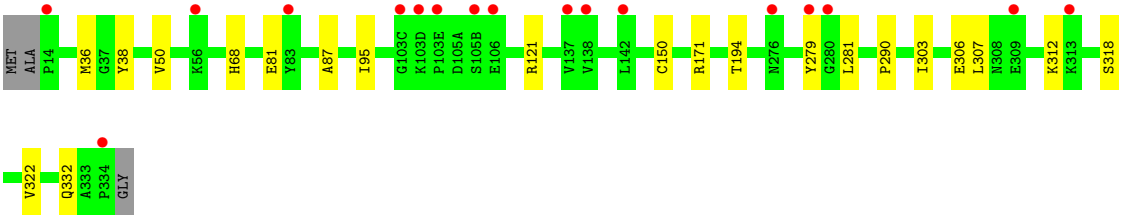
3 Residue-property plots (i)

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: lactate dehydrogenase

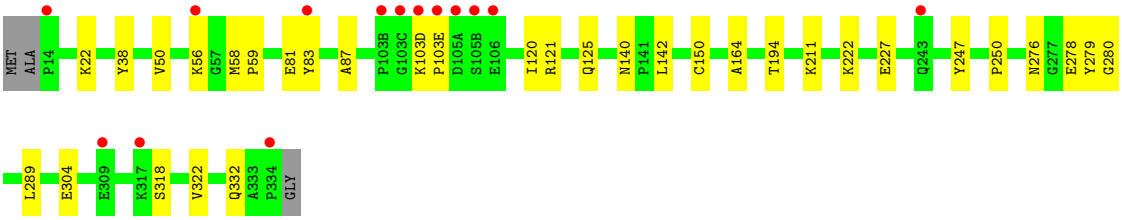
Chain A:





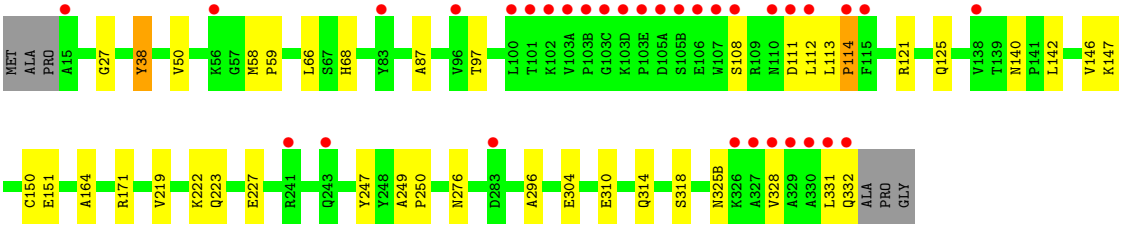
• Molecule 1: lactate dehydrogenase

Chain B:



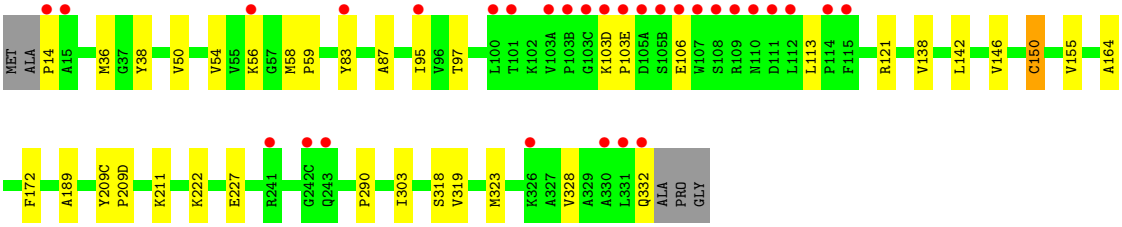
• Molecule 1: lactate dehydrogenase

Chain C:



• Molecule 1: lactate dehydrogenase

Chain D:


MET
ALA
P14
A15
M36
G37
Y38
V50
V54
V55
K56
G57
M58
P59
Y83
A87
I95
V96
T97
L100
T101
K102
V103A
P103B
G103C
K103D
P103E
D105A
S105B
E106
W107
S108
R109
N110
D111
L112
L113
P114
F115
R121
V138
L142
V146
C150
V155
A164
F172
A189
Y209C
P209D
K211
K222
E227
R241
G242C
Q243
P290
I303
S318
V319
M323
K326
A327
V328
A329
A330
L331
Q332
ALA
PRO
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.94Å 124.98Å 86.39Å 90.00° 105.94° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 28.95 – 1.60	Depositor EDS
% Data completeness (in resolution range)	91.8 (30.00-1.60) 91.8 (28.95-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 1.60Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.176 , 0.198 0.168 , 0.190	Depositor DCC
R_{free} test set	8417 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 45.1	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	0.97	EDS
Total number of atoms	10639	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, A3D, CME

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	0.46	0/2506	0.68	0/3389
1	B	0.46	0/2506	0.68	0/3389
1	C	0.46	0/2485	0.67	1/3359 (0.0%)
1	D	0.43	0/2493	0.67	0/3370
All	All	0.45	0/9990	0.68	1/13507 (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
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

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	C	27	GLY	N-CA-C	-5.02	100.55	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	38	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	38	TYR	Sidechain
1	C	38	TYR	Sidechain
1	D	38	TYR	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	2478	0	2533	12	0
1	B	2478	0	2533	21	0
1	C	2459	0	2513	26	0
1	D	2466	0	2521	22	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	44	0	27	0	0
3	B	44	0	27	0	0
3	C	44	0	27	1	0
3	D	44	0	27	2	0
4	A	160	0	0	1	0
4	B	149	0	0	0	0
4	C	121	0	0	0	0
4	D	132	0	0	0	0
All	All	10639	0	10208	76	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 4.

