



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:33 AM GMT

PDB ID : 3ME3
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 : 2010-03-31
Resolution : 1.95 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

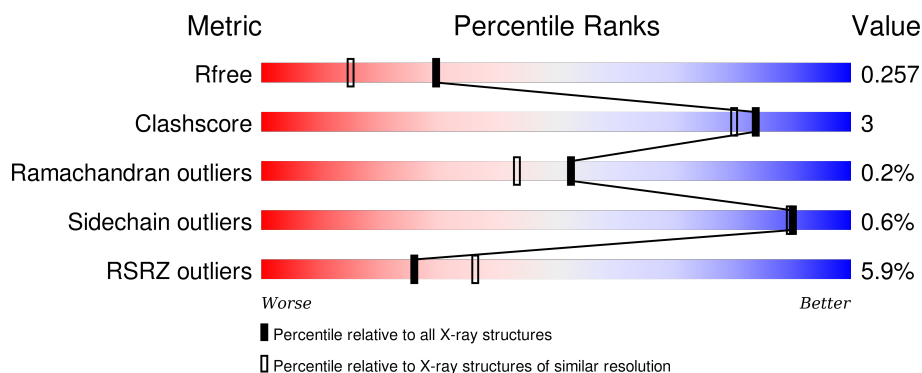
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	550	<div> <div>5%</div> <div>87%</div> <div>7%</div> <div>6%</div> </div>
1	B	550	<div> <div>8%</div> <div>83%</div> <div>7%</div> <div>9%</div> </div>
1	C	550	<div> <div>4%</div> <div>87%</div> <div>7%</div> <div>6%</div> </div>
1	D	550	<div> <div>4%</div> <div>84%</div> <div>7%</div> <div>8%</div> </div>

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
4	SO4	C	532	-	-	-	X
5	UNX	A	534	-	-	-	X
5	UNX	A	535	-	-	-	X
5	UNX	A	536	-	-	-	X
5	UNX	A	539	-	-	-	X
5	UNX	A	546	-	-	-	X
5	UNX	B	534	-	-	-	X
5	UNX	B	535	-	-	-	X
5	UNX	B	536	-	-	-	X
5	UNX	B	537	-	-	-	X
5	UNX	B	538	-	-	-	X
5	UNX	B	539	-	-	-	X
5	UNX	B	543	-	-	-	X
5	UNX	C	533	-	-	-	X
5	UNX	C	534	-	-	-	X
5	UNX	C	535	-	-	-	X
5	UNX	C	536	-	-	-	X
5	UNX	C	537	-	-	-	X
5	UNX	C	539	-	-	-	X
5	UNX	C	540	-	-	-	X
5	UNX	D	537	-	-	-	X
5	UNX	D	539	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16045 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	518	Total	C	N	O	S	0	0	0
			3854	2427	676	726	25			
1	B	498	Total	C	N	O	S	0	1	0
			3702	2323	664	691	24			
1	C	517	Total	C	N	O	S	0	0	0
			3866	2436	680	726	24			
1	D	504	Total	C	N	O	S	0	3	0
			3745	2360	663	698	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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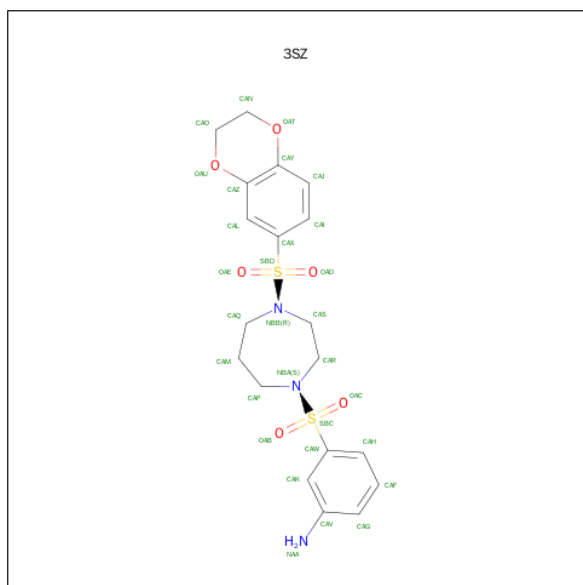
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	EXPRESSION TAG	UNP P14618
B	-15	SER	-	EXPRESSION TAG	UNP P14618
B	-14	HIS	-	EXPRESSION TAG	UNP P14618
B	-13	HIS	-	EXPRESSION TAG	UNP P14618
B	-12	HIS	-	EXPRESSION TAG	UNP P14618
B	-11	HIS	-	EXPRESSION TAG	UNP P14618
B	-10	HIS	-	EXPRESSION TAG	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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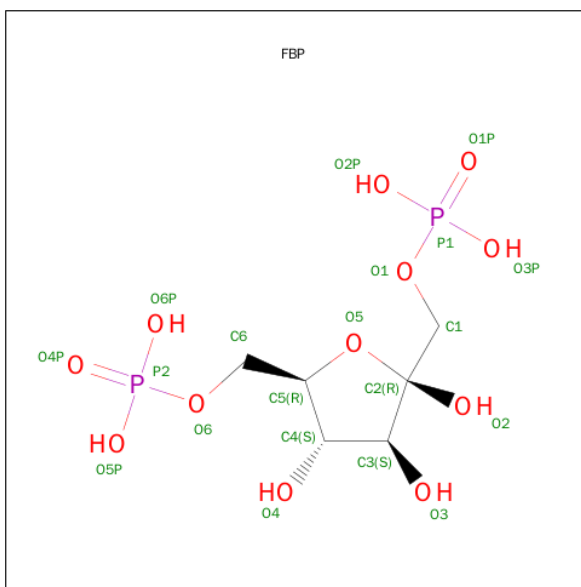
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	EXPRESSION TAG	UNP P14618
D	-11	HIS	-	EXPRESSION TAG	UNP P14618
D	-10	HIS	-	EXPRESSION TAG	UNP P14618
D	-9	HIS	-	EXPRESSION TAG	UNP P14618
D	-8	SER	-	EXPRESSION TAG	UNP P14618
D	-7	SER	-	EXPRESSION TAG	UNP P14618
D	-6	GLY	-	EXPRESSION TAG	UNP 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 3-{[4-(2,3-DIHYDRO-1,4-BENZODIOXIN-6-YLSULFONYL)-1,4-DIAZEPAN-1-YL]SULFONYL}ANILINE (three-letter code: 3SZ) (formula: C₁₉H₂₃N₃O₆S₂).



