



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 12, 2016 – 11:04 PM EDT

PDB ID : 5JBY
Title : Lys27-linked triubiquitin
Authors : Pan, M.; Gao, S.; Zheng, Y.
Deposited on : 2016-04-14
Resolution : 1.99 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at 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.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027790

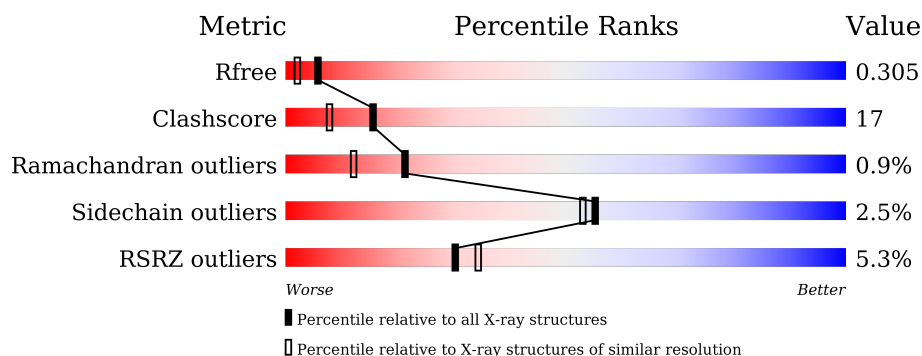
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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}	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	76	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>.</div> </div> </div>
1	C	76	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>28%</div> <div>5%</div> </div> </div>
1	E	76	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>21%</div> <div>5%</div> </div> </div>
2	B	76	<div> <div></div> <div> <div></div> <div>67%</div> <div>21%</div> <div>12%</div> </div> </div>
2	D	76	<div> <div></div> <div> <div></div> <div>54%</div> <div>34%</div> <div>12%</div> </div> </div>
2	F	76	<div> <div></div> <div> <div></div> <div>46%</div> <div>42%</div> <div>12%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6738 atoms, of which 3165 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 ubiquitin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	73	Total	C	H	N	O	S	0	0	0
			1190	366	608	102	113	1			
1	C	72	Total	C	H	N	O	S	0	0	0
			1167	360	594	100	112	1			
1	E	73	Total	C	H	N	O	S	0	0	0
			1186	366	604	102	113	1			

- Molecule 2 is a protein (with D amino acids) called D-ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	67	Total	C	H	N	O	0	0	0
			993	339	457	90	107			
2	D	67	Total	C	H	N	O	0	0	0
			993	339	457	90	107			
2	F	67	Total	C	H	N	O	0	0	0
			979	337	445	89	108			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	41	Total	O	0	0
			41	41		
3	C	41	Total	O	0	0
			41	41		
3	D	31	Total	O	0	0
			31	31		
3	E	42	Total	O	0	0
			42	42		
3	F	40	Total	O	0	0
			40	40		

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 errors 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.

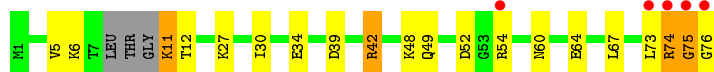
- Molecule 1: ubiquitin



- Molecule 1: ubiquitin



- Molecule 1: ubiquitin



- Molecule 2: D-ubiquitin



- Molecule 2: D-ubiquitin



- Molecule 2: D-ubiquitin



L1	Q2	I3	F4	V5	K6	T7	DLE	T9	GLY	DLY	T12	I13	T14	L15	E16	V17	E18		T22	I23		V26		E34		P38		Q41	R42		F45	A46		E51	D52	G53	R54	T55	L56			Y59	N60	I61	K63	E64	S65	T66	L67	H68	L69	V70	DLE	DAR	DLE	DAR	GLY	DAL
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.76Å 51.75Å 54.98Å 90.02° 118.15° 119.95°	Depositor
Resolution (Å)	22.57 – 1.99 22.57 – 1.99	Depositor EDS
% Data completeness (in resolution range)	79.6 (22.57-1.99) 75.7 (22.57-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.99Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.237 , 0.308 0.240 , 0.305	Depositor DCC
R_{free} test set	1410 reflections (6.22%)	DCC
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 21.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.59$, $\langle L^2 \rangle = 0.44$	Xtriage
Estimated twinning fraction	0.400 for k,-h-k,h+l 0.400 for -h-k,h,h+k+l 0.000 for -h-k,k,-l 0.000 for h,-h-k,-h-l 0.000 for k,h,-h-k-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6738	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, DNE, DTH, DPR, DHI, DAL, DVA, DGN, DGL, DSN, DTY, DLE, DAR, DAS, DPN, 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	0.66	0/587	0.81	0/787
1	C	0.64	0/578	0.78	0/776
1	E	0.69	0/587	0.80	2/787 (0.3%)
2	B	1.21	0/9	1.49	0/6
2	D	0.97	0/9	1.13	0/6
2	F	1.30	0/9	1.54	0/6
All	All	0.68	0/1779	0.80	2/2368 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	42	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	E	39	ASP	CB-CG-OD1	5.23	123.01	118.30

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	582	608	607	13	0
1	C	573	594	594	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	582	604	607	18	0
2	B	536	457	497	18	0
2	D	536	457	498	29	0
2	F	534	445	498	30	0
3	A	35	0	0	0	0
3	B	41	0	0	5	0
3	C	41	0	0	7	0
3	D	31	0	0	10	1
3	E	42	0	0	2	1
3	F	40	0	0	10	0
All	All	3573	3165	3301	114	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 17.

The worst 5 of 114 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:12:THR:N	3:C:101:HOH:O	1.82	1.09
1:C:25:ASN:ND2	3:C:102:HOH:O	1.94	1.00
2:B:54:DAR:NH2	3:B:101:HOH:O	1.96	0.97
1:A:74:ARG:NH2	1:E:52:ASP:OD1	2.01	0.94
2:F:7:DTH:O	2:F:9:DTH:N	2.03	0.91

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:D:126:HOH:O	3:E:134:HOH:O[1_445]	1.84	0.36

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	69/76 (91%)	66 (96%)	3 (4%)	0	100	100
1	C	68/76 (90%)	67 (98%)	1 (2%)	0	100	100
1	E	69/76 (91%)	65 (94%)	2 (3%)	2 (3%)	6	1
2	B	3/76 (4%)	2 (67%)	1 (33%)	0	100	100
2	D	3/76 (4%)	3 (100%)	0	0	100	100
2	F	3/76 (4%)	3 (100%)	0	0	100	100
All	All	215/456 (47%)	206 (96%)	7 (3%)	2 (1%)	21	12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	75	GLY
1	E	74	ARG

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	66/68 (97%)	63 (96%)	3 (4%)	34	26
1	C	65/68 (96%)	64 (98%)	1 (2%)	72	73
1	E	66/68 (97%)	65 (98%)	1 (2%)	72	73
All	All	197/204 (97%)	192 (98%)	5 (2%)	55	53

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	A	72	ARG
1	A	73	LEU
1	C	57	SER
1	E	11	LYS

