



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 16, 2017 – 07:39 am GMT

PDB ID : 4GLN  
Title : Crystal Structure of Chemically Synthesized Heterochiral {D-Protein Antagonist plus VEGF-A} Protein Complex in space group P21/n  
Authors : Mandal, K.; Uppalapati, M.; Ault-Riche, D.; Kenney, J.; Lowitz, J.; Sidhu, S.; Kent, S.B.H.  
Deposited on : 2012-08-14  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	<b>FAILED</b>
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28986

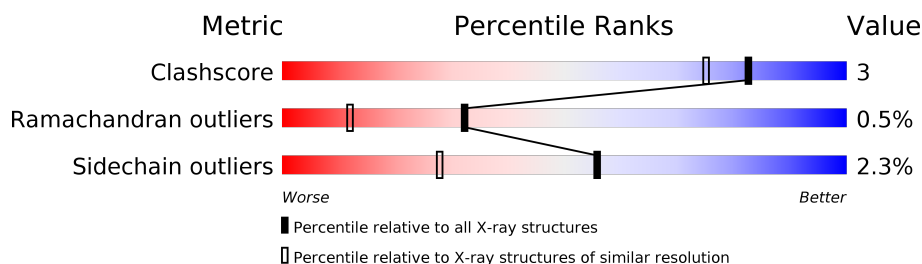
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 Å.

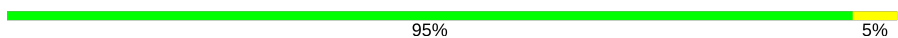
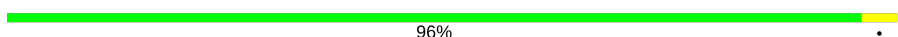


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	D	56	 95% 5%
1	H	56	 96% .
2	E	102	 82% 10% 7%
2	F	102	 84% 9% 7%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3060 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 (with D amino acids) called D-RFX001.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	D	56	Total	C	N	O	0	4	0
			470	305	65	100			
1	H	56	Total	C	N	O	0	6	0
			485	316	65	104			

- Molecule 2 is a protein called Vascular endothelial growth factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	95	Total	C	N	O	S	0	4	0
			781	493	129	146	13			
2	F	95	Total	C	N	O	S	0	6	0
			800	501	134	151	14			

- Molecule 3 is water.

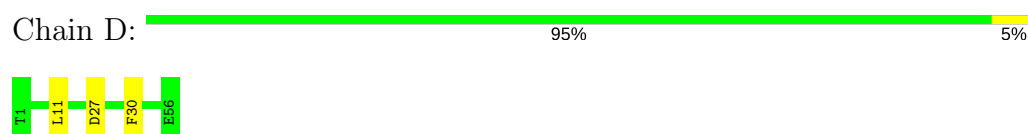
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	126	Total	O	0	0
			126	126		
3	E	132	Total	O	0	0
			132	132		
3	F	167	Total	O	0	0
			167	167		
3	H	99	Total	O	0	0
			99	99		

### 3 Residue-property plots [i](#)

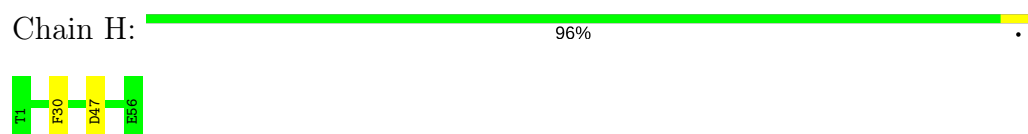
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS failed to run properly.