All (76) 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:112:LEU:C	1:C:114:PRO:HD2	1.82	0.99
1:C:113:LEU:N	1:C:114:PRO:HD2	1.87	0.90
1:C:113:LEU:HD11	1:C:328:VAL:HG12	1.60	0.83
1:C:113:LEU:HD11	1:C:328:VAL:CG1	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ARG:O	1:C:125:GLN:HG3	1.92	0.69
1:D:113:LEU:HD11	1:D:328:VAL:CG2	2.25	0.66
1:D:103(D):LYS:HE3	1:D:106:GLU:HB3	1.78	0.65
1:C:296:ALA:HB1	1:D:14:PRO:HB2	1.80	0.63
1:B:56:LYS:HE3	1:B:83:TYR:HD2	1.67	0.59
1:D:113:LEU:HD11	1:D:328:VAL:HG22	1.84	0.58
1:D:121:ARG:NH1	1:D:332:GLN:HB2	2.19	0.57
1:B:211:LYS:HE2	1:C:304:GLU:O	2.05	0.56
1:C:50:VAL:HG11	1:C:87:ALA:HA	1.87	0.56
1:C:113:LEU:N	1:C:114:PRO:CD	2.66	0.56
1:B:194:THR:HG21	1:B:322:VAL:HB	1.88	0.56
1:C:310:GLU:HG3	1:C:314:GLN:HE21	1.71	0.55
1:D:142:LEU:O	1:D:146:VAL:HG23	2.07	0.54
1:A:50:VAL:HG11	1:A:87:ALA:HA	1.90	0.53
1:B:22:LYS:HE3	1:B:50:VAL:HG21	1.90	0.53
1:D:290:PRO:HB2	1:D:303:ILE:HB	1.91	0.52
1:A:194:THR:HG21	1:A:322:VAL:HB	1.93	0.51
1:C:219:VAL:HG23	1:C:223:GLN:CD	2.30	0.51
1:A:121:ARG:NH1	1:A:332:GLN:HG2	2.25	0.51
1:B:222:LYS:O	1:B:227:GLU:HG3	2.10	0.51
1:B:50:VAL:HG13	1:B:81:GLU:HG2	1.93	0.51
1:B:56:LYS:HG3	1:B:83:TYR:CD2	2.46	0.51
1:B:121:ARG:NH1	1:B:332:GLN:HG3	2.25	0.51
1:A:290:PRO:HB2	1:A:303:ILE:HB	1.92	0.50
1:C:310:GLU:HG3	1:C:314:GLN:NE2	2.26	0.50
1:A:307:LEU:O	1:A:312:LYS:HE3	2.12	0.50
1:D:319:VAL:O	1:D:323:MET:HG3	2.11	0.50
1:B:22:LYS:HE3	1:B:50:VAL:CG2	2.42	0.50
1:C:147:LYS:O	1:C:151:GLU:HG3	2.12	0.50
1:D:50:VAL:HG11	1:D:87:ALA:HA	1.95	0.49
1:D:56:LYS:HA	1:D:83:TYR:CE2	2.49	0.48
1:C:108:SER:HB3	1:C:111:ASP:OD2	2.14	0.47
1:D:58:MET:HB3	1:D:59:PRO:HD3	1.97	0.47
1:B:279:TYR:CZ	1:B:304:GLU:HA	2.50	0.46
1:C:142:LEU:O	1:C:146:VAL:HG23	2.15	0.46
1:B:103(D):LYS:HA	1:B:103(E):PRO:HD3	1.86	0.45
1:C:140:ASN:HA	1:C:142:LEU:N	2.31	0.45
1:C:331:LEU:O	1:C:332:GLN:HB2	2.16	0.45
1:B:279:TYR:CE2	1:B:304:GLU:HA	2.52	0.45
1:D:222:LYS:O	1:D:227:GLU:HG3	2.17	0.44
1:D:150:CME:HE2	1:D:155:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:TYR:HB2	1:A:281:LEU:HG	1.99	0.44
1:B:278:GLU:C	1:B:280:GLY:H	2.21	0.44
1:B:278:GLU:C	1:B:280:GLY:N	2.71	0.44
1:C:222:LYS:O	1:C:227:GLU:HG3	2.18	0.44
1:D:36:MET:SD	1:D:95:ILE:HG21	2.58	0.44
1:B:279:TYR:CE2	1:B:289:LEU:HD22	2.53	0.43
1:B:121:ARG:O	1:B:125:GLN:HG3	2.17	0.43
1:C:97:THR:HB	3:C:605:A3D:H51N	1.99	0.43
1:D:103(D):LYS:HE3	1:D:106:GLU:CB	2.47	0.43
1:D:97:THR:HB	3:D:607:A3D:H51N	2.00	0.42
1:B:50:VAL:HG11	1:B:87:ALA:HA	2.00	0.42
1:D:172:PHE:CD2	1:D:189:ALA:HB1	2.54	0.42
1:A:306:GLU:HG3	1:D:211:LYS:HD3	2.00	0.42
1:B:58:MET:HB3	1:B:59:PRO:HD3	2.02	0.42
1:D:97:THR:HG22	1:D:138:VAL:HB	2.02	0.42
1:C:38:TYR:HA	1:C:66:LEU:HD22	2.01	0.42
1:D:54:VAL:HG13	3:D:607:A3D:N1A	2.35	0.42
1:A:171:ARG:HG2	1:C:68:HIS:CE1	2.55	0.41
1:D:209(C):TYR:HA	1:D:209(D):PRO:HD3	1.93	0.41
1:A:36:MET:SD	1:A:95:ILE:HG21	2.60	0.41
1:A:50:VAL:HG13	1:A:81:GLU:HG2	2.02	0.41
1:A:332:GLN:NE2	4:A:677:HOH:O	2.52	0.41
1:A:68:HIS:CE1	1:C:171:ARG:HG2	2.56	0.41
1:B:247:TYR:C	1:B:250:PRO:HD2	2.41	0.41
1:C:249:ALA:N	1:C:250:PRO:CD	2.83	0.41
1:C:58:MET:HB3	1:C:59:PRO:HD3	2.02	0.41
1:C:325(B):ASN:O	1:C:328:VAL:HG22	2.20	0.41
1:B:120:ILE:HD13	1:B:120:ILE:HA	1.94	0.40
1:B:140:ASN:HA	1:B:142:LEU:N	2.36	0.40
1:C:247:TYR:C	1:C:250:PRO:HD2	2.41	0.40
1:D:103(D):LYS:HA	1:D:103(E):PRO:HD3	1.98	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	325/331 (98%)	320 (98%)	5 (2%)	0	100	100
1	B	325/331 (98%)	319 (98%)	5 (2%)	1 (0%)	41	21
1	C	322/331 (97%)	314 (98%)	6 (2%)	2 (1%)	25	8
1	D	323/331 (98%)	318 (98%)	4 (1%)	1 (0%)	41	21
All	All	1295/1324 (98%)	1271 (98%)	20 (2%)	4 (0%)	41	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	114	PRO
1	B	164	ALA
1	D	164	ALA
1	C	164	ALA

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	269/270 (100%)	268 (100%)	1 (0%)	91	84
1	B	269/270 (100%)	267 (99%)	2 (1%)	84	73
1	C	267/270 (99%)	265 (99%)	2 (1%)	84	73
1	D	268/270 (99%)	267 (100%)	1 (0%)	91	84
All	All	1073/1080 (99%)	1067 (99%)	6 (1%)	86	77

