



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:57 am BST

PDB ID : 2XO2  
Title : Human Annexin V with incorporated Methionine analogue Azidohomoalanine  
Authors : Debela, M.; Merkel, L.; Goettig, P.; Budisa, N.  
Deposited on : 2010-08-09  
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

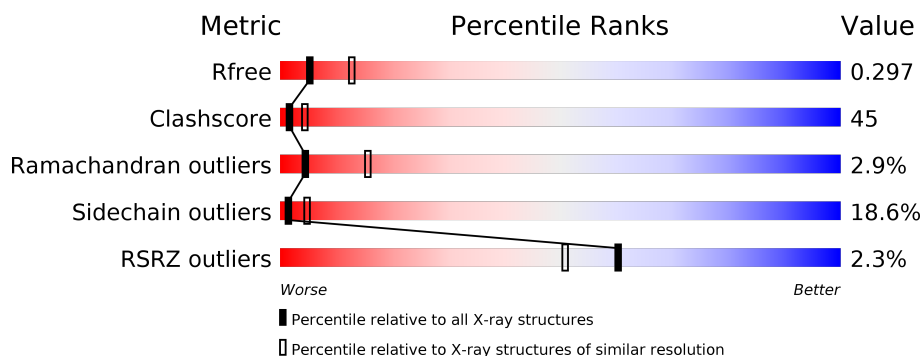
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	320	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	AZH	A	152	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2635 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 ANNEXIN A5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	95	0	1
			2512	1571	443	497	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	AZH	MET	engineered mutation	UNP P08758
A	28	AZH	MET	engineered mutation	UNP P08758
A	85	AZH	MET	engineered mutation	UNP P08758
A	152	AZH	MET	engineered mutation	UNP P08758
A	214	AZH	MET	engineered mutation	UNP P08758
A	259	AZH	MET	engineered mutation	UNP P08758
A	273	AZH	MET	engineered mutation	UNP P08758
A	299	AZH	MET	engineered mutation	UNP P08758

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

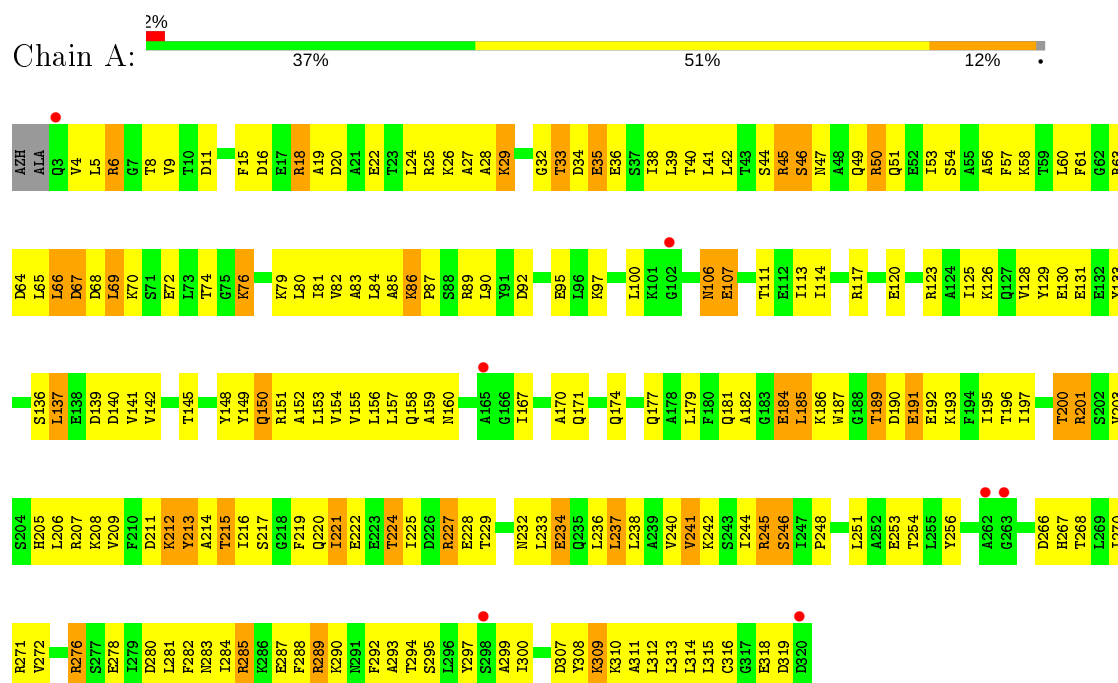
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	109	Total	O	0	0
			109	109		

### 3 Residue-property plots

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.