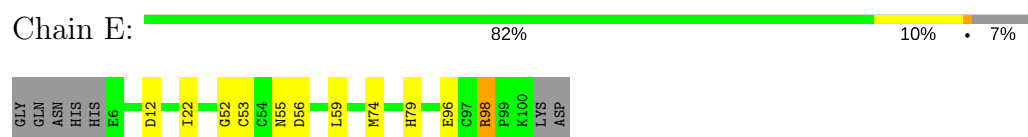
- Molecule 1: D-RFX001



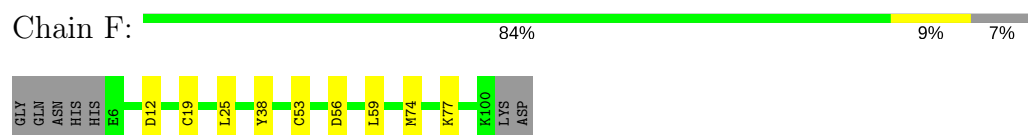
- Molecule 1: D-RFX001



- Molecule 2: Vascular endothelial growth factor A



- Molecule 2: Vascular endothelial growth factor A



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21/n 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.16Å 88.32Å 77.87Å 90.00° 99.98° 90.00°	Depositor
Resolution (Å)	32.22 – 1.60	Depositor
% Data completeness (in resolution range)	97.9 (32.22-1.60)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 1.60Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1128)	Depositor
R, $R_{free}$	0.229 , 0.264	Depositor
Wilson B-factor (Å <sup>2</sup> )	48.8	Xtriage
Anisotropy	-0.890	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *None*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DIL, DPN, DTH, DLE, DAL, DVA, DGL, DSN, DTY, DAS, DTR, DSG, DLY

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	D	0.36	0/6	0.36	0/4
1	H	0.43	0/6	0.18	0/4
2	E	0.34	0/811	0.51	0/1094
2	F	0.33	0/838	0.50	0/1129
All	All	0.34	0/1661	0.50	0/2231

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	470	0	391	3	0
1	H	485	0	404	2	0
2	E	781	0	750	8	0
2	F	800	0	759	6	0
3	D	126	0	0	0	0
3	E	132	0	0	1	0
3	F	167	0	0	2	1
3	H	99	0	0	0	0
All	All	3060	0	2304	14	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 3.

All (14) 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:E:96:GLU:OE1	2:E:98:ARG:NH1	2.15	0.79
2:E:12[B]:ASP:OD2	3:E:324:HOH:O	2.04	0.75
2:E:22[A]:ILE:HD13	2:F:25:LEU:HD12	1.79	0.64
1:D:30:DPN:HE2	2:F:74[B]:MET:SD	2.48	0.54
2:F:38:TYR:CE2	2:F:77:LYS:HG3	2.47	0.49
2:E:74:MET:SD	1:H:30:DPN:HE1	2.58	0.43
1:D:27:DAS:OD1	2:E:55:ASN:ND2	2.52	0.43
2:E:56:ASP:HB3	2:E:59:LEU:HG	2.00	0.43
2:F:56:ASP:HB3	2:F:59:LEU:HG	2.01	0.42
2:E:52:GLY:CA	2:F:25:LEU:HD13	2.49	0.42
2:F:12[A]:ASP:OD1	3:F:366:HOH:O	2.22	0.41
2:E:22[A]:ILE:HD11	3:F:233:HOH:O	2.22	0.40
1:D:11:DLE:HD12	1:D:11:DLE:C	2.52	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)
3:F:303:HOH:O	3:F:321:HOH:O[3_656]	2.17	0.03

## 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	D	2/56 (4%)	2 (100%)	0	0	100	100
1	H	2/56 (4%)	2 (100%)	0	0	100	100
2	E	97/102 (95%)	94 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	100/102 (98%)	98 (98%)	1 (1%)	1 (1%)	18	4
All	All	201/316 (64%)	196 (98%)	4 (2%)	1 (0%)	32	12

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	19	CYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	92/96 (96%)	89 (97%)	3 (3%)	43	16
2	F	96/96 (100%)	95 (99%)	1 (1%)	80	65
All	All	188/192 (98%)	184 (98%)	4 (2%)	56	32

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	53	CYS
2	E	79	HIS
2	E	98	ARG
2	F	53	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