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	SER
1	B	276	ASN
1	B	318	SER
1	C	276	ASN

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Mol	Chain	Res	Type
1	C	318	SER
1	D	318	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	332	GLN
1	B	276	ASN
1	C	276	ASN
1	C	314	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CME	C	150	1	8,9,10	1.23	1 (12%)	5,9,11	1.34	1 (20%)
1	CME	B	150	1	8,9,10	1.22	1 (12%)	5,9,11	1.24	1 (20%)
1	CME	D	150	1	8,9,10	1.31	1 (12%)	5,9,11	1.19	1 (20%)
1	CME	A	150	1	8,9,10	1.26	1 (12%)	5,9,11	1.23	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	C	150	1	-	0/5/8/10	-
1	CME	B	150	1	-	0/5/8/10	-
1	CME	D	150	1	-	2/5/8/10	-
1	CME	A	150	1	-	0/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	CME	OH-CZ	-3.32	1.25	1.42
1	D	150	CME	OH-CZ	-3.32	1.25	1.42
1	B	150	CME	OH-CZ	-3.21	1.25	1.42
1	C	150	CME	OH-CZ	-3.18	1.25	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	150	CME	OH-CZ-CE	2.51	120.73	110.83
1	B	150	CME	OH-CZ-CE	2.46	120.53	110.83
1	C	150	CME	OH-CZ-CE	2.33	120.04	110.83
1	A	150	CME	OH-CZ-CE	2.22	119.59	110.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	150	CME	SD-CE-CZ-OH
1	D	150	CME	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	150	CME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	SO4	B	604	-	4,4,4	0.41	0	6,6,6	0.45	0
3	A3D	C	605	-	42,48,48	2.00	12 (28%)	50,73,73	1.44	6 (12%)
3	A3D	A	601	-	42,48,48	1.89	11 (26%)	50,73,73	1.45	7 (14%)
3	A3D	B	603	-	42,48,48	2.08	11 (26%)	50,73,73	1.43	7 (14%)
2	SO4	D	608	-	4,4,4	0.26	0	6,6,6	0.34	0
3	A3D	D	607	-	42,48,48	2.03	12 (28%)	50,73,73	1.40	7 (14%)
2	SO4	C	606	-	4,4,4	0.33	0	6,6,6	0.35	0
2	SO4	A	602	-	4,4,4	0.29	0	6,6,6	0.83	0

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	A3D	A	601	-	-	5/26/62/62	0/5/5/5
3	A3D	C	605	-	-	5/26/62/62	0/5/5/5
3	A3D	B	603	-	-	5/26/62/62	0/5/5/5
3	A3D	D	607	-	-	5/26/62/62	0/5/5/5

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	A3D	C2A-N3A	4.98	1.40	1.32
3	B	603	A3D	C2D-C1D	-4.93	1.46	1.53
3	D	607	A3D	C2D-C1D	-4.81	1.46	1.53
3	D	607	A3D	C2A-N3A	4.77	1.39	1.32
3	C	605	A3D	C4N-C3N	4.74	1.47	1.39
3	D	607	A3D	C4N-C3N	4.67	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	A3D	C4N-C3N	4.64	1.47	1.39
3	B	603	A3D	C2N-N1N	4.55	1.40	1.35
3	A	601	A3D	C2D-C1D	-4.46	1.47	1.53
3	D	607	A3D	C2N-N1N	4.44	1.40	1.35
3	A	601	A3D	C2A-N3A	4.42	1.39	1.32
3	C	605	A3D	C2N-N1N	4.31	1.40	1.35
3	D	607	A3D	C2A-N1A	4.25	1.41	1.33
3	C	605	A3D	C2A-N3A	4.22	1.38	1.32
3	A	601	A3D	C4N-C3N	4.20	1.46	1.39
3	C	605	A3D	C2D-C1D	-4.15	1.47	1.53
3	B	603	A3D	C2A-N1A	4.13	1.41	1.33
3	C	605	A3D	O4D-C1D	3.94	1.46	1.41
3	C	605	A3D	C2A-N1A	3.88	1.41	1.33
3	A	601	A3D	C2A-N1A	3.85	1.41	1.33
3	A	601	A3D	C2N-N1N	3.71	1.39	1.35
3	C	605	A3D	C6N-N1N	3.57	1.44	1.35
3	B	603	A3D	C6N-N1N	3.55	1.44	1.35
3	D	607	A3D	C6N-N1N	3.32	1.43	1.35
3	A	601	A3D	C6N-N1N	3.31	1.43	1.35
3	B	603	A3D	O4D-C1D	3.24	1.45	1.41
3	D	607	A3D	PA-O1A	-2.90	1.40	1.50
3	C	605	A3D	C4A-N3A	2.88	1.39	1.35
3	D	607	A3D	C4A-N3A	2.76	1.39	1.35
3	A	601	A3D	O4D-C1D	2.71	1.44	1.41
3	B	603	A3D	C4A-N3A	2.67	1.39	1.35
3	A	601	A3D	C3B-C4B	2.53	1.59	1.53
3	B	603	A3D	C3B-C4B	2.47	1.59	1.53
3	D	607	A3D	C3B-C4B	2.46	1.59	1.53
3	B	603	A3D	PA-O1A	-2.42	1.42	1.50
3	A	601	A3D	C4A-N3A	2.40	1.39	1.35
3	C	605	A3D	O4B-C4B	2.36	1.50	1.45
3	C	605	A3D	C3B-C4B	2.27	1.58	1.53
3	A	601	A3D	PA-O1A	-2.21	1.43	1.50
3	C	605	A3D	PA-O1A	-2.20	1.43	1.50
3	D	607	A3D	O4D-C1D	2.19	1.44	1.41
3	D	607	A3D	C3D-C4D	2.13	1.58	1.53
3	A	601	A3D	C3D-C4D	2.11	1.58	1.53
3	C	605	A3D	C6N-C5N	2.10	1.43	1.38
3	B	603	A3D	C5N-C4N	2.05	1.43	1.38
3	D	607	A3D	C6N-C5N	2.05	1.43	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	605	A3D	C5A-C6A-N6A	4.55	127.27	120.35
3	A	601	A3D	C5A-C6A-N6A	4.33	126.93	120.35
3	D	607	A3D	C5A-C6A-N6A	4.09	126.57	120.35
3	B	603	A3D	N3A-C2A-N1A	-4.02	122.40	128.68
3	A	601	A3D	N3A-C2A-N1A	-4.01	122.42	128.68
3	D	607	A3D	N3A-C2A-N1A	-3.94	122.52	128.68
3	B	603	A3D	C5A-C6A-N6A	3.93	126.32	120.35
3	C	605	A3D	N3A-C2A-N1A	-3.82	122.71	128.68
3	B	603	A3D	O5B-C5B-C4B	-3.72	96.17	108.99
3	D	607	A3D	O5B-C5B-C4B	-3.70	96.24	108.99
3	A	601	A3D	O5B-C5B-C4B	-3.67	96.37	108.99
3	C	605	A3D	O5B-C5B-C4B	-3.46	97.09	108.99
3	C	605	A3D	C1B-N9A-C4A	-3.45	120.57	126.64
3	A	601	A3D	C1B-N9A-C4A	-3.12	121.15	126.64
3	D	607	A3D	C1B-N9A-C4A	-2.84	121.66	126.64
3	C	605	A3D	C2N-C3N-C4N	2.75	121.38	118.26
3	A	601	A3D	C2N-C3N-C4N	2.63	121.24	118.26
3	B	603	A3D	C1B-N9A-C4A	-2.62	122.03	126.64
3	D	607	A3D	C2N-C3N-C4N	2.55	121.14	118.26
3	B	603	A3D	C2N-C3N-C4N	2.53	121.13	118.26
3	A	601	A3D	C5N-C6N-N1N	-2.46	116.87	120.40
3	B	603	A3D	C5N-C6N-N1N	-2.41	116.94	120.40
3	D	607	A3D	C5N-C6N-N1N	-2.40	116.96	120.40
3	B	603	A3D	C6N-N1N-C2N	2.14	123.93	121.97
3	C	605	A3D	C5N-C4N-C3N	-2.05	117.92	120.34
3	D	607	A3D	C5N-C4N-C3N	-2.03	117.94	120.34
3	A	601	A3D	C5N-C4N-C3N	-2.02	117.95	120.34