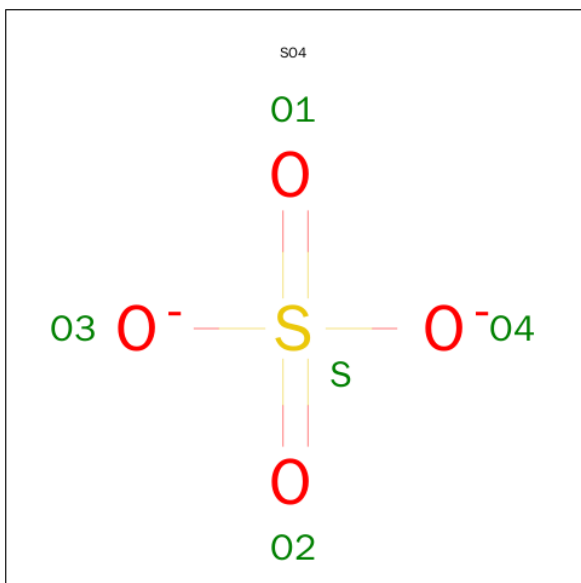
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			30	19	3	6	2		
2	D	1	Total	C	N	O	S	0	0
			30	19	3	6	2		

- Molecule 3 is SUGAR (BETA-FRUCTOSE-1,6-DIPHOSPHATE) (three-letter code: FBP) (formula: C₆H₁₄O₁₂P₂).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	10	Total X 10 10	0	0
5	A	14	Total X 14 14	0	0
5	D	7	Total X 7 7	0	0
5	C	11	Total X 11 11	0	0

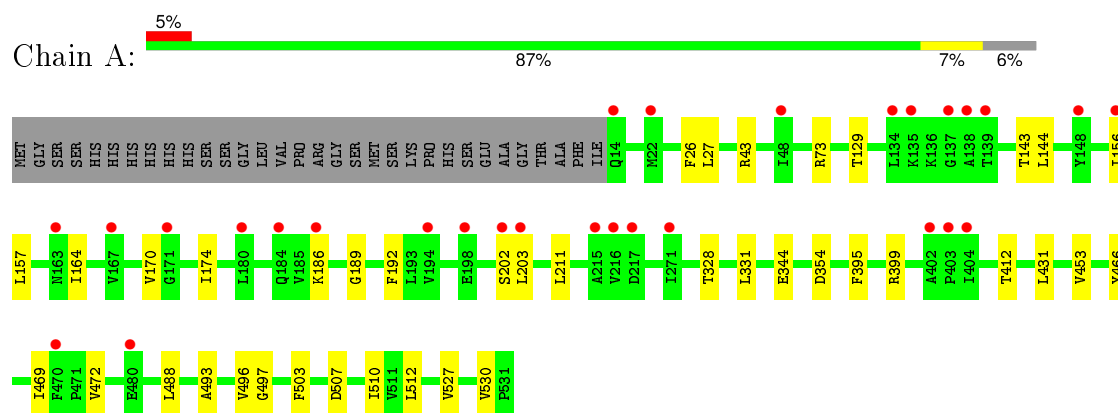
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	185	Total O 186 186	0	1
6	B	171	Total O 171 171	0	0
6	C	166	Total O 166 166	0	0
6	D	153	Total O 153 153	0	0

