Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:25 PM GMT

PDB ID	:	4RPP
Title	:	crystal structure of PKM2-K422R mutant bound with FBP
Authors	:	Wang, P.; Sun, C.; Zhu, T.; Xu, Y.
Deposited on	:	2014-10-31
Resolution	:	2.58 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:

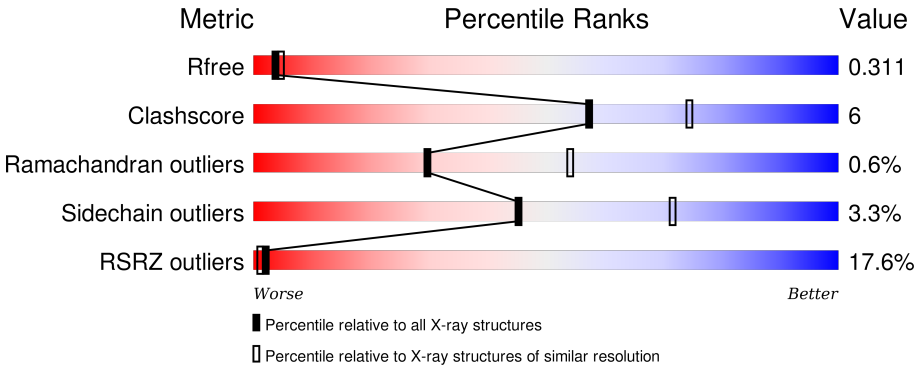
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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	536	10% 63% 13% • 23%
1	B	536	15% 63% 12% • 24%
1	C	536	15% 63% 11% 26%
1	D	536	13% 64% 11% • 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12596 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 PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3153	1978	568	586	21			
1	B	408	Total	C	N	O	S	0	0	0
			3140	1970	568	581	21			
1	C	396	Total	C	N	O	S	0	0	0
			3050	1912	552	565	21			
1	D	408	Total	C	N	O	S	0	0	0
			3143	1973	568	581	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PRO	-	EXPRESSION TAG	UNP P14618
A	-2	LEU	-	EXPRESSION TAG	UNP P14618
A	-1	GLY	-	EXPRESSION TAG	UNP P14618
A	0	SER	-	EXPRESSION TAG	UNP P14618
A	422	ARG	LYS	ENGINEERED MUTATION	UNP P14618
A	532	FBP	-	EXPRESSION TAG	UNP P14618
B	-3	PRO	-	EXPRESSION TAG	UNP P14618
B	-2	LEU	-	EXPRESSION TAG	UNP P14618
B	-1	GLY	-	EXPRESSION TAG	UNP P14618
B	0	SER	-	EXPRESSION TAG	UNP P14618
B	422	ARG	LYS	ENGINEERED MUTATION	UNP P14618
B	532	FBP	-	EXPRESSION TAG	UNP P14618
C	-3	PRO	-	EXPRESSION TAG	UNP P14618
C	-2	LEU	-	EXPRESSION TAG	UNP P14618
C	-1	GLY	-	EXPRESSION TAG	UNP P14618
C	0	SER	-	EXPRESSION TAG	UNP P14618
C	422	ARG	LYS	ENGINEERED MUTATION	UNP P14618
C	532	FBP	-	EXPRESSION TAG	UNP P14618
D	-3	PRO	-	EXPRESSION TAG	UNP P14618
D	-2	LEU	-	EXPRESSION TAG	UNP P14618
D	-1	GLY	-	EXPRESSION TAG	UNP P14618

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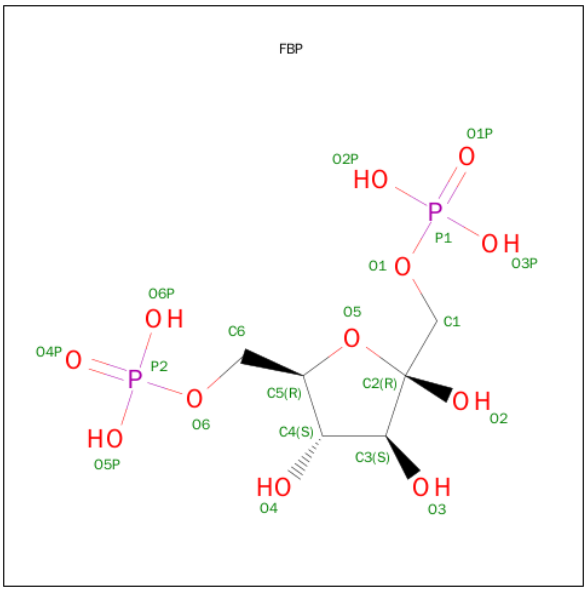
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	EXPRESSION TAG	UNP P14618
D	422	ARG	LYS	ENGINEERED MUTATION	UNP P14618
D	532	FBP	-	EXPRESSION TAG	UNP P14618