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	A3D	O4D-C1D-N1N-C2N
3	A	601	A3D	O4D-C1D-N1N-C6N
3	A	601	A3D	C2D-C1D-N1N-C2N
3	A	601	A3D	C2D-C1D-N1N-C6N
3	B	603	A3D	O4D-C1D-N1N-C2N
3	B	603	A3D	O4D-C1D-N1N-C6N
3	B	603	A3D	C2D-C1D-N1N-C2N
3	B	603	A3D	C2D-C1D-N1N-C6N
3	C	605	A3D	O4D-C1D-N1N-C2N
3	C	605	A3D	O4D-C1D-N1N-C6N
3	C	605	A3D	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
3	C	605	A3D	C2D-C1D-N1N-C6N
3	D	607	A3D	O4D-C1D-N1N-C2N
3	D	607	A3D	O4D-C1D-N1N-C6N
3	D	607	A3D	C2D-C1D-N1N-C2N
3	D	607	A3D	C2D-C1D-N1N-C6N
3	A	601	A3D	O4B-C4B-C5B-O5B
3	B	603	A3D	O4B-C4B-C5B-O5B
3	C	605	A3D	O4B-C4B-C5B-O5B
3	D	607	A3D	O4B-C4B-C5B-O5B

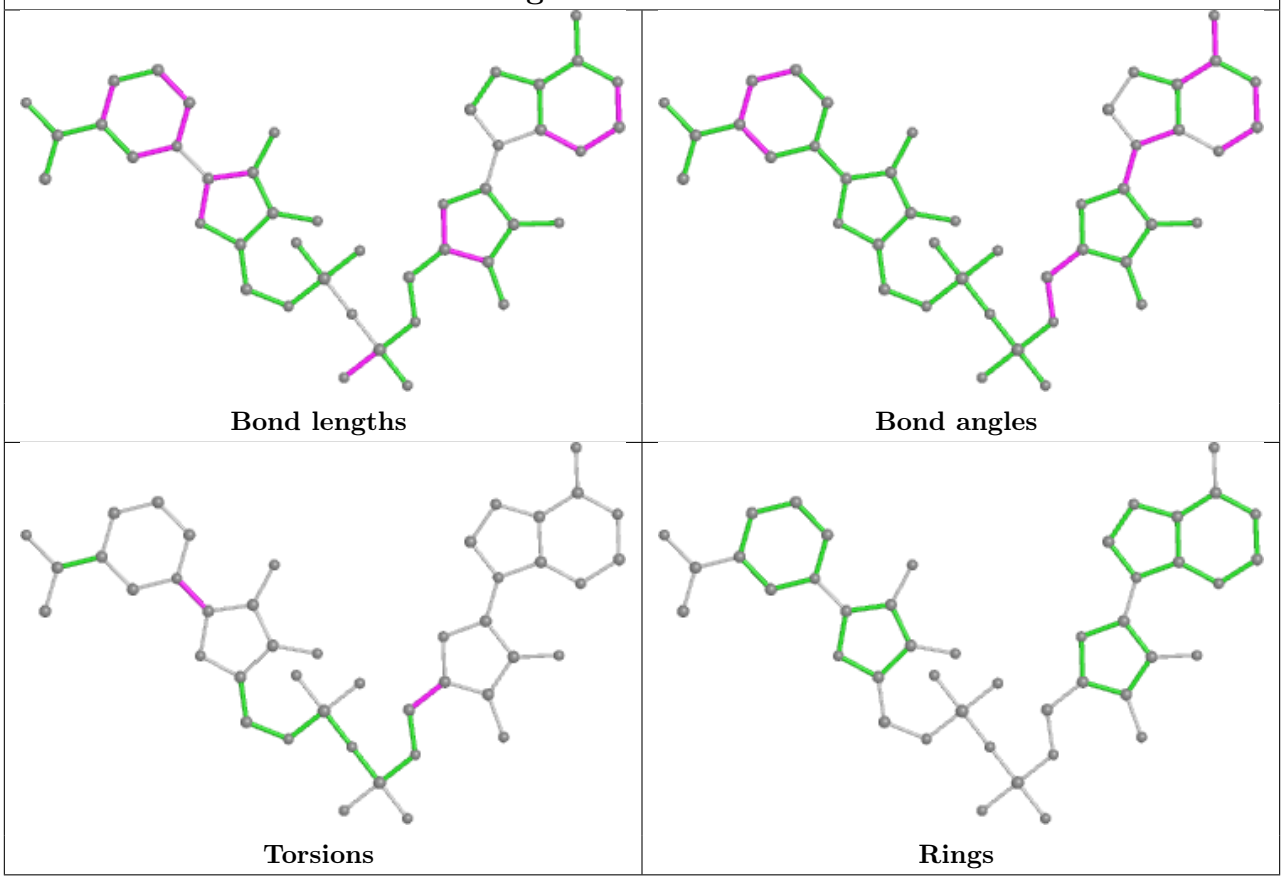
There are no ring outliers.