118 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	DTH	D	1	1	6,6,7	1.02	1 (16%)	6,7,9	0.93	0
1	DTH	D	10	1	6,6,7	1.10	1 (16%)	6,7,9	1.03	0
1	DLE	D	11	1	7,7,8	0.77	0	6,8,10	0.83	0
1	DLY	D	12	1	8,8,9	0.63	0	5,8,10	0.90	0
1	DGL	D	14	1	5,8,9	0.81	0	2,9,11	1.10	0
1	DTH	D	15[A]	-	6,6,7	0.92	0	6,7,9	0.79	0
1	DTH	D	15[B]	-	6,6,7	1.25	1 (16%)	6,7,9	0.96	1 (16%)
1	DTH	D	16	1	6,6,7	0.85	0	6,7,9	1.01	1 (16%)
1	DTH	D	17	1	6,6,7	0.89	0	6,7,9	0.93	0
1	DGL	D	18	1	5,8,9	1.32	1 (20%)	2,9,11	1.16	0
1	DAL	D	19	1	4,4,5	1.28	1 (25%)	1,4,6	0.23	0
1	DTY	D	2	1	12,12,13	0.51	0	14,15,17	0.64	0
1	DVA	D	20	1	6,6,7	1.03	1 (16%)	6,7,9	2.01	3 (50%)
1	DAS	D	21	1	4,7,8	1.23	1 (25%)	3,8,10	1.06	0
1	DVA	D	22[A]	1	6,6,7	1.08	1 (16%)	6,7,9	1.03	0
1	DVA	D	22[B]	1	6,6,7	0.85	0	6,7,9	1.24	1 (16%)
1	DPN	D	23	1	11,11,12	0.69	0	12,13,15	0.67	0
1	DAS	D	24	1	4,7,8	1.34	1 (25%)	3,8,10	0.98	0
1	DAL	D	25	1	4,4,5	1.32	1 (25%)	1,4,6	0.40	0
1	DPN	D	26	1	11,11,12	0.83	1 (9%)	12,13,15	0.62	0
1	DAS	D	27	1	4,7,8	1.12	0	3,8,10	1.10	0
1	DVA	D	28	1	6,6,7	0.90	0	6,7,9	1.29	1 (16%)
1	DPN	D	29	1	11,11,12	0.74	0	12,13,15	0.61	0
1	DLY	D	3	1	8,8,9	0.94	1 (12%)	5,8,10	0.87	0
1	DPN	D	30	1	11,11,12	0.73	1 (9%)	12,13,15	0.54	0
1	DVA	D	31	1	6,6,7	1.00	1 (16%)	6,7,9	1.10	0
1	DTY	D	32	1	12,12,13	0.79	1 (8%)	14,15,17	0.52	0
1	DAL	D	33	1	4,4,5	1.17	1 (25%)	1,4,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	DAL	D	34	1	4,4,5	1.22	1 (25%)	1,4,6	0.41	0
1	DSN	D	35[A]	-	5,5,6	1.14	1 (20%)	1,5,7	1.66	0
1	DSN	D	35[B]	-	5,5,6	1.14	1 (20%)	1,5,7	1.66	0
1	DSG	D	36	1	7,7,8	1.03	1 (14%)	7,8,10	0.81	0
1	DPN	D	37	1	11,11,12	0.68	0	12,13,15	0.91	1 (8%)
1	DSN	D	38	1	5,5,6	1.18	1 (20%)	1,5,7	1.59	0
1	DAS	D	39	1	4,7,8	1.26	1 (25%)	3,8,10	0.92	0
1	DLE	D	4	1	7,7,8	0.85	0	6,8,10	0.61	0
1	DPN	D	40	1	11,11,12	0.87	1 (9%)	12,13,15	0.99	1 (8%)
1	DAS	D	41	1	4,7,8	1.31	1 (25%)	3,8,10	1.01	0
1	DAS	D	42	1	4,7,8	1.15	0	3,8,10	0.85	0
1	DTR	D	43	1	14,15,16	0.77	0	13,20,22	0.92	0
1	DTH	D	44	1	6,6,7	0.98	1 (16%)	6,7,9	0.84	0
1	DTY	D	45	1	12,12,13	0.65	0	14,15,17	0.51	0
1	DAS	D	46	1	4,7,8	1.18	1 (25%)	3,8,10	1.25	0
1	DAS	D	47	1	4,7,8	1.25	1 (25%)	3,8,10	1.63	1 (33%)
1	DAL	D	48	1	4,4,5	1.26	1 (25%)	1,4,6	0.33	0
1	DTH	D	49	1	6,6,7	0.85	0	6,7,9	1.09	1 (16%)
1	DIL	D	5	1	7,7,8	0.74	0	6,8,10	1.28	1 (16%)
1	DLY	D	50	1	8,8,9	0.89	1 (12%)	5,8,10	0.62	0
1	DTH	D	51	1	6,6,7	0.82	0	6,7,9	0.83	0