- 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 20 6 12 2	0	0
2	B	1	Total C O P 20 6 12 2	0	0
2	C	1	Total C O P 20 6 12 2	0	0
2	D	1	Total C O P 20 6 12 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	7	Total O 7 7	0	0
3	B	7	Total O 7 7	0	0
3	C	8	Total O 8 8	0	0

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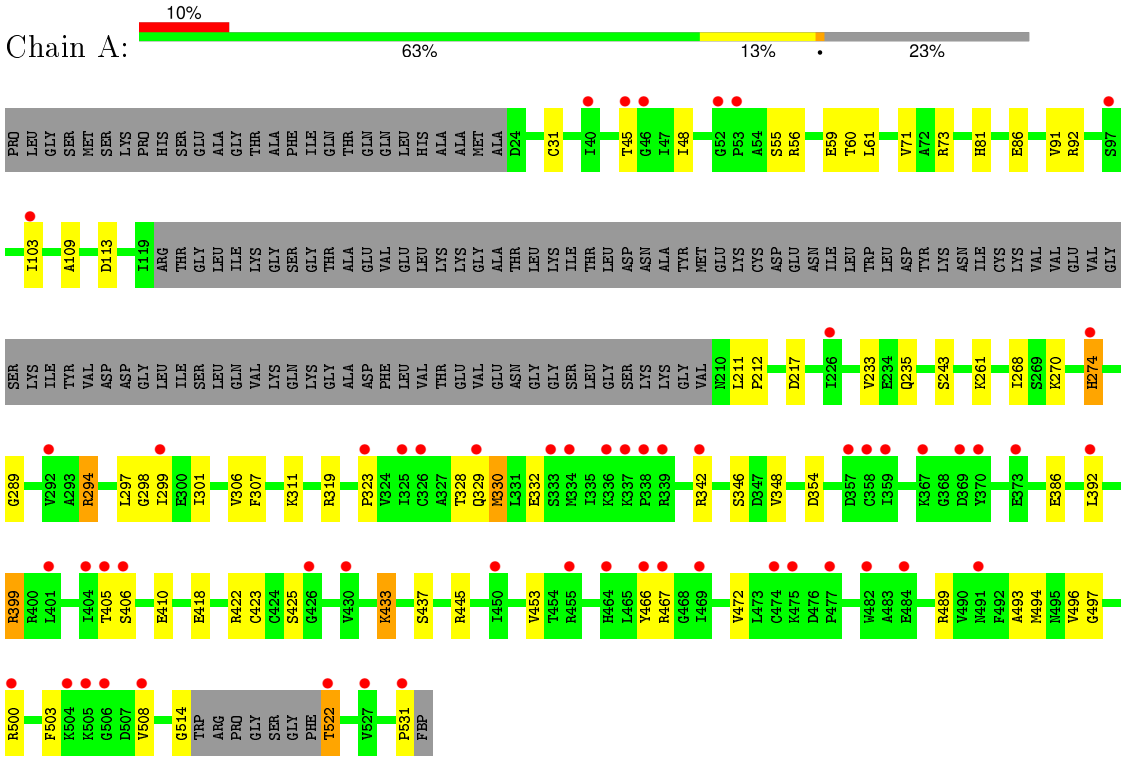
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	8	Total O 8 8	0	0

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.

