



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2017 – 12:40 AM EDT

PDB ID : 5HHC  
Title : Crystal Structure of Chemically Synthesized Heterochiral {RFX037 plus VEGF-A} Protein Complex in space group P21/n  
Authors : Uppalapati, M.; Lee, D.J.; Mandal, K.; Kent, S.B.H.; Sidhu, S.  
Deposited on : unknown  
Resolution : 2.10 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)	:	rb-20029824

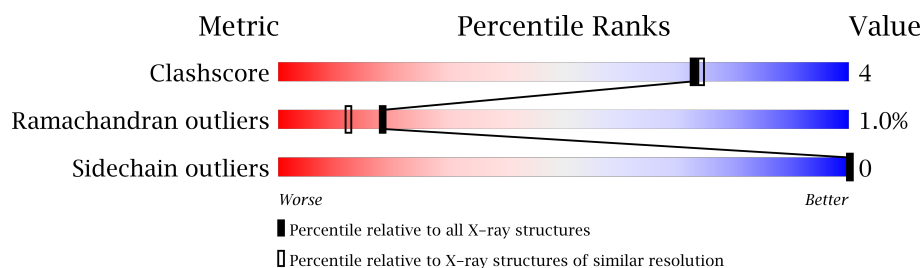
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.



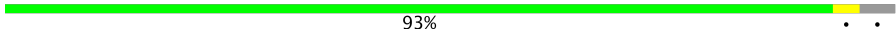

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)

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	A	102	
1	B	102	
2	C	69	
2	D	69	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2877 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 Vascular endothelial growth factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	95	Total	C	N	O	S	0	4	0
			800	502	134	151	13			
1	B	95	Total	C	N	O	S	0	3	0
			793	496	135	149	13			

- Molecule 2 is a protein (with D amino acids) called D- Vascular endothelial growth factor-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	66	Total	C	N	O	0	2	0
			544	344	91	109			
2	D	68	Total	C	N	O	0	1	0
			551	346	92	113			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	B	55	Total	O	0	0
			55	55		
4	C	31	Total	O	0	0
			31	31		
4	D	29	Total	O	0	0
			29	29		

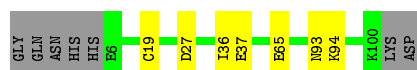
### 3 Residue-property plots [i](#)

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: Vascular endothelial growth factor A

Chain A: 



- Molecule 1: Vascular endothelial growth factor A

Chain B: 



- Molecule 2: D- Vascular endothelial growth factor-A

Chain C: 



- Molecule 2: D- Vascular endothelial growth factor-A

Chain D: 



## 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, $\alpha$ , $\beta$ , $\gamma$	55.29Å 87.24Å 81.34Å 90.00° 101.42° 90.00°	Depositor
Resolution (Å)	49.62 – 2.10	Depositor
% Data completeness (in resolution range)	98.8 (49.62-2.10)	Depositor
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.261 , 0.307	Depositor
Wilson B-factor (Å <sup>2</sup> )	49.7	Xtriage
Anisotropy	-0.752	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	2877	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	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, GOL, DTH, DLE, DAL, DPN, DVA, DGL, DSN, DTY, DAR, 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	A	0.53	0/821	0.57	0/1106
1	B	0.55	0/812	0.61	0/1095
2	C	0.40	0/20	0.36	0/18
2	D	0.33	0/20	0.91	0/18
All	All	0.54	0/1673	0.59	0/2237

