



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:58 AM GMT

PDB ID : 3GQY
Title : Activator-Bound Structure of Human Pyruvate Kinase M2
Authors : Hong, B.; Dimov, S.; Tempel, W.; Auld, D.; Thomas, C.; Boxer, M.; Jianq, J.-K.; Skoumbourdis, A.; Min, S.; Southall, N.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Bochkarev, A.; Inglese, J.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on : 2009-03-24
Resolution : 1.85 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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

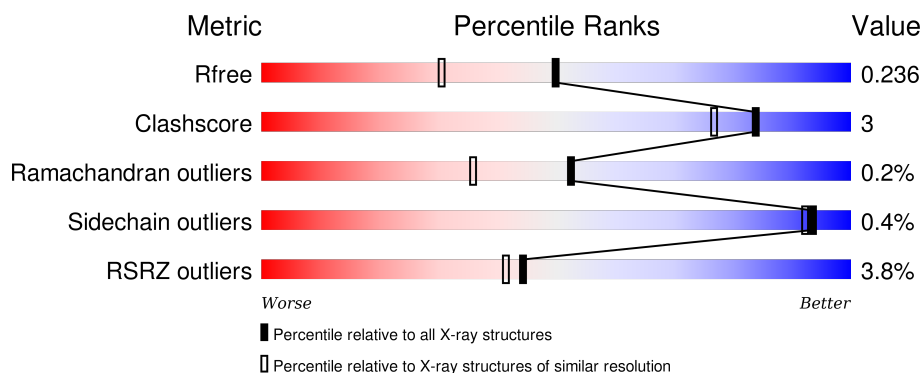
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	550	
1	B	550	
1	C	550	
1	D	550	

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
3	TLA	B	542	-	-	-	X
3	TLA	B	543	-	-	-	X
3	TLA	C	542	-	-	-	X
3	TLA	D	542	-	-	-	X
3	TLA	D	543	-	-	-	X
4	UNX	A	532	-	-	-	X
4	UNX	B	532	-	-	-	X
4	UNX	B	533	-	-	-	X
4	UNX	B	534	-	-	-	X
4	UNX	C	532	-	-	-	X
4	UNX	C	533	-	-	-	X
4	UNX	D	534	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15931 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 Pyruvate kinase isozymes M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			3819	2404	668	722	25			
1	B	504	Total	C	N	O	S	0	1	0
			3724	2344	658	698	24			
1	C	515	Total	C	N	O	S	0	0	0
			3805	2393	669	719	24			
1	D	505	Total	C	N	O	S	0	0	0
			3708	2333	656	695	24			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	EXPRESSION TAG	UNP P14618
A	-17	GLY	-	EXPRESSION TAG	UNP P14618
A	-16	SER	-	EXPRESSION TAG	UNP P14618
A	-15	SER	-	EXPRESSION TAG	UNP P14618
A	-14	HIS	-	EXPRESSION TAG	UNP P14618
A	-13	HIS	-	EXPRESSION TAG	UNP P14618
A	-12	HIS	-	EXPRESSION TAG	UNP P14618
A	-11	HIS	-	EXPRESSION TAG	UNP P14618
A	-10	HIS	-	EXPRESSION TAG	UNP P14618
A	-9	HIS	-	EXPRESSION TAG	UNP P14618
A	-8	SER	-	EXPRESSION TAG	UNP P14618
A	-7	SER	-	EXPRESSION TAG	UNP P14618
A	-6	GLY	-	EXPRESSION TAG	UNP P14618
A	-5	LEU	-	EXPRESSION TAG	UNP P14618
A	-4	VAL	-	EXPRESSION TAG	UNP P14618
A	-3	PRO	-	EXPRESSION TAG	UNP P14618
A	-2	ARG	-	EXPRESSION TAG	UNP P14618
A	-1	GLY	-	EXPRESSION TAG	UNP P14618
A	0	SER	-	EXPRESSION TAG	UNP P14618
B	-18	MET	-	EXPRESSION TAG	UNP P14618
B	-17	GLY	-	EXPRESSION TAG	UNP P14618