1	DPN	D	52	1	11,11,12	0.70	0	12,13,15	0.93	1 (8%)
1	DTH	D	53	1	6,6,7	0.82	0	6,7,9	0.82	0
1	DVA	D	54	1	6,6,7	0.91	0	6,7,9	0.78	0
1	DTH	D	55	1	6,6,7	0.81	0	6,7,9	0.90	1 (16%)
1	DGL	D	56	1	1,9,9	0.28	0	1,11,11	0.11	0
1	DLE	D	6	1	7,7,8	0.93	1 (14%)	6,8,10	0.57	0
1	DSG	D	7[A]	-	7,7,8	0.79	0	7,8,10	0.55	0
1	DSG	D	7[B]	-	7,7,8	0.79	0	7,8,10	0.77	0
1	DLY	D	9	1	8,8,9	0.90	1 (12%)	5,8,10	0.86	0
1	DTH	H	1	1	6,6,7	1.04	1 (16%)	6,7,9	0.88	0
1	DTH	H	10[A]	1	6,6,7	1.10	1 (16%)	6,7,9	0.89	0
1	DTH	H	10[B]	1	6,6,7	1.01	1 (16%)	6,7,9	1.13	1 (16%)
1	DLE	H	11	1	7,7,8	0.86	1 (14%)	6,8,10	0.71	0
1	DLY	H	12	1	8,8,9	0.64	0	5,8,10	0.75	0
1	DGL	H	14	1	5,8,9	0.77	0	2,9,11	1.27	0
1	DTH	H	15	1	6,6,7	0.93	0	6,7,9	1.05	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	DTH	H	16	1	6,6,7	0.88	0	6,7,9	0.88	0
1	DTH	H	17	1	6,6,7	0.84	0	6,7,9	0.85	0
1	DGL	H	18	1	5,8,9	1.07	1 (20%)	2,9,11	1.29	0
1	DAL	H	19	1	4,4,5	1.19	1 (25%)	1,4,6	0.13	0
1	DTY	H	2	1	12,12,13	0.56	0	14,15,17	0.58	0
1	DVA	H	20	1	6,6,7	1.11	1 (16%)	6,7,9	2.08	3 (50%)
1	DAS	H	21	1	4,7,8	1.09	0	3,8,10	1.08	0
1	DVA	H	22[A]	-	6,6,7	0.86	0	6,7,9	1.28	1 (16%)
1	DVA	H	22[B]	-	6,6,7	1.13	1 (16%)	6,7,9	0.93	0
1	DPN	H	23	1	11,11,12	0.67	0	12,13,15	0.69	0
1	DAS	H	24	1	4,7,8	1.28	1 (25%)	3,8,10	0.96	0
1	DAL	H	25	1	4,4,5	0.91	0	1,4,6	0.49	0
1	DPN	H	26	1	11,11,12	0.79	1 (9%)	12,13,15	0.58	0
1	DAS	H	27	1	4,7,8	1.26	1 (25%)	3,8,10	1.01	0
1	DVA	H	28	1	6,6,7	0.92	0	6,7,9	1.32	1 (16%)
1	DPN	H	29	1	11,11,12	0.85	1 (9%)	12,13,15	0.65	0
1	DLY	H	3	1	8,8,9	0.89	1 (12%)	5,8,10	0.89	0
1	DPN	H	30	1	11,11,12	0.74	1 (9%)	12,13,15	0.58	0
1	DVA	H	31	1	6,6,7	1.13	1 (16%)	6,7,9	0.94	0
1	DTY	H	32	1	12,12,13	0.78	1 (8%)	14,15,17	0.62	0
1	DAL	H	33	1	4,4,5	1.20	1 (25%)	1,4,6	0.45	0
1	DAL	H	34	1	4,4,5	1.23	1 (25%)	1,4,6	0.38	0
1	DSN	H	35[A]	-	5,5,6	1.06	1 (20%)	1,5,7	1.69	0
1	DSN	H	35[B]	-	5,5,6	0.94	0	1,5,7	1.47	0
1	DSG	H	36	1	7,7,8	0.88	1 (14%)	7,8,10	0.87	0
1	DPN	H	37	1	11,11,12	0.64	0	12,13,15	1.05	1 (8%)
1	DSN	H	38	1	5,5,6	1.13	1 (20%)	1,5,7	1.56	0
1	DAS	H	39[A]	1	4,7,8	1.22	1 (25%)	3,8,10	0.99	0
1	DAS	H	39[B]	1	4,7,8	1.17	1 (25%)	3,8,10	1.04	0
1	DLE	H	4	1	7,7,8	0.65	0	6,8,10	0.73	0
1	DPN	H	40	1	11,11,12	0.78	1 (9%)	12,13,15	0.98	1 (8%)
1	DAS	H	41	1	4,7,8	1.28	1 (25%)	3,8,10	1.00	0
1	DAS	H	42	1	4,7,8	1.12	0	3,8,10	0.83	0
1	DTR	H	43	1	14,15,16	0.76	0	13,20,22	0.90	0
1	DTH	H	44	1	6,6,7	0.91	0	6,7,9	0.85	0