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	A	800	0	763	4	0
1	B	793	0	744	5	0
2	C	544	0	460	2	0
2	D	551	0	455	10	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	62	0	0	1	0
4	B	55	0	0	2	0
4	C	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	29	0	0	1	0
All	All	2877	0	2438	20	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 (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASP:OD2	4:A:301:HOH:O	1.99	0.79
1:B:65:GLU:OE1	4:B:301:HOH:O	2.00	0.79
1:B:66:GLU:OE2	4:B:302:HOH:O	2.10	0.68
1:A:93:ASN:O	1:A:94:LYS:HD2	1.95	0.67
2:D:3:DAR:O	2:D:5:DAR:N	2.35	0.60
2:D:2:DAR:HA	2:D:26:DGL:HG3	1.87	0.57
2:D:5:DAR:HG2	2:D:6:GLY:H	1.71	0.56
1:A:65:GLU:OE1	1:A:94:LYS:HD3	2.10	0.52
2:D:11:DLY:HD2	2:D:22:DGL:OE2	2.13	0.49
2:D:5:DAR:C	2:D:7:GLY:H	2.25	0.48
2:D:17:DLY:HE3	4:D:121:HOH:O	2.13	0.48
2:D:51:DTR:HE1	2:D:60:DPN:HD1	1.79	0.47
1:B:38:TYR:CE1	1:B:77:LYS:HG3	2.49	0.47
1:A:36:ILE:HG13	1:A:37:GLU:HG2	1.97	0.46
2:D:2:DAR:O	2:D:3:DAR:NH2	2.48	0.46
2:D:5:DAR:HG2	2:D:6:GLY:N	2.31	0.45
2:D:1:DAR:HH12	2:D:32:DAS:CG	2.29	0.45
1:B:66:GLU:CD	1:B:90:LEU:HD21	2.41	0.41
2:C:37:DPN:HA	2:C:37:DPN:HD1	1.88	0.41
1:B:74:MET:SD	2:C:38:DPN:HE1	2.62	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	97/102 (95%)	96 (99%)	0	1 (1%)	18	12
1	B	96/102 (94%)	94 (98%)	1 (1%)	1 (1%)	18	12
2	C	5/69 (7%)	5 (100%)	0	0	100	100
2	D	6/69 (9%)	6 (100%)	0	0	100	100
All	All	204/342 (60%)	201 (98%)	1 (0%)	2 (1%)	18	12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	CYS
1	B	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	
1	A	94/96 (98%)	94 (100%)	0	100	100
1	B	92/96 (96%)	92 (100%)	0	100	100
All	All	186/192 (97%)	186 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 ⓘ

