



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 02:38 PM UTC

PDB ID : 3KV6 / pdb_00003kv6
Title : Structure of KIAA1718, human Jumonji demethylase, in complex with alpha-ketoglutarate
Authors : Horton, J.R.; Upadhyay, A.K.; Qi, H.H.; Zhang, X.; Shi, Y.; Cheng, X.
Deposited on : 2009-11-29
Resolution : 2.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

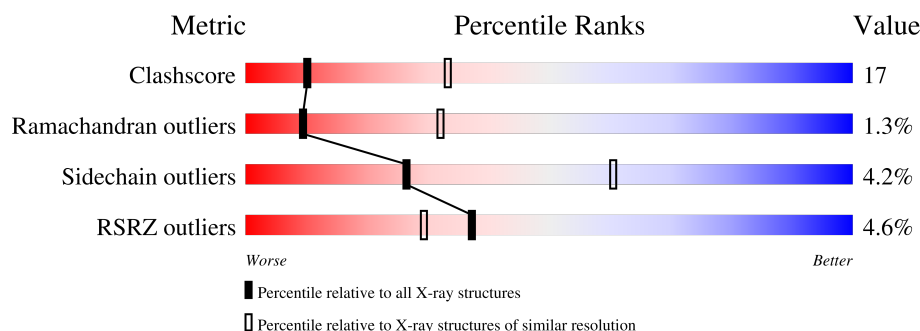
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	488	4% 58% 31% • 8%
1	D	488	4% 56% 33% • 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7389 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 JmjC domain-containing histone demethylation protein 1D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	3	0
			3580	2305	609	640	26			
1	D	448	Total	C	N	O	S	0	2	0
			3614	2327	608	653	26			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is FE (II) ION (CCD ID: FE2) (formula: Fe).

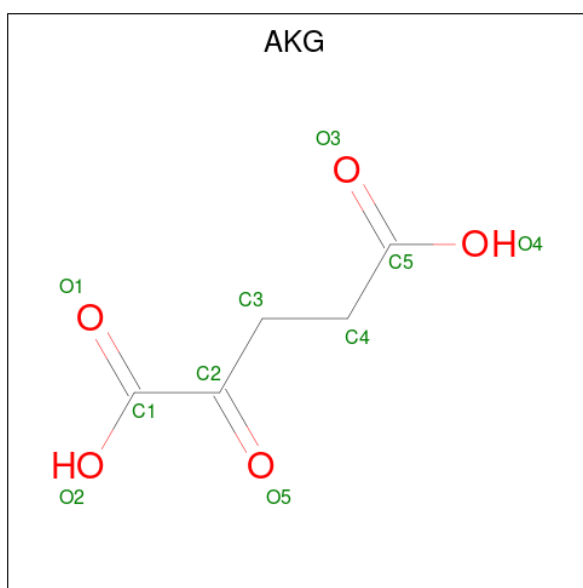
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	D	1	Total	Fe	0	0
			1	1		

- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			2	2		
4	D	1	Total	O	0	0
			2	2		

- Molecule 5 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	5	5		
5	D	1	Total	C	O	0	0
			10	5	5		

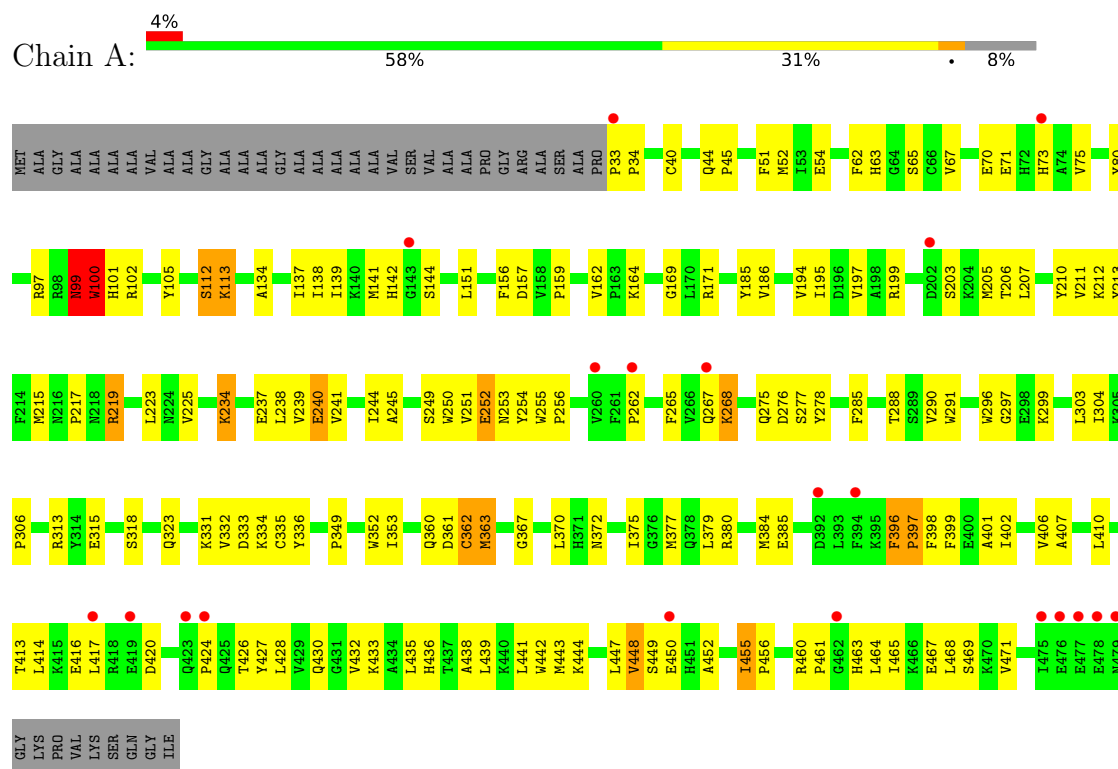
- Molecule 6 is water.