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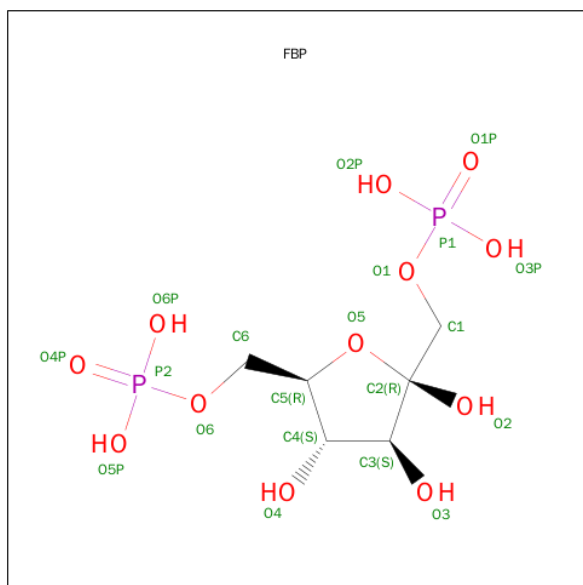
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	EXPRESSION TAG	UNP P14618
B	-15	SER	-	EXPRESSION TAG	UNP P14618
B	-14	HIS	-	EXPRESSION TAG	UNP P14618
B	-13	HIS	-	EXPRESSION TAG	UNP P14618
B	-12	HIS	-	EXPRESSION TAG	UNP P14618
B	-11	HIS	-	EXPRESSION TAG	UNP P14618
B	-10	HIS	-	EXPRESSION TAG	UNP P14618
B	-9	HIS	-	EXPRESSION TAG	UNP P14618
B	-8	SER	-	EXPRESSION TAG	UNP P14618
B	-7	SER	-	EXPRESSION TAG	UNP P14618
B	-6	GLY	-	EXPRESSION TAG	UNP P14618
B	-5	LEU	-	EXPRESSION TAG	UNP P14618
B	-4	VAL	-	EXPRESSION TAG	UNP P14618
B	-3	PRO	-	EXPRESSION TAG	UNP P14618
B	-2	ARG	-	EXPRESSION TAG	UNP P14618
B	-1	GLY	-	EXPRESSION TAG	UNP P14618
B	0	SER	-	EXPRESSION TAG	UNP P14618
C	-18	MET	-	EXPRESSION TAG	UNP P14618
C	-17	GLY	-	EXPRESSION TAG	UNP P14618
C	-16	SER	-	EXPRESSION TAG	UNP P14618
C	-15	SER	-	EXPRESSION TAG	UNP P14618
C	-14	HIS	-	EXPRESSION TAG	UNP P14618
C	-13	HIS	-	EXPRESSION TAG	UNP P14618
C	-12	HIS	-	EXPRESSION TAG	UNP P14618
C	-11	HIS	-	EXPRESSION TAG	UNP P14618
C	-10	HIS	-	EXPRESSION TAG	UNP P14618
C	-9	HIS	-	EXPRESSION TAG	UNP P14618
C	-8	SER	-	EXPRESSION TAG	UNP P14618
C	-7	SER	-	EXPRESSION TAG	UNP P14618
C	-6	GLY	-	EXPRESSION TAG	UNP P14618
C	-5	LEU	-	EXPRESSION TAG	UNP P14618
C	-4	VAL	-	EXPRESSION TAG	UNP P14618
C	-3	PRO	-	EXPRESSION TAG	UNP P14618
C	-2	ARG	-	EXPRESSION TAG	UNP P14618
C	-1	GLY	-	EXPRESSION TAG	UNP P14618
C	0	SER	-	EXPRESSION TAG	UNP P14618
D	-18	MET	-	EXPRESSION TAG	UNP P14618
D	-17	GLY	-	EXPRESSION TAG	UNP P14618
D	-16	SER	-	EXPRESSION TAG	UNP P14618
D	-15	SER	-	EXPRESSION TAG	UNP P14618
D	-14	HIS	-	EXPRESSION TAG	UNP P14618
D	-13	HIS	-	EXPRESSION TAG	UNP P14618

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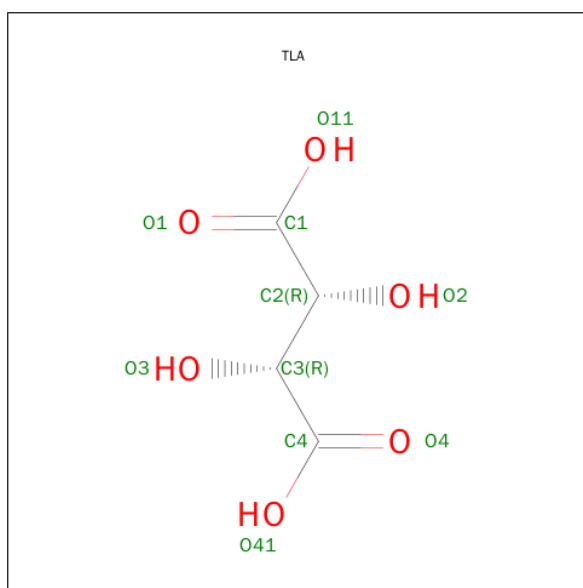
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	EXPRESSION TAG	UNP P14618
D	-11	HIS	-	EXPRESSION TAG	UNP P14618
D	-10	HIS	-	EXPRESSION TAG	UNP P14618
D	-9	HIS	-	EXPRESSION TAG	UNP P14618
D	-8	SER	-	EXPRESSION TAG	UNP P14618
D	-7	SER	-	EXPRESSION TAG	UNP P14618
D	-6	GLY	-	EXPRESSION TAG	UNP P14618
D	-5	LEU	-	EXPRESSION TAG	UNP P14618
D	-4	VAL	-	EXPRESSION TAG	UNP P14618
D	-3	PRO	-	EXPRESSION TAG	UNP P14618
D	-2	ARG	-	EXPRESSION TAG	UNP P14618
D	-1	GLY	-	EXPRESSION TAG	UNP P14618
D	0	SER	-	EXPRESSION TAG	UNP P14618