125 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$
2	DAR	C	1	2	10,10,11	0.83	1 (10%)	7,11,13	0.79	0
2	DTY	C	10	2	12,12,13	1.03	2 (16%)	14,15,17	0.53	0
2	DLY	C	11	2	8,8,9	0.96	1 (12%)	5,8,10	0.97	0
2	DLE	C	12	2	7,7,8	1.25	1 (14%)	6,8,10	0.68	0
2	DIL	C	13	2	7,7,8	0.85	0	6,8,10	1.71	2 (33%)
2	DLE	C	14	2	7,7,8	0.94	0	6,8,10	0.65	0
2	DSG	C	15[A]	2	7,7,8	0.62	0	7,8,10	0.94	0
2	DSG	C	15[B]	2	7,7,8	0.57	0	7,8,10	0.57	0
2	DLY	C	17	2	8,8,9	0.79	0	5,8,10	0.90	0
2	DTH	C	18	2	6,6,7	1.18	1 (16%)	6,7,9	1.25	1 (16%)
2	DLE	C	19	2	7,7,8	0.85	0	6,8,10	0.87	1 (16%)
2	DAR	C	2	2	10,10,11	0.86	1 (10%)	7,11,13	0.81	0
2	DLY	C	20	2	8,8,9	0.52	0	5,8,10	1.07	0
2	DGL	C	22	2	5,8,9	1.37	1 (20%)	2,9,11	1.42	0
2	DTH	C	23	2	6,6,7	1.50	1 (16%)	6,7,9	1.05	1 (16%)
2	DTH	C	24	2	6,6,7	0.65	0	6,7,9	0.90	1 (16%)
2	DTH	C	25	2	6,6,7	1.31	1 (16%)	6,7,9	0.86	0
2	DGL	C	26	2	5,8,9	0.71	0	2,9,11	1.53	0
2	DAL	C	27	2	4,4,5	1.16	0	1,4,6	0.39	0
2	DVA	C	28	2	6,6,7	1.10	1 (16%)	6,7,9	1.21	1 (16%)
2	DAS	C	29	2	4,7,8	1.16	0	3,8,10	0.94	0
2	DAR	C	3	2	10,10,11	0.72	0	7,11,13	0.60	0
2	DVA	C	30[A]	2	6,6,7	1.08	1 (16%)	6,7,9	0.81	0
2	DVA	C	30[B]	2	6,6,7	0.96	1 (16%)	6,7,9	1.11	0
2	DPN	C	31	2	11,11,12	0.89	1 (9%)	12,13,15	0.55	0
2	DAS	C	32	2	4,7,8	1.91	1 (25%)	3,8,10	1.20	0
2	DAL	C	33	2	4,4,5	1.70	1 (25%)	1,4,6	0.19	0
2	DPN	C	34	2	11,11,12	1.06	1 (9%)	12,13,15	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DAS	C	35	2	4,7,8	1.55	1 (25%)	3,8,10	1.20	0
2	DVA	C	36	2	6,6,7	1.21	1 (16%)	6,7,9	1.44	1 (16%)
2	DPN	C	37	2	11,11,12	1.30	1 (9%)	12,13,15	0.60	0
2	DPN	C	38	2	11,11,12	0.85	1 (9%)	12,13,15	0.59	0
2	DVA	C	39	2	6,6,7	1.04	1 (16%)	6,7,9	1.73	1 (16%)
2	DAR	C	4	2	10,10,11	0.65	0	7,11,13	0.75	0
2	DTY	C	40	2	12,12,13	0.88	1 (8%)	14,15,17	0.64	0
2	DAL	C	41	2	4,4,5	1.23	1 (25%)	1,4,6	0.28	0
2	DAL	C	42	2	4,4,5	1.11	1 (25%)	1,4,6	0.43	0
2	DSN	C	43	2	5,5,6	1.37	1 (20%)	1,5,7	1.49	0
2	DSG	C	44	2	7,7,8	0.74	0	7,8,10	0.93	0
2	DPN	C	45	2	11,11,12	0.52	0	12,13,15	0.92	1 (8%)
2	DSN	C	46	2	5,5,6	1.47	1 (20%)	1,5,7	1.52	0