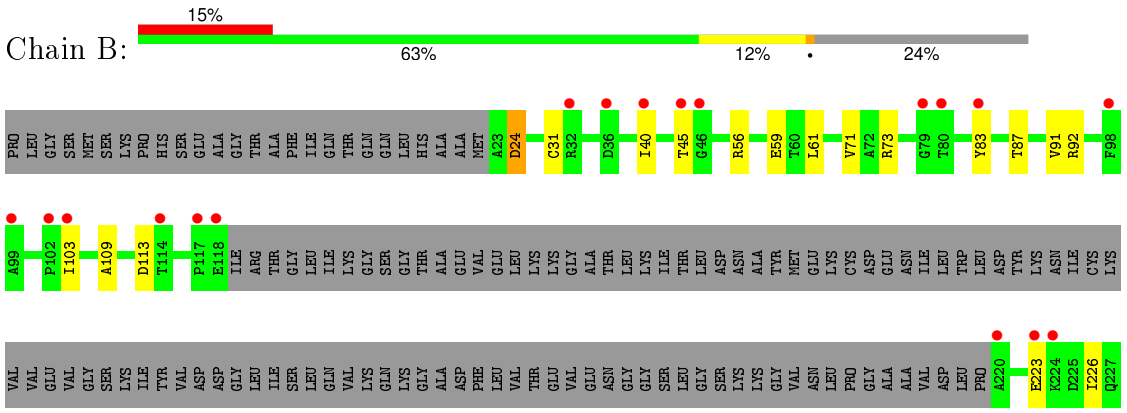
- Molecule 1: Pyruvate kinase PKM

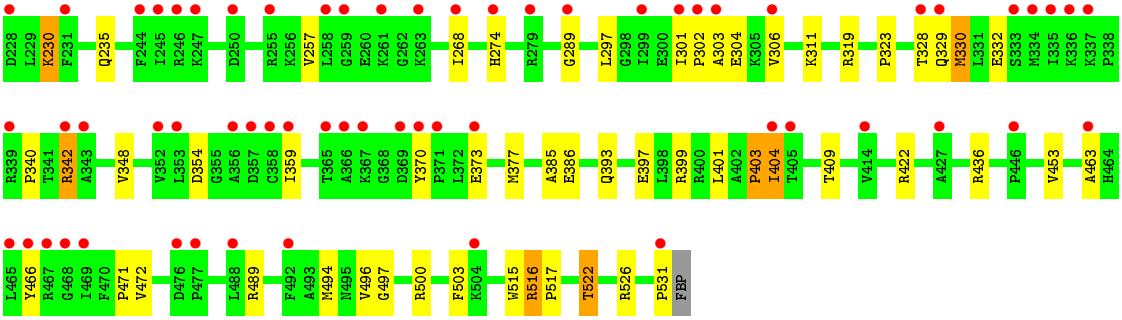
Chain A:



- Molecule 1: Pyruvate kinase PKM

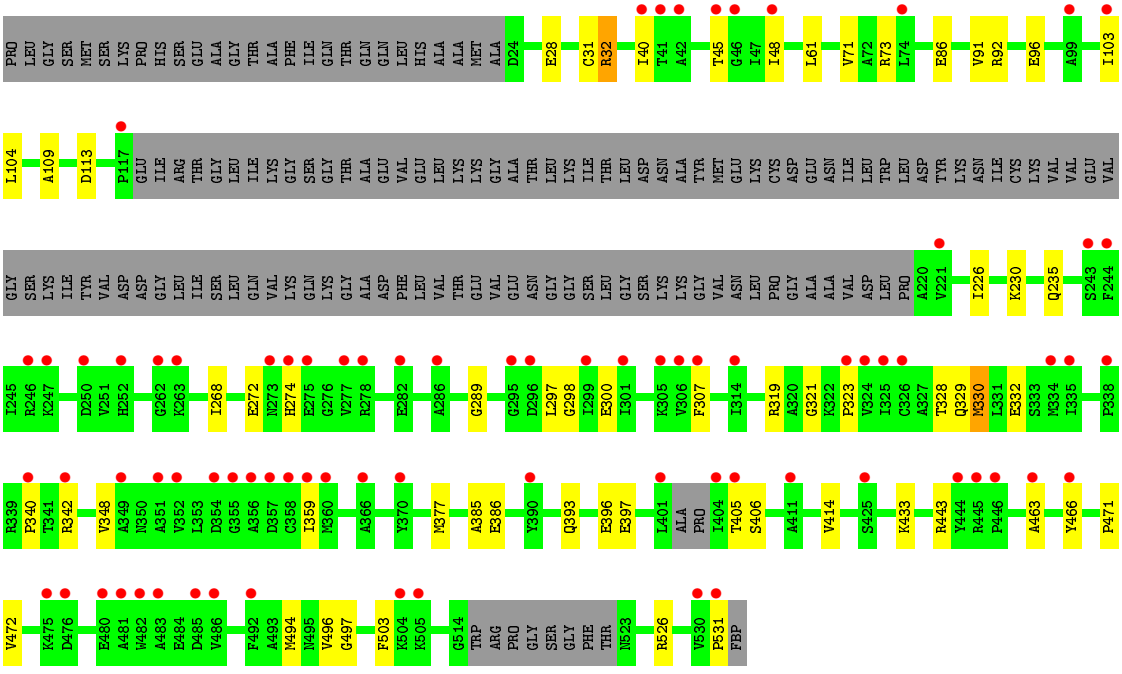
Chain B:





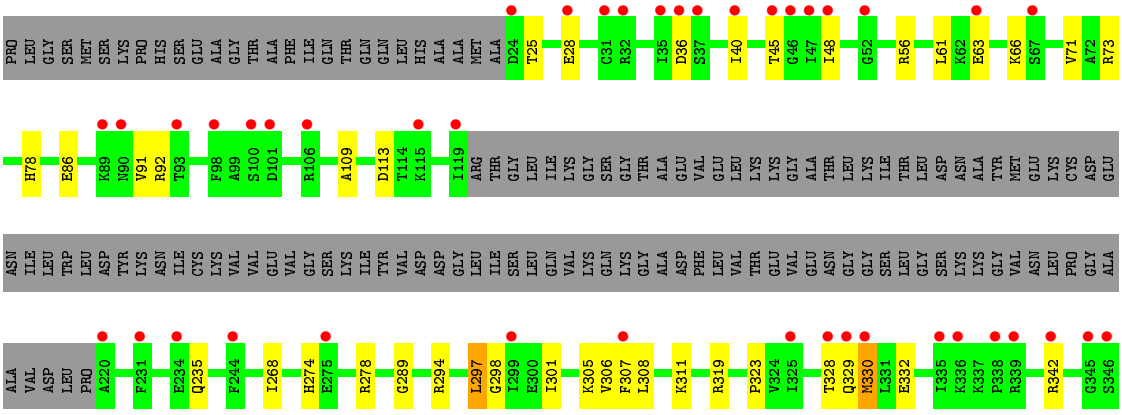
• Molecule 1: Pyruvate kinase PKM

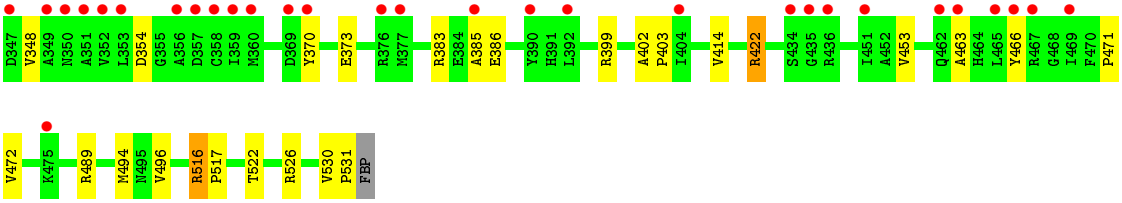
Chain C:



• Molecule 1: Pyruvate kinase PKM

Chain D:




D347
V348
A349
N350
A351
V352
L353
D354
G355
A356
D357
G358
I359
M360
D369
Y370
E373
R376
M377
R383
E384
A385
E386
Y390
H391
L392
R399
A402
P403
I404
V414
R422
S434
G435
R436
I451
A452
V453
Q462
A463
H464
L465
Y466
R467
G468
I469
F470
P471

V472
K475
R489
M494
N495
V496
R516
P517
T522
R526
V530
P531
PBP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.67Å 152.55Å 97.68Å 90.00° 104.24° 90.00°	Depositor
Resolution (Å)	38.31 – 2.58 38.31 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.6 (38.31-2.58) 97.6 (38.31-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.52 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.274 , 0.308 0.287 , 0.311	Depositor DCC
R_{free} test set	3472 reflections (5.16%)	DCC
Wilson B-factor (Å^2)	66.4	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	1 of 70704 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12596	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: FBP

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	0.24	0/3204	0.45	0/4330
1	B	0.23	0/3194	0.46	1/4315 (0.0%)
1	C	0.23	0/3097	0.43	0/4178
1	D	0.22	0/3197	0.41	0/4319
All	All	0.23	0/12692	0.44	1/17142 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	342	ARG	CG-CD-NE	-5.17	100.95	111.80

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	3153	0	3214	53	0
1	B	3140	0	3191	55	0
1	C	3050	0	3109	35	0
1	D	3143	0	3197	40	0
2	A	20	0	10	1	0
2	B	20	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	20	0	10	0	0
2	D	20	0	10	0	0
3	A	7	0	0	0	0
3	B	7	0	0	0	0
3	C	8	0	0	0	0
3	D	8	0	0	1	0
All	All	12596	0	12751	153	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 6.