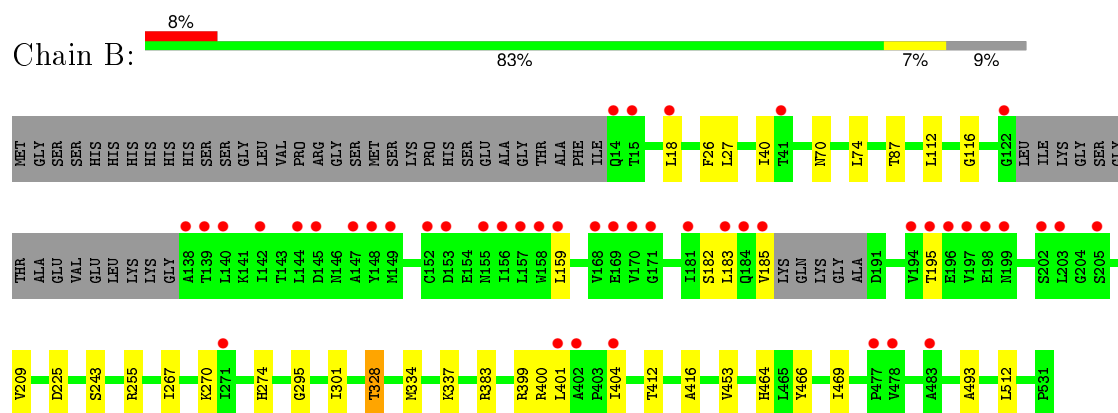
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

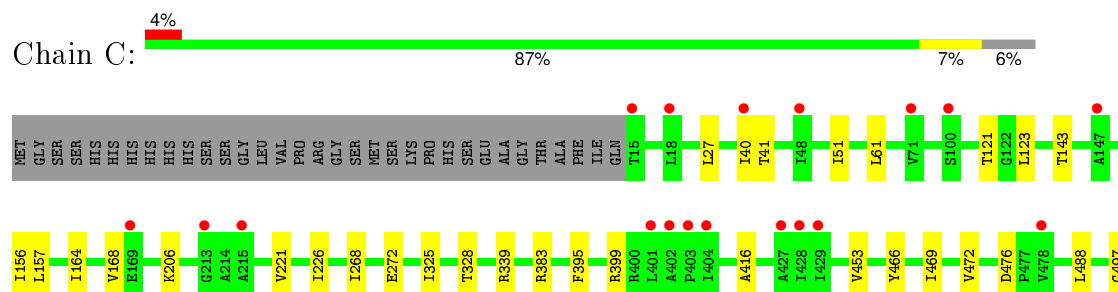
- Molecule 1: Pyruvate kinase isozymes M1/M2



- Molecule 1: Pyruvate kinase isozymes M1/M2

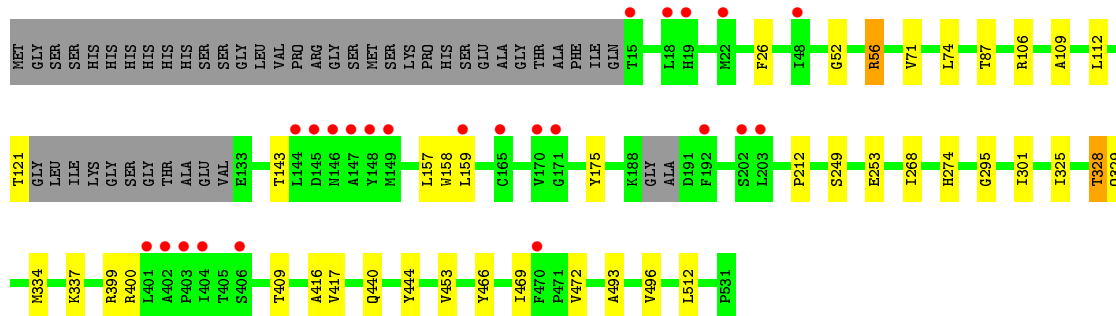
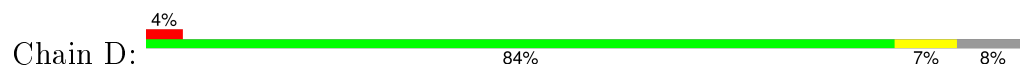


- Molecule 1: Pyruvate kinase isozymes M1/M2





- 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	80.88Å 152.56Å 93.04Å 90.00° 103.17° 90.00°	Depositor
Resolution (Å)	26.71 – 1.95 26.71 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (26.71-1.95) 99.7 (26.71-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.219 , 0.262 0.219 , 0.257	Depositor DCC
R_{free} test set	1917 reflections (1.22%)	DCC
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 158798 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16045	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, FBP, SO4, 3SZ