2	DAS	C	47	2	4,7,8	1.56	1 (25%)	3,8,10	1.06	0
2	DPN	C	48	2	11,11,12	0.88	1 (9%)	12,13,15	0.90	1 (8%)
2	DAS	C	49	2	4,7,8	1.38	1 (25%)	3,8,10	1.09	0
2	DAR	C	5	2	10,10,11	0.96	1 (10%)	7,11,13	0.83	0
2	DAS	C	50	2	4,7,8	1.10	0	3,8,10	0.81	0
2	DTR	C	51	2	14,15,16	0.85	0	13,20,22	0.85	0
2	DTH	C	52	2	6,6,7	1.26	1 (16%)	6,7,9	0.79	0
2	DTY	C	53	2	12,12,13	0.68	0	14,15,17	0.76	0
2	DAS	C	54	2	4,7,8	1.02	0	3,8,10	0.98	0
2	DAS	C	55	2	4,7,8	0.88	0	3,8,10	1.03	0
2	DAL	C	56	2	4,4,5	2.11	1 (25%)	1,4,6	0.24	0
2	DTH	C	57	2	6,6,7	0.97	1 (16%)	6,7,9	1.17	1 (16%)
2	DLY	C	58	2	8,8,9	1.09	1 (12%)	5,8,10	0.69	0
2	DTH	C	59	2	6,6,7	1.02	0	6,7,9	0.91	0
2	DPN	C	60	2	11,11,12	0.79	0	12,13,15	0.91	1 (8%)
2	DTH	C	61	2	6,6,7	0.94	0	6,7,9	0.84	0
2	DVA	C	62	2	6,6,7	1.40	1 (16%)	6,7,9	0.82	0
2	DTH	C	63	2	6,6,7	0.90	0	6,7,9	0.93	1 (16%)
2	DGL	C	64	2	5,8,9	1.25	1 (20%)	2,9,11	1.44	0
2	DSN	C	8	2	5,5,6	0.93	0	1,5,7	1.74	0
2	DTH	C	9	2	6,6,7	0.90	0	6,7,9	0.87	0
2	DAR	D	1	2	10,10,11	1.10	1 (10%)	7,11,13	0.84	0
2	DTY	D	10	2	12,12,13	1.02	1 (8%)	14,15,17	0.42	0
2	DLY	D	11	2	8,8,9	0.97	1 (12%)	5,8,10	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DLE	D	12	2	7,7,8	0.78	0	6,8,10	0.75	0
2	DIL	D	13	2	7,7,8	1.12	1 (14%)	6,8,10	0.80	0
2	DLE	D	14	2	7,7,8	0.78	0	6,8,10	0.62	0
2	DSG	D	15[A]	2	7,7,8	0.82	0	7,8,10	0.64	0
2	DSG	D	15[B]	2	7,7,8	0.76	0	7,8,10	0.62	0
2	DLY	D	17	2	8,8,9	1.15	1 (12%)	5,8,10	0.91	0
2	DTH	D	18	2	6,6,7	0.98	1 (16%)	6,7,9	0.94	1 (16%)
2	DLE	D	19	2	7,7,8	0.83	0	6,8,10	0.72	0
2	DAR	D	2	2	10,10,11	1.08	1 (10%)	7,11,13	0.58	0
2	DLY	D	20	2	8,8,9	0.70	0	5,8,10	0.88	0
2	DGL	D	22	2	5,8,9	0.76	0	2,9,11	0.99	0
2	DTH	D	23	2	6,6,7	0.95	0	6,7,9	1.13	1 (16%)
2	DTH	D	24	2	6,6,7	0.89	0	6,7,9	0.81	0
2	DTH	D	25	2	6,6,7	0.94	0	6,7,9	0.72	0
2	DGL	D	26	2	5,8,9	0.78	0	2,9,11	1.13	0
2	DAL	D	27	2	4,4,5	0.85	0	1,4,6	0.30	0
2	DVA	D	28	2	6,6,7	1.30	1 (16%)	6,7,9	0.95	0
2	DAS	D	29	2	4,7,8	1.27	1 (25%)	3,8,10	0.93	0
2	DAR	D	3	2	10,10,11	0.94	1 (10%)	7,11,13	0.83	0
2	DVA	D	30	2	6,6,7	1.22	1 (16%)	6,7,9	0.88	0