All (153) 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:306:VAL:HG11	1:B:342:ARG:HH22	1.37	0.88
1:A:342:ARG:NH2	1:B:302:PRO:O	2.06	0.88
1:B:56:ARG:NH2	1:B:83:TYR:O	2.17	0.75
1:A:494:MET:HG2	1:A:531:PRO:HD2	1.69	0.74
1:B:274:HIS:CE1	1:B:301:ILE:HG22	2.25	0.71
1:D:494:MET:HG2	1:D:531:PRO:HD2	1.73	0.70
1:A:422:ARG:HG3	1:C:414:VAL:HG11	1.72	0.70
1:A:306:VAL:HG11	1:B:342:ARG:NH2	2.06	0.70
1:C:494:MET:HG2	1:C:531:PRO:HD2	1.74	0.69
1:B:494:MET:HG2	1:B:531:PRO:HD2	1.75	0.68
1:B:301:ILE:HD11	1:B:306:VAL:HG22	1.76	0.67
1:A:298:GLY:HA3	1:B:342:ARG:NH1	2.10	0.67
1:A:342:ARG:NE	1:B:306:VAL:HB	2.11	0.66
1:A:342:ARG:CZ	1:B:306:VAL:H	2.08	0.66
1:C:298:GLY:HA3	1:D:342:ARG:NH2	2.10	0.66
1:B:399:ARG:HG2	1:D:422:ARG:HH22	1.61	0.66
1:A:342:ARG:NH2	1:B:306:VAL:H	1.94	0.66
1:A:294:ARG:HB3	1:B:342:ARG:HH21	1.61	0.63
1:D:25:THR:HG23	1:D:28:GLU:H	1.63	0.63
1:A:433:LYS:NZ	2:A:600:FBP:O3P	2.31	0.62
1:C:321:GLY:HA3	1:C:443:ARG:HD2	1.81	0.62
1:A:399:ARG:NH2	1:C:396:GLU:OE2	2.34	0.61
1:A:472:VAL:HG21	1:A:496:VAL:HG11	1.82	0.61
1:D:71:VAL:HG22	1:D:109:ALA:HB3	1.83	0.61
1:B:403:PRO:O	1:B:404:ILE:HG13	2.01	0.61
1:C:342:ARG:HH12	1:D:306:VAL:HG21	1.66	0.61
1:A:405:THR:O	1:A:406:SER:OG	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ARG:HH12	1:B:304:GLU:C	2.04	0.60
1:D:92:ARG:NH1	1:D:235:GLN:O	2.31	0.60
1:B:71:VAL:HG22	1:B:109:ALA:HB3	1.85	0.59
1:B:522:THR:HG22	2:B:600:FBP:H4	1.85	0.59
1:D:383:ARG:NH2	3:D:706:HOH:O	2.34	0.58
1:C:92:ARG:NH1	1:C:235:GLN:O	2.31	0.57
1:A:103:ILE:O	1:A:500:ARG:NH2	2.38	0.57
1:B:496:VAL:HG13	1:B:500:ARG:NH1	2.20	0.57
1:B:73:ARG:NH1	1:B:113:ASP:OD2	2.38	0.56
1:A:233:VAL:HG11	1:A:261:LYS:HB3	1.88	0.55
1:C:28:GLU:O	1:C:32:ARG:HG2	2.06	0.55
1:B:329:GLN:HA	1:B:332:GLU:HG2	1.88	0.54
1:B:56:ARG:NH2	1:B:87:THR:OG1	2.40	0.54
1:C:71:VAL:HG22	1:C:109:ALA:HB3	1.89	0.54
1:D:73:ARG:NH1	1:D:113:ASP:OD2	2.41	0.54
1:C:342:ARG:CD	1:D:294:ARG:HB3	2.39	0.53
1:A:445:ARG:HD2	1:A:467:ARG:HH21	1.73	0.53
1:A:342:ARG:O	1:A:346:SER:N	2.29	0.53
1:A:294:ARG:HB3	1:B:342:ARG:NH2	2.24	0.53
1:D:274:HIS:CD2	1:D:301:ILE:HG22	2.44	0.53
1:C:73:ARG:NH1	1:C:113:ASP:OD2	2.41	0.53
1:C:31:CYS:HB3	1:D:319:ARG:HH21	1.74	0.53
1:A:71:VAL:HG22	1:A:109:ALA:HB3	1.91	0.53
1:D:329:GLN:HA	1:D:332:GLU:HG2	1.91	0.52
1:A:298:GLY:HA3	1:B:342:ARG:HH12	1.74	0.52
1:B:393:GLN:O	1:B:397:GLU:HG3	2.09	0.52
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.44	0.52
1:A:31:CYS:HB3	1:B:319:ARG:HH21	1.73	0.52
1:C:342:ARG:HH22	1:D:298:GLY:HA3	1.75	0.52