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 ⓘ

192 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	DNE	B	1	2	5,7,8	0.75	0	5,7,9	0.89	0
2	DLY	B	11	2	6,8,9	0.53	0	6,8,10	0.90	1 (16%)
2	DTH	B	12	2	5,6,7	0.64	0	5,7,9	1.21	0
2	DIL	B	13	2	6,7,8	0.85	0	7,8,10	1.73	2 (28%)
2	DTH	B	14	2	5,6,7	1.09	0	5,7,9	0.99	0
2	DLE	B	15	2	5,7,8	0.45	0	6,8,10	0.75	0
2	DGL	B	16	2	3,8,9	0.53	0	4,9,11	0.85	0
2	DVA	B	17	2	5,6,7	0.66	0	5,7,9	0.65	0
2	DGL	B	18	2	3,8,9	0.66	0	4,9,11	1.16	1 (25%)
2	DPR	B	19	2	5,7,8	0.33	0	7,8,10	1.13	0
2	DGN	B	2	2	6,8,9	0.98	1 (16%)	7,9,11	0.95	0
2	DSN	B	20	2	3,5,6	0.42	0	3,5,7	1.32	1 (33%)
2	DAS	B	21	2	2,7,8	0.75	0	2,8,10	1.50	1 (50%)
2	DTH	B	22	2	5,6,7	0.56	0	5,7,9	0.94	0
2	DIL	B	23	2	6,7,8	0.90	0	7,8,10	1.27	1 (14%)
2	DGL	B	24	2	3,8,9	0.83	0	4,9,11	1.24	0
2	DSG	B	25	2	5,7,8	0.43	0	6,8,10	1.23	1 (16%)
2	DVA	B	26	2	5,6,7	0.58	0	5,7,9	0.95	0
2	DLY	B	27	2	6,8,9	0.64	0	6,8,10	0.78	0
2	DAL	B	28	2	1,4,5	0.77	0	1,4,6	0.44	0
2	DLY	B	29	2	6,8,9	0.52	0	6,8,10	0.86	0
2	DIL	B	3	2	6,7,8	0.46	0	7,8,10	0.90	1 (14%)
2	DIL	B	30	2	6,7,8	0.56	0	7,8,10	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DGN	B	31	2	6,8,9	0.57	0	7,9,11	0.61	0
2	DAS	B	32	2	2,7,8	0.53	0	2,8,10	1.52	0
2	DLY	B	33	2	6,8,9	0.49	0	6,8,10	0.77	0
2	DGL	B	34	2	3,8,9	0.48	0	4,9,11	1.04	1 (25%)
2	DIL	B	36	2	6,7,8	0.78	0	7,8,10	0.78	0
2	DPR	B	37	2	5,7,8	0.42	0	7,8,10	1.53	2 (28%)
2	DPR	B	38	2	5,7,8	0.72	0	7,8,10	1.36	1 (14%)
2	DAS	B	39	2	2,7,8	0.37	0	2,8,10	1.57	1 (50%)
2	DPN	B	4	2	9,11,12	0.56	0	11,13,15	0.66	1 (9%)
2	DGN	B	40	2	6,8,9	0.46	0	7,9,11	1.11	1 (14%)
2	DGN	B	41	2	6,8,9	0.37	0	7,9,11	0.41	0
2	DAR	B	42	2	8,10,11	0.56	0	9,11,13	0.94	1 (11%)
2	DLE	B	43	2	5,7,8	0.44	0	6,8,10	0.91	0
2	DIL	B	44	2	6,7,8	0.94	0	7,8,10	1.22	1 (14%)
2	DPN	B	45	2	9,11,12	0.59	0	11,13,15	0.67	0
2	DAL	B	46	2	1,4,5	0.78	0	1,4,6	0.63	0
2	DLY	B	48	2	6,8,9	0.62	0	6,8,10	0.81	0
2	DGN	B	49	2	6,8,9	0.86	0	7,9,11	1.26	1 (14%)
2	DVA	B	5	2	5,6,7	0.78	0	5,7,9	0.82	0
2	DLE	B	50	2	5,7,8	0.48	0	6,8,10	1.16	1 (16%)
2	DGL	B	51	2	3,8,9	0.62	0	4,9,11	1.32	1 (25%)
2	DAS	B	52	2	2,7,8	0.93	0	2,8,10	1.39	0
2	DAR	B	54	2	8,10,11	0.91	0	9,11,13	0.98	1 (11%)
2	DTH	B	55	2	5,6,7	0.38	0	5,7,9	1.49	1 (20%)
2	DLE	B	56	2	5,7,8	0.36	0	6,8,10	0.98	1 (16%)
2	DSN	B	57	2	3,5,6	0.68	0	3,5,7	1.52	1 (33%)
2	DAS	B	58	2	2,7,8	0.67	0	2,8,10	1.26	0
2	DTY	B	59	2	10,12,13	0.53	0	13,15,17	0.71	1 (7%)
2	DLY	B	6	2	6,8,9	0.74	0	6,8,10	1.00	1 (16%)
2	DSG	B	60	2	5,7,8	0.78	0	6,8,10	0.89	1 (16%)
2	DIL	B	61	2	6,7,8	0.71	0	7,8,10	1.21	1 (14%)
2	DGN	B	62	2	6,8,9	0.31	0	7,9,11	0.63	0
2	DLY	B	63	2	6,8,9	0.67	0	6,8,10	1.16	1 (16%)
2	DGL	B	64	2	3,8,9	1.02	0	4,9,11	1.28	1 (25%)
2	DSN	B	65	2	3,5,6	1.16	0	3,5,7	1.42	0
2	DTH	B	66	2	5,6,7	0.48	0	5,7,9	1.26	1 (20%)
2	DLE	B	67	2	5,7,8	0.36	0	6,8,10	1.37	1 (16%)
2	DHI	B	68	2	3,10,11	0.60	0	2,12,14	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DLE	B	69	2	5,7,8	0.42	0	6,8,10	1.21	1 (16%)
2	DTH	B	7	2	5,6,7	0.77	0	5,7,9	0.87	0
2	DVA	B	70	2	5,6,7	0.52	0	5,7,9	0.97	1 (20%)
2	DNE	D	1	2	5,7,8	0.65	0	5,7,9	0.86	0
2	DLY	D	11	2	6,8,9	0.64	0	6,8,10	0.81	0
2	DTH	D	12	2	5,6,7	0.50	0	5,7,9	1.00	0
2	DIL	D	13	2	6,7,8	0.61	0	7,8,10	1.49	2 (28%)
2	DTH	D	14	2	5,6,7	0.81	0	5,7,9	0.81	0
2	DLE	D	15	2	5,7,8	0.42	0	6,8,10	1.09	0
2	DGL	D	16	2	3,8,9	0.49	0	4,9,11	0.94	0
2	DVA	D	17	2	5,6,7	0.68	0	5,7,9	0.88	0
2	DGL	D	18	2	3,8,9	0.46	0	4,9,11	1.02	1 (25%)
2	DPR	D	19	2	5,7,8	0.50	0	7,8,10	1.23	0
2	DGN	D	2	2	6,8,9	1.14	1 (16%)	7,9,11	0.59	0
2	DSN	D	20	2	3,5,6	0.41	0	3,5,7	1.35	1 (33%)
2	DAS	D	21	2	2,7,8	0.68	0	2,8,10	1.55	1 (50%)
2	DTH	D	22	2	5,6,7	0.56	0	5,7,9	1.02	0
2	DIL	D	23	2	6,7,8	0.70	0	7,8,10	0.73	0
2	DGL	D	24	2	3,8,9	0.69	0	4,9,11	1.04	0
2	DSG	D	25	2	5,7,8	0.39	0	6,8,10	0.94	1 (16%)
2	DVA	D	26	2	5,6,7	0.73	0	5,7,9	1.12	1 (20%)
2	DLY	D	27	2	6,8,9	0.64	0	6,8,10	0.92	1 (16%)
2	DAL	D	28	2	1,4,5	0.79	0	1,4,6	0.34	0
2	DLY	D	29	2	6,8,9	0.48	0	6,8,10	0.79	0
2	DIL	D	3	2	6,7,8	0.56	0	7,8,10	0.62	0
2	DIL	D	30	2	6,7,8	0.46	0	7,8,10	0.80	0
2	DGN	D	31	2	6,8,9	0.69	0	7,9,11	0.77	0
2	DAS	D	32	2	2,7,8	0.48	0	2,8,10	1.35	0
2	DLY	D	33	2	6,8,9	0.49	0	6,8,10	0.99	1 (16%)
2	DGL	D	34	2	3,8,9	0.78	0	4,9,11	1.18	1 (25%)
2	DIL	D	36	2	6,7,8	0.88	0	7,8,10	0.88	0
2	DPR	D	37	2	5,7,8	0.54	0	7,8,10	1.54	2 (28%)
2	DPR	D	38	2	5,7,8	0.47	0	7,8,10	1.41	1 (14%)
2	DAS	D	39	2	2,7,8	0.41	0	2,8,10	1.59	1 (50%)
2	DPN	D	4	2	9,11,12	0.61	0	11,13,15	0.58	0