- Molecule 2 is SUGAR (BETA-FRUCTOSE-1,6-DIPHOSPHATE) (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			6	1	4	1		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



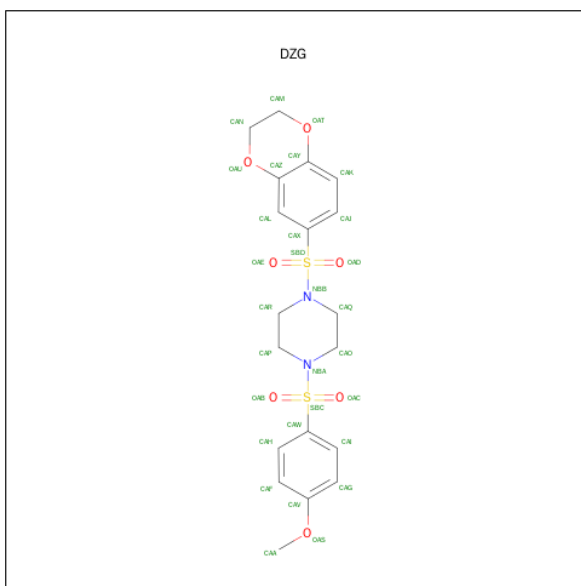
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	X	0	0
			3	3		
4	A	1	Total	X	0	0
			1	1		
4	D	3	Total	X	0	0
			3	3		
4	C	2	Total	X	0	0
			2	2		

- Molecule 5 is 1-(2,3-DIHYDRO-1,4-BENZODIOXIN-6-YLSULFONYL)-4-[(4-METHOXY

HENYL)SULFONYL]PIPERAZINE (three-letter code: DZG) (formula: C₁₉H₂₂N₂O₇S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total 30	C 19	N 2	O 7	S 2	0	0
5	C	1	Total 30	C 19	N 2	O 7	S 2	0	0

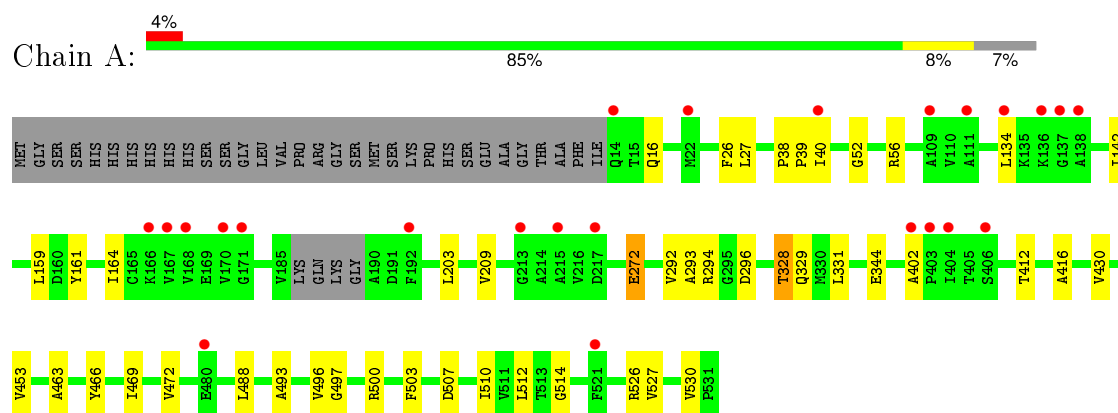
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	182	Total O 182 182	0	0
6	B	164	Total O 164 164	0	0
6	C	174	Total O 174 174	0	0
6	D	160	Total O 160 160	0	0