#### • Molecule 1: ANNEXIN A5



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.71 Å   152.71 Å   33.60 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	19.09 – 2.80 19.09 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.09-2.80) 99.9 (19.09-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.79 Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.274   ,   0.296 0.269   ,   0.297	Depositor DCC
$R_{free}$ test set	377 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.3	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29   ,   54.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2635	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: AZH, NA, CA, SO4, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.33	0/2476	0.55	1/3327 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	32	GLY	N-CA-C	-5.22	100.05	113.10

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	2512	0	2494	213	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	10	0	0	1	0
5	A	1	0	0	0	0
6	A	109	0	0	3	0
All	All	2635	0	2494	213	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 45.

All (213) 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:47:ASN:HA	1:A:50:ARG:HD2	1.35	1.05
1:A:27:ALA:HB1	1:A:34:ASP:HB3	1.40	0.99
1:A:129:TYR:HB3	1:A:137:LEU:HD12	1.57	0.87
1:A:212:LYS:HA	1:A:215:THR:HG23	1.58	0.84
1:A:64:ASP:HB3	1:A:67:ASP:HB2	1.61	0.82
1:A:242:LYS:HA	1:A:245:ARG:HD3	1.62	0.81
1:A:137:LEU:H	1:A:137:LEU:HD22	1.46	0.80
1:A:268:THR:HG22	1:A:271:ARG:NH2	1.96	0.80
1:A:182:ALA:HA	1:A:186:LYS:HZ1	1.46	0.80
1:A:24:LEU:HD23	1:A:65:LEU:HD11	1.66	0.78
1:A:137:LEU:HD13	1:A:137:LEU:N	1.97	0.77
1:A:137:LEU:O	1:A:141:VAL:HG23	1.85	0.76
1:A:25:ARG:HH12	1:A:63:ARG:NH2	1.84	0.76
1:A:27:ALA:CB	1:A:34:ASP:HB3	2.14	0.76
1:A:197:ILE:HA	1:A:201:ARG:HD3	1.67	0.75
1:A:285:ARG:NH2	1:A:319:ASP:HB2	2.03	0.74
1:A:100:LEU:HD13	1:A:140:ASP:HB3	1.70	0.73
1:A:50:ARG:HA	1:A:53:ILE:HD12	1.70	0.73
1:A:47:ASN:O	1:A:51:GLN:HG2	1.89	0.73
1:A:25:ARG:HH12	1:A:63:ARG:HH21	1.36	0.72
1:A:212:LYS:O	1:A:216:ILE:HG12	1.89	0.72