2	DGN	D	40	2	6,8,9	0.60	0	7,9,11	0.88	1 (14%)
2	DGN	D	41	2	6,8,9	0.60	0	7,9,11	0.75	0
2	DAR	D	42	2	8,10,11	0.50	0	9,11,13	0.86	1 (11%)
2	DLE	D	43	2	5,7,8	0.34	0	6,8,10	0.95	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DIL	D	44	2	6,7,8	0.66	0	7,8,10	0.88	0
2	DPN	D	45	2	9,11,12	0.50	0	11,13,15	0.56	0
2	DAL	D	46	2	1,4,5	0.82	0	1,4,6	0.28	0
2	DLY	D	48	2	6,8,9	1.10	0	6,8,10	0.81	0
2	DGN	D	49	2	6,8,9	0.58	0	7,9,11	0.87	1 (14%)
2	DVA	D	5	2	5,6,7	0.96	0	5,7,9	0.58	0
2	DLE	D	50	2	5,7,8	0.38	0	6,8,10	1.38	2 (33%)
2	DGL	D	51	2	3,8,9	0.49	0	4,9,11	1.49	1 (25%)
2	DAS	D	52	2	2,7,8	1.21	0	2,8,10	1.67	1 (50%)
2	DAR	D	54	2	8,10,11	0.74	0	9,11,13	0.91	1 (11%)
2	DTH	D	55	2	5,6,7	0.57	0	5,7,9	1.39	1 (20%)
2	DLE	D	56	2	5,7,8	0.34	0	6,8,10	1.17	0
2	DSN	D	57	2	3,5,6	0.32	0	3,5,7	1.31	1 (33%)
2	DAS	D	58	2	2,7,8	0.32	0	2,8,10	1.61	1 (50%)
2	DTY	D	59	2	10,12,13	0.71	0	13,15,17	0.56	0
2	DLY	D	6	2	6,8,9	0.52	0	6,8,10	1.22	1 (16%)
2	DSG	D	60	2	5,7,8	1.16	1 (20%)	6,8,10	0.71	0
2	DIL	D	61	2	6,7,8	0.46	0	7,8,10	0.85	0
2	DGN	D	62	2	6,8,9	0.71	0	7,9,11	0.17	0
2	DLY	D	63	2	6,8,9	0.71	0	6,8,10	0.96	1 (16%)
2	DGL	D	64	2	3,8,9	0.68	0	4,9,11	1.79	2 (50%)
2	DSN	D	65	2	3,5,6	0.85	0	3,5,7	0.88	0
2	DTH	D	66	2	5,6,7	0.31	0	5,7,9	1.16	1 (20%)
2	DLE	D	67	2	5,7,8	0.48	0	6,8,10	1.36	1 (16%)
2	DHI	D	68	2	3,10,11	0.63	0	2,12,14	1.58	1 (50%)
2	DLE	D	69	2	5,7,8	0.42	0	6,8,10	1.14	1 (16%)
2	DTH	D	7	2	5,6,7	0.68	0	5,7,9	1.38	0
2	DVA	D	70	2	5,6,7	0.61	0	5,7,9	1.06	1 (20%)
2	DNE	F	1	2	5,7,8	0.67	0	5,7,9	0.88	0
2	DTH	F	12	2	5,6,7	0.46	0	5,7,9	1.13	0
2	DIL	F	13	2	6,7,8	0.52	0	7,8,10	1.28	1 (14%)
2	DTH	F	14	2	5,6,7	0.69	0	5,7,9	0.89	0
2	DLE	F	15	2	5,7,8	0.35	0	6,8,10	1.13	1 (16%)
2	DGL	F	16	2	3,8,9	0.71	0	4,9,11	1.06	0
2	DVA	F	17	2	5,6,7	0.76	0	5,7,9	1.71	2 (40%)
2	DGL	F	18	2	3,8,9	0.53	0	4,9,11	0.93	0
2	DPR	F	19	2	5,7,8	0.55	0	7,8,10	1.27	0
2	DGN	F	2	2	6,8,9	0.61	0	7,9,11	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DSN	F	20	2	3,5,6	0.21	0	3,5,7	1.41	1 (33%)
2	DAS	F	21	2	2,7,8	0.59	0	2,8,10	1.37	0
2	DTH	F	22	2	5,6,7	0.64	0	5,7,9	1.25	1 (20%)
2	DIL	F	23	2	6,7,8	0.58	0	7,8,10	0.85	0
2	DGL	F	24	2	3,8,9	0.85	0	4,9,11	1.00	0
2	DSG	F	25	2	5,7,8	0.42	0	6,8,10	1.06	1 (16%)
2	DVA	F	26	2	5,6,7	0.95	0	5,7,9	1.23	1 (20%)
2	DLY	F	27	2	6,8,9	0.68	0	6,8,10	0.85	0
2	DAL	F	28	2	1,4,5	0.60	0	1,4,6	0.34	0
2	DLY	F	29	2	6,8,9	0.65	0	6,8,10	0.49	0
2	DIL	F	3	2	6,7,8	0.51	0	7,8,10	0.81	0
2	DIL	F	30	2	6,7,8	0.67	0	7,8,10	0.86	0
2	DGN	F	31	2	6,8,9	0.60	0	7,9,11	0.69	0
2	DAS	F	32	2	2,7,8	0.67	0	2,8,10	1.43	0
2	DLY	F	33	2	6,8,9	0.45	0	6,8,10	0.86	0
2	DGL	F	34	2	3,8,9	0.65	0	4,9,11	1.30	1 (25%)
2	DIL	F	36	2	6,7,8	0.57	0	7,8,10	1.11	1 (14%)
2	DPR	F	37	2	5,7,8	0.46	0	7,8,10	1.54	2 (28%)
2	DPR	F	38	2	5,7,8	0.54	0	7,8,10	1.35	1 (14%)
2	DAS	F	39	2	2,7,8	0.36	0	2,8,10	1.47	1 (50%)
2	DPN	F	4	2	9,11,12	0.50	0	11,13,15	0.58	0
2	DGN	F	40	2	6,8,9	0.66	0	7,9,11	0.90	1 (14%)
2	DGN	F	41	2	6,8,9	0.50	0	7,9,11	0.46	0
2	DAR	F	42	2	8,10,11	0.54	0	9,11,13	1.12	1 (11%)
2	DLE	F	43	2	5,7,8	0.47	0	6,8,10	0.81	0
2	DIL	F	44	2	6,7,8	1.00	0	7,8,10	0.98	1 (14%)
2	DPN	F	45	2	9,11,12	0.84	1 (11%)	11,13,15	0.78	1 (9%)
2	DAL	F	46	2	1,4,5	1.15	0	1,4,6	0.50	0
2	DLY	F	48	2	6,8,9	0.61	0	6,8,10	0.95	1 (16%)
2	DGN	F	49	2	6,8,9	0.63	0	7,9,11	0.91	1 (14%)
2	DVA	F	5	2	5,6,7	0.64	0	5,7,9	1.20	1 (20%)
2	DLE	F	50	2	5,7,8	0.37	0	6,8,10	1.34	2 (33%)
2	DGL	F	51	2	3,8,9	0.66	0	4,9,11	1.21	1 (25%)
2	DAS	F	52	2	2,7,8	0.97	0	2,8,10	1.89	1 (50%)
2	DAR	F	54	2	8,10,11	0.68	0	9,11,13	0.87	0
2	DTH	F	55	2	5,6,7	0.33	0	5,7,9	1.50	2 (40%)
2	DLE	F	56	2	5,7,8	0.64	0	6,8,10	0.97	0
2	DSN	F	57	2	3,5,6	0.35	0	3,5,7	1.80	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DAS	F	58	2	2,7,8	1.03	0	2,8,10	1.34	0
2	DTY	F	59	2	10,12,13	0.44	0	13,15,17	0.59	0
2	DLY	F	6	2	6,8,9	0.46	0	6,8,10	1.00	1 (16%)
2	DSG	F	60	2	5,7,8	0.54	0	6,8,10	0.76	0
2	DIL	F	61	2	6,7,8	0.53	0	7,8,10	1.30	1 (14%)
2	DGN	F	62	2	6,8,9	0.47	0	7,9,11	0.52	0
2	DLY	F	63	2	6,8,9	0.80	0	6,8,10	1.04	1 (16%)
2	DGL	F	64	2	3,8,9	0.94	0	4,9,11	1.68	1 (25%)
2	DSN	F	65	2	3,5,6	0.69	0	3,5,7	1.31	0
2	DTH	F	66	2	5,6,7	0.63	0	5,7,9	0.86	0
2	DLE	F	67	2	5,7,8	0.50	0	6,8,10	1.07	1 (16%)
2	DHI	F	68	2	3,10,11	0.61	0	2,12,14	0.97	0
2	DLE	F	69	2	5,7,8	0.34	0	6,8,10	1.32	1 (16%)
2	DTH	F	7	2	5,6,7	0.83	0	5,7,9	0.82	0
2	DVA	F	70	2	5,6,7	0.61	0	5,7,9	0.96	1 (20%)
2	DTH	F	9	-	5,6,7	0.71	0	5,7,9	1.71	2 (40%)