2 monomers are involved in 3 short contacts:

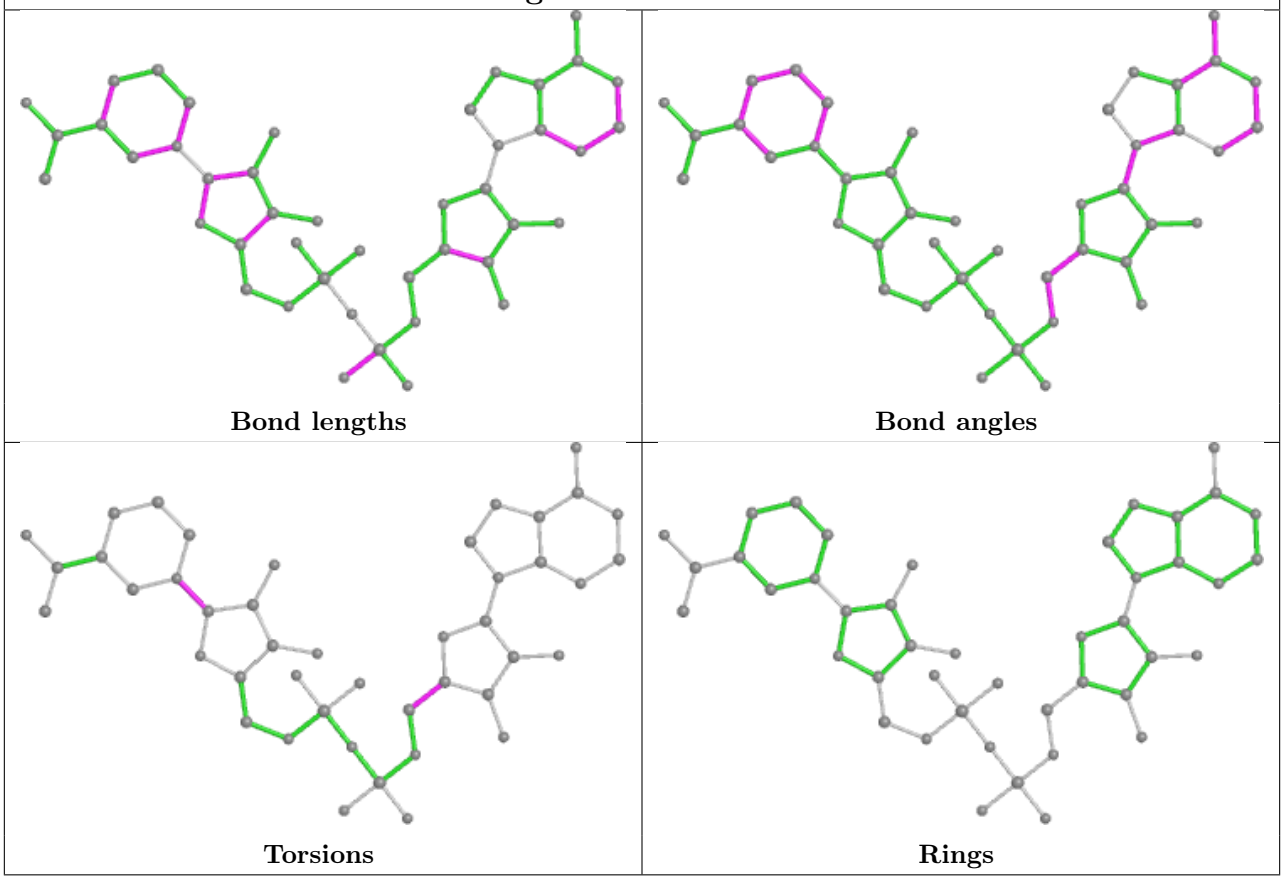
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	605	A3D	1	0
3	D	607	A3D	2	0

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.