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	0/3918	0.70	4/5311 (0.1%)
1	B	0.67	0/3765	0.72	0/5103
1	C	0.67	0/3930	0.68	0/5325
1	D	0.66	0/3816	0.68	0/5176
All	All	0.67	0/15429	0.70	4/20915 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	431	LEU	CA-CB-CG	6.12	129.37	115.30
1	A	354	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	43	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	3854	0	3804	19	0
1	B	3702	0	3627	26	0
1	C	3866	0	3846	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3745	0	3657	26	0
2	A	30	0	23	4	0
2	D	30	0	23	2	0
3	A	20	0	10	0	0
3	B	20	0	10	0	0
3	C	20	0	10	0	0
3	D	20	0	10	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	14	0	0	0	0
5	B	10	0	0	0	0
5	C	11	0	0	0	0
5	D	7	0	0	0	0
6	A	186	0	0	0	0
6	B	171	0	0	1	0
6	C	166	0	0	0	0
6	D	153	0	0	1	0
All	All	16045	0	15020	91	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 (91) 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:395:PHE:CZ	1:C:399:ARG:HD2	2.07	0.88
1:C:416:ALA:HB2	1:C:512:LEU:HD21	1.76	0.67
1:D:409:THR:CG2	1:D:440:GLN:OE1	2.42	0.67
1:A:144:LEU:HD11	1:A:164:ILE:HG22	1.79	0.64
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.79	0.63
1:A:395:PHE:CZ	1:A:399:ARG:HD2	2.34	0.63
1:B:112:LEU:C	1:B:112:LEU:HD23	2.20	0.62
1:D:409:THR:HG21	1:D:440:GLN:OE1	1.99	0.62
1:B:399:ARG:NH2	1:D:399:ARG:CD	2.65	0.60
1:B:182:SER:O	1:B:183:LEU:HD23	2.02	0.60
1:C:416:ALA:CB	1:C:512:LEU:HD21	2.33	0.58
1:C:488:LEU:O	1:C:488:LEU:HD23	2.06	0.56
1:A:27:LEU:HD23	1:B:401:LEU:HD12	1.87	0.55
1:D:328:THR:HG22	1:D:329:GLN:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106[B]:ARG:CG	6:D:605:HOH:O	2.55	0.54
1:B:412:THR:HG22	1:B:512:LEU:HD22	1.89	0.54
1:C:466:TYR:HB2	1:C:469:ILE:HD12	1.90	0.53
2:A:540:3SZ:CAN	1:B:27:LEU:HD13	2.37	0.53
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.45	0.52
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.92	0.52
1:D:249:SER:O	1:D:253:GLU:HG3	2.09	0.51
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.93	0.51
1:C:395:PHE:CE2	1:C:399:ARG:HD2	2.45	0.50
1:C:488:LEU:C	1:C:488:LEU:HD23	2.32	0.50
1:B:116:GLY:HA2	1:B:225:ASP:OD2	2.12	0.50
1:B:453:VAL:HG21	1:B:493:ALA:HB2	1.93	0.50
1:C:395:PHE:CE1	1:C:399:ARG:HD2	2.47	0.49
1:C:121:THR:HB	1:C:157:LEU:HD11	1.95	0.49
1:D:274:HIS:CE1	1:D:301:ILE:HG22	2.48	0.49
1:C:123:LEU:HD21	1:C:206:LYS:HE3	1.95	0.48
1:A:453:VAL:HG21	1:A:493:ALA:HB2	1.97	0.47
1:C:453:VAL:HG22	1:C:472:VAL:CG2	2.45	0.47
2:A:540:3SZ:HAMA	1:B:26:PHE:CZ	2.49	0.46
1:D:175:TYR:CE1	1:D:212:PRO:HG3	2.51	0.46
1:B:255:ARG:CZ	1:B:267:ILE:HD12	2.45	0.46
1:D:74:LEU:HD21	1:D:87:THR:HG21	1.97	0.46
1:A:507:ASP:O	1:A:530:VAL:HG23	2.16	0.46
1:C:27:LEU:HD13	2:D:540:3SZ:CAN	2.46	0.46
1:D:268:ILE:HG21	1:D:325:ILE:HD12	1.97	0.46
1:C:476:ASP:OD2	1:C:488:LEU:HD21	2.16	0.46
1:A:143:THR:HG21	1:A:156:ILE:HD11	1.97	0.45
1:B:112:LEU:CD2	1:B:112:LEU:C	2.85	0.45
1:A:510:ILE:HD12	1:A:527:VAL:HG22	1.98	0.45
1:D:121:THR:HB	1:D:157:LEU:HD11	1.99	0.45
1:B:416:ALA:HB2	1:B:512:LEU:HD21	1.98	0.45
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.97	0.45
1:D:409:THR:HG22	1:D:440:GLN:OE1	2.13	0.45
1:C:516:ARG:HB2	1:C:517:PRO:CD	2.47	0.45
1:D:52:GLY:O	1:D:56:ARG:HB3	2.17	0.45
1:A:412:THR:HG22	1:A:512:LEU:CD2	2.48	0.44
1:D:295:GLY:CA	1:D:328:THR:HG21	2.48	0.44
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.99	0.44
1:C:268:ILE:HG21	1:C:325:ILE:HD12	1.99	0.44
1:B:404:ILE:HD12	1:B:404:ILE:N	2.33	0.44
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.54	0.43
1:C:51:ILE:HD12	1:C:61:LEU:HD21	2.01	0.43
1:D:417:VAL:HG21	1:D:444:TYR:HB2	1.99	0.43
1:A:157:LEU:HD13	1:A:203:LEU:HD21	2.01	0.43
1:B:185:VAL:HA	1:B:195:THR:HG22	1.99	0.43
1:B:40:ILE:O	1:B:383:ARG:HD2	2.18	0.43
1:A:26:PHE:CE1	2:A:540:3SZ:HAPA	2.54	0.43
1:B:274:HIS:HB2	6:B:594:HOH:O	2.18	0.42
1:A:453:VAL:CG2	1:A:493:ALA:HB2	2.48	0.42
1:A:174:ILE:HG12	1:A:211:LEU:HD22	2.02	0.42
1:B:453:VAL:CG2	1:B:493:ALA:HB2	2.49	0.42
1:B:334:MET:HA	1:B:337:LYS:O	2.20	0.42
1:D:334:MET:HA	1:D:337:LYS:O	2.20	0.42
1:C:143:THR:CG2	1:C:156:ILE:HD11	2.50	0.42
1:D:453:VAL:HG21	1:D:493:ALA:HB2	2.00	0.42
1:B:18:LEU:HA	1:B:18:LEU:HD23	1.84	0.42
1:C:164:ILE:O	1:C:168:VAL:HG22	2.19	0.42
1:A:170:VAL:HG13	1:A:186:LYS:O	2.20	0.41
1:A:189:GLY:HA3	1:A:192:PHE:CZ	2.56	0.41
1:D:26:PHE:CG	2:D:540:3SZ:HAR	2.55	0.41
1:D:143:THR:O	1:D:158:TRP:HA	2.20	0.41
1:D:121:THR:HG22	1:D:159:LEU:CD2	2.51	0.41
1:C:40:ILE:O	1:C:383:ARG:HD2	2.21	0.41
1:C:221:VAL:HG12	1:C:226:ILE:HG13	2.03	0.41
1:D:71:VAL:HG22	1:D:109:ALA:HB3	2.02	0.41
1:B:295:GLY:CA	1:B:328:THR:HG21	2.51	0.41
1:D:112:LEU:HD23	1:D:112:LEU:C	2.41	0.40
1:A:488:LEU:C	1:A:488:LEU:HD23	2.41	0.40
1:B:74:LEU:HD21	1:B:87:THR:CG2	2.50	0.40
1:A:331:LEU:HD23	1:A:344:GLU:HB3	2.03	0.40
1:D:453:VAL:CG2	1:D:493:ALA:HB2	2.51	0.40
1:C:41:THR:HG21	1:C:500:ARG:O	2.20	0.40
1:B:70:ASN:HB3	1:B:464:HIS:CG	2.56	0.40
1:B:159:LEU:CD2	1:B:209:VAL:HG21	2.51	0.40
2:A:540:3SZ:HAS	1:B:26:PHE:CG	2.56	0.40
1:B:243:SER:HA	1:B:270:LYS:HD3	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	516/550 (94%)	504 (98%)	11 (2%)	1 (0%)	52	43
1	B	493/550 (90%)	482 (98%)	10 (2%)	1 (0%)	52	43
1	C	515/550 (94%)	505 (98%)	9 (2%)	1 (0%)	52	43
1	D	501/550 (91%)	490 (98%)	10 (2%)	1 (0%)	52	43
All	All	2025/2200 (92%)	1981 (98%)	40 (2%)	4 (0%)	52	43