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	DNE	B	1	2	-	0/4/6/8	0/0/0/0
2	DLY	B	11	2	-	0/5/7/9	0/0/0/0
2	DTH	B	12	2	-	0/4/6/8	0/0/0/0
2	DIL	B	13	2	-	0/6/8/10	0/0/0/0
2	DTH	B	14	2	-	0/4/6/8	0/0/0/0
2	DLE	B	15	2	-	0/4/6/8	0/0/0/0
2	DGL	B	16	2	-	0/3/7/9	0/0/0/0
2	DVA	B	17	2	-	0/4/6/8	0/0/0/0
2	DGL	B	18	2	-	0/3/7/9	0/0/0/0
2	DPR	B	19	2	-	0/0/9/11	0/1/1/1
2	DGN	B	2	2	-	0/5/7/9	0/0/0/0
2	DSN	B	20	2	-	0/2/4/6	0/0/0/0
2	DAS	B	21	2	-	0/2/6/8	0/0/0/0
2	DTH	B	22	2	-	0/4/6/8	0/0/0/0
2	DIL	B	23	2	-	0/6/8/10	0/0/0/0
2	DGL	B	24	2	-	0/3/7/9	0/0/0/0
2	DSG	B	25	2	-	0/4/6/8	0/0/0/0
2	DVA	B	26	2	-	0/4/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DLY	B	27	2	-	0/5/7/9	0/0/0/0
2	DAL	B	28	2	-	0/0/2/4	0/0/0/0
2	DLY	B	29	2	-	0/5/7/9	0/0/0/0
2	DIL	B	3	2	-	0/6/8/10	0/0/0/0
2	DIL	B	30	2	-	0/6/8/10	0/0/0/0
2	DGN	B	31	2	-	0/5/7/9	0/0/0/0
2	DAS	B	32	2	-	0/2/6/8	0/0/0/0
2	DLY	B	33	2	-	0/5/7/9	0/0/0/0
2	DGL	B	34	2	-	0/3/7/9	0/0/0/0
2	DIL	B	36	2	-	0/6/8/10	0/0/0/0
2	DPR	B	37	2	-	0/0/9/11	0/1/1/1
2	DPR	B	38	2	-	0/0/9/11	0/1/1/1
2	DAS	B	39	2	-	0/2/6/8	0/0/0/0
2	DPN	B	4	2	-	0/4/6/8	0/1/1/1
2	DGN	B	40	2	-	0/5/7/9	0/0/0/0
2	DGN	B	41	2	-	0/5/7/9	0/0/0/0
2	DAR	B	42	2	-	0/7/9/11	0/0/0/0
2	DLE	B	43	2	-	0/4/6/8	0/0/0/0
2	DIL	B	44	2	-	0/6/8/10	0/0/0/0
2	DPN	B	45	2	-	0/4/6/8	0/1/1/1
2	DAL	B	46	2	-	0/0/2/4	0/0/0/0
2	DLY	B	48	2	-	0/5/7/9	0/0/0/0
2	DGN	B	49	2	-	0/5/7/9	0/0/0/0
2	DVA	B	5	2	-	0/4/6/8	0/0/0/0
2	DLE	B	50	2	-	0/4/6/8	0/0/0/0
2	DGL	B	51	2	-	0/3/7/9	0/0/0/0
2	DAS	B	52	2	-	0/2/6/8	0/0/0/0
2	DAR	B	54	2	-	0/7/9/11	0/0/0/0
2	DTH	B	55	2	-	0/4/6/8	0/0/0/0
2	DLE	B	56	2	-	0/4/6/8	0/0/0/0
2	DSN	B	57	2	-	0/2/4/6	0/0/0/0
2	DAS	B	58	2	-	0/2/6/8	0/0/0/0
2	DTY	B	59	2	-	0/4/6/8	0/1/1/1
2	DLY	B	6	2	-	0/5/7/9	0/0/0/0
2	DSG	B	60	2	-	0/4/6/8	0/0/0/0
2	DIL	B	61	2	-	0/6/8/10	0/0/0/0
2	DGN	B	62	2	-	0/5/7/9	0/0/0/0
2	DLY	B	63	2	-	0/5/7/9	0/0/0/0
2	DGL	B	64	2	-	0/3/7/9	0/0/0/0
2	DSN	B	65	2	-	0/2/4/6	0/0/0/0
2	DTH	B	66	2	-	0/4/6/8	0/0/0/0
2	DLE	B	67	2	-	0/4/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DHI	B	68	2	-	0/3/6/8	0/1/1/1
2	DLE	B	69	2	-	0/4/6/8	0/0/0/0
2	DTH	B	7	2	-	0/4/6/8	0/0/0/0
2	DVA	B	70	2	-	0/4/6/8	0/0/0/0
2	DNE	D	1	2	-	0/4/6/8	0/0/0/0
2	DLY	D	11	2	-	0/5/7/9	0/0/0/0
2	DTH	D	12	2	-	0/4/6/8	0/0/0/0
2	DIL	D	13	2	-	0/6/8/10	0/0/0/0
2	DTH	D	14	2	-	0/4/6/8	0/0/0/0
2	DLE	D	15	2	-	0/4/6/8	0/0/0/0
2	DGL	D	16	2	-	0/3/7/9	0/0/0/0
2	DVA	D	17	2	-	0/4/6/8	0/0/0/0
2	DGL	D	18	2	-	0/3/7/9	0/0/0/0
2	DPR	D	19	2	-	0/0/9/11	0/1/1/1
2	DGN	D	2	2	-	0/5/7/9	0/0/0/0
2	DSN	D	20	2	-	0/2/4/6	0/0/0/0
2	DAS	D	21	2	-	0/2/6/8	0/0/0/0
2	DTH	D	22	2	-	0/4/6/8	0/0/0/0
2	DIL	D	23	2	-	0/6/8/10	0/0/0/0
2	DGL	D	24	2	-	0/3/7/9	0/0/0/0
2	DSG	D	25	2	-	0/4/6/8	0/0/0/0
2	DVA	D	26	2	-	0/4/6/8	0/0/0/0
2	DLY	D	27	2	-	0/5/7/9	0/0/0/0
2	DAL	D	28	2	-	0/0/2/4	0/0/0/0
2	DLY	D	29	2	-	0/5/7/9	0/0/0/0
2	DIL	D	3	2	-	0/6/8/10	0/0/0/0
2	DIL	D	30	2	-	0/6/8/10	0/0/0/0
2	DGN	D	31	2	-	0/5/7/9	0/0/0/0
2	DAS	D	32	2	-	0/2/6/8	0/0/0/0
2	DLY	D	33	2	-	0/5/7/9	0/0/0/0
2	DGL	D	34	2	-	0/3/7/9	0/0/0/0
2	DIL	D	36	2	-	0/6/8/10	0/0/0/0
2	DPR	D	37	2	-	0/0/9/11	0/1/1/1
2	DPR	D	38	2	-	0/0/9/11	0/1/1/1
2	DAS	D	39	2	-	0/2/6/8	0/0/0/0
2	DPN	D	4	2	-	0/4/6/8	0/1/1/1
2	DGN	D	40	2	-	0/5/7/9	0/0/0/0
2	DGN	D	41	2	-	0/5/7/9	0/0/0/0