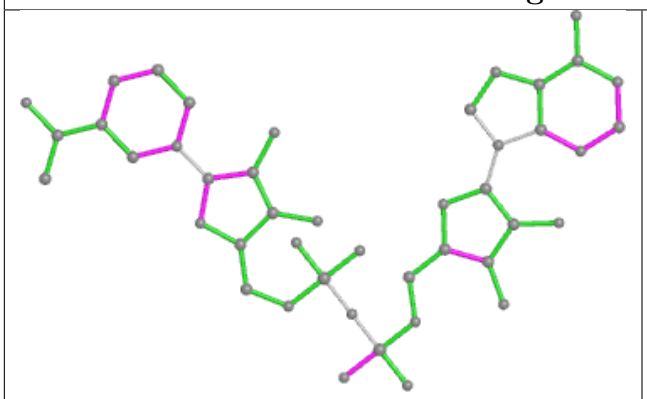
Ligand A3D C 605



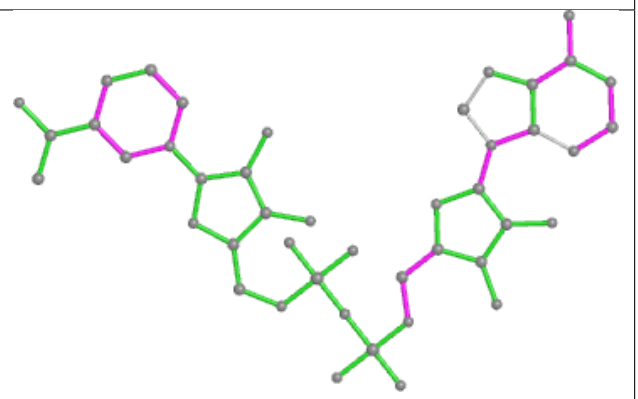
Ligand A3D A 601



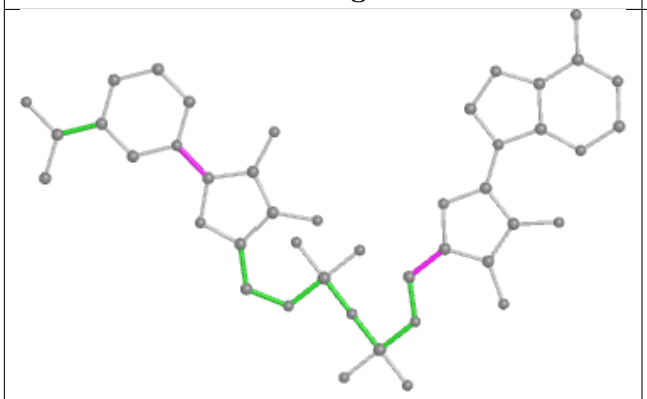
Ligand A3D B 603



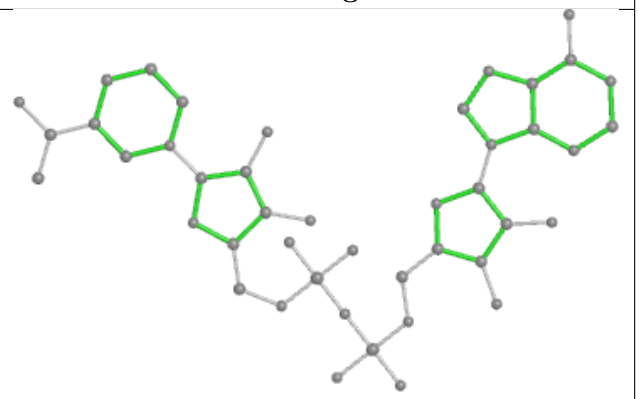
Bond lengths



Bond angles

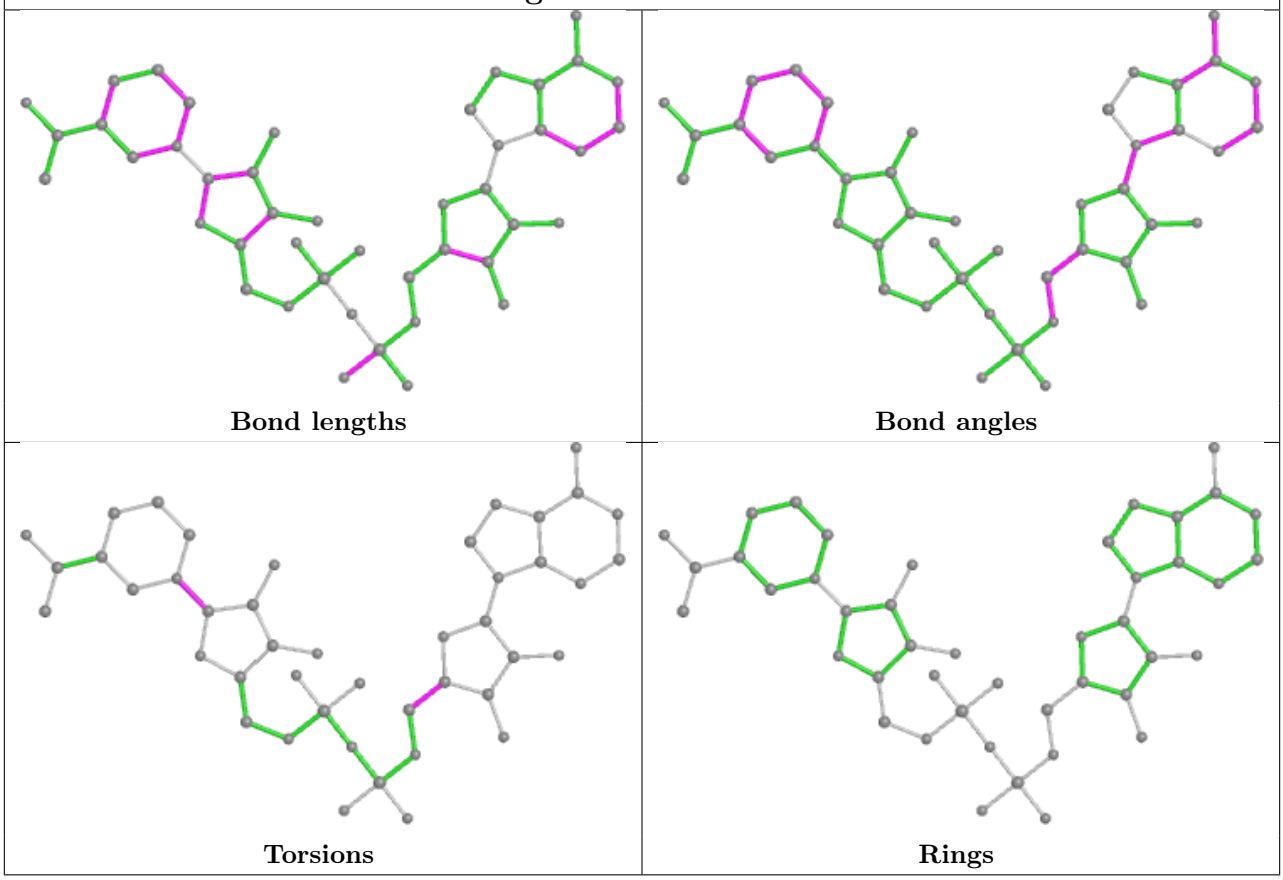


Torsions



Rings

Ligand A3D D 607



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	327/331 (98%)	-0.01	17 (5%)	27	24	12, 17, 34, 47	0
1	B	327/331 (98%)	0.05	14 (4%)	35	32	13, 19, 36, 52	0
1	C	324/331 (97%)	0.40	33 (10%)	6	5	12, 20, 48, 61	0
1	D	325/331 (98%)	0.28	30 (9%)	9	7	13, 20, 43, 59	0
All	All	1303/1324 (98%)	0.18	94 (7%)	15	14	12, 19, 39, 61	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	103(E)	PRO	9.9
1	C	115	PHE	9.7
1	C	103(C)	GLY	7.8
1	C	105(B)	SER	7.8
1	C	103(B)	PRO	7.3
1	D	103(A)	VAL	6.6
1	C	107	TRP	6.4
1	B	83	TYR	6.2
1	D	103(B)	PRO	6.0
1	D	103(E)	PRO	5.9
1	C	331	LEU	5.9
1	C	330	ALA	5.6
1	D	115	PHE	5.5
1	C	108	SER	5.3
1	C	106	GLU	5.2
1	C	332	GLN	5.1
1	D	103(C)	GLY	5.1
1	C	105(A)	ASP	5.1
1	C	103(D)	LYS	5.1
1	A	56	LYS	4.9
1	B	105(B)	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	112	LEU	4.8
1	D	103(D)	LYS	4.6
1	A	103(C)	GLY	4.6
1	D	56	LYS	4.6
1	D	331	LEU	4.6
1	C	15	ALA	4.4
1	C	100	LEU	4.4
1	A	83	TYR	4.4
1	C	101	THR	4.4
1	D	83	TYR	4.3
1	C	56	LYS	4.2
1	D	330	ALA	4.2
1	C	103(A)	VAL	4.1
1	D	332	GLN	4.1
1	C	328	VAL	4.0
1	B	103(B)	PRO	4.0
1	C	110	ASN	4.0
1	B	103(C)	GLY	4.0
1	B	103(E)	PRO	3.9
1	B	309	GLU	3.8
1	A	280	GLY	3.8
1	D	243	GLN	3.7
1	D	108	SER	3.6
1	A	14	PRO	3.6
1	D	241	ARG	3.6
1	D	105(B)	SER	3.6
1	D	100	LEU	3.6
1	D	105(A)	ASP	3.6
1	D	107	TRP	3.6