1:B:422:ARG:HG3	1:D:414:VAL:HG11	1.93	0.51
1:A:342:ARG:CD	1:B:306:VAL:HB	2.41	0.51
1:A:330:MET:HG3	1:A:348:VAL:HG22	1.92	0.51
1:A:243:SER:HA	1:A:270:LYS:HD3	1.92	0.51
1:A:472:VAL:HG11	1:A:496:VAL:HG21	1.91	0.51
1:B:472:VAL:HG21	1:B:496:VAL:HG11	1.92	0.51
1:D:40:ILE:HG22	1:D:40:ILE:O	2.11	0.51
1:C:385:ALA:HA	1:D:307:PHE:HZ	1.76	0.51
1:D:330:MET:HG3	1:D:348:VAL:HG22	1.93	0.51
1:B:24:ASP:N	1:B:24:ASP:OD1	2.43	0.50
1:C:329:GLN:HA	1:C:332:GLU:HG2	1.93	0.50
1:B:340:PRO:HG3	1:B:377:MET:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:VAL:HG13	1:A:500:ARG:NH1	2.27	0.49
1:A:493:ALA:HA	1:A:496:VAL:HB	1.95	0.49
1:D:61:LEU:HD13	1:D:91:VAL:HA	1.95	0.49
1:C:342:ARG:NH1	1:D:306:VAL:HG21	2.28	0.48
1:D:516:ARG:NE	1:D:517:PRO:O	2.41	0.48
1:D:274:HIS:O	1:D:278:ARG:HG3	2.13	0.47
1:C:272:GLU:O	1:C:300:GLU:HG3	2.14	0.47
1:A:307:PHE:HZ	1:B:385:ALA:HA	1.78	0.47
1:C:48:ILE:HG12	1:C:71:VAL:HB	1.97	0.47
1:C:319:ARG:O	1:C:443:ARG:NH1	2.35	0.47
1:C:393:GLN:O	1:C:397:GLU:HG3	2.15	0.47
1:B:496:VAL:HG13	1:B:500:ARG:HH11	1.79	0.46
1:D:311:LYS:NZ	1:D:354:ASP:OD1	2.48	0.46
1:C:307:PHE:HZ	1:D:385:ALA:HA	1.80	0.46
1:C:61:LEU:HD13	1:C:91:VAL:HA	1.98	0.46
1:A:61:LEU:HD13	1:A:91:VAL:HA	1.96	0.46
1:D:63:GLU:HA	1:D:66:LYS:HE3	1.97	0.46
1:A:211:LEU:HD13	1:A:299:ILE:HG21	1.98	0.46
1:C:268:ILE:HD13	1:C:289:GLY:HA3	1.98	0.46
1:A:405:THR:HG21	1:A:410:GLU:HG2	1.99	0.45
1:A:319:ARG:HH21	1:B:31:CYS:HB3	1.80	0.45
1:A:48:ILE:HG12	1:A:71:VAL:HB	1.97	0.45
1:B:453:VAL:HG11	1:B:489:ARG:HB3	1.98	0.45
1:B:463:ALA:HB3	1:B:471:PRO:HB3	1.98	0.45
1:A:56:ARG:NH2	1:A:86:GLU:HB3	2.32	0.45
1:A:329:GLN:HA	1:A:332:GLU:HG2	1.98	0.45
1:A:268:ILE:HD13	1:A:289:GLY:HA3	1.99	0.45
1:A:437:SER:OG	1:A:522:THR:HG21	2.16	0.45
1:A:274:HIS:CE1	1:A:301:ILE:HG22	2.51	0.45
1:A:453:VAL:HG11	1:A:489:ARG:HB3	1.99	0.45
1:A:342:ARG:O	1:A:342:ARG:HG2	2.17	0.45
1:B:61:LEU:HD13	1:B:91:VAL:HA	1.98	0.45
1:B:268:ILE:HD13	1:B:289:GLY:HA3	1.99	0.45
1:C:472:VAL:HG21	1:C:496:VAL:HG11	1.98	0.44
1:C:298:GLY:HA3	1:D:342:ARG:HH21	1.82	0.44
1:A:73:ARG:NH1	1:A:113:ASP:OD2	2.50	0.44
1:D:297:LEU:O	1:D:301:ILE:HG12	2.18	0.44
1:B:92:ARG:NH1	1:B:235:GLN:O	2.40	0.44
1:C:340:PRO:HG3	1:C:377:MET:HG2	1.99	0.44
1:D:402:ALA:HA	1:D:403:PRO:HD3	1.87	0.44
1:D:472:VAL:HG21	1:D:496:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:GLU:HA	1:B:226:ILE:HD12	2.00	0.43
1:A:92:ARG:NH1	1:A:235:GLN:O	2.40	0.43
1:A:311:LYS:NZ	1:A:354:ASP:OD1	2.51	0.43
1:B:409:THR:HG23	1:B:522:THR:OG1	2.18	0.43