2	DAR	D	42	2	-	0/7/9/11	0/0/0/0
2	DLE	D	43	2	-	0/4/6/8	0/0/0/0
2	DIL	D	44	2	-	0/6/8/10	0/0/0/0
2	DPN	D	45	2	-	0/4/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DAL	D	46	2	-	0/0/2/4	0/0/0/0
2	DLY	D	48	2	-	0/5/7/9	0/0/0/0
2	DGN	D	49	2	-	0/5/7/9	0/0/0/0
2	DVA	D	5	2	-	0/4/6/8	0/0/0/0
2	DLE	D	50	2	-	0/4/6/8	0/0/0/0
2	DGL	D	51	2	-	0/3/7/9	0/0/0/0
2	DAS	D	52	2	-	0/2/6/8	0/0/0/0
2	DAR	D	54	2	-	0/7/9/11	0/0/0/0
2	DTH	D	55	2	-	0/4/6/8	0/0/0/0
2	DLE	D	56	2	-	0/4/6/8	0/0/0/0
2	DSN	D	57	2	-	0/2/4/6	0/0/0/0
2	DAS	D	58	2	-	0/2/6/8	0/0/0/0
2	DTY	D	59	2	-	0/4/6/8	0/1/1/1
2	DLY	D	6	2	-	0/5/7/9	0/0/0/0
2	DSG	D	60	2	-	0/4/6/8	0/0/0/0
2	DIL	D	61	2	-	0/6/8/10	0/0/0/0
2	DGN	D	62	2	-	0/5/7/9	0/0/0/0
2	DLY	D	63	2	-	0/5/7/9	0/0/0/0
2	DGL	D	64	2	-	0/3/7/9	0/0/0/0
2	DSN	D	65	2	-	0/2/4/6	0/0/0/0
2	DTH	D	66	2	-	0/4/6/8	0/0/0/0
2	DLE	D	67	2	-	0/4/6/8	0/0/0/0
2	DHI	D	68	2	-	0/3/6/8	0/1/1/1
2	DLE	D	69	2	-	0/4/6/8	0/0/0/0
2	DTH	D	7	2	-	0/4/6/8	0/0/0/0
2	DVA	D	70	2	-	0/4/6/8	0/0/0/0
2	DNE	F	1	2	-	0/4/6/8	0/0/0/0
2	DTH	F	12	2	-	0/4/6/8	0/0/0/0
2	DIL	F	13	2	-	0/6/8/10	0/0/0/0
2	DTH	F	14	2	-	0/4/6/8	0/0/0/0
2	DLE	F	15	2	-	0/4/6/8	0/0/0/0
2	DGL	F	16	2	-	0/3/7/9	0/0/0/0
2	DVA	F	17	2	-	0/4/6/8	0/0/0/0
2	DGL	F	18	2	-	0/3/7/9	0/0/0/0
2	DPR	F	19	2	-	0/0/9/11	0/1/1/1
2	DGN	F	2	2	-	0/5/7/9	0/0/0/0
2	DSN	F	20	2	-	0/2/4/6	0/0/0/0
2	DAS	F	21	2	-	0/2/6/8	0/0/0/0
2	DTH	F	22	2	-	0/4/6/8	0/0/0/0
2	DIL	F	23	2	-	0/6/8/10	0/0/0/0
2	DGL	F	24	2	-	0/3/7/9	0/0/0/0
2	DSG	F	25	2	-	0/4/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DVA	F	26	2	-	0/4/6/8	0/0/0/0
2	DLY	F	27	2	-	0/5/7/9	0/0/0/0
2	DAL	F	28	2	-	0/0/2/4	0/0/0/0
2	DLY	F	29	2	-	0/5/7/9	0/0/0/0
2	DIL	F	3	2	-	0/6/8/10	0/0/0/0
2	DIL	F	30	2	-	0/6/8/10	0/0/0/0
2	DGN	F	31	2	-	0/5/7/9	0/0/0/0
2	DAS	F	32	2	-	0/2/6/8	0/0/0/0
2	DLY	F	33	2	-	0/5/7/9	0/0/0/0
2	DGL	F	34	2	-	0/3/7/9	0/0/0/0
2	DIL	F	36	2	-	0/6/8/10	0/0/0/0
2	DPR	F	37	2	-	0/0/9/11	0/1/1/1
2	DPR	F	38	2	-	0/0/9/11	0/1/1/1
2	DAS	F	39	2	-	0/2/6/8	0/0/0/0
2	DPN	F	4	2	-	0/4/6/8	0/1/1/1
2	DGN	F	40	2	-	0/5/7/9	0/0/0/0
2	DGN	F	41	2	-	0/5/7/9	0/0/0/0
2	DAR	F	42	2	-	0/7/9/11	0/0/0/0
2	DLE	F	43	2	-	0/4/6/8	0/0/0/0
2	DIL	F	44	2	-	0/6/8/10	0/0/0/0
2	DPN	F	45	2	-	0/4/6/8	0/1/1/1
2	DAL	F	46	2	-	0/0/2/4	0/0/0/0
2	DLY	F	48	2	-	0/5/7/9	0/0/0/0
2	DGN	F	49	2	-	0/5/7/9	0/0/0/0
2	DVA	F	5	2	-	0/4/6/8	0/0/0/0
2	DLE	F	50	2	-	0/4/6/8	0/0/0/0
2	DGL	F	51	2	-	0/3/7/9	0/0/0/0
2	DAS	F	52	2	-	0/2/6/8	0/0/0/0
2	DAR	F	54	2	-	0/7/9/11	0/0/0/0
2	DTH	F	55	2	-	0/4/6/8	0/0/0/0
2	DLE	F	56	2	-	0/4/6/8	0/0/0/0
2	DSN	F	57	2	-	0/2/4/6	0/0/0/0
2	DAS	F	58	2	-	0/2/6/8	0/0/0/0
2	DTY	F	59	2	-	0/4/6/8	0/1/1/1
2	DLY	F	6	2	-	0/5/7/9	0/0/0/0
2	DSG	F	60	2	-	0/4/6/8	0/0/0/0
2	DIL	F	61	2	-	0/6/8/10	0/0/0/0
2	DGN	F	62	2	-	0/5/7/9	0/0/0/0
2	DLY	F	63	2	-	0/5/7/9	0/0/0/0
2	DGL	F	64	2	-	0/3/7/9	0/0/0/0
2	DSN	F	65	2	-	0/2/4/6	0/0/0/0
2	DTH	F	66	2	-	0/4/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DLE	F	67	2	-	0/4/6/8	0/0/0/0
2	DHI	F	68	2	-	0/3/6/8	0/1/1/1
2	DLE	F	69	2	-	0/4/6/8	0/0/0/0
2	DTH	F	7	2	-	0/4/6/8	0/0/0/0
2	DVA	F	70	2	-	0/4/6/8	0/0/0/0
2	DTH	F	9	-	-	0/4/6/8	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	45	DPN	CE1-CD1	-2.07	1.34	1.38
2	D	60	DSG	CB-CG	-2.04	1.46	1.51
2	B	2	DGN	CB-CA	2.06	1.56	1.53
2	D	2	DGN	CB-CA	2.23	1.56	1.53