2	DPN	D	31	2	11,11,12	0.92	1 (9%)	12,13,15	0.61	0
2	DAS	D	32	2	4,7,8	1.86	1 (25%)	3,8,10	1.17	0
2	DAL	D	33	2	4,4,5	1.12	1 (25%)	1,4,6	0.40	0
2	DPN	D	34	2	11,11,12	0.75	0	12,13,15	0.66	0
2	DAS	D	35	2	4,7,8	1.28	1 (25%)	3,8,10	1.36	0
2	DVA	D	36	2	6,6,7	1.16	1 (16%)	6,7,9	1.44	1 (16%)
2	DPN	D	37	2	11,11,12	1.00	1 (9%)	12,13,15	0.56	0
2	DPN	D	38	2	11,11,12	1.10	1 (9%)	12,13,15	0.59	0
2	DVA	D	39	2	6,6,7	1.50	1 (16%)	6,7,9	0.77	0
2	DAR	D	4	2	10,10,11	1.16	1 (10%)	7,11,13	0.75	0
2	DTY	D	40	2	12,12,13	1.20	1 (8%)	14,15,17	0.54	0
2	DAL	D	41	2	4,4,5	1.38	1 (25%)	1,4,6	0.29	0
2	DAL	D	42	2	4,4,5	1.06	0	1,4,6	0.49	0
2	DSN	D	43	2	5,5,6	1.09	1 (20%)	1,5,7	1.60	0
2	DSG	D	44	2	7,7,8	0.73	0	7,8,10	0.88	0
2	DPN	D	45	2	11,11,12	0.72	0	12,13,15	0.88	1 (8%)
2	DSN	D	46	2	5,5,6	1.60	1 (20%)	1,5,7	1.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DAS	D	47	2	4,7,8	1.55	1 (25%)	3,8,10	1.16	0
2	DPN	D	48	2	11,11,12	1.08	1 (9%)	12,13,15	0.97	1 (8%)
2	DAS	D	49	2	4,7,8	0.84	0	3,8,10	1.61	1 (33%)
2	DAR	D	5	2	10,10,11	1.17	1 (10%)	7,11,13	0.78	0
2	DAS	D	50	2	4,7,8	1.00	0	3,8,10	0.85	0
2	DTR	D	51	2	14,15,16	0.86	0	13,20,22	0.94	0
2	DTH	D	52	2	6,6,7	0.89	0	6,7,9	1.00	0
2	DTY	D	53	2	12,12,13	0.77	0	14,15,17	0.59	0
2	DAS	D	54	2	4,7,8	1.01	0	3,8,10	0.90	0
2	DAS	D	55	2	4,7,8	1.25	1 (25%)	3,8,10	1.15	0
2	DAL	D	56	2	4,4,5	1.42	1 (25%)	1,4,6	0.12	0
2	DTH	D	57	2	6,6,7	1.11	1 (16%)	6,7,9	1.00	0
2	DLY	D	58	2	8,8,9	1.31	1 (12%)	5,8,10	0.78	0
2	DTH	D	59	2	6,6,7	0.77	0	6,7,9	1.10	1 (16%)
2	DPN	D	60	2	11,11,12	0.89	0	12,13,15	0.77	1 (8%)
2	DTH	D	61	2	6,6,7	0.66	0	6,7,9	0.96	0
2	DVA	D	62	2	6,6,7	0.88	0	6,7,9	0.95	0
2	DTH	D	63	2	6,6,7	0.81	0	6,7,9	0.86	0
2	DGL	D	64	2	5,8,9	0.96	0	2,9,11	1.25	0
2	DSN	D	67	2	5,5,6	1.10	1 (20%)	1,5,7	1.59	0
2	DAS	D	68	2	4,7,8	1.61	1 (25%)	3,8,10	0.79	0
2	DSN	D	8	2	5,5,6	1.31	1 (20%)	1,5,7	1.52	0
2	DTH	D	9	2	6,6,7	0.92	0	6,7,9	0.90	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
2	DAR	C	1	2	-	0/7/9/11	0/0/0/0
2	DTY	C	10	2	-	0/4/6/8	0/1/1/1