1:A:251:LEU:HD13	1:A:276:ARG:HD2	1.71	0.72
1:A:41:LEU:O	1:A:45:ARG:HD2	1.90	0.71
1:A:282:PHE:HD1	1:A:285:ARG:HH12	1.36	0.71
1:A:221:ILE:O	1:A:225:ILE:HG13	1.90	0.71
1:A:196:THR:O	1:A:200:THR:HG23	1.91	0.70
1:A:309:LYS:HD3	1:A:310:LYS:H	1.57	0.70
1:A:182:ALA:HA	1:A:186:LYS:NZ	2.07	0.69
1:A:39:LEU:HD21	1:A:311:ALA:HA	1.74	0.69
1:A:152:AZH:HB2C	1:A:236:LEU:HD23	1.74	0.68
1:A:4:VAL:HG13	1:A:4:VAL:O	1.94	0.67
1:A:234:GLU:O	1:A:238:LEU:HB2	1.95	0.67
1:A:285:ARG:CZ	1:A:319:ASP:HB2	2.25	0.66
1:A:51:GLN:HE22	1:A:86:LYS:C	1.98	0.66
1:A:137:LEU:H	1:A:137:LEU:HD13	1.61	0.65
1:A:126:LYS:CA	1:A:137:LEU:HG	2.27	0.65
1:A:148:TYR:HA	1:A:151:ARG:HG3	1.79	0.64
1:A:310:LYS:O	1:A:314:LEU:HD13	1.96	0.64
1:A:191:GLU:O	1:A:195:ILE:HG13	1.97	0.64
1:A:90:LEU:O	1:A:90:LEU:HD23	1.96	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LYS:HB2	1:A:137:LEU:HG	1.80	0.64
1:A:136:SER:HB3	1:A:139:ASP:HB2	1.79	0.63
1:A:25:ARG:NH2	4:A:1331:SO4:O4	2.31	0.63
1:A:42:LEU:HD23	1:A:81:ILE:HG23	1.81	0.63
1:A:129:TYR:CD1	1:A:137:LEU:HD12	2.34	0.63
1:A:184:GLU:OE2	1:A:224:THR:HB	1.99	0.62
1:A:289:ARG:HH11	1:A:289:ARG:HG3	1.62	0.62
1:A:141:VAL:HG21	1:A:157:LEU:HD22	1.81	0.62
1:A:270:ILE:HD11	1:A:308:TYR:HE1	1.65	0.62
1:A:92:ASP:HB2	1:A:125:ILE:HG12	1.81	0.62
1:A:129:TYR:CB	1:A:137:LEU:HD12	2.30	0.62
1:A:65:LEU:O	1:A:69:LEU:HD22	2.00	0.61
1:A:233:LEU:O	1:A:237:LEU:HD22	1.99	0.61
1:A:238:LEU:O	1:A:242:LYS:HG2	2.00	0.61
1:A:248:PRO:HA	1:A:284:ILE:HD13	1.82	0.61
1:A:126:LYS:HA	1:A:137:LEU:HG	1.83	0.60
1:A:45:ARG:HB3	1:A:45:ARG:NH1	2.16	0.60
1:A:197:ILE:O	1:A:201:ARG:HG2	2.02	0.60
1:A:57:PHE:HE2	1:A:63:ARG:HB2	1.65	0.60
1:A:153:LEU:O	1:A:157:LEU:HB2	2.03	0.59
1:A:203:VAL:HG13	1:A:244:ILE:HG23	1.84	0.59
1:A:126:LYS:O	1:A:137:LEU:HD11	2.03	0.59
1:A:142:VAL:HG13	1:A:150:GLN:HE22	1.68	0.59
1:A:22:GLU:HB3	1:A:61:PHE:HZ	1.68	0.59
1:A:129:TYR:HB3	1:A:137:LEU:CD1	2.32	0.59
1:A:282:PHE:CD1	1:A:285:ARG:NH1	2.71	0.59
1:A:177:GLN:O	1:A:181:GLN:HG3	2.03	0.58
1:A:117:ARG:NH2	6:A:2053:HOH:O	2.31	0.58
1:A:51:GLN:HE22	1:A:87:PRO:N	2.01	0.58