1	C	329	ALA	3.6
1	C	326	LYS	3.5
1	D	14	PRO	3.5
1	B	103(D)	LYS	3.4
1	C	114	PRO	3.4
1	D	106	GLU	3.3
1	C	327	ALA	3.3
1	C	111	ASP	3.2
1	A	106	GLU	3.2
1	B	14	PRO	3.2
1	D	101	THR	3.1
1	A	105(B)	SER	3.1
1	D	112	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	56	LYS	3.0
1	B	334	PRO	2.9
1	B	106	GLU	2.9
1	C	83	TYR	2.9
1	A	103(E)	PRO	2.9
1	D	326	LYS	2.9
1	A	309	GLU	2.7
1	D	114	PRO	2.7
1	D	110	ASN	2.6
1	C	243	GLN	2.6
1	A	334	PRO	2.5
1	B	243	GLN	2.5
1	A	276	ASN	2.5
1	A	279	TYR	2.5
1	A	103(D)	LYS	2.5
1	D	15	ALA	2.4
1	D	111	ASP	2.4
1	C	241	ARG	2.3
1	A	313	LYS	2.3
1	D	242(C)	GLY	2.3
1	B	317	LYS	2.3
1	C	96	VAL	2.2
1	A	137	VAL	2.2
1	A	142	LEU	2.2
1	C	138	VAL	2.1
1	B	105(A)	ASP	2.1
1	C	102	LYS	2.0
1	A	138	VAL	2.0
1	D	109	ARG	2.0
1	D	95	ILE	2.0
1	C	283	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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	B-factors(Å^2)	Q<0.9
1	CME	C	150	10/11	0.93	0.11	22,25,38,39	0
1	CME	B	150	10/11	0.95	0.08	19,22,34,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CME	A	150	10/11	0.95	0.08	15,18,31,31	0
1	CME	D	150	10/11	0.96	0.08	19,25,34,34	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

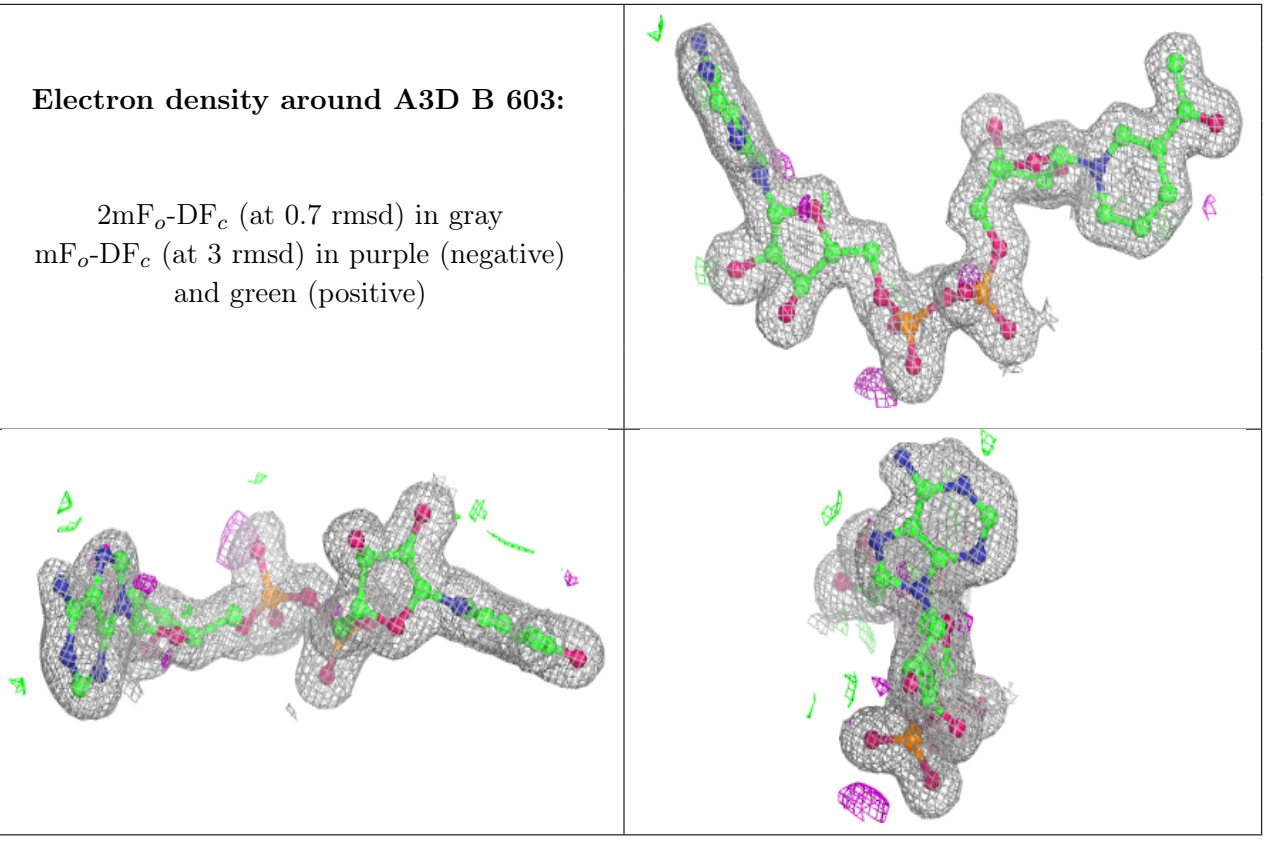
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	602	5/5	0.95	0.09	22,22,25,28	0
2	SO4	C	606	5/5	0.95	0.08	23,25,28,30	0
3	A3D	B	603	44/44	0.95	0.09	16,18,29,32	0
3	A3D	C	605	44/44	0.95	0.08	19,24,31,33	0
3	A3D	D	607	44/44	0.95	0.08	19,22,32,35	0
3	A3D	A	601	44/44	0.96	0.09	14,17,29,33	0
2	SO4	B	604	5/5	0.96	0.09	23,24,27,29	0
2	SO4	D	608	5/5	0.98	0.05	24,26,27,29	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.