2	DLY	C	11	2	-	0/5/7/9	0/0/0/0
2	DLE	C	12	2	-	0/4/6/8	0/0/0/0
2	DIL	C	13	2	-	0/7/8/10	0/0/0/0
2	DLE	C	14	2	-	0/4/6/8	0/0/0/0
2	DSG	C	15[A]	2	-	0/4/6/8	0/0/0/0
2	DSG	C	15[B]	2	-	0/4/6/8	0/0/0/0
2	DLY	C	17	2	-	0/5/7/9	0/0/0/0
2	DTH	C	18	2	-	0/4/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DLE	C	19	2	-	0/4/6/8	0/0/0/0
2	DAR	C	2	2	-	0/7/9/11	0/0/0/0
2	DLY	C	20	2	-	0/5/7/9	0/0/0/0
2	DGL	C	22	2	-	0/3/7/9	0/0/0/0
2	DTH	C	23	2	-	0/4/6/8	0/0/0/0
2	DTH	C	24	2	-	0/4/6/8	0/0/0/0
2	DTH	C	25	2	-	0/4/6/8	0/0/0/0
2	DGL	C	26	2	-	0/3/7/9	0/0/0/0
2	DAL	C	27	2	-	0/0/2/4	0/0/0/0
2	DVA	C	28	2	-	0/5/6/8	0/0/0/0
2	DAS	C	29	2	-	0/2/6/8	0/0/0/0
2	DAR	C	3	2	-	0/7/9/11	0/0/0/0
2	DVA	C	30[A]	2	-	0/5/6/8	0/0/0/0
2	DVA	C	30[B]	2	-	0/5/6/8	0/0/0/0
2	DPN	C	31	2	-	0/4/6/8	0/1/1/1
2	DAS	C	32	2	-	0/2/6/8	0/0/0/0
2	DAL	C	33	2	-	0/0/2/4	0/0/0/0
2	DPN	C	34	2	-	0/4/6/8	0/1/1/1
2	DAS	C	35	2	-	0/2/6/8	0/0/0/0
2	DVA	C	36	2	-	0/5/6/8	0/0/0/0
2	DPN	C	37	2	-	0/4/6/8	0/1/1/1
2	DPN	C	38	2	-	0/4/6/8	0/1/1/1
2	DVA	C	39	2	-	0/5/6/8	0/0/0/0
2	DAR	C	4	2	-	0/7/9/11	0/0/0/0
2	DTY	C	40	2	-	0/4/6/8	0/1/1/1
2	DAL	C	41	2	-	0/0/2/4	0/0/0/0
2	DAL	C	42	2	-	0/0/2/4	0/0/0/0
2	DSN	C	43	2	-	0/2/4/6	0/0/0/0
2	DSG	C	44	2	-	0/4/6/8	0/0/0/0
2	DPN	C	45	2	-	0/4/6/8	0/1/1/1
2	DSN	C	46	2	-	0/2/4/6	0/0/0/0
2	DAS	C	47	2	-	0/2/6/8	0/0/0/0
2	DPN	C	48	2	-	0/4/6/8	0/1/1/1
2	DAS	C	49	2	-	0/2/6/8	0/0/0/0
2	DAR	C	5	2	-	0/7/9/11	0/0/0/0
2	DAS	C	50	2	-	0/2/6/8	0/0/0/0
2	DTR	C	51	2	-	0/3/6/8	0/2/2/2
2	DTH	C	52	2	-	0/4/6/8	0/0/0/0
2	DTY	C	53	2	-	0/4/6/8	0/1/1/1
2	DAS	C	54	2	-	0/2/6/8	0/0/0/0
2	DAS	C	55	2	-	0/2/6/8	0/0/0/0
2	DAL	C	56	2	-	0/0/2/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTH	C	57	2	-	0/4/6/8	0/0/0/0
2	DLY	C	58	2	-	0/5/7/9	0/0/0/0
2	DTH	C	59	2	-	0/4/6/8	0/0/0/0
2	DPN	C	60	2	-	0/4/6/8	0/1/1/1
2	DTH	C	61	2	-	0/4/6/8	0/0/0/0
2	DVA	C	62	2	-	0/5/6/8	0/0/0/0
2	DTH	C	63	2	-	0/4/6/8	0/0/0/0
2	DGL	C	64	2	-	0/3/7/9	0/0/0/0
2	DSN	C	8	2	-	0/2/4/6	0/0/0/0
2	DTH	C	9	2	-	0/4/6/8	0/0/0/0
2	DAR	D	1	2	-	0/7/9/11	0/0/0/0