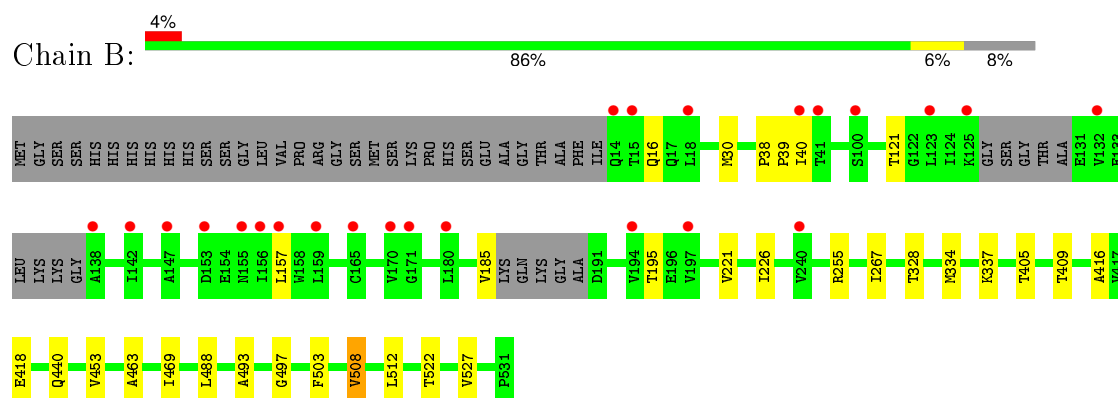
3 Residue-property plots [i](#)

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.

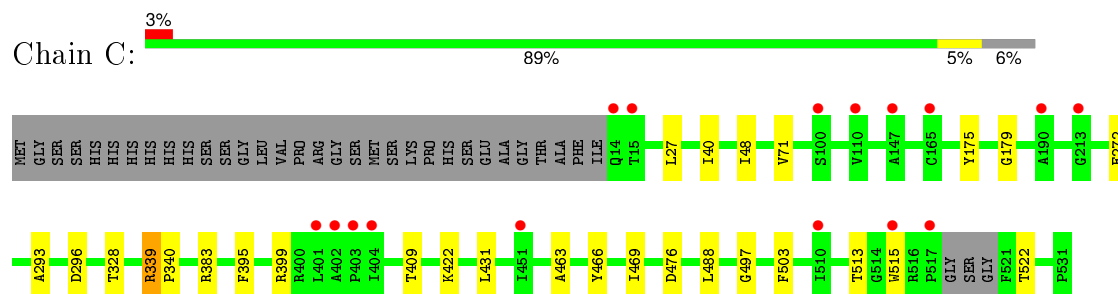
- Molecule 1: Pyruvate kinase isozymes M1/M2



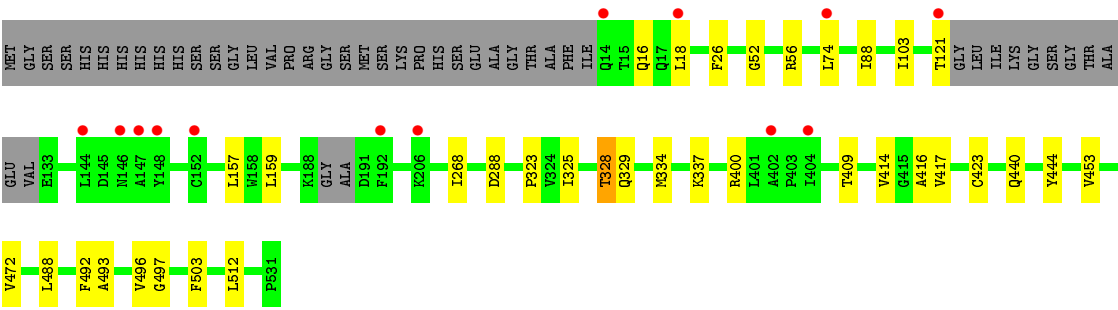
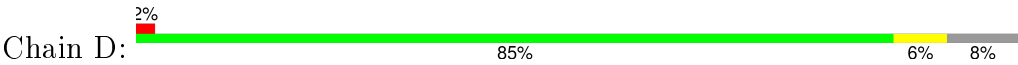
- Molecule 1: Pyruvate kinase isozymes M1/M2



- Molecule 1: Pyruvate kinase isozymes M1/M2



- Molecule 1: Pyruvate kinase isozymes M1/M2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.15Å 152.95Å 93.16Å 90.00° 103.28° 90.00°	Depositor
Resolution (Å)	25.00 – 1.85 24.89 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.7 (25.00-1.85) 96.7 (24.89-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.213 , 0.238 0.213 , 0.236	Depositor DCC
R_{free} test set	2125 reflections (1.18%)	DCC
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 181605 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15931	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: UNX, TLA, FBP, DZG

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	0.51	0/3882	0.53	0/5264
1	B	0.50	0/3786	0.52	0/5134
1	C	0.49	0/3866	0.53	0/5246
1	D	0.50	0/3770	0.51	0/5117
All	All	0.50	0/15304	0.52	0/20761

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3819	0	3754	31	0
1	B	3724	0	3636	22	0
1	C	3805	0	3735	18	0
1	D	3708	0	3578	23	0
2	A	20	0	10	1	0
2	B	20	0	10	0	0
2	C	6	0	0	0	0
2	D	20	0	10	0	0
3	A	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	8	0	0
3	C	10	0	4	0	0
3	D	20	0	8	0	0
4	A	1	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
5	B	30	0	22	4	0
5	C	30	0	22	3	0
6	A	182	0	0	0	0
6	B	164	0	0	0	0
6	C	174	0	0	0	0
6	D	160	0	0	0	0
All	All	15931	0	14801	89	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 3.