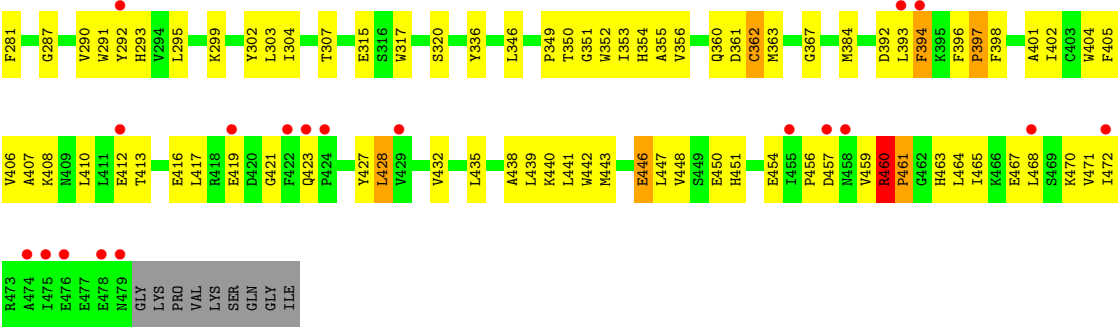
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	82	Total 82	O 82	0	0
6	D	83	Total 83	O 83	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: JmjC domain-containing histone demethylation protein 1D





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.40Å 125.20Å 206.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.54 – 2.89 34.54 – 2.89	Depositor EDS
% Data completeness (in resolution range)	93.3 (34.54-2.89) 93.1 (34.54-2.89)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.253 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7389	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.35% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OXY, AKG, FE2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	0/3684	0.96	9/5007 (0.2%)
1	D	0.48	0/3720	1.00	27/5056 (0.5%)
All	All	0.47	0/7404	0.98	36/10063 (0.4%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	396	PHE	CA-C-N	7.25	128.90	119.84
1	D	396	PHE	C-N-CA	7.25	128.90	119.84
1	D	113	LYS	CA-C-N	6.25	126.77	120.14
1	D	113	LYS	C-N-CA	6.25	126.77	120.14
1	D	460	ARG	CA-C-N	6.21	127.60	119.84
1	D	460	ARG	C-N-CA	6.21	127.60	119.84
1	D	255	TRP	CA-C-N	6.18	126.20	119.90
1	D	255	TRP	C-N-CA	6.18	126.20	119.90
1	D	457	ASP	N-CA-C	-6.15	105.63	113.01
1	A	455	ILE	N-CA-C	6.06	113.84	108.63
1	A	277	SER	N-CA-C	-5.89	101.76	110.48
1	D	423	GLN	CA-C-N	5.89	125.90	119.89
1	D	423	GLN	C-N-CA	5.89	125.90	119.89
1	A	169	GLY	N-CA-C	-5.86	107.15	115.30
1	A	396	PHE	CA-C-N	5.85	127.15	119.84
1	A	396	PHE	C-N-CA	5.85	127.15	119.84
1	D	351	GLY	N-CA-C	5.85	123.12	115.40
1	D	254	TYR	N-CA-C	5.74	122.10	114.12
1	D	447	LEU	N-CA-C	5.71	117.18	111.07
1	D	454	GLU	N-CA-C	5.49	117.07	111.14
1	D	394	PHE	N-CA-C	-5.48	105.95	113.30
1	D	44	GLN	CA-C-N	5.31	125.25	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	44	GLN	C-N-CA	5.31	125.25	119.78
1	A	206	THR	N-CA-C	-5.30	102.63	110.48
1	D	230	PHE	N-CA-C	5.30	118.76	112.72
1	D	362	CYS	N-CA-C	5.26	117.38	109.23
1	A	334	LYS	N-CA-C	5.26	116.99	108.26
1	D	54	GLU	N-CA-C	5.21	117.74	109.24
1	D	197	VAL	N-CA-C	5.21	120.17	109.34
1	A	112	SER	N-CA-C	-5.16	103.73	110.53
1	D	162	VAL	CA-C-N	5.14	126.27	119.84
1	D	162	VAL	C-N-CA	5.14	126.27	119.84
1	D	253	ASN	N-CA-C	5.14	118.02	111.69
1	D	307	THR	N-CA-C	-5.13	103.92	110.53
1	D	277	SER	N-CA-C	-5.09	102.17	110.20
1	A	99	ASN	N-CA-C	5.05	117.95	109.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3580	0	3440	117	0
1	D	3614	0	3475	126	0
2	A	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	A	10	0	4	1	0
5	D	10	0	4	1	0
6	A	82	0	0	4	0
6	D	83	0	0	2	0
All	All	7389	0	6923	243	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 17.