All (4) Ramachandran outliers are listed below:

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

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	392/452 (87%)	390 (100%)	2 (0%)	92	91
1	B	372/452 (82%)	370 (100%)	2 (0%)	92	91
1	C	397/452 (88%)	394 (99%)	3 (1%)	86	85
1	D	374/452 (83%)	372 (100%)	2 (0%)	92	91
All	All	1535/1808 (85%)	1526 (99%)	9 (1%)	90	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	THR
1	A	202	SER
1	B	301	ILE
1	B	400	ARG
1	C	272	GLU
1	C	339	ARG
1	C	519	SER
1	D	56	ARG
1	D	400	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	184	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 42 are unknown - leaving 10 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	532	-	4,4,4	0.14	0	6,6,6	0.38	0
2	3SZ	A	540	-	33,33,33	2.10	4 (12%)	47,49,49	2.04	11 (23%)
3	FBP	A	541	-	18,20,20	0.86	1 (5%)	21,32,32	1.14	2 (9%)
4	SO4	B	532	-	4,4,4	0.27	0	6,6,6	0.30	0
3	FBP	B	541	-	18,20,20	0.75	0	21,32,32	1.07	1 (4%)
4	SO4	C	532	-	4,4,4	0.20	0	6,6,6	0.27	0
3	FBP	C	541	-	18,20,20	0.96	1 (5%)	21,32,32	1.11	2 (9%)
4	SO4	D	532	-	4,4,4	0.10	0	6,6,6	0.33	0
2	3SZ	D	540	-	33,33,33	2.22	9 (27%)	47,49,49	1.79	11 (23%)
3	FBP	D	541	-	18,20,20	0.89	1 (5%)	21,32,32	1.16	2 (9%)