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	49	DGN	O-C-CA	-3.27	116.94	125.72
2	D	13	DIL	O-C-CA	-3.01	117.46	125.69
2	B	13	DIL	O-C-CA	-2.96	117.61	125.69
2	F	17	DVA	C-CA-N	-2.95	103.43	109.95
2	B	13	DIL	C-CA-N	-2.94	103.46	109.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

70 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	DNE	1	0
2	B	14	DTH	2	0
2	B	16	DGL	1	0
2	B	17	DVA	1	0
2	B	2	DGN	1	0
2	B	24	DGL	1	0
2	B	4	DPN	2	0
2	B	42	DAR	3	0
2	B	45	DPN	2	0
2	B	46	DAL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	52	DAS	1	0
2	B	54	DAR	5	0
2	B	65	DSN	1	0
2	B	67	DLE	1	0
2	B	70	DVA	1	0
2	D	1	DNE	1	0
2	D	11	DLY	1	0
2	D	13	DIL	3	0
2	D	15	DLE	1	0
2	D	16	DGL	3	0
2	D	17	DVA	1	0
2	D	18	DGL	1	0
2	D	2	DGN	5	0
2	D	27	DLY	1	0
2	D	34	DGL	1	0
2	D	41	DGN	1	0
2	D	42	DAR	5	0
2	D	45	DPN	1	0
2	D	46	DAL	2	0
2	D	49	DGN	1	0
2	D	5	DVA	2	0
2	D	51	DGL	2	0
2	D	54	DAR	3	0
2	D	59	DTY	1	0
2	D	63	DLY	1	0
2	D	64	DGL	1	0
2	D	67	DLE	1	0
2	D	7	DTH	1	0
2	D	70	DVA	2	0
2	F	1	DNE	1	0
2	F	13	DIL	3	0
2	F	15	DLE	1	0
2	F	17	DVA	1	0
2	F	18	DGL	3	0
2	F	2	DGN	1	0
2	F	22	DTH	1	0
2	F	23	DIL	1	0
2	F	26	DVA	1	0
2	F	34	DGL	1	0
2	F	38	DPR	1	0
2	F	4	DPN	1	0
2	F	41	DGN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	42	DAR	1	0
2	F	45	DPN	1	0
2	F	46	DAL	1	0
2	F	5	DVA	2	0
2	F	51	DGL	2	0
2	F	54	DAR	4	0
2	F	56	DLE	1	0
2	F	59	DTY	2	0
2	F	61	DIL	1	0
2	F	63	DLY	1	0
2	F	64	DGL	2	0
2	F	65	DSN	2	0
2	F	67	DLE	1	0
2	F	68	DHI	1	0
2	F	69	DLE	1	0
2	F	7	DTH	2	0
2	F	70	DVA	1	0
2	F	9	DTH	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	73/76 (96%)	0.47	3 (4%) 41 45	19, 28, 46, 73	0
1	C	72/76 (94%)	0.42	4 (5%) 28 32	20, 29, 44, 54	0
1	E	73/76 (96%)	0.41	5 (6%) 20 24	19, 28, 50, 67	0
2	B	3/76 (3%)	0.93	0 100 100	25, 25, 42, 53	0
2	D	3/76 (3%)	1.09	0 100 100	27, 27, 41, 52	0
2	F	3/76 (3%)	0.66	0 100 100	29, 29, 42, 44	0
All	All	227/456 (49%)	0.45	12 (5%) 30 34	19, 29, 52, 73	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	ARG	5.6
1	A	75	GLY	5.5
1	E	73	LEU	4.7
1	E	75	GLY	3.7
1	C	72	ARG	3.4

