Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:46 PM GMT

PDB ID	:	4G1N
Title	:	PKM2 in complex with an activator
Authors	:	Kung, C.; Hixon, J.; Dang, L.; DeLaBarre, B.; Qian, K.C.
Deposited on	:	2012-07-10
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

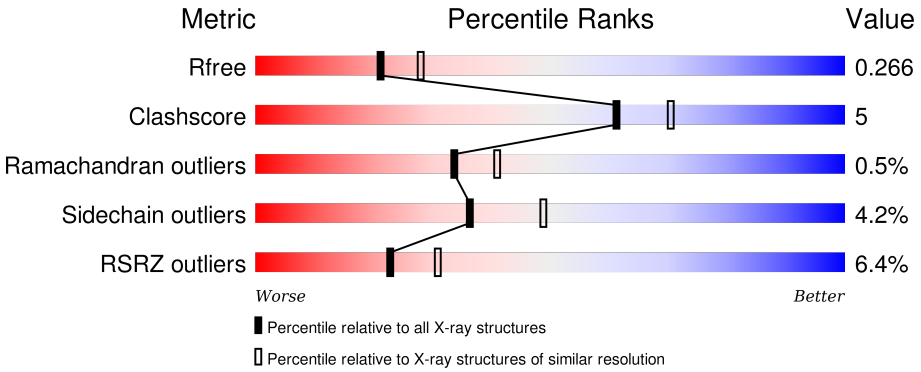
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 <=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	518	3%, 86%, 13%
1	B	518	14%, 85%, 13%
1	C	518	4%, 86%, 13%
1	D	518	5%, 86%, 13%

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	NZT	D	603[A]	-	-	-	X
4	NZT	D	603[B]	-	-	-	X

2 Entry composition

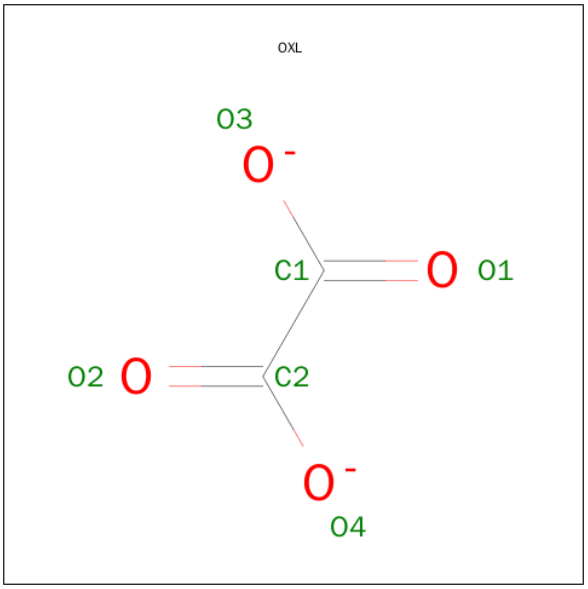
There are 5 unique types of molecules in this entry. The entry contains 16230 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			3965	2492	704	744	25			
1	B	518	Total	C	N	O	S	0	2	0
			3978	2501	707	744	26			
1	C	518	Total	C	N	O	S	0	1	0
			3970	2496	704	744	26			
1	D	518	Total	C	N	O	S	0	0	0
			3965	2492	704	744	25			

- Molecule 2 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



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

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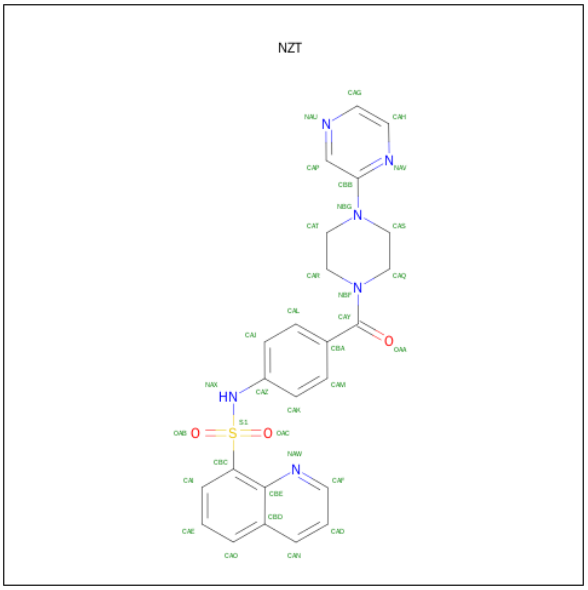
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 6 2 4	0	0
2	D	1	Total C O 6 2 4	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is N-(4-{[4-(PYRAZIN-2-YL)PIPERAZIN-1-YL]CARBONYL}PHENYL)QUINOLINE-8-SULFONAMIDE (three-letter code: NZT) (formula: $C_{24}H_{22}N_6O_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 34 24 6 3 1	0	1
4	D	1	Total C N O S 68 48 12 6 2	0	1

- Molecule 5 is water.