2	DTY	D	10	2	-	0/4/6/8	0/1/1/1
2	DLY	D	11	2	-	0/5/7/9	0/0/0/0
2	DLE	D	12	2	-	0/4/6/8	0/0/0/0
2	DIL	D	13	2	-	0/7/8/10	0/0/0/0
2	DLE	D	14	2	-	0/4/6/8	0/0/0/0
2	DSG	D	15[A]	2	-	0/4/6/8	0/0/0/0
2	DSG	D	15[B]	2	-	0/4/6/8	0/0/0/0
2	DLY	D	17	2	-	0/5/7/9	0/0/0/0
2	DTH	D	18	2	-	0/4/6/8	0/0/0/0
2	DLE	D	19	2	-	0/4/6/8	0/0/0/0
2	DAR	D	2	2	-	0/7/9/11	0/0/0/0
2	DLY	D	20	2	-	0/5/7/9	0/0/0/0
2	DGL	D	22	2	-	0/3/7/9	0/0/0/0
2	DTH	D	23	2	-	0/4/6/8	0/0/0/0
2	DTH	D	24	2	-	0/4/6/8	0/0/0/0
2	DTH	D	25	2	-	0/4/6/8	0/0/0/0
2	DGL	D	26	2	-	0/3/7/9	0/0/0/0
2	DAL	D	27	2	-	0/0/2/4	0/0/0/0
2	DVA	D	28	2	-	0/5/6/8	0/0/0/0
2	DAS	D	29	2	-	0/2/6/8	0/0/0/0
2	DAR	D	3	2	-	0/7/9/11	0/0/0/0
2	DVA	D	30	2	-	0/5/6/8	0/0/0/0
2	DPN	D	31	2	-	0/4/6/8	0/1/1/1
2	DAS	D	32	2	-	0/2/6/8	0/0/0/0
2	DAL	D	33	2	-	0/0/2/4	0/0/0/0
2	DPN	D	34	2	-	0/4/6/8	0/1/1/1
2	DAS	D	35	2	-	0/2/6/8	0/0/0/0
2	DVA	D	36	2	-	0/5/6/8	0/0/0/0
2	DPN	D	37	2	-	0/4/6/8	0/1/1/1
2	DPN	D	38	2	-	0/4/6/8	0/1/1/1
2	DVA	D	39	2	-	0/5/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DAR	D	4	2	-	0/7/9/11	0/0/0/0
2	DTY	D	40	2	-	0/4/6/8	0/1/1/1
2	DAL	D	41	2	-	0/0/2/4	0/0/0/0
2	DAL	D	42	2	-	0/0/2/4	0/0/0/0
2	DSN	D	43	2	-	0/2/4/6	0/0/0/0
2	DSG	D	44	2	-	0/4/6/8	0/0/0/0
2	DPN	D	45	2	-	0/4/6/8	0/1/1/1
2	DSN	D	46	2	-	0/2/4/6	0/0/0/0
2	DAS	D	47	2	-	0/2/6/8	0/0/0/0
2	DPN	D	48	2	-	0/4/6/8	0/1/1/1
2	DAS	D	49	2	-	0/2/6/8	0/0/0/0
2	DAR	D	5	2	-	0/7/9/11	0/0/0/0
2	DAS	D	50	2	-	0/2/6/8	0/0/0/0
2	DTR	D	51	2	-	0/3/6/8	0/2/2/2
2	DTH	D	52	2	-	0/4/6/8	0/0/0/0
2	DTY	D	53	2	-	0/4/6/8	0/1/1/1
2	DAS	D	54	2	-	0/2/6/8	0/0/0/0
2	DAS	D	55	2	-	0/2/6/8	0/0/0/0
2	DAL	D	56	2	-	0/0/2/4	0/0/0/0
2	DTH	D	57	2	-	0/4/6/8	0/0/0/0
2	DLY	D	58	2	-	0/5/7/9	0/0/0/0
2	DTH	D	59	2	-	0/4/6/8	0/0/0/0
2	DPN	D	60	2	-	0/4/6/8	0/1/1/1
2	DTH	D	61	2	-	0/4/6/8	0/0/0/0
2	DVA	D	62	2	-	0/5/6/8	0/0/0/0
2	DTH	D	63	2	-	0/4/6/8	0/0/0/0
2	DGL	D	64	2	-	0/3/7/9	0/0/0/0
2	DSN	D	67	2	-	0/2/4/6	0/0/0/0
2	DAS	D	68	2	-	0/2/6/8	0/0/0/0
2	DSN	D	8	2	-	0/2/4/6	0/0/0/0
2	DTH	D	9	2	-	0/4/6/8	0/0/0/0