1:A:270:ILE:HD11	1:A:308:TYR:CE1	2.39	0.58
1:A:282:PHE:HD1	1:A:285:ARG:NH1	2.02	0.58
1:A:24:LEU:O	1:A:28:AZH:HB2C	2.04	0.58
1:A:190:ASP:C	1:A:192:GLU:H	2.07	0.57
1:A:141:VAL:HG21	1:A:157:LEU:CD2	2.35	0.57
1:A:20:ASP:O	1:A:24:LEU:HD13	2.05	0.57
1:A:186:LYS:HG2	1:A:187:TRP:N	2.20	0.56
1:A:84:LEU:HD21	1:A:315:LEU:HD12	1.87	0.56
1:A:85:AZH:O	1:A:85:AZH:HG2C	2.04	0.56
1:A:300:ILE:HG21	1:A:312:LEU:HB3	1.86	0.56
1:A:128:VAL:HA	1:A:131:GLU:HG2	1.85	0.56
1:A:234:GLU:HG3	1:A:238:LEU:HD22	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:PHE:CE2	1:A:63:ARG:HB2	2.40	0.56
1:A:152:AZH:HB2C	1:A:236:LEU:CD2	2.35	0.56
1:A:251:LEU:HD13	1:A:276:ARG:CD	2.36	0.56
1:A:18:ARG:O	1:A:22:GLU:HG2	2.06	0.56
1:A:33:THR:HG23	1:A:72:GLU:OE1	2.06	0.56
1:A:114:ILE:HD12	1:A:153:LEU:HD22	1.87	0.56
1:A:87:PRO:HB2	1:A:90:LEU:HB3	1.89	0.55
1:A:137:LEU:H	1:A:137:LEU:CD2	2.09	0.55
1:A:287:GLU:HA	1:A:290:LYS:HG2	1.89	0.55
1:A:56:ALA:O	1:A:60:LEU:HB2	2.07	0.55
1:A:25:ARG:O	1:A:29:LYS:HG3	2.06	0.55
1:A:107:GLU:HG3	1:A:232:ASN:OD1	2.07	0.54
1:A:181:GLN:HA	1:A:185:LEU:HB2	1.89	0.54
1:A:76:LYS:HB2	1:A:308:TYR:CE1	2.43	0.53
1:A:309:LYS:HD3	1:A:310:LYS:N	2.24	0.53
1:A:47:ASN:HA	1:A:50:ARG:CD	2.24	0.53
1:A:129:TYR:CG	1:A:137:LEU:HD12	2.44	0.53
1:A:5:LEU:H	1:A:5:LEU:HD22	1.74	0.52
1:A:76:LYS:NZ	6:A:2039:HOH:O	2.41	0.52
1:A:222:GLU:HA	1:A:225:ILE:HD12	1.91	0.52
1:A:9:VAL:HG12	1:A:46:SER:HA	1.91	0.52
1:A:137:LEU:HD22	1:A:137:LEU:N	2.19	0.52
1:A:126:LYS:CB	1:A:137:LEU:HG	2.39	0.52
1:A:197:ILE:O	1:A:206:LEU:HD21	2.10	0.52
1:A:113:ILE:O	1:A:117:ARG:HG2	2.10	0.51
1:A:149:TYR:CD2	1:A:232:ASN:ND2	2.78	0.51
1:A:309:LYS:NZ	1:A:310:LYS:HD2	2.25	0.51
1:A:84:LEU:HD21	1:A:315:LEU:CD1	2.39	0.51
1:A:266:ASP:O	1:A:270:ILE:HG12	2.10	0.51
1:A:253:GLU:HB2	1:A:292:PHE:HZ	1.75	0.51
1:A:26:LYS:O	1:A:29:LYS:HB2	2.11	0.51
1:A:5:LEU:HB3	1:A:280:ASP:HB3	1.93	0.51
1:A:248:PRO:HA	1:A:284:ILE:CD1	2.39	0.51
1:A:15:PHE:HE1	1:A:53:ILE:HD11	1.76	0.51
1:A:111:THR:HG23	1:A:236:LEU:HA	1.93	0.51
1:A:151:ARG:O	1:A:155:VAL:HG23	2.11	0.51
1:A:186:LYS:HE2	1:A:190:ASP:HB2	1.93	0.50