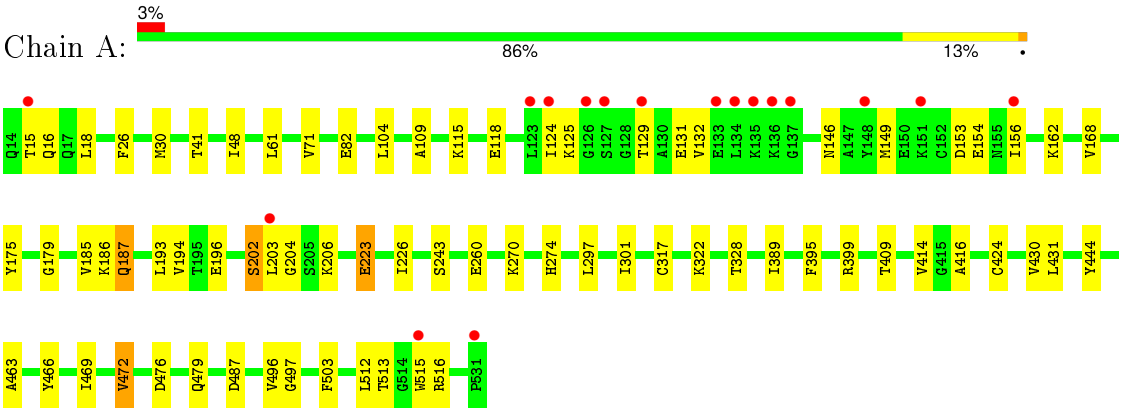
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	66	Total O 66 66	0	0
5	B	71	Total O 71 71	0	0
5	C	48	Total O 48 48	0	0
5	D	37	Total O 37 37	0	0

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.

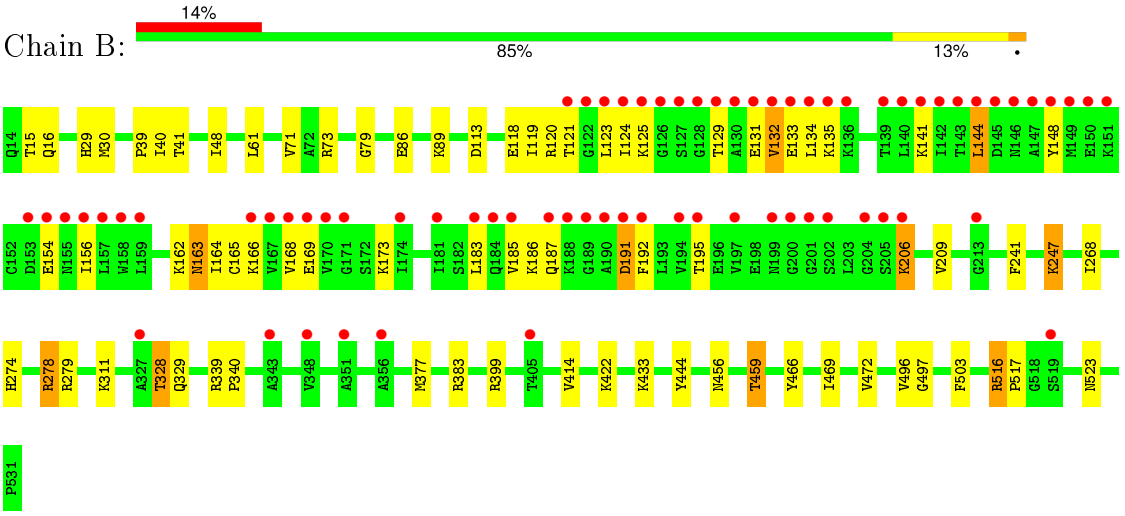
- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain A:



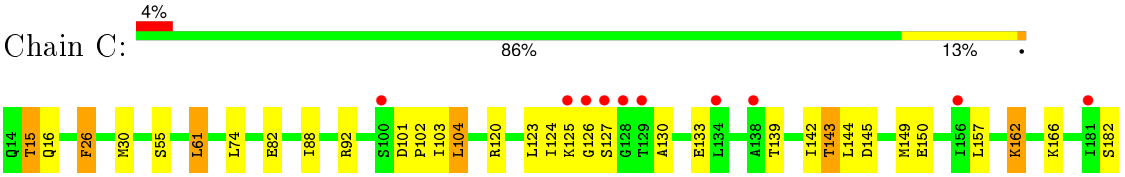
- Molecule 1: Pyruvate kinase isozymes M1/M2

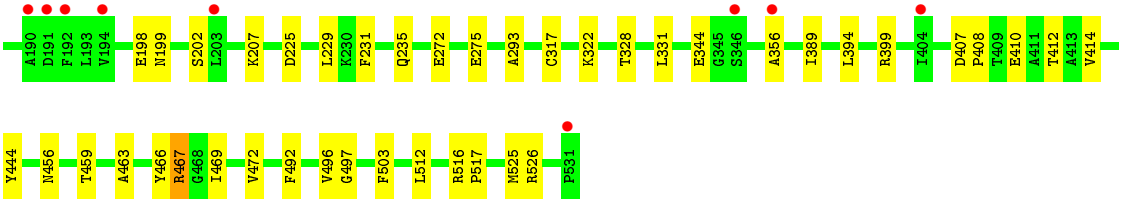
Chain B:



- Molecule 1: Pyruvate kinase isozymes M1/M2

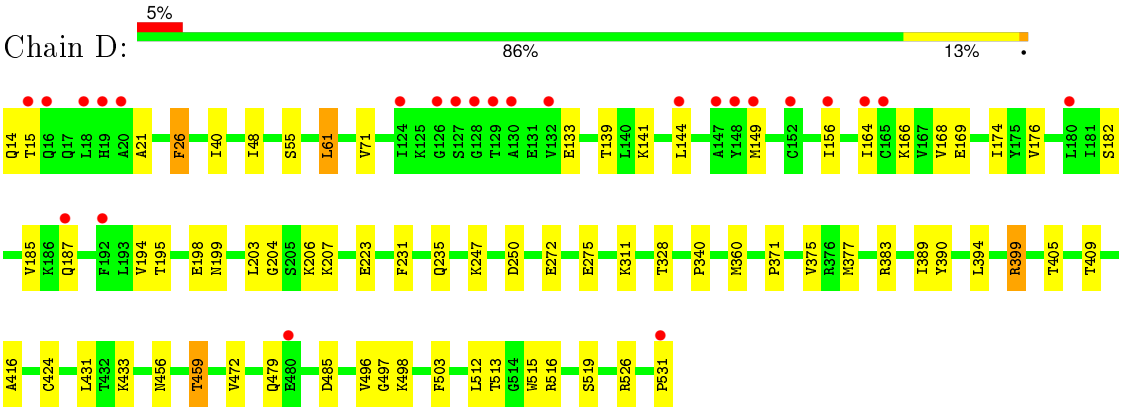
Chain C:





- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.12Å 94.14Å 146.15Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	40.24 – 2.30 40.24 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.24-2.30) 98.1 (40.24-2.28)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.211 , 0.266 0.211 , 0.266	Depositor DCC
R_{free} test set	4985 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	3 of 100811 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16230	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: OXL, MG, NZT

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	0.49	0/4029	0.65	0/5441
1	B	0.50	0/4048	0.65	0/5465
1	C	0.47	0/4037	0.62	0/5451
1	D	0.46	0/4029	0.63	0/5441
All	All	0.48	0/16143	0.63	0/21798

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

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	3965	0	4049	32	0
1	B	3978	0	4071	61	0
1	C	3970	0	4058	49	0
1	D	3965	0	4049	41	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	34	0	22	1	0
4	D	68	0	44	14	0
5	A	66	0	0	0	0
5	B	71	0	0	2	0
5	C	48	0	0	1	0
5	D	37	0	0	1	0
All	All	16230	0	16293	176	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 5.