All (89) 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:159:LEU:HD21	1:A:209:VAL:HG21	1.46	0.94
1:A:496:VAL:O	1:A:500:ARG:HG2	1.91	0.70
1:A:159:LEU:CD2	1:A:209:VAL:HG21	2.21	0.69
1:B:409[A]:THR:HG22	1:B:440:GLN:OE1	1.95	0.66
1:A:16:GLN:HG2	1:A:40:ILE:HG23	1.78	0.65
1:A:526:ARG:HD3	1:C:515:TRP:CD2	2.36	0.61
1:D:409:THR:CG2	1:D:440:GLN:OE1	2.49	0.61
1:B:453:VAL:HG21	1:B:493:ALA:HB2	1.84	0.59
1:B:409[A]:THR:CG2	1:B:440:GLN:OE1	2.52	0.58
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.86	0.57
1:A:416:ALA:HB2	1:A:512:LEU:HD21	1.86	0.57
1:C:466:TYR:HB2	1:C:469:ILE:HD12	1.87	0.56
1:C:395:PHE:CZ	1:C:399:ARG:HD2	2.42	0.55
1:C:27:LEU:HD13	5:C:540:DZG:HAM	1.90	0.54
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.89	0.54
1:C:476:ASP:OD2	1:C:488:LEU:HD21	2.08	0.53
1:B:463:ALA:HB1	1:B:469:ILE:HG21	1.90	0.53
1:A:27:LEU:HD13	5:B:540:DZG:HAM	1.90	0.53
1:D:409:THR:HG21	1:D:440:GLN:OE1	2.09	0.53
1:A:526:ARG:HD3	1:C:515:TRP:CE3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:VAL:CG2	1:B:493:ALA:HB2	2.39	0.52
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.91	0.52
1:B:508:VAL:HG21	1:B:527:VAL:CG1	2.40	0.52
1:B:508:VAL:CG2	1:B:527:VAL:CG1	2.89	0.50
1:D:488:LEU:HD23	1:D:488:LEU:C	2.31	0.50
1:B:508:VAL:CG2	1:B:527:VAL:HG13	2.42	0.49
1:B:416:ALA:HB2	1:B:512:LEU:HD21	1.95	0.49
1:A:134:LEU:HD11	1:A:203:LEU:HD22	1.94	0.48
1:B:185:VAL:HA	1:B:195:THR:HG22	1.95	0.48
1:A:430:VAL:HG22	1:A:512:LEU:HD12	1.95	0.48
1:B:409[A]:THR:HG23	1:B:522:THR:HB	1.96	0.47
1:C:27:LEU:HD13	5:C:540:DZG:CAM	2.44	0.47
1:B:121:THR:HB	1:B:157:LEU:HD11	1.96	0.47
1:C:488:LEU:C	1:C:488:LEU:HD23	2.35	0.47
1:B:221:VAL:HG12	1:B:226:ILE:HG13	1.97	0.47
1:C:339:ARG:HB2	1:C:340:PRO:HD2	1.97	0.47
1:A:412:THR:HG22	1:A:512:LEU:HD22	1.96	0.47
1:A:27:LEU:HD13	5:B:540:DZG:CAM	2.46	0.46
1:A:161:TYR:CE1	1:A:164:ILE:HA	2.50	0.46
1:D:103:ILE:HD13	1:D:492:PHE:CE1	2.50	0.46
1:C:175:TYR:HB3	1:C:179:GLY:HA2	1.97	0.46
1:A:510:ILE:CD1	1:A:527:VAL:HG22	2.46	0.46
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.51	0.46
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.51	0.45
1:A:328:THR:HG22	1:A:329:GLN:HG3	1.99	0.45
1:A:514:GLY:HA3	2:A:541:FBP:O3	2.17	0.45
1:A:272:GLU:HG2	1:A:293:ALA:HB3	1.99	0.45
1:C:463:ALA:HB1	1:C:469:ILE:HG21	1.99	0.45
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.52	0.45
1:D:453:VAL:CG2	1:D:493:ALA:HB2	2.47	0.44
1:A:142:ILE:N	1:A:142:ILE:HD12	2.32	0.44
1:D:52:GLY:O	1:D:56:ARG:HB2	2.18	0.44
1:C:48:ILE:HG12	1:C:71:VAL:HB	2.00	0.44
1:D:74:LEU:HD11	1:D:88:ILE:HG13	2.00	0.44
1:B:16:GLN:NE2	1:B:40:ILE:HD13	2.32	0.44
1:D:121:THR:HA	1:D:159:LEU:HD23	1.98	0.44
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.52	0.44
1:D:16:GLN:HG3	1:D:18:LEU:HG	2.00	0.44
1:D:453:VAL:HG21	1:D:493:ALA:HB2	2.00	0.44
1:D:334:MET:HA	1:D:337:LYS:O	2.18	0.44
1:D:288:ASP:O	1:D:323:PRO:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:540:DZG:HAP	1:D:26:PHE:CE1	2.53	0.43
1:B:334:MET:HA	1:B:337:LYS:O	2.19	0.43
1:D:409:THR:HG22	1:D:440:GLN:OE1	2.19	0.43
1:C:409:THR:HG22	1:C:522:THR:O	2.19	0.43
1:D:328:THR:HG22	1:D:329:GLN:HG3	2.00	0.43
1:A:463:ALA:HB1	1:A:469:ILE:HG21	2.01	0.43
1:A:331:LEU:HD23	1:A:344:GLU:HB3	2.00	0.42
1:A:26:PHE:CE1	5:B:540:DZG:HARA	2.54	0.42
1:A:292:VAL:HG12	1:A:294:ARG:HG2	2.02	0.42
1:A:466:TYR:HB2	1:A:469:ILE:HD12	2.02	0.42
1:B:255:ARG:CZ	1:B:267:ILE:HD12	2.50	0.42
1:B:418:GLU:HG3	1:D:414:VAL:HG13	2.00	0.42
1:B:38:PRO:HA	1:B:39:PRO:HD3	1.97	0.42
1:B:30:MET:SD	5:B:540:DZG:HAAB	2.60	0.42
1:A:38:PRO:HA	1:A:39:PRO:HD3	1.94	0.42
1:B:488:LEU:HD23	1:B:488:LEU:C	2.40	0.42
1:C:40:ILE:O	1:C:383:ARG:HD2	2.20	0.42
1:D:417:VAL:HG21	1:D:444:TYR:HB2	2.02	0.41
1:A:507:ASP:O	1:A:530:VAL:HG23	2.20	0.41
1:A:52:GLY:O	1:A:56:ARG:HB2	2.21	0.41
1:D:121:THR:HB	1:D:157:LEU:HD11	2.02	0.41
1:A:453:VAL:HG21	1:A:493:ALA:HB2	2.03	0.41
1:C:272:GLU:HB3	1:C:293:ALA:HB3	2.02	0.41
1:D:268:ILE:HG21	1:D:325:ILE:HD12	2.03	0.40
1:B:405:THR:O	1:D:423:CYS:HA	2.21	0.40
1:A:402:ALA:HB1	1:C:422:LYS:NZ	2.36	0.40
1:C:431:LEU:HG	1:C:513:THR:HG22	2.03	0.40
1:A:488:LEU:C	1:A:488:LEU:HD23	2.41	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	510/550 (93%)	502 (98%)	7 (1%)	1 (0%)	52	36
1	B	497/550 (90%)	490 (99%)	6 (1%)	1 (0%)	52	36
1	C	511/550 (93%)	503 (98%)	7 (1%)	1 (0%)	52	36
1	D	499/550 (91%)	492 (99%)	6 (1%)	1 (0%)	52	36
All	All	2017/2200 (92%)	1987 (98%)	26 (1%)	4 (0%)	52	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	328	THR
1	A	328	THR
1	C	328	THR
1	D	328	THR