1:A:83:ALA:HA	1:A:86:LYS:HD2	1.94	0.50
1:A:150:GLN:O	1:A:154:VAL:HG23	2.12	0.50
1:A:179:LEU:HD11	1:A:197:ILE:HG21	1.94	0.50
1:A:156:LEU:HA	6:A:2071:HOH:O	2.11	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:SER:C	1:A:45:ARG:HH11	2.16	0.49
1:A:8:THR:HG21	1:A:316:CYS:O	2.12	0.49
1:A:16:ASP:OD2	1:A:19:ALA:HB2	2.12	0.49
1:A:25:ARG:O	1:A:29:LYS:CG	2.60	0.49
1:A:189:THR:HB	1:A:191:GLU:OE1	2.12	0.49
1:A:42:LEU:CD2	1:A:81:ILE:HG23	2.41	0.49
1:A:82:VAL:O	1:A:86:LYS:HD2	2.13	0.49
1:A:197:ILE:O	1:A:206:LEU:HD11	2.13	0.49
1:A:80:LEU:HD22	1:A:312:LEU:CD1	2.43	0.49
1:A:126:LYS:HB2	1:A:137:LEU:CG	2.43	0.49
1:A:192:GLU:HG2	1:A:192:GLU:O	2.13	0.49
1:A:80:LEU:HD22	1:A:312:LEU:HD12	1.95	0.49
1:A:222:GLU:O	1:A:225:ILE:HB	2.13	0.48
1:A:281:LEU:HD12	1:A:284:ILE:HB	1.94	0.48
1:A:51:GLN:NE2	1:A:87:PRO:N	2.60	0.48
1:A:97:LYS:HD3	1:A:133:TYR:CZ	2.47	0.48
1:A:15:PHE:CE1	1:A:53:ILE:HD11	2.47	0.48
1:A:39:LEU:HD12	1:A:307:ASP:HB3	1.94	0.48
1:A:58:LYS:HB3	1:A:63:ARG:O	2.13	0.48
1:A:309:LYS:O	1:A:313:LEU:HG	2.14	0.48
1:A:285:ARG:HH21	1:A:319:ASP:N	2.11	0.48
1:A:186:LYS:HB2	1:A:186:LYS:HZ2	1.79	0.48
1:A:126:LYS:NZ	1:A:158:GLN:HA	2.29	0.47
1:A:242:LYS:HA	1:A:245:ARG:CD	2.36	0.47
1:A:256:TYR:HA	1:A:299:AZH:NZ	2.29	0.47
1:A:5:LEU:HD22	1:A:5:LEU:N	2.29	0.47
1:A:253:GLU:HA	1:A:292:PHE:CE2	2.49	0.47
1:A:97:LYS:HD3	1:A:133:TYR:CE1	2.48	0.47
1:A:148:TYR:O	1:A:152:AZH:HG2C	2.14	0.47
1:A:220:GLN:O	1:A:224:THR:HG23	2.14	0.47
1:A:15:PHE:HZ	1:A:53:ILE:HG13	1.80	0.46
1:A:5:LEU:HA	1:A:283:ASN:HD21	1.79	0.46
1:A:236:LEU:O	1:A:240:VAL:HG23	2.16	0.46
1:A:284:ILE:O	1:A:288:PHE:HB2	2.15	0.46
1:A:289:ARG:O	1:A:293:ALA:HA	2.15	0.46
1:A:251:LEU:O	1:A:254:THR:HB	2.15	0.46
1:A:145:THR:OG1	1:A:150:GLN:HB2	2.15	0.46
1:A:285:ARG:HH21	1:A:319:ASP:HB2	1.81	0.46
1:A:174:GLN:O	1:A:177:GLN:HG3	2.15	0.46
1:A:297:TYR:HB2	1:A:319:ASP:O	2.15	0.46
1:A:6:ARG:O	1:A:282:PHE:HB3	2.14	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LYS:O	1:A:137:LEU:CD1	2.65	0.45
1:A:237:LEU:O	1:A:241:VAL:HG23	2.16	0.45
1:A:315:LEU:HD23	1:A:315:LEU:O	2.16	0.45