1:D:323:PRO:HD3	1:D:466:TYR:CE2	2.54	0.43
1:C:323:PRO:HD3	1:C:466:TYR:CE2	2.54	0.43
1:C:330:MET:HG3	1:C:348:VAL:HG22	2.00	0.43
1:B:230:LYS:HE3	1:B:257:VAL:O	2.19	0.43
1:A:423:CYS:SG	1:A:425:SER:OG	2.77	0.43
1:B:401:LEU:HD23	1:B:401:LEU:HA	1.89	0.43
1:C:274:HIS:CE1	1:D:36:ASP:OD1	2.72	0.42
1:B:515:TRP:CZ3	1:B:516:ARG:HG3	2.54	0.42
1:B:302:PRO:C	1:B:304:GLU:H	2.22	0.42
1:A:418:GLU:O	1:A:422:ARG:HG2	2.20	0.42
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.55	0.42
1:C:463:ALA:HB3	1:C:471:PRO:HB3	2.02	0.42
1:C:226:ILE:HG22	1:C:230:LYS:NZ	2.35	0.42
1:B:311:LYS:NZ	1:B:354:ASP:OD1	2.52	0.42
1:D:274:HIS:NE2	1:D:301:ILE:HG22	2.34	0.42
1:D:453:VAL:HG11	1:D:489:ARG:HB3	2.02	0.42
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.55	0.42
1:A:298:GLY:CA	1:B:342:ARG:HH12	2.33	0.42
1:B:370:TYR:HB3	1:B:373:GLU:HB2	2.01	0.41
1:A:514:GLY:CA	1:A:522:THR:HA	2.50	0.41
1:C:40:ILE:HG22	1:C:40:ILE:O	2.21	0.41
1:B:56:ARG:HH22	1:B:83:TYR:C	2.19	0.41
1:A:55:SER:HA	1:A:60:THR:HG21	2.03	0.41
1:C:92:ARG:O	1:C:96:GLU:HG2	2.20	0.41
1:B:436:ARG:HE	1:B:436:ARG:HB2	1.67	0.41
1:D:463:ALA:HB3	1:D:471:PRO:HB3	2.03	0.41
1:B:330:MET:HG3	1:B:348:VAL:HG22	2.01	0.41
1:D:494:MET:HG3	1:D:530:VAL:HG13	2.02	0.41
1:A:323:PRO:HD3	1:A:466:TYR:CE2	2.55	0.41
1:D:268:ILE:HD13	1:D:289:GLY:HA3	2.03	0.41
1:B:302:PRO:O	1:B:304:GLU:N	2.53	0.40
1:D:48:ILE:HG12	1:D:71:VAL:HB	2.03	0.40
1:B:103:ILE:O	1:B:500:ARG:NH1	2.48	0.40
1:B:40:ILE:HG22	1:B:40:ILE:O	2.22	0.40
1:A:392:LEU:HD13	1:A:392:LEU:HA	1.83	0.40
1:B:323:PRO:HD3	1:B:466:TYR:CE2	2.56	0.40
1:D:305:LYS:O	1:D:308:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ILE:HG23	1:C:104:LEU:HG	2.03	0.40
1:D:370:TYR:HB3	1:D:373:GLU:HB2	2.03	0.40
1:D:56:ARG:NH2	1:D:86:GLU:HB3	2.37	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	405/536 (76%)	393 (97%)	10 (2%)	2 (0%)	34	58
1	B	404/536 (75%)	391 (97%)	8 (2%)	5 (1%)	16	33
1	C	388/536 (72%)	380 (98%)	6 (2%)	2 (0%)	34	58
1	D	404/536 (75%)	397 (98%)	6 (2%)	1 (0%)	52	75
All	All	1601/2144 (75%)	1561 (98%)	30 (2%)	10 (1%)	30	54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	404	ILE
1	B	303	ALA
1	B	403	PRO
1	C	406	SER
1	A	212	PRO
1	A	328	THR
1	B	328	THR
1	C	328	THR
1	D	328	THR
1	B	517	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/439 (77%)	326 (96%)	13 (4%)	40	67
1	B	336/439 (76%)	325 (97%)	11 (3%)	45	71
1	C	328/439 (75%)	318 (97%)	10 (3%)	48	75
1	D	337/439 (77%)	327 (97%)	10 (3%)	48	75
All	All	1340/1756 (76%)	1296 (97%)	44 (3%)	45	71