All (176) 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:30[B]:MET:SD	4:D:603[B]:NZT:H17	1.80	1.23
1:D:48:ILE:HB	1:D:360:MET:HG3	1.58	0.84
1:B:516:ARG:HB2	1:B:517:PRO:HD2	1.63	0.78
1:B:73:ARG:NH1	1:B:113:ASP:OD1	2.18	0.77
1:B:414:VAL:HG12	1:B:444:TYR:CE2	2.20	0.77
1:C:55:SER:O	1:C:61:LEU:HD13	1.84	0.76
1:A:414:VAL:HG12	1:A:444:TYR:CE2	2.21	0.75
1:C:389:ILE:HD11	1:C:467:ARG:HH21	1.53	0.72
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.71	0.71
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.77	0.67
1:B:29:HIS:HD2	1:B:30[B]:MET:CE	2.09	0.65
4:D:603[B]:NZT:OAB	4:D:603[B]:NZT:H10	1.96	0.65
1:A:15:THR:HG23	1:A:16:GLN:HG2	1.78	0.65
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.79	0.64
1:D:55:SER:O	1:D:61:LEU:HD13	1.98	0.64
1:D:231:PHE:CE2	1:D:235:GLN:HG3	2.33	0.63
1:C:394:LEU:HD13	4:D:603[A]:NZT:CAG	2.29	0.62
1:D:390:TYR:HB3	4:D:603[A]:NZT:H1	1.81	0.62
1:B:133:GLU:HG2	1:B:134:LEU:N	2.14	0.62
1:C:389:ILE:HD11	1:C:467:ARG:NH2	2.15	0.62
1:B:185:VAL:HA	1:B:195:THR:HG22	1.81	0.62
1:B:48:ILE:HG12	1:B:71:VAL:HB	1.81	0.61
1:A:203:LEU:HD23	1:A:204:GLY:O	2.01	0.61
1:D:185:VAL:HA	1:D:195:THR:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:ARG:HH21	1:D:399:ARG:NH2	1.98	0.60
1:B:183:LEU:HD13	1:B:195:THR:HG21	1.82	0.60
1:D:141:LYS:HE3	1:D:156:ILE:HD12	1.84	0.60
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.83	0.60
1:C:389:ILE:HG23	4:D:603[B]:NZT:OAC	2.02	0.59
1:B:121:THR:O	1:B:206:LYS:HD3	2.02	0.59
1:C:127:SER:HB2	1:C:130:ALA:HB2	1.84	0.59
1:B:132:VAL:HG13	1:B:133:GLU:N	2.16	0.59
1:A:515:TRP:CE3	1:C:526:ARG:HD3	2.37	0.58
1:C:82:GLU:HG3	5:C:724:HOH:O	2.03	0.58
1:A:131:GLU:OE1	1:A:202:SER:HB2	2.03	0.57
1:A:146:ASN:O	1:A:149:MET:HB3	2.04	0.57
1:D:231:PHE:CZ	1:D:235:GLN:HG3	2.39	0.57
4:D:603[B]:NZT:CAM	4:D:603[B]:NZT:H18	2.33	0.57
1:B:132:VAL:HG13	1:B:133:GLU:H	1.69	0.57
1:B:133:GLU:O	1:B:154:GLU:HB3	2.04	0.57
4:D:603[B]:NZT:CAJ	4:D:603[B]:NZT:OAB	2.52	0.56
1:D:433:LYS:O	1:D:459:THR:HG21	2.04	0.56
1:C:123:LEU:HD12	1:C:150:GLU:HG2	1.87	0.56
1:D:247:LYS:O	1:D:250:ASP:HB2	2.05	0.56
1:C:472:VAL:HG21	1:C:496:VAL:HG11	1.87	0.56
1:C:143:THR:HG22	1:C:145:ASP:H	1.69	0.56
1:B:168:VAL:HG12	1:B:169:GLU:N	2.21	0.55
1:B:124:ILE:HD12	1:B:132:VAL:HG12	1.88	0.55
1:B:39:PRO:HB2	1:B:383:ARG:HG2	1.89	0.55
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.43	0.54
1:C:356:ALA:O	1:C:467:ARG:NH1	2.36	0.54
1:C:231:PHE:CE2	1:C:235:GLN:HG3	2.43	0.54
1:B:399:ARG:HH21	1:D:399:ARG:HH21	1.56	0.54
1:C:124:ILE:C	1:C:126:GLY:H	2.12	0.54
1:D:479:GLN:HB2	1:D:485:ASP:HB2	1.91	0.53
1:D:174:ILE:CD1	1:D:185:VAL:HG23	2.39	0.53
1:C:389:ILE:CD1	1:C:467:ARG:HH21	2.19	0.53
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.44	0.53
1:A:223:GLU:HA	1:A:226:ILE:HD12	1.90	0.52
1:B:433:LYS:O	1:B:459:THR:HG21	2.09	0.52
1:B:134:LEU:HD13	1:B:154:GLU:HB2	1.91	0.52
1:B:186:LYS:H	1:B:195:THR:HA	1.74	0.52
1:D:431:LEU:HD22	1:D:513:THR:HG22	1.92	0.52
1:C:103:ILE:HG22	1:C:104:LEU:HD13	1.90	0.52
1:A:431:LEU:HD22	1:A:513:THR:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LEU:HD22	1:B:191:ASP:HB2	1.92	0.52
1:B:340:PRO:HG3	1:B:377:MET:HG2	1.92	0.52
1:D:456:ASN:HB3	1:D:459:THR:HG23	1.91	0.51
1:B:29:HIS:CD2	1:B:30[B]:MET:HE2	2.45	0.51
1:B:399:ARG:NH2	1:D:399:ARG:HH21	2.09	0.51
1:C:516:ARG:HB2	1:C:517:PRO:HD2	1.93	0.51
1:C:26:PHE:O	1:C:30[A]:MET:HG2	2.11	0.51
1:A:472:VAL:HG21	1:A:496:VAL:HG11	1.93	0.51
1:B:29:HIS:HD2	1:B:30[B]:MET:HE3	1.74	0.51
1:C:225:ASP:O	1:C:229:LEU:HG	2.10	0.50
1:C:410:GLU:O	1:C:414:VAL:HG23	2.11	0.50
1:B:164:ILE:O	1:B:168:VAL:HG23	2.12	0.50
1:A:71:VAL:HG22	1:A:109:ALA:HB3	1.94	0.50
1:C:456:ASN:CG	1:C:459:THR:HG23	2.32	0.50
1:A:395:PHE:CZ	1:A:399:ARG:HD2	2.47	0.49
1:A:175:TYR:HB3	1:A:179:GLY:HA2	1.94	0.49
1:C:15:THR:HG23	1:C:16:GLN:HG2	1.92	0.49
1:C:414:VAL:HG22	1:C:444:TYR:CZ	2.48	0.49
1:C:394:LEU:CD1	4:D:603[A]:NZT:H23	2.41	0.49
1:A:515:TRP:CD2	1:C:526:ARG:HD3	2.48	0.49
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.48	0.49
1:D:204:GLY:HA3	1:D:207:LYS:HE2	1.93	0.49
1:C:124:ILE:O	1:C:126:GLY:N	2.45	0.49
1:B:29:HIS:HD2	1:B:30[B]:MET:HE2	1.77	0.48