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	388/452 (86%)	386 (100%)	2 (0%)	92	90
1	B	372/452 (82%)	371 (100%)	1 (0%)	94	94
1	C	384/452 (85%)	382 (100%)	2 (0%)	92	90
1	D	365/452 (81%)	364 (100%)	1 (0%)	94	94
All	All	1509/1808 (84%)	1503 (100%)	6 (0%)	93	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	GLU
1	A	296	ASP
1	B	508	VAL
1	C	296	ASP
1	C	339	ARG
1	D	400	ARG

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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 9 are unknown - leaving 12 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
2	FBP	A	541	-	18,20,20	0.98	1 (5%)	21,32,32	0.61	0
3	TLA	A	542	-	3,9,9	0.23	0	6,12,12	1.04	0
5	DZG	B	540	-	33,33,33	2.55	6 (18%)	49,49,49	2.13	9 (18%)
2	FBP	B	541	-	18,20,20	0.87	1 (5%)	21,32,32	0.72	0
3	TLA	B	542	-	3,9,9	0.79	0	6,12,12	1.27	2 (33%)
3	TLA	B	543	-	3,9,9	0.37	0	6,12,12	0.92	0
5	DZG	C	540	-	33,33,33	2.35	6 (18%)	49,49,49	2.07	8 (16%)
2	FBP	C	541	-	5,5,20	0.66	0	5,7,32	0.61	0
3	TLA	C	542	-	3,9,9	0.52	0	6,12,12	1.25	1 (16%)
2	FBP	D	541	-	18,20,20	0.89	1 (5%)	21,32,32	0.75	0
3	TLA	D	542	-	3,9,9	0.61	0	6,12,12	1.41	2 (33%)
3	TLA	D	543	-	3,9,9	0.68	0	6,12,12	1.20	1 (16%)