All (243) 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:234:LYS:H	1:A:234:LYS:HD2	1.24	1.00
1:D:315:GLU:HB2	1:D:384:MET:HE2	1.49	0.94
1:D:460:ARG:HD3	1:D:460:ARG:N	1.83	0.93
1:A:75:VAL:HG11	1:A:199:ARG:HH11	1.37	0.89
1:D:70:GLU:H	1:D:73[B]:HIS:HD2	1.22	0.88
1:A:185:TYR:O	1:A:234:LYS:HD3	1.78	0.84
1:D:408:LYS:HA	1:D:464:LEU:HD11	1.61	0.81
1:D:398:PHE:HB3	1:D:401:ALA:HB3	1.66	0.78
1:D:99:ASN:ND2	1:D:102:ARG:H	1.84	0.76
1:A:215:MET:HE2	1:A:215:MET:HA	1.66	0.75
1:D:443:MET:HE2	1:D:461:PRO:HB2	1.66	0.75
1:A:234:LYS:H	1:A:234:LYS:CD	1.93	0.75
1:A:234:LYS:HD2	1:A:234:LYS:N	2.01	0.75
1:D:392:ASP:C	1:D:394:PHE:H	1.94	0.75
1:A:416:GLU:O	1:A:420:ASP:HB2	1.88	0.74
1:D:159:PRO:HG2	1:D:303:LEU:HD13	1.69	0.74
1:D:460:ARG:HG2	1:D:463:HIS:HB3	1.68	0.73
1:D:148:GLN:OE1	1:D:247:LYS:HE3	1.88	0.73
1:A:297:GLY:HA3	1:A:362:CYS:HB2	1.71	0.72
1:D:299:LYS:HE2	1:D:362:CYS:SG	2.30	0.71
1:A:304:ILE:HD12	1:A:332:VAL:HG21	1.72	0.70
1:A:99:ASN:HD21	1:A:102:ARG:HG2	1.56	0.70
1:D:467:GLU:O	1:D:471:VAL:HG23	1.92	0.70
1:D:349:PRO:HG2	1:D:352:TRP:CD1	2.29	0.68
1:D:467:GLU:HA	1:D:470:LYS:HG2	1.76	0.67
1:D:99:ASN:HD21	1:D:102:ARG:H	1.42	0.67
1:A:75:VAL:HG11	1:A:199:ARG:NH1	2.07	0.66
1:A:398:PHE:HB3	1:A:401:ALA:HB3	1.78	0.66
1:A:249:SER:HB3	1:A:252:GLU:HB2	1.79	0.65
1:D:254:TYR:CD2	1:D:406:VAL:HG22	2.33	0.64
1:A:443:MET:HE2	1:A:461:PRO:HB2	1.78	0.64
1:D:81:HIS:H	1:D:92:SER:HB3	1.61	0.63
1:D:110:ASP:O	1:D:112:SER:N	2.32	0.63
1:A:318:SER:HA	1:A:323:GLN:NE2	2.13	0.63
1:D:138:ILE:HG22	1:D:159:PRO:HB2	1.79	0.63
1:D:142:HIS:HB3	6:D:496:HOH:O	2.00	0.62
1:D:464:LEU:O	1:D:468:LEU:HB2	2.00	0.62
1:D:211:VAL:O	1:D:215:MET:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:LYS:HE3	1:D:460:ARG:HH12	1.64	0.61
1:A:100:TRP:HA	1:A:100:TRP:CE3	2.35	0.61
1:D:72:HIS:HD2	1:D:221:LYS:NZ	1.98	0.61
1:A:304:ILE:HB	1:A:353:ILE:HB	1.83	0.60
1:D:295:LEU:HD23	1:D:363:MET:HE2	1.83	0.60
1:A:137:ILE:HG13	1:A:138:ILE:N	2.17	0.60
1:D:80:TYR:HA	1:D:92:SER:HB3	1.82	0.59
1:A:213:TYR:CE2	1:A:223:LEU:HB2	2.37	0.59
1:A:99:ASN:HB2	1:A:105:TYR:HA	1.82	0.59
1:A:349:PRO:HG2	1:A:352:TRP:CD1	2.37	0.59
1:A:417:LEU:HD12	1:A:424:PRO:HG3	1.85	0.59
1:A:112:SER:O	1:A:113:LYS:HB2	2.01	0.59
1:A:306:PRO:HG3	1:A:352:TRP:HA	1.85	0.58
1:D:392:ASP:O	1:D:394:PHE:N	2.37	0.58
1:A:159:PRO:HG2	1:A:303:LEU:HD13	1.85	0.57
1:D:287:GLY:O	1:D:350:THR:HG23	2.04	0.57