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
4	SO4	A	532	-	-	0/0/0/0	0/0/0/0
2	3SZ	A	540	-	-	0/24/42/42	0/3/4/4
3	FBP	A	541	-	-	0/13/32/32	0/1/1/1
4	SO4	B	532	-	-	0/0/0/0	0/0/0/0
3	FBP	B	541	-	-	0/13/32/32	0/1/1/1
4	SO4	C	532	-	-	0/0/0/0	0/0/0/0
3	FBP	C	541	-	-	0/13/32/32	0/1/1/1
4	SO4	D	532	-	-	0/0/0/0	0/0/0/0
2	3SZ	D	540	-	-	0/24/42/42	0/3/4/4
3	FBP	D	541	-	-	0/13/32/32	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	540	3SZ	CAX-SBD	-3.95	1.70	1.76
2	D	540	3SZ	CAW-SBC	-3.00	1.72	1.76
2	D	540	3SZ	CAP-NBA	-2.18	1.45	1.47
2	D	540	3SZ	OAT-CAN	2.11	1.48	1.43
3	A	541	FBP	O2-C2	2.19	1.44	1.41
3	D	541	FBP	O2-C2	2.99	1.45	1.41
3	C	541	FBP	O2-C2	3.16	1.46	1.41
2	D	540	3SZ	SBC-NBA	3.95	1.69	1.63
2	D	540	3SZ	OAE-SBD	4.04	1.48	1.43
2	D	540	3SZ	OAC-SBC	4.45	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	540	3SZ	OAC-SBC	4.78	1.49	1.43
2	D	540	3SZ	OAD-SBD	5.22	1.50	1.43
2	A	540	3SZ	OAE-SBD	5.43	1.50	1.43
2	A	540	3SZ	OAB-SBC	5.92	1.51	1.43
2	D	540	3SZ	OAB-SBC	6.05	1.51	1.43
2	A	540	3SZ	OAD-SBD	6.05	1.51	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	540	3SZ	OAC-SBC-OAB	-6.17	108.83	119.47
2	A	540	3SZ	OAE-SBD-OAD	-5.10	110.67	119.47
2	D	540	3SZ	OAE-SBD-OAD	-3.92	112.70	119.47
2	D	540	3SZ	CAS-CAR-NBA	-3.87	108.86	113.13
2	D	540	3SZ	OAC-SBC-OAB	-3.50	113.42	119.47
2	D	540	3SZ	CAH-CAW-SBC	-3.45	115.98	119.79
2	A	540	3SZ	CAS-CAR-NBA	-3.44	109.34	113.13
2	D	540	3SZ	CAM-CAP-NBA	-3.27	106.57	112.28
3	D	541	FBP	O1-P1-O1P	-2.44	100.92	107.14
2	D	540	3SZ	CAV-CAK-CAW	-2.35	117.94	120.30
2	A	540	3SZ	CAM-CAP-NBA	-2.34	108.19	112.28
3	D	541	FBP	O3P-P1-O2P	2.02	115.07	107.38
3	A	541	FBP	O6-P2-O4P	2.04	112.33	107.14
2	A	540	3SZ	CAK-CAW-SBC	2.09	121.99	119.41
3	C	541	FBP	O5-C5-C6	2.10	114.28	109.49
2	A	540	3SZ	OAC-SBC-CAW	2.18	110.84	108.00
2	A	540	3SZ	OAB-SBC-NBA	2.34	109.00	106.69
2	D	540	3SZ	OAD-SBD-NBB	2.38	109.04	106.69
3	C	541	FBP	O6-P2-O4P	2.57	113.68	107.14
2	A	540	3SZ	CAM-CAQ-NBB	2.68	116.96	112.28
2	D	540	3SZ	OAC-SBC-CAW	2.88	111.74	108.00
2	D	540	3SZ	CAK-CAW-SBC	2.93	123.01	119.41
3	A	541	FBP	O3P-P1-O1P	3.19	120.85	110.58
3	B	541	FBP	O6-P2-O4P	3.23	115.36	107.14
2	D	540	3SZ	CAW-SBC-NBA	3.50	111.63	107.32
2	D	540	3SZ	OAE-SBD-CAX	3.71	112.82	108.00
2	A	540	3SZ	CAX-SBD-NBB	3.74	111.93	107.32
2	A	540	3SZ	OAD-SBD-NBB	4.00	110.64	106.69
2	A	540	3SZ	CAW-SBC-NBA	6.11	114.85	107.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	540	3SZ	4	0