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	FBP	A	541	-	-	0/13/32/32	0/1/1/1
3	TLA	A	542	-	-	0/4/12/12	0/0/0/0
5	DZG	B	540	-	-	0/26/43/43	0/4/4/4
2	FBP	B	541	-	-	0/13/32/32	0/1/1/1
3	TLA	B	542	-	-	0/4/12/12	0/0/0/0
3	TLA	B	543	-	-	0/4/12/12	0/0/0/0
5	DZG	C	540	-	-	0/26/43/43	0/4/4/4
2	FBP	C	541	-	-	0/1/3/32	0/0/0/1
3	TLA	C	542	-	-	0/4/12/12	0/0/0/0
2	FBP	D	541	-	-	0/13/32/32	0/1/1/1
3	TLA	D	542	-	-	0/4/12/12	0/0/0/0
3	TLA	D	543	-	-	0/4/12/12	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	541	FBP	O2-C2	2.86	1.45	1.41
2	D	541	FBP	O2-C2	2.87	1.45	1.41
2	A	541	FBP	O2-C2	3.40	1.46	1.41
5	C	540	DZG	OAD-SBD	4.33	1.49	1.43
5	C	540	DZG	OAB-SBC	4.75	1.49	1.43
5	B	540	DZG	OAD-SBD	4.93	1.49	1.43
5	C	540	DZG	OAC-SBC	5.24	1.50	1.43
5	B	540	DZG	OAC-SBC	5.29	1.50	1.43
5	B	540	DZG	OAB-SBC	5.41	1.50	1.43
5	C	540	DZG	SBD-NBB	5.50	1.71	1.63
5	C	540	DZG	SBC-NBA	5.55	1.71	1.63
5	B	540	DZG	SBD-NBB	5.61	1.71	1.63
5	B	540	DZG	OAE-SBD	5.71	1.50	1.43
5	C	540	DZG	OAE-SBD	5.76	1.50	1.43
5	B	540	DZG	SBC-NBA	7.13	1.74	1.63