1:A:142[A]:HIS:HD2	1:A:144:SER:OG	1.88	0.57
1:A:267[A]:GLN:HG3	1:A:268:LYS:HG2	1.87	0.56
1:A:304:ILE:HD13	1:A:335:CYS:HA	1.86	0.56
1:D:412:GLU:O	1:D:416:GLU:HG3	2.05	0.56
1:D:435:LEU:O	1:D:439:LEU:HD13	2.05	0.56
1:D:468:LEU:O	1:D:472:ILE:HG13	2.05	0.56
1:A:414:LEU:HD11	1:A:432:VAL:HG21	1.87	0.56
1:A:100:TRP:HA	1:A:100:TRP:HE3	1.70	0.56
1:A:461:PRO:O	1:A:465:ILE:HG13	2.06	0.56
1:D:410:LEU:HD13	1:D:432:VAL:HG22	1.86	0.56
1:D:360:GLN:O	1:D:361:ASP:C	2.49	0.55
1:D:254:TYR:HD2	1:D:406:VAL:HG22	1.69	0.55
1:A:151:LEU:HD12	1:A:244:ILE:HD11	1.87	0.55
1:D:72:HIS:HD2	1:D:221:LYS:HZ1	1.54	0.55
1:D:446:GLU:H	1:D:446:GLU:CD	2.15	0.55
1:A:254:TYR:CD2	1:A:406:VAL:HG22	2.43	0.54
1:A:290:VAL:HG23	1:A:367:GLY:O	2.08	0.54
1:A:399:PHE:O	1:A:402:ILE:HG22	2.08	0.54
1:D:356:VAL:HG21	5:D:701:AKG:H41	1.90	0.54
1:A:435:LEU:O	1:A:439:LEU:HD13	2.07	0.53
1:A:197:VAL:HG11	1:A:278:TYR:H	1.74	0.53
1:A:379:LEU:HD13	1:A:438:ALA:HB2	1.90	0.53
1:D:207:LEU:O	1:D:211:VAL:HG23	2.08	0.53
1:D:408:LYS:CE	1:D:460:ARG:HH12	2.21	0.53
1:A:290:VAL:HG22	1:A:291:TRP:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ASP:OD1	1:D:112:SER:CB	2.57	0.53
1:D:98:ARG:HD2	1:D:106:THR:O	2.09	0.52
1:A:99:ASN:HD22	1:A:101:HIS:H	1.57	0.52
1:D:70:GLU:H	1:D:73[B]:HIS:CD2	2.13	0.52
1:D:290:VAL:HG23	1:D:367:GLY:O	2.10	0.52
1:D:410:LEU:HD13	1:D:432:VAL:CG2	2.39	0.52
1:D:54:GLU:HB2	1:D:61:TRP:CE2	2.45	0.52
1:D:402:ILE:HA	1:D:405:PHE:HD1	1.74	0.52
1:A:313:ARG:HD3	1:A:331:LYS:O	2.09	0.52
1:D:292[A]:TYR:HE2	1:D:299:LYS:HG3	1.73	0.52
1:A:306:PRO:HB2	1:A:377:MET:HE3	1.91	0.52
1:A:413:THR:O	1:A:417:LEU:HG	2.10	0.52
1:D:81:HIS:N	1:D:92:SER:HB3	2.24	0.51
1:A:241:VAL:HG22	6:A:561:HOH:O	2.11	0.51
1:A:194:VAL:HG21	1:A:205:MET:SD	2.50	0.51
1:D:292[A]:TYR:OH	1:D:299:LYS:HE3	2.09	0.51
1:D:459:VAL:HG23	1:D:460:ARG:N	2.25	0.51
1:D:427:TYR:CG	1:D:428:LEU:N	2.78	0.51
1:D:460:ARG:HD3	1:D:460:ARG:H	1.70	0.51
1:D:456:PRO:HB2	1:D:459:VAL:HG13	1.94	0.50
1:A:285:PHE:HA	1:A:385:GLU:OE1	2.11	0.50
1:A:185:TYR:CE2	1:A:238:LEU:HD11	2.45	0.50
1:A:315:GLU:HB2	1:A:384:MET:HE2	1.94	0.50
1:D:404:TRP:CD1	1:D:456:PRO:HD3	2.47	0.50
1:A:99:ASN:HD21	1:A:102:ARG:CG	2.22	0.49
1:A:162:VAL:HG12	1:A:164:LYS:O	2.12	0.49
1:A:171:ARG:NH2	1:A:237:GLU:O	2.45	0.49
1:D:134:ALA:O	1:D:138:ILE:HG12	2.13	0.49
1:D:254:TYR:O	1:D:256:PRO:HD3	2.11	0.49
1:A:52:MET:HA	1:A:62:PHE:O	2.13	0.49