1:A:212:LYS:HA	1:A:215:THR:CG2	2.39	0.45
1:A:190:ASP:C	1:A:192:GLU:N	2.70	0.45
1:A:205:HIS:O	1:A:209:VAL:HG23	2.16	0.45
1:A:309:LYS:HZ3	1:A:310:LYS:HD2	1.80	0.45
1:A:152:AZH:ND	1:A:195:ILE:HG12	2.32	0.45
1:A:217:SER:OG	1:A:219:PHE:HD1	2.00	0.45
1:A:190:ASP:O	1:A:192:GLU:N	2.50	0.44
1:A:149:TYR:CE2	1:A:153:LEU:HD11	2.53	0.44
1:A:219:PHE:CE2	1:A:227:ARG:NH1	2.85	0.44
1:A:267:HIS:ND1	1:A:271:ARG:NH1	2.65	0.44
1:A:271:ARG:HG3	1:A:272:VAL:N	2.32	0.44
1:A:308:TYR:O	1:A:312:LEU:HD13	2.17	0.44
1:A:285:ARG:NE	1:A:319:ASP:HB2	2.33	0.44
1:A:276:ARG:O	1:A:281:LEU:HB2	2.17	0.44
1:A:213:TYR:CE1	1:A:224:THR:HG21	2.53	0.43
1:A:41:LEU:O	1:A:45:ARG:CD	2.62	0.43
1:A:51:GLN:HE21	1:A:87:PRO:HA	1.83	0.43
1:A:95:GLU:OE2	1:A:271:ARG:HD3	2.19	0.43
1:A:219:PHE:HB2	1:A:224:THR:HG22	2.00	0.43
1:A:214:AZH:HA	1:A:219:PHE:O	2.19	0.43
1:A:245:ARG:O	1:A:246:SER:HB2	2.18	0.43
1:A:201:ARG:HE	1:A:201:ARG:HB3	1.74	0.42
1:A:45:ARG:HB3	1:A:45:ARG:CZ	2.48	0.42
1:A:136:SER:HB3	1:A:139:ASP:CB	2.47	0.42
1:A:289:ARG:NH1	1:A:289:ARG:HG3	2.31	0.42
1:A:38:ILE:HG22	1:A:42:LEU:HD22	2.00	0.42
1:A:35:GLU:O	1:A:39:LEU:HB2	2.20	0.42
1:A:189:THR:HG21	1:A:228:GLU:O	2.20	0.42
1:A:41:LEU:C	1:A:41:LEU:HD23	2.40	0.42
1:A:9:VAL:CG1	1:A:46:SER:HA	2.50	0.42
1:A:51:GLN:NE2	1:A:87:PRO:HA	2.34	0.42
1:A:149:TYR:CG	1:A:232:ASN:ND2	2.87	0.41
1:A:66:LEU:O	1:A:70:LYS:HG2	2.20	0.41
1:A:211:ASP:O	1:A:214:AZH:HB1C	2.20	0.41
1:A:294:THR:HG22	1:A:295:SER:N	2.35	0.41
1:A:85:AZH:O	1:A:85:AZH:CG	2.68	0.41
1:A:271:ARG:HG3	1:A:272:VAL:H	1.86	0.41
1:A:36:GLU:O	1:A:40:THR:HG23	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:HG21	1:A:195:ILE:HG21	2.03	0.41
1:A:201:ARG:H	1:A:201:ARG:HD2	1.84	0.41
1:A:197:ILE:HA	1:A:201:ARG:CD	2.46	0.41
1:A:248:PRO:CA	1:A:284:ILE:HD13	2.49	0.41
1:A:123:ARG:HA	1:A:126:LYS:HG2	2.02	0.40
1:A:240:VAL:O	1:A:244:ILE:HG13	2.21	0.40
1:A:276:ARG:HB3	1:A:276:ARG:CZ	2.50	0.40
1:A:137:LEU:O	1:A:141:VAL:CG2	2.62	0.40
1:A:170:ALA:O	1:A:174:GLN:HB2	2.22	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	309/320 (97%)	262 (85%)	38 (12%)	9 (3%)	4	15