1	DTY	H	45	1	12,12,13	0.71	1 (8%)	14,15,17	0.50	0
1	DAS	H	46	1	4,7,8	1.05	0	3,8,10	1.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	DAS	H	47[A]	-	4,7,8	1.10	0	3,8,10	1.01	0
1	DAS	H	47[B]	-	4,7,8	1.41	1 (25%)	3,8,10	0.97	0
1	DAL	H	48	1	4,4,5	1.34	1 (25%)	1,4,6	0.17	0
1	DTH	H	49	1	6,6,7	0.91	0	6,7,9	0.95	0
1	DIL	H	5[A]	-	7,7,8	0.78	0	6,8,10	1.73	2 (33%)
1	DIL	H	5[B]	-	7,7,8	0.74	0	6,8,10	1.06	0
1	DLY	H	50	1	8,8,9	0.82	1 (12%)	5,8,10	0.62	0
1	DTH	H	51	1	6,6,7	0.89	0	6,7,9	0.86	0
1	DPN	H	52	1	11,11,12	0.64	0	12,13,15	0.89	1 (8%)
1	DTH	H	53	1	6,6,7	0.88	0	6,7,9	0.83	0
1	DVA	H	54	1	6,6,7	0.84	0	6,7,9	0.85	0
1	DTH	H	55	1	6,6,7	0.71	0	6,7,9	0.87	0
1	DGL	H	56	1	1,9,9	0.24	0	1,11,11	0.01	0
1	DLE	H	6	1	7,7,8	0.72	0	6,8,10	0.75	0
1	DSG	H	7	1	7,7,8	0.75	0	7,8,10	0.59	0
1	DLY	H	9	1	8,8,9	0.90	1 (12%)	5,8,10	0.94	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
1	DTH	D	1	1	-	0/4/6/8	0/0/0/0
1	DTH	D	10	1	-	0/4/6/8	0/0/0/0
1	DLE	D	11	1	-	0/4/6/8	0/0/0/0
1	DLY	D	12	1	-	0/5/7/9	0/0/0/0
1	DGL	D	14	1	-	0/3/7/9	0/0/0/0
1	DTH	D	15[A]	-	-	0/4/6/8	0/0/0/0
1	DTH	D	15[B]	-	-	0/4/6/8	0/0/0/0
1	DTH	D	16	1	-	0/4/6/8	0/0/0/0
1	DTH	D	17	1	-	0/4/6/8	0/0/0/0
1	DGL	D	18	1	-	0/3/7/9	0/0/0/0
1	DAL	D	19	1	-	0/0/2/4	0/0/0/0
1	DTY	D	2	1	-	0/4/6/8	0/1/1/1
1	DVA	D	20	1	-	0/5/6/8	0/0/0/0
1	DAS	D	21	1	-	0/2/6/8	0/0/0/0
1	DVA	D	22[A]	1	-	0/5/6/8	0/0/0/0
1	DVA	D	22[B]	1	-	0/5/6/8	0/0/0/0
1	DPN	D	23	1	-	0/4/6/8	0/1/1/1
1	DAS	D	24	1	-	0/2/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DAL	D	25	1	-	0/0/2/4	0/0/0/0
1	DPN	D	26	1	-	0/4/6/8	0/1/1/1
1	DAS	D	27	1	-	0/2/6/8	0/0/0/0
1	DVA	D	28	1	-	0/5/6/8	0/0/0/0
1	DPN	D	29	1	-	0/4/6/8	0/1/1/1
1	DLY	D	3	1	-	0/5/7/9	0/0/0/0
1	DPN	D	30	1	-	0/4/6/8	0/1/1/1
1	DVA	D	31	1	-	0/5/6/8	0/0/0/0
1	DTY	D	32	1	-	0/4/6/8	0/1/1/1
1	DAL	D	33	1	-	0/0/2/4	0/0/0/0
1	DAL	D	34	1	-	0/0/2/4	0/0/0/0
1	DSN	D	35[A]	-	-	0/2/4/6	0/0/0/0
1	DSN	D	35[B]	-	-	0/2/4/6	0/0/0/0
1	DSG	D	36	1	-	0/4/6/8	0/0/0/0
1	DPN	D	37	1	-	0/4/6/8	0/1/1/1
1	DSN	D	38	1	-	0/2/4/6	0/0/0/0
1	DAS	D	39	1	-	0/2/6/8	0/0/0/0
1	DLE	D	4	1	-	0/4/6/8	0/0/0/0
1	DPN	D	40	1	-	0/4/6/8	0/1/1/1
1	DAS	D	41	1	-	0/2/6/8	0/0/0/0
1	DAS	D	42	1	-	0/2/6/8	0/0/0/0
1	DTR	D	43	1	-	0/3/6/8	0/2/2/2
1	DTH	D	44	1	-	0/4/6/8	0/0/0/0
1	DTY	D	45	1	-	0/4/6/8	0/1/1/1
1	DAS	D	46	1	-	0/2/6/8	0/0/0/0
1	DAS	D	47	1	-	0/2/6/8	0/0/0/0
1	DAL	D	48	1	-	0/0/2/4	0/0/0/0
1	DTH	D	49	1	-	0/4/6/8	0/0/0/0