1:A:219:ARG:NH2	1:A:361:ASP:OD2	2.46	0.49
1:A:262:PRO:HD2	1:A:398:PHE:CE2	2.48	0.48
1:A:288:THR:HG22	1:A:370:LEU:CD2	2.42	0.48
1:D:137:ILE:HD13	1:D:336:TYR:CD2	2.48	0.48
1:D:110:ASP:OD1	1:D:112:SER:HB2	2.13	0.48
1:D:122:PHE:HD2	1:D:123:ILE:HD12	1.79	0.48
1:D:103:HIS:O	1:D:199:ARG:HG2	2.14	0.48
1:D:240:GLU:CD	1:D:246:LYS:NZ	2.71	0.48
1:D:408:LYS:HA	1:D:464:LEU:CD1	2.39	0.48
1:D:413:THR:O	1:D:417:LEU:HG	2.14	0.48
1:D:229:GLU:HA	1:D:268:LYS:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:VAL:HG12	1:D:291:TRP:HZ2	1.78	0.47
1:D:256:PRO:HG2	1:D:405:PHE:CE2	2.48	0.47
1:A:63:HIS:O	1:A:67:VAL:HG22	2.15	0.47
1:A:251:VAL:HG23	6:A:504:HOH:O	2.14	0.47
1:A:112:SER:O	1:A:113:LYS:CB	2.62	0.47
1:D:239:VAL:HG12	1:D:240:GLU:N	2.30	0.47
1:A:360:GLN:O	1:A:361:ASP:C	2.58	0.47
1:D:141:MET:HE2	1:D:146:LEU:CA	2.45	0.47
1:D:194:VAL:HG12	1:D:195:ILE:N	2.30	0.47
1:D:215:MET:HE3	1:D:215:MET:HA	1.97	0.47
1:D:240:GLU:HA	1:D:240:GLU:OE1	2.14	0.47
1:A:290:VAL:CG2	1:A:291:TRP:N	2.78	0.47
1:D:177:PHE:HD2	1:D:363:MET:HE1	1.79	0.47
1:D:219:ARG:NH1	1:D:274:VAL:HB	2.29	0.47
1:D:281:PHE:CD1	1:D:355:ALA:HB2	2.49	0.46
1:A:443:MET:O	1:A:448:VAL:HB	2.15	0.46
1:D:185:TYR:HB3	1:D:235:MET:HB2	1.97	0.46
1:A:427:TYR:CG	1:A:428:LEU:N	2.84	0.46
1:A:448:VAL:O	1:A:452:ALA:HB2	2.15	0.46
1:A:139:ILE:HG21	1:A:141:MET:HE2	1.97	0.46
1:D:275:GLN:O	1:D:276:ASP:HB2	2.16	0.46
1:A:219:ARG:NH2	1:A:361:ASP:CG	2.73	0.46
1:D:99:ASN:HD22	1:D:101:HIS:H	1.63	0.46
1:A:70:GLU:O	1:A:73[B]:HIS:HB2	2.16	0.46
1:A:134:ALA:HA	1:A:336:TYR:HB3	1.98	0.46
1:D:101:HIS:HD2	6:D:513:HOH:O	1.99	0.46
1:A:44:GLN:OE1	1:A:45:PRO:HD2	2.16	0.46
1:A:250:TRP:CD2	1:A:406:VAL:HG21	2.51	0.46
1:A:288:THR:HG22	1:A:370:LEU:HG	1.97	0.46
1:D:281:PHE:HA	1:D:354:HIS:O	2.16	0.46
1:D:460:ARG:HG2	1:D:460:ARG:O	2.16	0.46
1:A:75:VAL:CG1	1:A:199:ARG:HH11	2.20	0.45
1:A:464:LEU:O	1:A:468:LEU:HB2	2.16	0.45
1:A:296:TRP:HB3	6:A:503:HOH:O	2.16	0.45
1:D:460:ARG:HA	1:D:461:PRO:HD2	1.70	0.45
1:A:467:GLU:O	1:A:471:VAL:HG23	2.16	0.45
1:A:244:ILE:HG23	1:A:245:ALA:N	2.32	0.45
1:A:275:GLN:O	1:A:276:ASP:HB2	2.16	0.45
1:A:407:ALA:HB2	1:A:435:LEU:HD21	1.98	0.45
1:D:410:LEU:CD1	1:D:432:VAL:HG22	2.45	0.45
1:A:194:VAL:HG12	1:A:195:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:SER:C	1:D:176:THR:H	2.25	0.45
1:A:447:LEU:O	1:A:449:SER:N	2.50	0.45
1:D:230:PHE:CG	1:D:235:MET:HE2	2.52	0.45