1:D:182:SER:HB3	1:D:198:GLU:HB2	1.94	0.48
1:C:394:LEU:HD13	4:D:603[A]:NZT:H23	1.95	0.48
1:B:40:ILE:O	1:B:383:ARG:HD2	2.12	0.48
1:C:414:VAL:HG22	1:C:444:TYR:CE2	2.49	0.48
1:C:463:ALA:HB1	1:C:469:ILE:HG21	1.94	0.48
1:C:272:GLU:HB3	1:C:293:ALA:HB3	1.96	0.48
1:C:182:SER:HB3	1:C:198:GLU:HB2	1.94	0.48
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.95	0.48
1:B:241:PHE:HD1	1:B:268:ILE:HB	1.79	0.48
1:B:168:VAL:CG1	1:B:169:GLU:N	2.77	0.48
1:B:247:LYS:HD2	1:B:279:ARG:NH2	2.28	0.48
1:B:274:HIS:CD2	1:B:278:ARG:HD3	2.49	0.48
1:D:144:LEU:HD21	1:D:164:ILE:HG22	1.95	0.48
4:D:603[A]:NZT:H18	4:D:603[A]:NZT:CAM	2.42	0.48
1:D:389:ILE:HG23	4:D:603[A]:NZT:OAC	2.14	0.47
1:B:123:LEU:HB3	1:B:129:THR:HB	1.95	0.47
1:B:414:VAL:HG12	1:B:444:TYR:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:VAL:CG1	1:C:492:PHE:CE2	2.97	0.47
1:A:389:ILE:HG23	4:A:603[A]:NZT:OAC	2.14	0.47
1:B:422:LYS:HE3	1:D:405:THR:HG22	1.96	0.47
1:B:516:ARG:HD3	1:B:516:ARG:C	2.34	0.47
1:C:30[A]:MET:HE1	1:D:311:LYS:HD3	1.97	0.47
1:A:30:MET:CE	1:B:311:LYS:HB3	2.45	0.47
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.49	0.47
1:B:516:ARG:HB2	1:B:517:PRO:CD	2.40	0.47
1:B:29:HIS:CD2	1:B:30[B]:MET:CE	2.93	0.46
1:B:274:HIS:HD2	1:B:278:ARG:HD3	1.80	0.46
1:A:16:GLN:HG3	1:A:18:LEU:HG	1.98	0.46
1:B:119:ILE:HG22	1:B:209:VAL:HB	1.97	0.46
1:C:162:LYS:CD	1:C:162:LYS:H	2.28	0.46
1:B:164:ILE:HG23	1:B:165:CYS:N	2.30	0.46
1:C:142:ILE:HA	1:C:157:LEU:O	2.16	0.46
1:D:394:LEU:HD13	4:D:603[B]:NZT:CAG	2.46	0.45
1:A:463:ALA:HB1	1:A:469:ILE:HG21	1.98	0.45
1:B:162:LYS:O	1:B:164:ILE:N	2.42	0.45
1:B:456:ASN:CG	1:B:459:THR:HG23	2.37	0.45
1:C:412:THR:HG22	1:C:512:LEU:HD21	1.99	0.45
1:D:40:ILE:O	1:D:383:ARG:HD2	2.17	0.45
1:C:120:ARG:HA	1:C:207:LYS:O	2.17	0.45
1:B:16:GLN:HA	5:B:762:HOH:O	2.16	0.45
1:A:430:VAL:HG22	1:A:512:LEU:HD12	1.99	0.45
1:D:456:ASN:CG	1:D:459:THR:HG23	2.38	0.44
1:C:88:ILE:O	1:C:92:ARG:HG3	2.17	0.44
1:C:407:ASP:HA	1:C:408:PRO:HD3	1.88	0.44
1:A:416:ALA:HB2	1:A:512:LEU:HD21	2.00	0.44
1:D:187:GLN:HB3	1:D:194:VAL:HB	1.99	0.43
1:D:498:LYS:NZ	1:D:531:PRO:O	2.51	0.43
1:A:317:CYS:HB3	1:A:322:LYS:O	2.18	0.43
1:B:123:LEU:HB3	1:B:124:ILE:H	1.75	0.43
1:A:162:LYS:HA	1:A:162:LYS:HD2	1.73	0.43
1:A:153:ASP:HB2	1:A:154:GLU:OE1	2.18	0.43
1:B:141:LYS:O	1:B:156:ILE:HA	2.18	0.43
1:B:144:LEU:HD11	1:B:164:ILE:HG21	1.99	0.43
1:A:243:SER:HA	1:A:270:LYS:HD3	2.01	0.43
4:D:603[B]:NZT:CAR	4:D:603[B]:NZT:CAM	2.97	0.42
1:B:134:LEU:HD12	1:B:135:LYS:H	1.84	0.42
1:C:317:CYS:HB3	1:C:322:LYS:O	2.19	0.42
1:B:144:LEU:HD21	1:B:164:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LYS:HD2	1:A:196:GLU:HB2	2.00	0.42
1:B:121:THR:O	1:B:206:LYS:HA	2.19	0.42
1:A:48:ILE:HG12	1:A:71:VAL:HB	2.01	0.42
1:C:166:LYS:HE2	1:C:166:LYS:HB3	1.79	0.42
1:A:297:LEU:O	1:A:301:ILE:HG12	2.20	0.42
1:B:328:THR:HG22	1:B:329:GLN:HG3	2.01	0.42
1:D:176:VAL:HG11	1:D:203:LEU:HD11	2.02	0.42
1:D:340:PRO:HG3	1:D:377:MET:HG2	2.02	0.42
1:C:466:TYR:HB2	1:C:469:ILE:HD12	2.02	0.41
1:A:115:LYS:O	1:A:118:GLU:HG3	2.19	0.41
1:B:15:THR:HG23	1:B:16:GLN:HG2	2.02	0.41
1:D:515:TRP:CH2	1:D:516:ARG:HD2	2.56	0.41
1:B:79:GLY:HA2	5:B:754:HOH:O	2.21	0.41
1:D:371:PRO:O	1:D:375:VAL:HG23	2.21	0.41
1:C:101:ASP:HA	1:C:102:PRO:HD2	1.95	0.41
1:A:187:GLN:HB2	1:A:194:VAL:HB	2.02	0.41
1:C:74:LEU:HD11	1:C:88:ILE:HG13	2.02	0.40
1:D:21:ALA:HB1	5:D:711:HOH:O	2.20	0.40
1:D:14:GLN:HB3	1:D:15:THR:H	1.60	0.40
1:D:26:PHE:CE2	4:D:603[A]:NZT:H20	2.56	0.40
1:B:399:ARG:NH2	1:D:399:ARG:HE	2.18	0.40
1:B:118:GLU:OE2	1:B:120:ARG:HD2	2.20	0.40
1:D:168:VAL:CG1	1:D:169:GLU:N	2.84	0.40
1:D:48:ILE:HG12	1:D:71:VAL:HB	2.03	0.40
1:A:399:ARG:CZ	1:C:399:ARG:HH21	2.34	0.40
1:B:86:GLU:O	1:B:89:LYS:HB3	2.20	0.40
1:A:399:ARG:NH2	1:C:399:ARG:NH2	2.69	0.40
1:C:331:LEU:HD23	1:C:344:GLU:HB3	2.04	0.40
1:B:523:ASN:O	1:D:526:ARG:HA	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	516/518 (100%)	499 (97%)	15 (3%)	2 (0%)	39	48
1	B	518/518 (100%)	493 (95%)	20 (4%)	5 (1%)	19	21
1	C	517/518 (100%)	497 (96%)	18 (4%)	2 (0%)	39	48
1	D	516/518 (100%)	492 (95%)	22 (4%)	2 (0%)	39	48
All	All	2067/2072 (100%)	1981 (96%)	75 (4%)	11 (0%)	34	41