1	DIL	D	5	1	-	0/7/8/10	0/0/0/0
1	DLY	D	50	1	-	0/5/7/9	0/0/0/0
1	DTH	D	51	1	-	0/4/6/8	0/0/0/0
1	DPN	D	52	1	-	0/4/6/8	0/1/1/1
1	DTH	D	53	1	-	0/4/6/8	0/0/0/0
1	DVA	D	54	1	-	0/5/6/8	0/0/0/0
1	DTH	D	55	1	-	0/4/6/8	0/0/0/0
1	DGL	D	56	1	-	0/3/9/9	0/0/0/0
1	DLE	D	6	1	-	0/4/6/8	0/0/0/0
1	DSG	D	7[A]	-	-	0/4/6/8	0/0/0/0
1	DSG	D	7[B]	-	-	0/4/6/8	0/0/0/0
1	DLY	D	9	1	-	0/5/7/9	0/0/0/0
1	DTH	H	1	1	-	0/4/6/8	0/0/0/0
1	DTH	H	10[A]	1	-	0/4/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DTH	H	10[B]	1	-	0/4/6/8	0/0/0/0
1	DLE	H	11	1	-	0/4/6/8	0/0/0/0
1	DLY	H	12	1	-	0/5/7/9	0/0/0/0
1	DGL	H	14	1	-	0/3/7/9	0/0/0/0
1	DTH	H	15	1	-	0/4/6/8	0/0/0/0
1	DTH	H	16	1	-	0/4/6/8	0/0/0/0
1	DTH	H	17	1	-	0/4/6/8	0/0/0/0
1	DGL	H	18	1	-	0/3/7/9	0/0/0/0
1	DAL	H	19	1	-	0/0/2/4	0/0/0/0
1	DTY	H	2	1	-	0/4/6/8	0/1/1/1
1	DVA	H	20	1	-	0/5/6/8	0/0/0/0
1	DAS	H	21	1	-	0/2/6/8	0/0/0/0
1	DVA	H	22[A]	-	-	0/5/6/8	0/0/0/0
1	DVA	H	22[B]	-	-	0/5/6/8	0/0/0/0
1	DPN	H	23	1	-	0/4/6/8	0/1/1/1
1	DAS	H	24	1	-	0/2/6/8	0/0/0/0
1	DAL	H	25	1	-	0/0/2/4	0/0/0/0
1	DPN	H	26	1	-	0/4/6/8	0/1/1/1
1	DAS	H	27	1	-	0/2/6/8	0/0/0/0
1	DVA	H	28	1	-	0/5/6/8	0/0/0/0
1	DPN	H	29	1	-	0/4/6/8	0/1/1/1
1	DLY	H	3	1	-	0/5/7/9	0/0/0/0
1	DPN	H	30	1	-	0/4/6/8	0/1/1/1
1	DVA	H	31	1	-	0/5/6/8	0/0/0/0
1	DTY	H	32	1	-	0/4/6/8	0/1/1/1
1	DAL	H	33	1	-	0/0/2/4	0/0/0/0
1	DAL	H	34	1	-	0/0/2/4	0/0/0/0
1	DSN	H	35[A]	-	-	0/2/4/6	0/0/0/0
1	DSN	H	35[B]	-	-	0/2/4/6	0/0/0/0
1	DSG	H	36	1	-	0/4/6/8	0/0/0/0
1	DPN	H	37	1	-	0/4/6/8	0/1/1/1
1	DSN	H	38	1	-	0/2/4/6	0/0/0/0
1	DAS	H	39[A]	1	-	0/2/6/8	0/0/0/0
1	DAS	H	39[B]	1	-	0/2/6/8	0/0/0/0
1	DLE	H	4	1	-	0/4/6/8	0/0/0/0
1	DPN	H	40	1	-	0/4/6/8	0/1/1/1
1	DAS	H	41	1	-	0/2/6/8	0/0/0/0
1	DAS	H	42	1	-	0/2/6/8	0/0/0/0
1	DTR	H	43	1	-	0/3/6/8	0/2/2/2
1	DTH	H	44	1	-	0/4/6/8	0/0/0/0
1	DTY	H	45	1	-	0/4/6/8	0/1/1/1
1	DAS	H	46	1	-	0/2/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DAS	H	47[A]	-	-	0/2/6/8	0/0/0/0
1	DAS	H	47[B]	-	-	0/2/6/8	0/0/0/0
1	DAL	H	48	1	-	0/0/2/4	0/0/0/0
1	DTH	H	49	1	-	0/4/6/8	0/0/0/0
1	DIL	H	5[A]	-	-	0/7/8/10	0/0/0/0
1	DIL	H	5[B]	-	-	0/7/8/10	0/0/0/0
1	DLY	H	50	1	-	0/5/7/9	0/0/0/0
1	DTH	H	51	1	-	0/4/6/8	0/0/0/0
1	DPN	H	52	1	-	0/4/6/8	0/1/1/1
1	DTH	H	53	1	-	0/4/6/8	0/0/0/0
1	DVA	H	54	1	-	0/5/6/8	0/0/0/0
1	DTH	H	55	1	-	0/4/6/8	0/0/0/0
1	DGL	H	56	1	-	0/3/9/9	0/0/0/0
1	DLE	H	6	1	-	0/4/6/8	0/0/0/0
1	DSG	H	7	1	-	0/4/6/8	0/0/0/0
1	DLY	H	9	1	-	0/5/7/9	0/0/0/0