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	185	LEU
1	A	159	ALA
1	A	191	GLU
1	A	246	SER
1	A	46	SER
1	A	221	ILE
1	A	167	ILE
1	A	241	VAL

### 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	263 / 264 (100%)	214 (81%)	49 (19%)	<b>1</b> <b>5</b>

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	11	ASP
1	A	18	ARG
1	A	29	LYS
1	A	33	THR
1	A	35	GLU
1	A	45	ARG
1	A	49	GLN
1	A	50	ARG
1	A	54	SER
1	A	66	LEU
1	A	67	ASP
1	A	68	ASP
1	A	69	LEU
1	A	74	THR
1	A	76	LYS
1	A	79	LYS
1	A	86	LYS
1	A	89	ARG
1	A	106	ASN
1	A	107	GLU
1	A	120	GLU
1	A	130	GLU
1	A	137	LEU
1	A	150	GLN
1	A	160	ASN
1	A	171	GLN
1	A	184	GLU
1	A	189	THR
1	A	193	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	200	THR
1	A	201	ARG
1	A	207	ARG
1	A	208	LYS
1	A	212	LYS
1	A	213	TYR
1	A	215	THR
1	A	224	THR
1	A	227	ARG
1	A	229	THR
1	A	234	GLU
1	A	237	LEU
1	A	245	ARG
1	A	276	ARG
1	A	278	GLU
1	A	285	ARG
1	A	289	ARG
1	A	309	LYS
1	A	318	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	160	ASN
1	A	283	ASN
1	A	291	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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	AZH	A	152	1	6,8,9	1.16	1 (16%)	3,8,10	0.87	0
1	AZH	A	85	1	6,8,9	1.13	1 (16%)	3,8,10	0.53	0
1	AZH	A	259	1	6,8,9	1.14	1 (16%)	3,8,10	0.60	0
1	AZH	A	28	1,2	6,8,9	1.21	1 (16%)	3,8,10	0.62	0
1	AZH	A	299	1	6,8,9	1.15	1 (16%)	3,8,10	0.57	0
1	AZH	A	273	1	6,8,9	1.14	1 (16%)	3,8,10	0.57	0
1	AZH	A	214	1	6,8,9	1.22	1 (16%)	3,8,10	0.95	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	AZH	A	152	1	-	2/6/7/9	-
1	AZH	A	85	1	-	1/6/7/9	-
1	AZH	A	259	1	-	1/6/7/9	-
1	AZH	A	28	1,2	-	4/6/7/9	-
1	AZH	A	299	1	-	3/6/7/9	-
1	AZH	A	273	1	-	1/6/7/9	-
1	AZH	A	214	1	-	3/6/7/9	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	AZH	NE-ND	2.74	1.30	1.23
1	A	28	AZH	NE-ND	2.71	1.30	1.23
1	A	152	AZH	NE-ND	2.63	1.30	1.23
1	A	85	AZH	NE-ND	2.57	1.30	1.23
1	A	273	AZH	NE-ND	2.56	1.30	1.23
1	A	299	AZH	NE-ND	2.55	1.30	1.23
1	A	259	AZH	NE-ND	2.54	1.30	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
1	A	28	AZH	N-CA-CB-CG
1	A	28	AZH	C-CA-CB-CG
1	A	28	AZH	O-C-CA-CB
1	A	28	AZH	CA-CB-CG-ND
1	A	299	AZH	CA-CB-CG-ND
1	A	214	AZH	C-CA-CB-CG
1	A	214	AZH	CA-CB-CG-ND
1	A	259	AZH	CG-ND-NE-NZ
1	A	299	AZH	CG-ND-NE-NZ
1	A	152	AZH	CA-CB-CG-ND
1	A	214	AZH	N-CA-CB-CG
1	A	299	AZH	C-CA-CB-CG
1	A	152	AZH	N-CA-CB-CG
1	A	85	AZH	CG-ND-NE-NZ
1	A	273	AZH	CG-ND-NE-NZ

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	152	AZH	4	0
1	A	85	AZH	2	0
1	A	28	AZH	1	0
1	A	299	AZH	1	0
1	A	214	AZH	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	A	1331	-	4,4,4	0.32	0	6,6,6	0.22	0
4	SO4	A	1330	2	4,4,4	0.29	0	6,6,6	0.07	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1331	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	311/320 (97%)	0.30	7 (2%) 60 51	46, 62, 77, 80	33 (10%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	320	ASP	4.7
1	A	263	GLY	4.2
1	A	262	ALA	4.1
1	A	102	GLY	3.3
1	A	165	ALA	3.2
1	A	3	GLN	2.6
1	A	298	SER	2.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	AZH	A	28	9/10	0.77	0.26	74,74,75,75	4
1	AZH	A	214	9/10	0.81	0.21	59,59,60,60	4
1	AZH	A	85	9/10	0.82	0.25	52,53,54,54	3
1	AZH	A	299	9/10	0.88	0.21	78,79,79,79	0
1	AZH	A	273	9/10	0.90	0.28	51,52,53,53	0
1	AZH	A	152	9/10	0.91	0.23	54,54,55,55	2
1	AZH	A	259	9/10	0.92	0.14	65,65,66,66	1

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	1327	1/1	0.76	0.13	61,61,61,61	0
2	CA	A	1328	1/1	0.83	0.08	85,85,85,85	0
4	SO4	A	1331	5/5	0.85	0.24	97,97,97,97	0
4	SO4	A	1330	5/5	0.94	0.14	74,74,74,74	0
5	CL	A	1332	1/1	0.95	0.10	76,76,76,76	0
3	NA	A	1329	1/1	0.95	0.10	33,33,33,33	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.