2	D	540	3SZ	2	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	518/550 (94%)	0.38	29 (5%)	28	39	16, 26, 54, 64	0
1	B	498/550 (90%)	0.49	45 (9%)	12	19	16, 26, 67, 79	0
1	C	517/550 (94%)	0.33	23 (4%)	38	49	17, 27, 43, 53	0
1	D	504/550 (91%)	0.34	24 (4%)	34	45	17, 27, 53, 65	0
All	All	2037/2200 (92%)	0.38	121 (5%)	26	36	16, 27, 54, 79	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	ALA	7.9
1	A	404	ILE	6.8
1	C	404	ILE	6.2
1	C	401	LEU	5.6
1	A	403	PRO	5.5
1	A	134	LEU	5.5
1	C	403	PRO	5.4
1	A	217	ASP	5.3
1	B	170	VAL	5.3
1	B	197	VAL	5.1
1	D	148	TYR	5.1
1	B	203	LEU	5.0
1	D	147	ALA	4.8
1	D	170	VAL	4.7
1	B	148	TYR	4.7
1	D	404	ILE	4.6
1	B	156	ILE	4.3
1	A	215	ALA	4.3
1	B	138	ALA	4.2
1	C	213	GLY	4.1
1	B	194	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	153	ASP	4.0
1	B	122	GLY	4.0
1	B	184	GLN	4.0
1	A	138	ALA	3.9
1	B	41	THR	3.9
1	A	137	GLY	3.9
1	B	205	SER	3.9
1	C	402	ALA	3.9
1	A	171	GLY	3.8
1	B	155	ASN	3.8
1	C	215	ALA	3.7
1	D	402	ALA	3.7
1	D	192	PHE	3.7
1	B	140	LEU	3.7
1	B	171	GLY	3.5
1	A	139	THR	3.5
1	D	22	MET	3.5
1	B	14	GLN	3.4
1	A	148	TYR	3.4
1	C	147	ALA	3.3
1	D	171	GLY	3.2
1	D	144	LEU	3.2
1	A	167	VAL	3.2
1	B	159	LEU	3.2
1	A	480	GLU	3.1
1	D	203	LEU	3.1
1	C	18	LEU	3.1
1	B	15	THR	3.1
1	B	196	GLU	3.0
1	B	18	LEU	3.0
1	A	470	PHE	2.9
1	B	202	SER	2.9
1	B	144	LEU	2.9
1	C	100	SER	2.9
1	B	145	ASP	2.9
1	D	149	MET	2.8
1	C	511	VAL	2.8
1	B	402	ALA	2.8
1	D	403	PRO	2.8
1	B	169	GLU	2.8
1	A	198	GLU	2.7
1	B	181	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	521	PHE	2.7
1	A	184	GLN	2.7
1	C	169	GLU	2.7
1	D	146	ASN	2.7
1	A	402	ALA	2.6
1	C	15	THR	2.6
1	C	510	ILE	2.6
1	D	15	THR	2.6
1	A	194	VAL	2.5
1	C	428	ILE	2.5
1	A	22	MET	2.5
1	C	525	MET	2.5
1	B	152	CYS	2.5
1	B	477	PRO	2.5
1	A	14	GLN	2.4
1	B	195	THR	2.4
1	A	163	ASN	2.4
1	B	183	LEU	2.4
1	A	202	SER	2.4
1	B	168	VAL	2.4
1	B	185	VAL	2.4
1	B	139	THR	2.4
1	B	149	MET	2.4
1	A	156	ILE	2.3
1	A	135	LYS	2.3
1	A	186	LYS	2.3
1	D	145	ASP	2.3
1	A	180	LEU	2.3
1	B	401	LEU	2.3
1	D	406	SER	2.3
1	B	158	TRP	2.3
1	C	48	ILE	2.3
1	A	48	ILE	2.3
1	D	202	SER	2.2
1	A	203	LEU	2.2
1	D	401	LEU	2.2
1	C	40	ILE	2.2
1	B	157	LEU	2.2
1	A	216	VAL	2.2
1	B	478	VAL	2.2
1	C	527	VAL	2.2
1	D	165	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	19	HIS	2.2
1	B	271	ILE	2.1
1	C	478	VAL	2.1
1	C	429	ILE	2.1
1	D	48	ILE	2.1
1	D	18	LEU	2.1
1	C	427	ALA	2.1
1	A	271	ILE	2.1
1	B	142	ILE	2.1
1	B	198	GLU	2.1
1	B	199	ASN	2.0
1	D	470	PHE	2.0
1	C	71	VAL	2.0
1	B	483	ALA	2.0
1	D	159	LEU	2.0