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	40	DPN	CA-C	2.00	1.52	1.50
1	H	36	DSG	CA-C	2.01	1.52	1.50
1	D	30	DPN	CA-C	2.02	1.52	1.50
1	H	50	DLY	CA-C	2.02	1.52	1.50
1	H	45	DTY	CA-C	2.06	1.53	1.50
1	H	35[A]	DSN	CA-C	2.07	1.53	1.50
1	D	44	DTH	CA-C	2.07	1.53	1.50
1	H	11	DLE	CA-C	2.07	1.53	1.50
1	H	18	DGL	CA-C	2.09	1.53	1.50
1	H	30	DPN	CA-C	2.10	1.53	1.50
1	H	39[B]	DAS	CA-C	2.10	1.53	1.50
1	D	26	DPN	CA-C	2.11	1.53	1.50
1	D	6	DLE	CA-C	2.11	1.53	1.50
1	D	46	DAS	CA-C	2.12	1.53	1.50
1	H	3	DLY	CA-C	2.12	1.53	1.50
1	D	33	DAL	CA-C	2.13	1.53	1.50
1	D	31	DVA	CA-C	2.13	1.53	1.50
1	D	3	DLY	CA-C	2.14	1.53	1.50
1	H	33	DAL	CA-C	2.15	1.53	1.50
1	H	19	DAL	CA-C	2.17	1.53	1.50
1	H	39[A]	DAS	CA-C	2.17	1.53	1.50
1	D	1	DTH	CA-C	2.19	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	50	DLY	CA-C	2.19	1.53	1.50
1	D	34	DAL	CA-C	2.20	1.53	1.50
1	H	26	DPN	CA-C	2.20	1.53	1.50
1	H	34	DAL	CA-C	2.21	1.53	1.50
1	H	27	DAS	CA-C	2.21	1.53	1.50
1	H	9	DLY	CA-C	2.21	1.53	1.50
1	D	21	DAS	CA-C	2.22	1.53	1.50
1	D	9	DLY	CA-C	2.22	1.53	1.50
1	H	29	DPN	CA-C	2.22	1.53	1.50
1	D	35[B]	DSN	CA-C	2.24	1.53	1.50
1	D	35[A]	DSN	CA-C	2.24	1.53	1.50
1	D	39	DAS	CA-C	2.25	1.53	1.50
1	H	10[B]	DTH	CA-C	2.26	1.53	1.50
1	H	1	DTH	CA-C	2.27	1.53	1.50
1	D	47	DAS	CA-C	2.29	1.53	1.50
1	D	48	DAL	CA-C	2.29	1.53	1.50
1	H	38	DSN	CA-C	2.30	1.53	1.50
1	H	24	DAS	CA-C	2.31	1.53	1.50
1	D	20	DVA	CA-C	2.34	1.53	1.50
1	H	41	DAS	CA-C	2.34	1.53	1.50
1	D	19	DAL	CA-C	2.35	1.53	1.50
1	D	41	DAS	CA-C	2.39	1.53	1.50
1	H	32	DTY	CA-C	2.40	1.53	1.50
1	D	32	DTY	CA-C	2.40	1.53	1.50
1	D	10	DTH	CA-C	2.41	1.53	1.50
1	D	25	DAL	CA-C	2.41	1.53	1.50
1	D	36	DSG	CA-C	2.44	1.53	1.50
1	D	38	DSN	CA-C	2.45	1.53	1.50
1	D	22[A]	DVA	CA-C	2.45	1.53	1.50
1	H	48	DAL	CA-C	2.45	1.53	1.50
1	D	24	DAS	CA-C	2.46	1.53	1.50
1	H	31	DVA	CA-C	2.48	1.53	1.50
1	D	40	DPN	CA-C	2.49	1.53	1.50
1	H	10[A]	DTH	CA-C	2.50	1.53	1.50
1	H	20	DVA	CA-C	2.54	1.53	1.50
1	H	22[B]	DVA	CA-C	2.57	1.53	1.50
1	H	47[B]	DAS	CA-C	2.60	1.53	1.50
1	D	15[B]	DTH	CA-C	2.62	1.53	1.50
1	D	18	DGL	CA-C	2.70	1.53	1.50