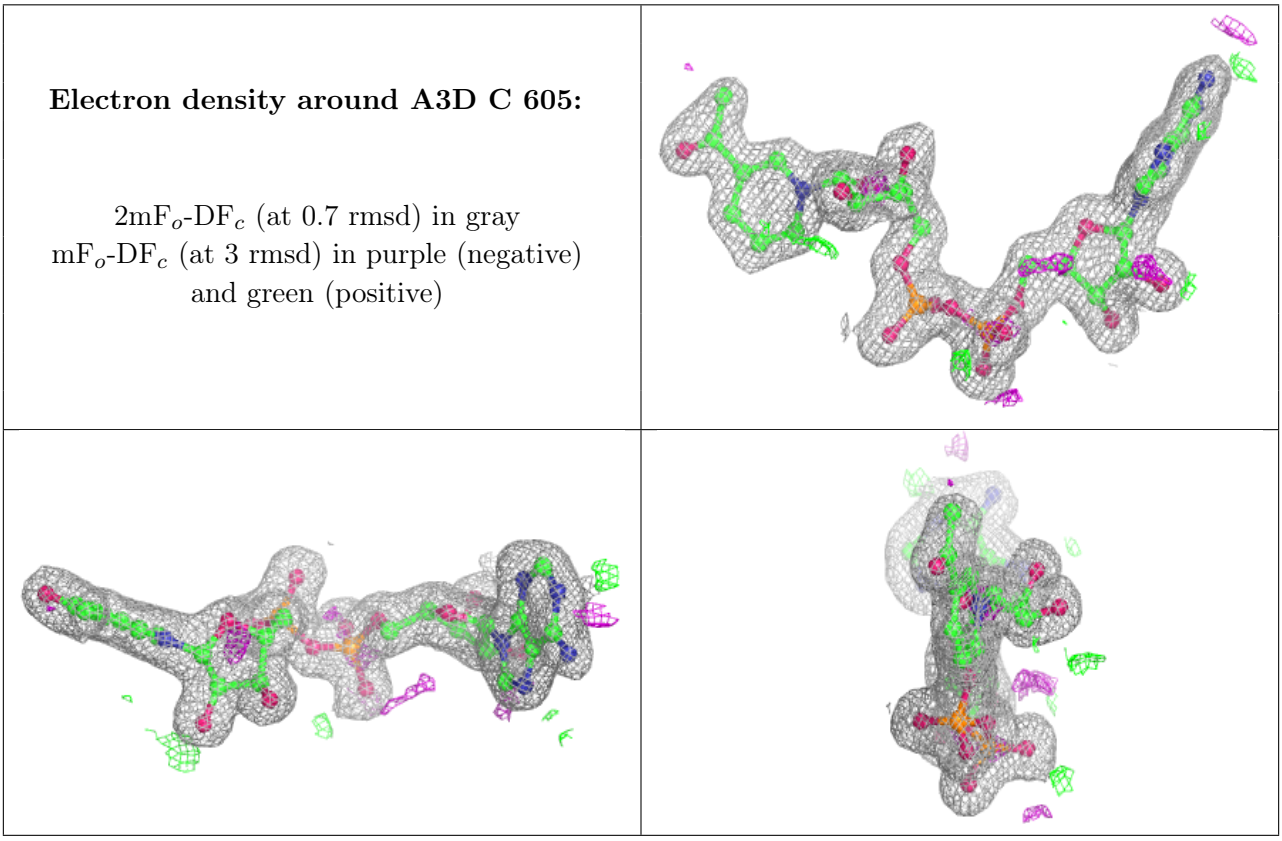
Electron density around A3D B 603:

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



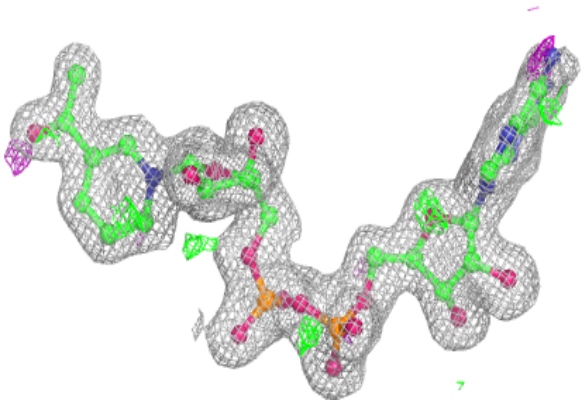
Electron density around A3D C 605:

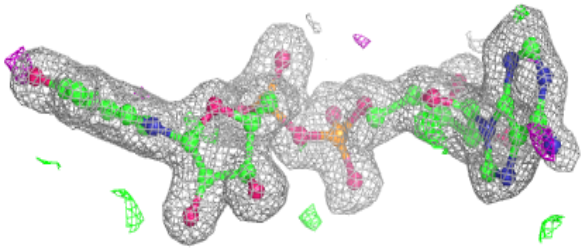
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

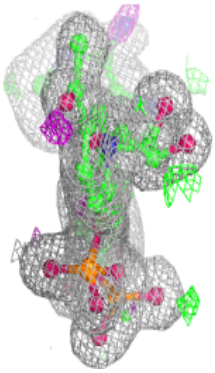


Electron density around A3D D 607:

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

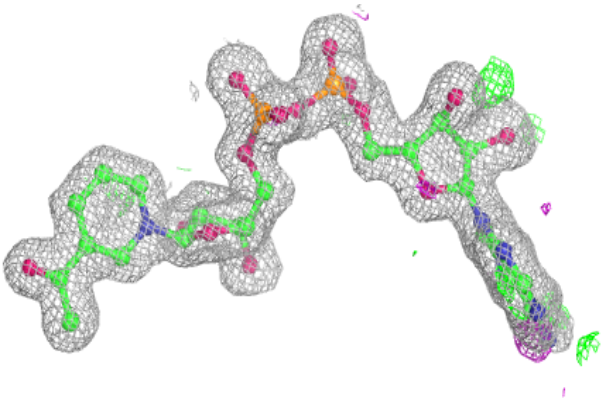


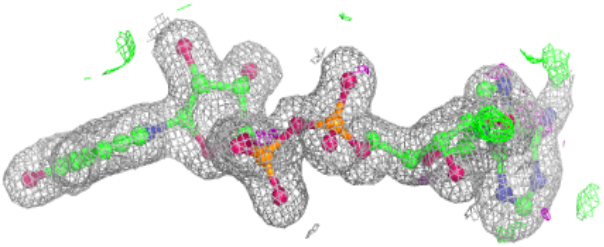




Electron density around A3D A 601:

$2mF_o$-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.