1:D:317:TRP:O	1:D:320:SER:HB3	2.17	0.45
1:D:165:LEU:HD21	1:D:293:HIS:CE1	2.52	0.45
1:D:63:HIS:O	1:D:64:GLY:C	2.59	0.44
1:D:292[A]:TYR:CE2	1:D:299:LYS:HG3	2.53	0.44
1:A:75:VAL:CG1	1:A:199:ARG:NH1	2.78	0.44
1:A:442:TRP:O	1:A:448:VAL:HA	2.18	0.44
1:D:302:TYR:HB2	1:D:355:ALA:HB3	2.00	0.44
1:A:396:PHE:HA	1:A:397:PRO:HD2	1.71	0.44
1:D:127:ARG:HG2	1:D:127:ARG:HH11	1.82	0.44
1:D:102:ARG:CZ	1:D:113:LYS:HB3	2.48	0.44
1:D:110:ASP:C	1:D:112:SER:H	2.26	0.44
1:D:141:MET:HE2	1:D:146:LEU:HB2	2.00	0.44
1:D:172:LEU:HB3	1:D:173:PRO:HD2	2.00	0.44
1:D:440:LYS:HG2	1:D:465:ILE:HG21	1.98	0.44
1:A:255:TRP:HA	1:A:256:PRO:HD3	1.85	0.44
1:D:258:ASP:O	1:D:259:SER:C	2.59	0.44
1:A:54:GLU:O	1:A:80:TYR:HB3	2.18	0.43
1:D:239:VAL:CG1	1:D:240:GLU:N	2.81	0.43
1:D:230:PHE:HB2	1:D:233:THR:OG1	2.19	0.43
1:A:372:ASN:O	1:A:375:ILE:HG13	2.18	0.43
1:D:265:PHE:HA	1:D:267:GLN:HE22	1.83	0.43
1:D:407:ALA:HB3	1:D:464:LEU:HD21	1.99	0.43
1:A:99:ASN:ND2	1:A:102:ARG:HG2	2.26	0.43
1:A:241:VAL:HG12	1:A:291:TRP:HZ2	1.82	0.43
1:A:207:LEU:O	1:A:211:VAL:HG23	2.19	0.43
1:A:410:LEU:HD13	1:A:432:VAL:HG22	2.01	0.43
1:A:213:TYR:CZ	1:A:223:LEU:HB2	2.54	0.43
1:A:239:VAL:CG1	1:A:240:GLU:N	2.81	0.43
1:A:33:PRO:N	1:A:34:PRO:HD3	2.34	0.42
1:A:210:TYR:CZ	1:A:225:VAL:HG23	2.54	0.42
1:A:296:TRP:CZ2	1:A:363:MET:HB2	2.54	0.42
1:D:35:PRO:HB2	1:D:36:PRO:HD2	2.00	0.42
1:A:253:ASN:O	1:A:254:TYR:CD1	2.72	0.42
1:A:455:ILE:HA	1:A:456:PRO:HD3	1.91	0.42
1:A:44:GLN:CD	1:A:45:PRO:HD2	2.44	0.42
1:A:460:ARG:HB2	1:A:463:HIS:HB3	2.01	0.42
1:A:97:ARG:NH1	1:A:100:TRP:CE3	2.87	0.42
1:A:215:MET:HA	1:A:215:MET:CE	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:PHE:HA	1:A:267[B]:GLN:OE1	2.20	0.42
1:A:433:LYS:HE3	1:A:433:LYS:HB2	1.86	0.42
1:D:113:LYS:HA	1:D:114:PRO:HD3	1.79	0.42
1:A:197:VAL:HG11	1:A:278:TYR:N	2.35	0.42
1:D:35:PRO:HB2	1:D:36:PRO:CD	2.50	0.42
1:A:441:LEU:O	1:A:447:LEU:HD12	2.20	0.42
1:D:141:MET:CE	1:D:146:LEU:HA	2.49	0.42
1:D:213:TYR:CE2	1:D:223:LEU:HB2	2.54	0.42
1:A:186:VAL:O	1:A:234:LYS:HE2	2.18	0.42
1:D:467:GLU:HA	1:D:470:LYS:HE3	2.01	0.42
1:D:98:ARG:HG3	1:D:107:GLU:O	2.20	0.41
1:D:210:TYR:O	1:D:213:TYR:HB3	2.19	0.41
1:A:99:ASN:ND2	1:A:102:ARG:N	2.69	0.41
1:A:426:THR:O	1:A:430:GLN:HG3	2.21	0.41
1:A:151:LEU:HD22	1:A:156:PHE:HB2	2.02	0.41
1:A:333:ASP:HB2	6:A:502:HOH:O	2.19	0.41
1:D:404:TRP:O	1:D:405:PHE:C	2.64	0.41