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	540	DZG	OAD-SBD-OAE	-6.30	108.60	119.47
5	B	540	DZG	OAD-SBD-OAE	-6.06	109.00	119.47
5	B	540	DZG	OAC-SBC-OAB	-6.04	109.06	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	540	DZG	OAC-SBC-OAB	-6.01	109.10	119.47
3	D	542	TLA	C4-C3-C2	-2.69	107.83	113.35
3	C	542	TLA	C1-C2-C3	-2.44	108.34	113.35
5	C	540	DZG	CAO-NBA-SBC	-2.23	112.83	117.12
3	B	542	TLA	C4-C3-C2	-2.21	108.82	113.35
5	B	540	DZG	OAE-SBD-CAX	-2.18	105.17	108.00
3	D	543	TLA	C4-C3-C2	-2.14	108.96	113.35
3	D	542	TLA	C1-C2-C3	-2.04	109.17	113.35
3	B	542	TLA	C1-C2-C3	-2.02	109.21	113.35
5	C	540	DZG	CAP-CAR-NBB	2.10	110.72	109.02
5	B	540	DZG	OAE-SBD-NBB	2.25	108.92	106.69
5	C	540	DZG	OAD-SBD-NBB	2.33	109.00	106.69
5	B	540	DZG	CAP-CAR-NBB	2.38	110.95	109.02
5	C	540	DZG	OAC-SBC-NBA	2.72	109.38	106.69
5	B	540	DZG	OAD-SBD-NBB	3.20	109.85	106.69
5	B	540	DZG	CAR-CAP-NBA	3.64	111.97	109.02
5	C	540	DZG	CAW-SBC-NBA	5.75	114.41	107.32
5	B	540	DZG	CAX-SBD-NBB	6.37	115.16	107.32
5	B	540	DZG	CAW-SBC-NBA	6.47	115.29	107.32
5	C	540	DZG	CAX-SBD-NBB	6.63	115.49	107.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	541	FBP	1	0
5	B	540	DZG	4	0
5	C	540	DZG	3	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	514/550 (93%)	0.10	24 (4%) 35 33	19, 30, 57, 64	0
1	B	504/550 (91%)	0.06	24 (4%) 34 32	19, 30, 64, 80	0
1	C	515/550 (93%)	-0.01	16 (3%) 52 49	20, 30, 46, 61	0
1	D	505/550 (91%)	0.01	13 (2%) 59 57	20, 30, 56, 70	0
All	All	2038/2200 (92%)	0.04	77 (3%) 44 41	19, 30, 57, 80	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	404	ILE	8.4
1	A	404	ILE	6.2
1	A	403	PRO	6.1
1	C	515	TRP	5.9
1	C	403	PRO	5.8
1	B	147	ALA	5.5
1	D	147	ALA	5.3
1	C	402	ALA	4.7
1	B	170	VAL	4.2
1	A	217	ASP	4.2
1	D	148	TYR	3.9
1	D	192	PHE	3.8
1	C	401	LEU	3.7
1	A	171	GLY	3.6
1	B	132	VAL	3.5
1	C	190	ALA	3.5
1	C	517	PRO	3.4
1	D	144	LEU	3.3
1	B	18	LEU	3.2
1	A	137	GLY	3.2
1	A	480	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	197	VAL	3.2
1	A	213	GLY	3.2
1	A	215	ALA	3.1
1	A	166	LYS	3.1
1	D	14	GLN	3.1
1	B	14	GLN	3.1
1	A	22	MET	3.1
1	B	41	THR	3.0
1	B	142	ILE	3.0
1	B	194	VAL	2.9
1	C	213	GLY	2.9
1	C	100	SER	2.9
1	C	147	ALA	2.9
1	A	134	LEU	2.8
1	D	74	LEU	2.8
1	A	192	PHE	2.8
1	A	136	LYS	2.7
1	B	100	SER	2.7
1	B	156	ILE	2.7
1	B	159	LEU	2.6
1	A	111	ALA	2.6
1	A	138	ALA	2.6
1	A	402	ALA	2.6
1	B	153	ASP	2.6
1	A	168	VAL	2.6
1	D	206	LYS	2.5
1	D	402	ALA	2.5
1	B	180	LEU	2.5
1	B	138	ALA	2.5
1	D	18	LEU	2.4
1	A	167	VAL	2.4
1	A	109	ALA	2.4
1	D	404	ILE	2.4
1	B	125	LYS	2.3
1	C	15	THR	2.3
1	B	171	GLY	2.3
1	B	123	LEU	2.3
1	A	14	GLN	2.3
1	C	510	ILE	2.3
1	B	157	LEU	2.2
1	D	152	CYS	2.2
1	A	521	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	15	THR	2.2
1	C	165	CYS	2.2
1	A	40	ILE	2.2
1	A	406	SER	2.2
1	B	240	VAL	2.2
1	D	146	ASN	2.1
1	B	40	ILE	2.1
1	C	451	ILE	2.1
1	B	165	CYS	2.1
1	C	14	GLN	2.1
1	A	170	VAL	2.1
1	B	155	ASN	2.0
1	D	121	THR	2.0
1	C	110	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
4	UNX	B	533	1/1	0.70	2.98	161.19	2,2,2,2	1
4	UNX	A	532	1/1	0.51	2.81	122.95	2,2,2,2	1
4	UNX	C	533	1/1	0.64	2.66	113.68	2,2,2,2	1
4	UNX	B	534	1/1	0.35	2.73	91.36	2,2,2,2	1
4	UNX	D	534	1/1	-0.27	1.96	77.17	2,2,2,2	1
4	UNX	C	532	1/1	0.06	1.23	31.59	2,2,2,2	1
4	UNX	B	532	1/1	-0.69	1.33	30.94	2,2,2,2	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	TLA	D	543	10/10	0.77	0.25	8.27	47,49,49,49	0
3	TLA	B	543	10/10	0.90	0.20	6.09	42,43,44,44	0
3	TLA	B	542	10/10	0.83	0.17	2.81	34,37,37,37	0
3	TLA	D	542	10/10	0.89	0.17	2.56	39,39,40,40	0
3	TLA	C	542	10/10	0.84	0.15	2.46	32,38,40,40	0
2	FBP	C	541	6/20	0.95	0.14	1.48	44,45,46,47	0
5	DZG	C	540	30/30	0.90	0.14	1.29	40,44,47,47	0
5	DZG	B	540	30/30	0.92	0.11	1.04	39,41,42,44	0
3	TLA	A	542	10/10	0.93	0.09	0.15	31,35,36,36	0
2	FBP	A	541	20/20	0.95	0.12	0.07	30,35,39,39	0
2	FBP	B	541	20/20	0.96	0.08	-0.03	21,27,31,32	0
2	FBP	D	541	20/20	0.98	0.07	-0.78	21,22,24,25	0
4	UNX	D	532	1/1	-0.04	1.24	-	2,2,2,2	1
4	UNX	D	533	1/1	-0.67	2.11	-	2,2,2,2	1

6.5 Other polymers [i](#)

There are no such residues in this entry.