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	DLE	B	43	8/9	0.90	0.17	-	25,31,45,47	0
2	DLY	D	6	9/10	0.91	0.17	-	31,51,77,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	DTH	F	9	7/8	0.77	0.20	-	40,47,58,59	0
2	DLE	B	69	8/9	0.94	0.13	-	25,35,42,43	0
2	DPR	D	37	7/8	0.93	0.16	-	26,36,43,43	0
2	DTH	F	12	7/8	0.79	0.18	-	28,40,45,54	0
2	DHI	B	68	10/11	0.91	0.16	-	20,30,39,41	0
2	DIL	D	13	8/9	0.90	0.12	-	35,43,50,50	0
2	DLE	B	67	8/9	0.91	0.14	-	22,29,41,41	0
2	DAS	D	52	8/9	0.75	0.16	-	36,44,50,56	0
2	DVA	D	26	7/8	0.80	0.22	-	27,34,39,41	0
2	DTH	B	22	7/8	0.88	0.14	-	29,33,36,39	0
2	DVA	B	26	7/8	0.81	0.23	-	29,35,37,40	0
2	DAS	D	21	8/9	0.83	0.17	-	29,42,50,53	0
2	DGN	B	41	9/10	0.87	0.15	-	29,37,47,54	0
2	DLY	F	6	9/10	0.93	0.19	-	31,55,78,92	0
2	DGN	B	31	9/10	0.82	0.16	-	30,38,50,50	0
2	DIL	B	61	8/9	0.92	0.15	-	22,33,41,42	0
2	DGL	B	18	9/10	0.89	0.10	-	28,36,46,46	0
2	DPN	D	4	11/12	0.91	0.12	-	25,40,55,55	0
2	DGN	B	62	9/10	0.89	0.15	-	24,39,50,51	0
2	DNE	B	1	8/9	0.88	0.15	-	22,36,47,55	0
2	DNE	D	1	8/9	0.89	0.15	-	30,41,50,50	0
2	DLY	F	48	9/10	0.91	0.12	-	22,33,48,56	0
2	DGL	F	24	9/10	0.83	0.18	-	28,48,66,78	0
2	DVA	F	5	7/8	0.93	0.15	-	27,35,39,39	0
2	DVA	D	70	7/8	0.86	0.18	-	31,37,52,52	0
2	DPR	F	37	7/8	0.93	0.12	-	24,30,40,40	0
2	DLY	D	33	9/10	0.82	0.22	-	43,55,66,68	0
2	DTY	B	59	12/13	0.90	0.13	-	17,26,32,34	0
2	DGN	D	62	9/10	0.87	0.16	-	29,48,63,66	0
2	DLE	F	67	8/9	0.93	0.16	-	25,36,39,43	0
2	DGL	B	64	9/10	0.83	0.20	-	30,45,66,71	0
2	DSN	D	57	6/7	0.88	0.19	-	21,26,40,48	0
2	DLE	F	56	8/9	0.88	0.21	-	21,25,32,32	0
2	DSN	F	57	6/7	0.93	0.12	-	20,24,31,37	0
2	DIL	B	23	8/9	0.91	0.16	-	27,36,49,49	0
2	DLY	B	6	9/10	0.94	0.16	-	28,42,83,100	0
2	DNE	F	1	8/9	0.93	0.13	-	26,34,41,41	0
2	DLY	D	29	9/10	0.88	0.18	-	28,41,56,58	0
2	DTY	D	59	12/13	0.87	0.13	-	22,31,39,41	0
2	DLY	F	33	9/10	0.82	0.26	-	44,60,72,82	0
2	DGL	F	51	9/10	0.91	0.14	-	27,42,69,69	0
2	DTH	D	66	7/8	0.91	0.13	-	24,26,27,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	DAR	D	42	11/12	0.86	0.30	-	24,68,88,94	0
2	DGN	F	31	9/10	0.79	0.17	-	30,47,57,57	0
2	DLE	F	50	8/9	0.90	0.14	-	24,29,38,40	0
2	DSN	B	65	6/7	0.86	0.17	-	24,36,51,51	0
2	DPR	F	19	7/8	0.88	0.17	-	23,27,36,38	0
2	DAL	B	46	5/6	0.95	0.10	-	14,19,24,25	0
2	DPR	D	19	7/8	0.94	0.12	-	26,32,33,43	0
2	DLY	F	27	9/10	0.94	0.10	-	26,33,42,48	0
2	DAS	B	32	8/9	0.82	0.20	-	38,48,56,60	0
2	DAR	D	54	11/12	0.87	0.15	-	28,42,50,58	0
2	DSN	F	20	6/7	0.90	0.13	-	26,30,36,37	0
2	DIL	B	30	8/9	0.91	0.15	-	26,35,42,43	0
2	DGL	B	24	9/10	0.85	0.24	-	36,56,81,95	0
2	DTH	D	22	7/8	0.95	0.12	-	29,31,35,43	0
2	DAS	D	39	8/9	0.88	0.14	-	35,43,59,61	0
2	DLE	D	15	8/9	0.89	0.12	-	25,32,37,39	0
2	DLE	D	56	8/9	0.94	0.16	-	22,31,41,41	0
2	DLE	B	56	8/9	0.94	0.17	-	19,27,32,32	0
2	DAL	D	28	5/6	0.91	0.16	-	29,31,38,44	0
2	DAR	B	54	11/12	0.91	0.15	-	30,37,46,53	0
2	DPN	B	45	11/12	0.89	0.12	-	15,25,31,36	0
2	DIL	B	36	8/9	0.90	0.13	-	22,33,38,43	0
2	DGN	F	41	9/10	0.93	0.11	-	28,36,42,50	0
2	DGN	B	49	9/10	0.86	0.23	-	26,39,60,60	0
2	DGN	D	41	9/10	0.91	0.11	-	23,31,42,50	0
2	DLE	D	50	8/9	0.89	0.16	-	30,36,44,44	0
2	DSN	D	20	6/7	0.89	0.14	-	26,32,39,47	0
2	DLE	F	43	8/9	0.93	0.14	-	25,33,46,46	0
2	DGN	D	40	9/10	0.87	0.20	-	35,53,78,78	0
2	DGL	B	34	9/10	0.83	0.21	-	33,52,65,73	0
2	DTH	D	14	7/8	0.92	0.15	-	29,34,48,51	0
2	DIL	F	30	8/9	0.92	0.16	-	28,36,46,52	0
2	DGL	D	24	9/10	0.89	0.21	-	28,52,75,88	0
2	DGL	F	34	9/10	0.86	0.13	-	42,48,61,73	0
2	DLY	B	29	9/10	0.94	0.11	-	26,37,49,52	0
2	DVA	F	17	7/8	0.88	0.15	-	28,38,45,46	0
2	DLY	B	33	9/10	0.81	0.26	-	31,45,54,54	0
2	DAL	F	46	5/6	0.93	0.11	-	19,21,26,26	0
2	DGN	F	2	9/10	0.94	0.10	-	29,43,52,58	0
2	DGL	D	64	9/10	0.83	0.19	-	29,47,71,71	0
2	DGL	F	64	9/10	0.88	0.15	-	27,54,70,70	0
2	DIL	B	13	8/9	0.87	0.17	-	29,39,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	DSN	B	20	6/7	0.90	0.14	-	24,29,33,34	0
2	DTH	F	22	7/8	0.94	0.10	-	21,34,37,43	0
2	DTH	D	7	7/8	0.88	0.15	-	39,53,59,61	0
2	DPR	F	38	7/8	0.96	0.12	-	28,30,38,38	0
2	DVA	D	5	7/8	0.94	0.10	-	21,33,45,45	0
2	DAS	D	58	8/9	0.92	0.11	-	23,30,39,47	0
2	DPR	B	19	7/8	0.91	0.14	-	25,28,39,40	0
2	DAS	F	58	8/9	0.92	0.12	-	17,25,33,39	0
2	DAS	F	32	8/9	0.79	0.23	-	48,58,64,73	0