1:D:110:ASP:OD1	1:D:112:SER:HB3	2.21	0.41
1:D:110:ASP:C	1:D:112:SER:N	2.77	0.41
1:D:179:VAL:HG12	1:D:272:MET:SD	2.61	0.41
1:D:467:GLU:CA	1:D:470:LYS:HG2	2.48	0.41
1:D:121:THR:O	1:D:125:GLU:HG3	2.21	0.41
1:D:160:ILE:O	1:D:346:LEU:HD12	2.20	0.41
1:D:177:PHE:CE1	1:D:181:ASP:HB3	2.55	0.41
1:D:246:LYS:HE3	1:D:246:LYS:HB2	1.90	0.41
1:D:255:TRP:HA	1:D:256:PRO:HD3	1.90	0.41
1:A:51:PHE:CG	1:A:71:GLU:HG2	2.55	0.41
1:D:137:ILE:HD13	1:D:336:TYR:CE2	2.56	0.41
1:A:99:ASN:ND2	1:A:102:ARG:H	2.19	0.40
1:A:215:MET:O	1:A:217:PRO:HD3	2.20	0.40
1:D:72:HIS:CE1	1:D:223:LEU:HD11	2.56	0.40
1:D:461:PRO:O	1:D:465:ILE:HG13	2.21	0.40
1:D:438:ALA:O	1:D:441:LEU:HB3	2.21	0.40
1:D:442:TRP:HB3	1:D:451:HIS:CG	2.56	0.40
1:A:436:HIS:HE1	1:A:465:ILE:O	2.04	0.40
1:A:75:VAL:O	1:A:75:VAL:HG22	2.20	0.40
1:A:254:TYR:HD2	1:A:406:VAL:HG22	1.85	0.40
1:D:127:ARG:HG2	1:D:127:ARG:NH1	2.36	0.40
1:A:299:LYS:HE3	5:A:702:AKG:O4	2.22	0.40
1:A:443:MET:O	1:A:444:LYS:C	2.64	0.40
1:D:304:ILE:HB	1:D:353:ILE:HB	2.03	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	448/488 (92%)	404 (90%)	39 (9%)	5 (1%)	11	36
1	D	448/488 (92%)	401 (90%)	40 (9%)	7 (2%)	7	27
All	All	896/976 (92%)	805 (90%)	79 (9%)	12 (1%)	9	32

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	111	GLY
1	A	100	TRP
1	A	397	PRO
1	D	448	VAL
1	A	40	CYS
1	D	393	LEU
1	A	113	LYS
1	A	448	VAL
1	D	112	SER
1	D	397	PRO
1	D	421	GLY
1	D	461	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/424 (92%)	372 (96%)	16 (4%)	27	61
1	D	396/424 (93%)	379 (96%)	17 (4%)	26	60
All	All	784/848 (92%)	751 (96%)	33 (4%)	26	60

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	SER
1	A	99	ASN
1	A	100	TRP
1	A	157	ASP
1	A	203	SER
1	A	212	LYS
1	A	219	ARG
1	A	234	LYS
1	A	240	GLU
1	A	252	GLU
1	A	268	LYS
1	A	362	CYS
1	A	363	MET
1	A	380	ARG
1	A	450	GLU
1	A	469	SER
1	D	83	PRO
1	D	87	VAL
1	D	92	SER
1	D	93	LEU
1	D	120	ARG
1	D	152	GLU
1	D	191	VAL
1	D	202	ASP
1	D	234	LYS
1	D	257	ASP
1	D	271	LEU
1	D	397	PRO
1	D	419	GLU
1	D	428	LEU
1	D	446	GLU
1	D	450	GLU
1	D	460	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	323	GLN
1	A	368	ASN
1	A	409	ASN
1	A	458	ASN
1	D	49	ASN
1	D	72	HIS
1	D	99	ASN
1	D	101	HIS
1	D	200	GLN
1	D	224	ASN
1	D	253	ASN
1	D	267	GLN
1	D	275	GLN
1	D	310	ASN
1	D	323	GLN
1	D	368	ASN
1	D	430	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	OXY	A	492	-	1,1,1	1.16	0	-		