1	B	404	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 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. 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(\AA^2)	Q<0.9
5	UNX	A	535	1/1	0.24	3.44	170.00	2,2,2,2	1
5	UNX	C	540	1/1	0.17	2.94	166.53	2,2,2,2	1
5	UNX	C	536	1/1	-0.00	3.10	156.03	2,2,2,2	1
5	UNX	A	536	1/1	-0.05	3.36	152.32	2,2,2,2	1
5	UNX	A	546	1/1	0.13	3.17	146.69	2,2,2,2	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	UNX	B	539	1/1	0.34	2.19	129.34	2,2,2,2	1
5	UNX	B	535	1/1	0.56	2.49	115.13	2,2,2,2	1
5	UNX	A	539	1/1	-0.18	3.08	114.19	2,2,2,2	1
5	UNX	B	543	1/1	0.05	2.63	113.25	2,2,2,2	1
5	UNX	B	536	1/1	0.74	1.70	107.85	2,2,2,2	1
5	UNX	B	537	1/1	0.58	2.31	107.81	2,2,2,2	1
5	UNX	C	535	1/1	0.11	2.76	101.32	2,2,2,2	1
5	UNX	A	534	1/1	-0.30	2.06	101.09	2,2,2,2	1
5	UNX	C	533	1/1	-0.07	2.23	79.74	2,2,2,2	1
5	UNX	D	539	1/1	0.35	1.93	74.21	2,2,2,2	1
5	UNX	C	534	1/1	0.41	2.01	69.17	2,2,2,2	1
5	UNX	B	534	1/1	-0.42	2.57	68.36	2,2,2,2	1
5	UNX	C	537	1/1	0.38	1.88	66.45	2,2,2,2	1
5	UNX	B	538	1/1	-0.42	1.35	64.16	2,2,2,2	1
5	UNX	C	539	1/1	0.17	1.45	55.42	2,2,2,2	1
5	UNX	D	537	1/1	-0.30	1.77	48.53	2,2,2,2	1
4	SO4	C	532	5/5	0.94	0.28	4.05	60,61,62,62	0
2	3SZ	A	540	30/30	0.91	0.14	1.55	25,32,35,37	0
2	3SZ	D	540	30/30	0.94	0.12	0.20	27,32,35,36	0
3	FBP	C	541	20/20	0.97	0.13	0.13	24,28,34,34	0
4	SO4	D	532	5/5	0.95	0.13	0.04	51,51,53,53	0
3	FBP	B	541	20/20	0.96	0.10	-0.02	19,21,27,29	0
4	SO4	B	532	5/5	0.96	0.08	-1.00	44,45,47,48	0
3	FBP	A	541	20/20	0.98	0.07	-1.16	22,26,29,29	0
3	FBP	D	541	20/20	0.98	0.06	-1.67	17,19,22,23	0
5	UNX	D	538	1/1	0.28	1.94	-	2,2,2,2	1
5	UNX	A	542	1/1	-0.16	2.10	-	2,2,2,2	1
5	UNX	D	534	1/1	0.32	2.03	-	2,2,2,2	1
5	UNX	A	543	1/1	0.36	2.24	-	2,2,2,2	1
4	SO4	A	532	5/5	0.90	0.25	-	53,53,56,56	0
5	UNX	A	547	1/1	-0.61	1.69	-	2,2,2,2	1
5	UNX	C	543	1/1	-0.28	2.36	-	2,2,2,2	1
5	UNX	D	535	1/1	0.58	1.76	-	2,2,2,2	1
5	UNX	B	540	1/1	0.17	2.55	-	2,2,2,2	1
5	UNX	A	544	1/1	0.14	2.67	-	2,2,2,2	1
5	UNX	A	538	1/1	-0.01	2.27	-	2,2,2,2	1
5	UNX	A	533	1/1	0.54	2.11	-	2,2,2,2	1
5	UNX	A	548	1/1	-0.76	1.98	-	2,2,2,2	1
5	UNX	D	533	1/1	0.17	2.23	-	2,2,2,2	1
5	UNX	A	537	1/1	0.31	4.16	-	2,2,2,2	1
5	UNX	C	542	1/1	-0.61	1.87	-	2,2,2,2	1
5	UNX	A	545	1/1	0.59	2.20	-	2,2,2,2	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	UNX	C	538	1/1	0.49	3.37	-	2,2,2,2	1
5	UNX	C	544	1/1	0.62	1.93	-	2,2,2,2	1
5	UNX	B	533	1/1	-0.37	1.68	-	2,2,2,2	1
5	UNX	D	536	1/1	-0.07	1.74	-	2,2,2,2	1
5	UNX	B	542	1/1	-0.45	1.90	-	2,2,2,2	1

6.5 Other polymers [i](#)

There are no such residues in this entry.