All (26) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	5[A]	DIL	CB-CA-C	-3.56	107.33	112.84
1	H	20	DVA	CB-CA-C	-3.14	108.66	112.96
1	H	37	DPN	CB-CA-C	-3.04	105.55	111.41
1	D	20	DVA	CB-CA-C	-2.84	109.07	112.96
1	H	28	DVA	CB-CA-C	-2.77	109.17	112.96
1	D	28	DVA	CB-CA-C	-2.72	109.23	112.96
1	H	40	DPN	CB-CA-C	-2.54	106.51	111.41
1	D	52	DPN	CB-CA-C	-2.52	106.55	111.41
1	D	40	DPN	CB-CA-C	-2.49	106.61	111.41
1	H	52	DPN	CB-CA-C	-2.48	106.63	111.41
1	D	37	DPN	CB-CA-C	-2.41	106.77	111.41
1	H	20	DVA	O-C-CA	-2.36	119.64	125.15
1	D	20	DVA	O-C-CA	-2.35	119.68	125.15
1	D	16	DTH	O-C-CA	-2.34	119.70	125.15
1	D	47	DAS	CB-CA-C	-2.28	107.03	111.41
1	H	22[A]	DVA	CB-CA-C	-2.26	109.87	112.96
1	D	22[B]	DVA	CB-CA-C	-2.23	109.91	112.96
1	H	5[A]	DIL	O-C-CA	-2.22	119.97	125.15
1	D	49	DTH	O-C-CA	-2.19	120.04	125.15
1	H	15	DTH	O-C-CA	-2.19	120.05	125.15
1	D	5	DIL	O-C-CA	-2.13	120.18	125.15
1	H	10[B]	DTH	O-C-CA	-2.09	120.28	125.15
1	D	15[B]	DTH	O-C-CA	-2.08	120.31	125.15
1	D	55	DTH	O-C-CA	-2.01	120.47	125.15
1	H	20	DVA	C-CA-N	3.24	116.39	109.86
1	D	20	DVA	C-CA-N	3.26	116.45	109.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	11	DLE	1	0
1	D	27	DAS	1	0
1	D	30	DPN	1	0
1	H	30	DPN	1	0
1	H	47[B]	DAS	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.