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	163	ASN
1	A	328	THR
1	A	125	LYS
1	B	328	THR
1	C	125	LYS
1	C	328	THR
1	D	328	THR
1	B	125	LYS
1	B	191	ASP
1	D	399	ARG
1	B	132	VAL

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	426/426 (100%)	401 (94%)	25 (6%)	24	32
1	B	428/426 (100%)	412 (96%)	16 (4%)	41	55
1	C	427/426 (100%)	412 (96%)	15 (4%)	43	58
1	D	426/426 (100%)	411 (96%)	15 (4%)	43	58
All	All	1707/1704 (100%)	1636 (96%)	71 (4%)	36	49

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	PHE
1	A	41	THR
1	A	61	LEU
1	A	82	GLU
1	A	104	LEU
1	A	124	ILE
1	A	129	THR
1	A	132	VAL
1	A	156	ILE
1	A	168	VAL
1	A	185	VAL
1	A	187	GLN
1	A	193	LEU
1	A	202	SER
1	A	206	LYS
1	A	223	GLU
1	A	260	GLU
1	A	274	HIS
1	A	409	THR
1	A	424	CYS
1	A	472	VAL
1	A	476	ASP
1	A	479	GLN
1	A	487	ASP
1	A	516	ARG
1	B	41	THR
1	B	61	LEU
1	B	131	GLU
1	B	144	LEU
1	B	148	TYR
1	B	163	ASN
1	B	166	LYS
1	B	173	LYS
1	B	187	GLN
1	B	192	PHE
1	B	206	LYS
1	B	247	LYS
1	B	278	ARG
1	B	339	ARG
1	B	459	THR
1	B	516	ARG
1	C	15	THR
1	C	26	PHE

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Mol	Chain	Res	Type
1	C	61	LEU
1	C	104	LEU
1	C	133	GLU
1	C	139	THR
1	C	143	THR
1	C	144	LEU
1	C	149	MET
1	C	162	LYS
1	C	199	ASN
1	C	202	SER
1	C	275	GLU
1	C	467	ARG
1	C	525	MET
1	D	26	PHE
1	D	61	LEU
1	D	133	GLU
1	D	139	THR
1	D	149	MET
1	D	166	LYS
1	D	199	ASN
1	D	206	LYS
1	D	223	GLU
1	D	272	GLU
1	D	275	GLU
1	D	409	THR
1	D	424	CYS
1	D	459	THR
1	D	519	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	393	GLN
1	B	29	HIS
1	B	393	GLN
1	D	440	GLN

5.3.3 RNA

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 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	OXL	A	601	3	0,5,5	0.00	-	0,6,6	0.00	-
4	NZT	A	603[A]	-	38,38,38	2.88	15 (39%)	49,54,54	1.87	10 (20%)
2	OXL	B	601	3	0,5,5	0.00	-	0,6,6	0.00	-
2	OXL	C	601	3	0,5,5	0.00	-	0,6,6	0.00	-
2	OXL	D	601	3	0,5,5	0.00	-	0,6,6	0.00	-
4	NZT	D	603[A]	-	38,38,38	2.95	12 (31%)	49,54,54	1.97	9 (18%)
4	NZT	D	603[B]	-	38,38,38	3.10	11 (28%)	49,54,54	1.84	9 (18%)