2	DTH	B	55	7/8	0.95	0.15	-	24,26,34,41	0
2	DSN	F	65	6/7	0.89	0.14	-	21,36,43,51	0
2	DIL	D	30	8/9	0.87	0.18	-	28,35,39,46	0
2	DSG	F	60	8/9	0.92	0.10	-	23,30,42,42	0
2	DIL	B	44	8/9	0.90	0.16	-	24,32,59,59	0
2	DAL	B	28	5/6	0.92	0.13	-	25,30,39,43	0
2	DIL	B	3	8/9	0.87	0.17	-	21,30,46,55	0
2	DGL	D	16	9/10	0.86	0.12	-	33,42,52,52	0
2	DIL	D	3	8/9	0.96	0.10	-	23,30,42,50	0
2	DTH	F	66	7/8	0.93	0.12	-	25,26,28,36	0
2	DTH	B	12	7/8	0.87	0.17	-	24,32,35,49	0
2	DHI	F	68	10/11	0.90	0.11	-	18,27,36,38	0
2	DAS	B	39	8/9	0.89	0.13	-	28,38,46,47	0
2	DLY	D	11	9/10	0.79	0.26	-	36,60,103,108	0
2	DLE	D	69	8/9	0.88	0.12	-	26,33,48,48	0
2	DGN	F	49	9/10	0.88	0.14	-	26,39,52,52	0
2	DPR	B	38	7/8	0.94	0.11	-	26,31,35,38	0
2	DGN	D	49	9/10	0.83	0.22	-	26,39,53,53	0
2	DLY	F	63	9/10	0.86	0.29	-	37,69,76,90	0
2	DSG	B	25	8/9	0.71	0.29	-	32,44,53,53	0
2	DGN	B	2	9/10	0.81	0.18	-	30,47,53,64	0
2	DLY	B	27	9/10	0.95	0.10	-	25,33,43,52	0
2	DAS	F	21	8/9	0.87	0.15	-	24,35,42,51	0
2	DIL	F	3	8/9	0.92	0.13	-	28,35,44,50	0
2	DTH	F	7	7/8	0.74	0.17	-	37,56,56,58	0
2	DSG	D	60	8/9	0.89	0.14	-	23,34,51,51	0
2	DIL	F	36	8/9	0.93	0.11	-	21,28,47,47	0
2	DAR	F	42	11/12	0.84	0.25	-	26,53,75,91	0
2	DIL	D	61	8/9	0.92	0.15	-	31,38,48,56	0
2	DGL	D	51	9/10	0.87	0.19	-	25,40,67,67	0
2	DGL	D	34	9/10	0.88	0.19	-	31,61,70,74	0
2	DSG	B	60	8/9	0.94	0.12	-	21,28,37,37	0
2	DSG	D	25	8/9	0.89	0.12	-	32,41,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	DGL	D	18	9/10	0.92	0.21	-	29,44,56,64	0
2	DPN	D	45	11/12	0.91	0.11	-	21,26,33,39	0
2	DVA	D	17	7/8	0.88	0.16	-	30,36,40,47	0
2	DIL	F	13	8/9	0.84	0.18	-	39,47,52,55	0
2	DVA	B	5	7/8	0.92	0.14	-	26,32,38,44	0
2	DVA	F	26	7/8	0.85	0.20	-	29,37,46,46	0
2	DSN	D	65	6/7	0.89	0.13	-	25,35,45,48	0
2	DGL	B	16	9/10	0.89	0.16	-	25,39,47,47	0
2	DLE	F	69	8/9	0.94	0.10	-	19,25,33,44	0
2	DAS	B	21	8/9	0.84	0.14	-	22,27,40,48	0
2	DLY	B	63	9/10	0.91	0.21	-	33,58,70,74	0
2	DTH	B	66	7/8	0.91	0.14	-	22,23,31,35	0
2	DGN	F	40	9/10	0.87	0.14	-	34,44,55,55	0
2	DAR	B	42	11/12	0.84	0.34	-	28,66,90,91	0
2	DIL	F	23	8/9	0.92	0.13	-	25,33,40,40	0
2	DPN	F	4	11/12	0.89	0.15	-	32,38,50,57	0
2	DTY	F	59	12/13	0.94	0.08	-	18,27,34,39	0
2	DPR	D	38	7/8	0.97	0.13	-	22,28,34,34	0
2	DIL	D	36	8/9	0.92	0.14	-	27,35,45,45	0
2	DLY	F	29	9/10	0.89	0.20	-	29,39,49,52	0
2	DVA	B	70	7/8	0.92	0.17	-	28,49,63,63	0
2	DIL	F	44	8/9	0.90	0.15	-	25,31,49,49	0
2	DAR	F	54	11/12	0.87	0.12	-	23,34,45,53	0
2	DVA	B	17	7/8	0.90	0.12	-	29,35,40,47	0
2	DAS	F	39	8/9	0.92	0.16	-	26,34,58,67	0
2	DLY	B	11	9/10	0.80	0.35	-	37,72,97,105	0
2	DLE	B	15	8/9	0.89	0.19	-	22,29,38,38	0
2	DTH	F	55	7/8	0.90	0.13	-	17,26,31,36	0
2	DGN	B	40	9/10	0.82	0.23	-	41,52,70,70	0
2	DGL	B	51	9/10	0.80	0.23	-	30,41,62,65	0
2	DPN	F	45	11/12	0.87	0.14	-	22,28,36,38	0
2	DAS	F	52	8/9	0.68	0.25	-	44,53,62,63	0
2	DSG	F	25	8/9	0.77	0.22	-	31,46,57,57	0
2	DPR	B	37	7/8	0.93	0.11	-	30,38,46,46	0
2	DAL	F	28	5/6	0.91	0.15	-	26,35,38,45	0
2	DGL	F	16	9/10	0.88	0.13	-	29,38,45,48	0
2	DTH	B	7	7/8	0.81	0.20	-	35,42,49,50	0
2	DHI	D	68	10/11	0.85	0.17	-	20,30,43,44	0
2	DPN	B	4	11/12	0.92	0.15	-	32,40,48,56	0
2	DTH	F	14	7/8	0.81	0.19	-	30,36,50,51	0
2	DTH	D	55	7/8	0.92	0.12	-	27,30,33,44	0
2	DLY	D	48	9/10	0.90	0.17	-	24,52,66,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	DTH	D	12	7/8	0.82	0.15	-	32,36,43,55	0
2	DLE	B	50	8/9	0.86	0.16	-	23,29,35,39	0
2	DGN	D	2	9/10	0.73	0.16	-	27,47,60,60	0
2	DAS	B	52	8/9	0.74	0.18	-	43,51,55,61	0
2	DIL	D	23	8/9	0.89	0.18	-	27,37,46,46	0
2	DSN	B	57	6/7	0.90	0.17	-	15,26,34,41	0
2	DIL	D	44	8/9	0.94	0.14	-	25,35,51,51	0
2	DGN	D	31	9/10	0.82	0.19	-	32,43,52,56	0
2	DLE	F	15	8/9	0.90	0.16	-	30,40,48,48	0
2	DGL	F	18	9/10	0.88	0.14	-	28,34,44,44	0
2	DLY	B	48	9/10	0.91	0.14	-	25,33,52,59	0
2	DVA	F	70	7/8	0.91	0.17	-	27,40,57,57	0
2	DLY	D	63	9/10	0.77	0.31	-	38,56,71,81	0
2	DAS	B	58	8/9	0.92	0.14	-	19,23,35,42	0
2	DAL	D	46	5/6	0.90	0.14	-	16,22,22,23	0
2	DAS	D	32	8/9	0.84	0.18	-	39,53,62,63	0
2	DGN	F	62	9/10	0.91	0.15	-	29,37,50,58	0
2	DLE	D	67	8/9	0.88	0.16	-	23,33,39,39	0
2	DLE	D	43	8/9	0.92	0.15	-	23,30,37,39	0
2	DIL	F	61	8/9	0.90	0.24	-	27,33,42,50	0
2	DLY	D	27	9/10	0.89	0.13	-	25,34,40,41	0
2	DTH	B	14	7/8	0.83	0.20	-	26,39,52,58	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.