5	AKG	A	702	3	9,9,9	1.20	1 (11%)	11,11,11	1.62	4 (36%)
4	OXY	D	492	-	1,1,1	1.17	0	-		
5	AKG	D	701	3	9,9,9	1.06	0	11,11,11	1.69	4 (36%)

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
5	AKG	A	702	3	-	0/9/9/9	-
5	AKG	D	701	3	-	0/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	702	AKG	C3-C2	2.24	1.53	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	701	AKG	O2-C1-O1	-2.85	117.11	123.90
5	D	701	AKG	O2-C1-C2	2.69	121.06	113.59
5	A	702	AKG	C3-C2-C1	2.42	119.97	115.86
5	A	702	AKG	O2-C1-O1	-2.41	118.15	123.90
5	D	701	AKG	C3-C2-C1	2.18	119.56	115.86
5	A	702	AKG	O2-C1-C2	2.17	119.62	113.59
5	A	702	AKG	O4-C5-O3	-2.15	117.81	123.33
5	D	701	AKG	O4-C5-O3	-2.11	117.89	123.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	702	AKG	1	0
5	D	701	AKG	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, 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	447/488 (91%)	0.18	20 (4%) 38 30	13, 32, 55, 84	3 (0%)
1	D	448/488 (91%)	0.14	21 (4%) 36 28	13, 31, 55, 84	2 (0%)
All	All	895/976 (91%)	0.16	41 (4%) 37 29	13, 32, 55, 84	5 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	479	ASN	7.2
1	A	479	ASN	5.9
1	A	33	PRO	4.8
1	A	267[A]	GLN	4.6
1	D	478	GLU	4.3
1	A	478	GLU	3.7
1	D	32	PRO	3.2
1	D	475	ILE	3.1
1	D	457	ASP	3.1
1	A	423	GLN	3.1
1	D	393	LEU	3.1
1	D	422	PHE	3.0
1	A	424	PRO	3.0
1	D	458	ASN	3.0
1	A	477	GLU	3.0
1	A	73[A]	HIS	3.0
1	A	260	VAL	2.9
1	D	429	VAL	2.8
1	D	292[A]	TYR	2.8
1	A	462	GLY	2.7
1	A	475	ILE	2.6
1	A	262	PRO	2.6
1	D	424	PRO	2.6
1	A	392	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	143	GLY	2.3
1	D	259	SER	2.3
1	A	450	GLU	2.3
1	D	468	LEU	2.2
1	A	476	GLU	2.2
1	D	476	GLU	2.2
1	A	202	ASP	2.2
1	D	394	PHE	2.2
1	A	417	LEU	2.2
1	D	412	GLU	2.1
1	D	455	ILE	2.1
1	D	419	GLU	2.1
1	D	423	GLN	2.0
1	D	474	ALA	2.0
1	A	419	GLU	2.0
1	A	394	PHE	2.0
1	D	472	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	OXY	D	492	2/2	0.61	0.36	72,72,72,73	0
4	OXY	A	492	2/2	0.87	0.28	61,61,61,61	0
5	AKG	A	702	10/10	0.88	0.25	97,97,99,99	0
5	AKG	D	701	10/10	0.89	0.26	102,103,103,103	0
3	FE2	A	491	1/1	0.97	0.04	65,65,65,65	0
3	FE2	D	491	1/1	0.99	0.03	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	D	489	1/1	1.00	0.01	30,30,30,30	0
2	ZN	D	490	1/1	1.00	0.01	27,27,27,27	0
2	ZN	A	489	1/1	1.00	0.02	21,21,21,21	0
2	ZN	A	490	1/1	1.00	0.01	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.