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	OXL	A	601	3	-	0/0/4/4	0/0/0/0
4	NZT	A	603[A]	-	-	0/23/33/33	0/5/5/5
2	OXL	B	601	3	-	0/0/4/4	0/0/0/0
2	OXL	C	601	3	-	0/0/4/4	0/0/0/0
2	OXL	D	601	3	-	0/0/4/4	0/0/0/0
4	NZT	D	603[A]	-	-	0/23/33/33	0/5/5/5
4	NZT	D	603[B]	-	-	0/23/33/33	0/5/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603[A]	NZT	CBC-CBE	-7.16	1.38	1.42
4	D	603[A]	NZT	CBA-CAY	-6.12	1.40	1.50
4	D	603[B]	NZT	CAZ-NAX	-5.94	1.33	1.43
4	D	603[B]	NZT	CBA-CAY	-5.90	1.40	1.50
4	D	603[A]	NZT	CBC-CBE	-5.82	1.39	1.42
4	D	603[A]	NZT	CAZ-NAX	-5.20	1.34	1.43
4	D	603[A]	NZT	CBC-S1	-5.06	1.72	1.77
4	D	603[B]	NZT	CBC-S1	-4.84	1.72	1.77
4	D	603[B]	NZT	CBC-CBE	-4.81	1.39	1.42
4	A	603[A]	NZT	CBA-CAY	-4.50	1.42	1.50
4	D	603[B]	NZT	S1-NAX	-4.43	1.56	1.63
4	A	603[A]	NZT	CAZ-NAX	-4.32	1.36	1.43
4	A	603[A]	NZT	CBE-NAW	-2.29	1.33	1.37
4	A	603[A]	NZT	CAT-NBG	2.01	1.49	1.46
4	D	603[A]	NZT	CAI-CBC	2.04	1.39	1.37
4	D	603[A]	NZT	CAS-NBG	2.09	1.49	1.46
4	A	603[A]	NZT	CAQ-NBF	2.10	1.50	1.47
4	A	603[A]	NZT	S1-NAX	2.16	1.67	1.63
4	A	603[A]	NZT	CAG-NAU	2.21	1.40	1.33
4	A	603[A]	NZT	CAH-NAV	2.36	1.39	1.34
4	D	603[B]	NZT	CAG-NAU	2.49	1.41	1.33
4	D	603[A]	NZT	CAG-NAU	2.51	1.41	1.33
4	A	603[A]	NZT	CAS-NBG	2.63	1.50	1.46
4	D	603[A]	NZT	CAP-NAU	2.75	1.40	1.34
4	D	603[B]	NZT	CAH-NAV	2.85	1.40	1.34
4	D	603[B]	NZT	CAP-NAU	2.93	1.40	1.34
4	A	603[A]	NZT	CAR-NBF	2.97	1.52	1.47
4	D	603[A]	NZT	CAH-NAV	2.98	1.41	1.34
4	A	603[A]	NZT	CAP-NAU	3.53	1.41	1.34
4	A	603[A]	NZT	CAF-NAW	4.17	1.40	1.32
4	D	603[B]	NZT	CAF-NAW	4.33	1.41	1.32
4	D	603[A]	NZT	CAF-NAW	4.95	1.42	1.32
4	A	603[A]	NZT	OAC-S1	6.84	1.51	1.43
4	D	603[A]	NZT	OAC-S1	7.31	1.51	1.43
4	D	603[B]	NZT	OAC-S1	8.60	1.52	1.43
4	D	603[A]	NZT	OAB-S1	8.61	1.53	1.43
4	A	603[A]	NZT	OAB-S1	9.11	1.53	1.43
4	D	603[B]	NZT	OAB-S1	9.40	1.53	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	603[A]	NZT	OAB-S1-OAC	-8.11	108.78	119.54
4	A	603[A]	NZT	OAB-S1-OAC	-7.08	110.15	119.54
4	D	603[B]	NZT	OAB-S1-OAC	-6.56	110.84	119.54
4	A	603[A]	NZT	CAI-CBC-CBE	-3.47	119.08	121.24
4	D	603[A]	NZT	CAG-CAH-NAV	-3.31	118.15	122.25
4	A	603[A]	NZT	CAG-CAH-NAV	-2.68	118.93	122.25
4	D	603[A]	NZT	CAD-CAF-NAW	-2.57	119.92	123.94
4	D	603[B]	NZT	CAG-CAH-NAV	-2.54	119.10	122.25
4	D	603[B]	NZT	CAD-CAF-NAW	-2.32	120.31	123.94
4	D	603[A]	NZT	OAB-S1-CBC	2.10	111.59	108.01
4	D	603[A]	NZT	CAR-NBF-CAQ	2.15	116.54	112.56
4	A	603[A]	NZT	CBA-CAY-NBF	2.27	121.78	118.76
4	D	603[A]	NZT	CAF-NAW-CBE	2.44	120.27	117.37
4	D	603[B]	NZT	CAR-NBF-CAQ	2.49	117.17	112.56
4	A	603[A]	NZT	CAT-NBG-CBB	2.51	126.18	120.22
4	A	603[A]	NZT	CAT-CAR-NBF	2.64	116.50	110.49
4	D	603[B]	NZT	OAB-S1-CBC	2.66	112.54	108.01
4	A	603[A]	NZT	CAT-NBG-CAS	2.70	117.27	111.59
4	A	603[A]	NZT	CAI-CBC-S1	2.74	120.68	117.05
4	D	603[B]	NZT	CAF-NAW-CBE	2.80	120.70	117.37
4	D	603[B]	NZT	CAI-CBC-S1	3.08	121.14	117.05
4	D	603[B]	NZT	CAH-NAV-CBB	3.22	121.09	116.92
4	D	603[A]	NZT	CAH-NAV-CBB	3.37	121.28	116.92
4	A	603[A]	NZT	CAH-NAV-CBB	3.43	121.37	116.92
4	D	603[A]	NZT	CAI-CBC-S1	3.50	121.70	117.05
4	A	603[A]	NZT	CAR-NBF-CAQ	3.97	119.92	112.56
4	D	603[B]	NZT	CAT-NBG-CAS	4.87	121.82	111.59
4	D	603[A]	NZT	CAT-NBG-CAS	5.04	122.17	111.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603[A]	NZT	1	0
4	D	603[A]	NZT	7	0