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	48	DPN	CA-C	2.02	1.52	1.50
2	D	10	DTY	CA-C	2.05	1.52	1.50
2	C	42	DAL	CA-C	2.05	1.52	1.50
2	D	18	DTH	CA-C	2.07	1.53	1.50
2	D	33	DAL	CA-C	2.08	1.53	1.50
2	C	10	DTY	CA-C	2.14	1.53	1.50
2	C	30[B]	DVA	CA-C	2.15	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	11	DLY	CA-C	2.15	1.53	1.50
2	D	55	DAS	CA-C	2.17	1.53	1.50
2	C	10	DTY	CE1-CD1	2.19	1.42	1.38
2	C	41	DAL	CA-C	2.19	1.53	1.50
2	D	29	DAS	CA-C	2.22	1.53	1.50
2	D	35	DAS	CA-C	2.22	1.53	1.50
2	C	57	DTH	CA-C	2.24	1.53	1.50
2	C	1	DAR	CA-C	2.25	1.53	1.50
2	D	43	DSN	CA-C	2.25	1.53	1.50
2	D	67	DSN	CA-C	2.25	1.53	1.50
2	D	57	DTH	CA-C	2.26	1.53	1.50
2	C	11	DLY	CA-C	2.28	1.53	1.50
2	C	39	DVA	CA-C	2.28	1.53	1.50
2	C	64	DGL	CA-C	2.30	1.53	1.50
2	C	38	DPN	CA-C	2.32	1.53	1.50
2	C	30[A]	DVA	CA-C	2.43	1.53	1.50
2	C	2	DAR	CA-C	2.43	1.53	1.50
2	C	28	DVA	CA-C	2.46	1.53	1.50
2	C	40	DTY	CA-C	2.47	1.53	1.50
2	C	49	DAS	CA-C	2.49	1.53	1.50
2	D	13	DIL	CA-C	2.50	1.53	1.50
2	D	36	DVA	CA-C	2.51	1.53	1.50
2	C	36	DVA	CA-C	2.55	1.53	1.50
2	C	25	DTH	CA-C	2.55	1.53	1.50
2	C	37	DPN	CA-C	2.56	1.53	1.50
2	D	37	DPN	CA-C	2.58	1.53	1.50
2	D	8	DSN	CA-C	2.61	1.53	1.50
2	D	41	DAL	CA-C	2.61	1.53	1.50
2	C	22	DGL	CA-C	2.61	1.53	1.50
2	D	30	DVA	CA-C	2.63	1.53	1.50
2	D	3	DAR	CA-C	2.64	1.53	1.50
2	D	56	DAL	CA-C	2.65	1.53	1.50
2	C	52	DTH	CA-C	2.66	1.53	1.50
2	C	31	DPN	CA-C	2.68	1.53	1.50
2	D	31	DPN	CA-C	2.70	1.53	1.50
2	C	58	DLY	CA-C	2.75	1.53	1.50
2	C	5	DAR	CA-C	2.75	1.53	1.50
2	C	18	DTH	CA-C	2.78	1.53	1.50
2	D	47	DAS	CA-C	2.79	1.53	1.50
2	D	17	DLY	CA-C	2.80	1.53	1.50
2	C	47	DAS	CA-C	2.81	1.53	1.50
2	D	5	DAR	CA-C	2.86	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	28	DVA	CA-C	2.91	1.54	1.50
2	C	62	DVA	CA-C	2.92	1.54	1.50
2	C	34	DPN	CA-C	2.93	1.54	1.50
2	C	35	DAS	CA-C	2.95	1.54	1.50
2	C	12	DLE	CA-C	2.96	1.54	1.50
2	C	43	DSN	CA-C	2.97	1.54	1.50
2	D	68	DAS	CA-C	3.04	1.54	1.50
2	C	46	DSN	CA-C	3.12	1.54	1.50
2	D	48	DPN	CA-C	3.14	1.54	1.50
2	C	33	DAL	CA-C	3.17	1.54	1.50
2	D	2	DAR	CA-C	3.18	1.54	1.50
2	D	1	DAR	CA-C	3.18	1.54	1.50
2	D	38	DPN	CA-C	3.22	1.54	1.50
2	D	39	DVA	CA-C	3.37	1.54	1.50
2	C	23	DTH	CA-C	3.42	1.54	1.50
2	D	46	DSN	CA-C	3.43	1.54	1.50
2	D	58	DLY	CA-C	3.44	1.54	1.50
2	D	4	DAR	CA-C	3.45	1.54	1.50
2	D	32	DAS	CA-C	3.51	1.54	1.50
2	C	32	DAS	CA-C	3.57	1.54	1.50
2	D	40	DTY	CA-C	3.85	1.55	1.50
2	C	56	DAL	CA-C	4.04	1.55	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	39	DVA	CB-CA-C	-3.81	107.74	112.96
2	C	13	DIL	CB-CA-C	-3.18	107.93	112.84
2	C	36	DVA	CB-CA-C	-3.17	108.61	112.96
2	D	36	DVA	CB-CA-C	-3.06	108.78	112.96
2	D	48	DPN	CB-CA-C	-2.60	106.39	111.41
2	C	60	DPN	CB-CA-C	-2.49	106.61	111.41
2	C	45	DPN	CB-CA-C	-2.32	106.95	111.41
2	C	57	DTH	O-C-CA	-2.31	119.76	125.15
2	C	23	DTH	O-C-CA	-2.29	119.81	125.15
2	C	48	DPN	CB-CA-C	-2.24	107.09	111.41
2	C	18	DTH	O-C-CA	-2.20	120.03	125.15
2	C	28	DVA	CB-CA-C	-2.18	109.98	112.96
2	D	60	DPN	CB-CA-C	-2.16	107.25	111.41
2	D	45	DPN	CB-CA-C	-2.14	107.28	111.41
2	D	49	DAS	CB-CA-C	-2.14	107.29	111.41
2	C	24	DTH	O-C-CA	-2.13	120.19	125.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	63	DTH	O-C-CA	-2.05	120.37	125.15
2	D	59	DTH	O-C-CA	-2.04	120.39	125.15
2	C	13	DIL	O-C-CA	-2.04	120.40	125.15
2	D	18	DTH	O-C-CA	-2.02	120.44	125.15
2	C	19	DLE	O-C-CA	-2.01	119.46	125.02
2	D	23	DTH	O-C-CA	-2.00	120.48	125.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	37	DPN	1	0
2	C	38	DPN	1	0
2	D	1	DAR	1	0
2	D	11	DLY	1	0
2	D	17	DLY	1	0
2	D	2	DAR	2	0
2	D	22	DGL	1	0
2	D	26	DGL	1	0
2	D	3	DAR	2	0
2	D	32	DAS	1	0
2	D	5	DAR	4	0
2	D	51	DTR	1	0
2	D	60	DPN	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	$\# Z  > 2$
3	GOL	A	201	-	5,5,5	0.43	0	5,5,5	0.39	0
3	GOL	B	201	-	5,5,5	0.34	0	5,5,5	0.24	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	GOL	A	201	-	-	0/4/4/4	0/0/0/0
3	GOL	B	201	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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.