4	D	603[B]	NZT	7	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^{th} 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	518/518 (100%)	0.25	17 (3%) 50 59	23, 41, 72, 114	0
1	B	518/518 (100%)	0.69	71 (13%) 4 6	22, 39, 122, 177	0
1	C	518/518 (100%)	0.34	19 (3%) 45 54	26, 43, 77, 122	0
1	D	518/518 (100%)	0.38	25 (4%) 34 43	27, 45, 78, 124	0
All	All	2072/2072 (100%)	0.42	132 (6%) 23 31	22, 42, 89, 177	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	128	GLY	18.7
1	B	127	SER	11.6
1	B	157	LEU	9.9
1	B	132	VAL	9.2
1	B	189	GLY	7.6
1	B	140	LEU	6.8
1	B	143	THR	6.8
1	B	126	GLY	6.6
1	B	125	LYS	6.4
1	B	190	ALA	6.4
1	A	126	GLY	6.3
1	B	202	SER	5.9
1	B	158	TRP	5.9
1	B	130	ALA	5.8
1	C	531	PRO	5.8
1	D	127	SER	5.7
1	B	129	THR	5.6
1	C	126	GLY	5.5
1	B	142	ILE	5.5
1	B	146	ASN	5.4
1	B	156	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	149	MET	5.4
1	B	195	THR	5.4
1	B	131	GLU	5.4
1	B	144	LEU	5.3
1	B	170	VAL	5.3
1	B	123	LEU	5.2
1	B	159	LEU	5.2
1	D	130	ALA	5.0
1	A	127	SER	5.0
1	A	129	THR	4.8
1	B	134	LEU	4.8
1	B	136	LYS	4.7
1	B	194	VAL	4.2
1	B	139	THR	4.2
1	A	134	LEU	4.1
1	B	153	ASP	4.0
1	B	205	SER	4.0
1	B	192	PHE	4.0
1	B	204	GLY	3.9
1	D	126	GLY	3.9
1	B	150	GLU	3.9
1	C	138	ALA	3.8
1	D	18	LEU	3.8
1	D	149	MET	3.8
1	A	203	LEU	3.7
1	C	129	THR	3.7
1	B	197	VAL	3.7
1	B	199	ASN	3.7
1	B	141	LYS	3.6
1	A	133	GLU	3.6
1	B	201	GLY	3.6
1	B	135	LYS	3.6
1	B	185	VAL	3.6
1	B	187	GLN	3.5
1	C	127	SER	3.5
1	B	188	LYS	3.4
1	B	133	GLU	3.4
1	B	191	ASP	3.4
1	B	124	ILE	3.4
1	D	144	LEU	3.4
1	D	19	HIS	3.4
1	C	192	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	148	TYR	3.3
1	B	169	GLU	3.2
1	D	480	GLU	3.2
1	B	356	ALA	3.2
1	B	145	ASP	3.2
1	A	156	ILE	3.1
1	B	174	ILE	3.1
1	B	167	VAL	3.1
1	C	125	LYS	3.0
1	D	192	PHE	3.0
1	D	16	GLN	2.9
1	D	147	ALA	2.9
1	C	190	ALA	2.8
1	B	171	GLY	2.8
1	A	151	LYS	2.8
1	D	148	TYR	2.8
1	A	124	ILE	2.8
1	C	128	GLY	2.8
1	A	137	GLY	2.7
1	B	147	ALA	2.7
1	A	148	TYR	2.7
1	C	404	ILE	2.6
1	D	156	ILE	2.6
1	B	154	GLU	2.5
1	B	200	GLY	2.5
1	A	15	THR	2.5
1	D	129	THR	2.5
1	B	168	VAL	2.5
1	B	519	SER	2.5
1	C	156	ILE	2.5
1	A	123	LEU	2.5
1	D	164	ILE	2.5
1	B	184	GLN	2.5
1	B	348	VAL	2.5
1	B	166	LYS	2.4
1	D	180	LEU	2.4
1	A	135	LYS	2.4
1	A	515	TRP	2.4
1	C	191	ASP	2.4
1	B	181	ILE	2.4
1	C	100	SER	2.4
1	D	165	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	122	GLY	2.4
1	C	346	SER	2.4
1	B	183	LEU	2.3
1	B	351	ALA	2.3
1	D	187	GLN	2.3
1	B	327	ALA	2.3
1	C	134	LEU	2.3
1	B	405	THR	2.3
1	D	15	THR	2.3
1	C	356	ALA	2.2
1	A	136	LYS	2.2
1	C	203	LEU	2.2
1	D	531	PRO	2.2
1	B	343	ALA	2.2
1	C	181	ILE	2.2
1	D	128	GLY	2.2
1	B	213	GLY	2.1
1	D	124	ILE	2.1
1	C	194	VAL	2.1
1	D	132	VAL	2.1
1	D	152	CYS	2.1
1	B	155	ASN	2.1
1	D	20	ALA	2.1
1	A	531	PRO	2.0
1	B	151	LYS	2.0
1	B	206	LYS	2.0
1	B	121	THR	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, 95^{th} 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	NZT	D	603[A]	34/34	0.85	0.35	6.21	31,34,47,48	34
4	NZT	D	603[B]	34/34	0.85	0.35	6.12	33,36,47,48	34
4	NZT	A	603[A]	34/34	0.89	0.19	1.26	34,42,57,60	0
2	OXL	A	601	6/6	0.92	0.16	-0.18	50,56,61,64	0
2	OXL	D	601	6/6	0.91	0.14	-0.92	45,49,52,54	0
2	OXL	B	601	6/6	0.94	0.13	-1.09	39,44,49,49	0
2	OXL	C	601	6/6	0.96	0.10	-2.18	45,47,48,49	0
3	MG	A	602	1/1	0.96	0.10	-	47,47,47,47	0
3	MG	B	602	1/1	0.96	0.11	-	39,39,39,39	0
3	MG	D	602	1/1	0.92	0.10	-	45,45,45,45	0
3	MG	C	602	1/1	0.92	0.09	-	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.