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	59	GLU
1	A	81	HIS
1	A	217	ASP
1	A	274	HIS
1	A	294	ARG
1	A	297	LEU
1	A	330	MET
1	A	386	GLU
1	A	399	ARG
1	A	433	LYS
1	A	508	VAL
1	A	522	THR
1	B	24	ASP
1	B	45	THR
1	B	59	GLU
1	B	230	LYS
1	B	297	LEU
1	B	330	MET
1	B	359	ILE
1	B	386	GLU
1	B	516	ARG
1	B	522	THR
1	B	526	ARG

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Mol	Chain	Res	Type
1	C	32	ARG
1	C	45	THR
1	C	86	GLU
1	C	297	LEU
1	C	330	MET
1	C	359	ILE
1	C	386	GLU
1	C	405	THR
1	C	433	LYS
1	C	526	ARG
1	D	45	THR
1	D	78	HIS
1	D	297	LEU
1	D	330	MET
1	D	386	GLU
1	D	399	ARG
1	D	422	ARG
1	D	516	ARG
1	D	522	THR
1	D	526	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	379	HIS

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)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FBP	A	600	-	18,20,20	0.90	1 (5%)	21,32,32	0.61	0
2	FBP	B	600	-	18,20,20	0.91	1 (5%)	21,32,32	0.66	0
2	FBP	C	600	-	18,20,20	0.90	1 (5%)	21,32,32	0.63	0
2	FBP	D	600	-	18,20,20	0.90	1 (5%)	21,32,32	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	A	600	-	-	0/13/32/32	0/1/1/1
2	FBP	B	600	-	-	0/13/32/32	0/1/1/1
2	FBP	C	600	-	-	0/13/32/32	0/1/1/1
2	FBP	D	600	-	-	0/13/32/32	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FBP	O2-C2	2.68	1.45	1.41
2	C	600	FBP	O2-C2	2.70	1.45	1.41
2	D	600	FBP	O2-C2	2.71	1.45	1.41
2	A	600	FBP	O2-C2	2.72	1.45	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FBP	1	0
2	B	600	FBP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	411/536 (76%)	0.91	56 (13%)	4 3	47, 80, 131, 203	0
1	B	408/536 (76%)	1.18	79 (19%)	1 1	55, 88, 134, 167	0
1	C	396/536 (73%)	1.16	79 (19%)	1 1	68, 95, 130, 167	0
1	D	408/536 (76%)	1.02	72 (17%)	2 1	50, 82, 121, 155	0
All	All	1623/2144 (75%)	1.07	286 (17%)	2 1	47, 87, 129, 203	0

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	LYS	9.7
1	D	40	ILE	8.1
1	B	244	PHE	7.9
1	C	41	THR	7.8
1	B	303	ALA	7.5
1	B	117	PRO	7.4
1	B	228	ASP	5.8
1	D	335	ILE	5.7
1	C	404	ILE	5.6
1	C	40	ILE	5.2
1	B	118	GLU	5.1
1	C	326	CYS	5.1
1	B	333	SER	4.8
1	B	302	PRO	4.8
1	A	527	VAL	4.7
1	C	340	PRO	4.7
1	A	334	MET	4.5
1	B	335	ILE	4.5
1	A	326	CYS	4.5
1	B	231	PHE	4.5
1	A	338	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	102	PRO	4.4
1	D	345	GLY	4.4
1	D	370	TYR	4.3
1	C	505	LYS	4.3
1	B	306	VAL	4.3
1	A	336	LYS	4.2
1	A	504	LYS	4.2
1	A	342	ARG	4.1
1	B	83	TYR	4.1
1	B	466	TYR	4.1
1	D	220	ALA	4.1
1	C	342	ARG	4.0
1	A	370	TYR	4.0
1	D	46	GLY	4.0
1	A	40	ILE	4.0
1	B	365	THR	4.0
1	B	258	LEU	4.0
1	D	244	PHE	4.0
1	C	244	PHE	3.9
1	A	505	LYS	3.9
1	A	339	ARG	3.9
1	D	358	CYS	3.8
1	C	475	LYS	3.8
1	D	119	ILE	3.8
1	B	274	HIS	3.8
1	B	250	ASP	3.8
1	C	355	GLY	3.8
1	D	342	ARG	3.7
1	C	466	TYR	3.7
1	A	53	PRO	3.7
1	C	531	PRO	3.7
1	B	463	ALA	3.7
1	D	392	LEU	3.7
1	C	48	ILE	3.6
1	C	262	GLY	3.6
1	D	346	SER	3.6
1	A	531	PRO	3.6
1	A	45	THR	3.6
1	C	334	MET	3.6
1	A	358	CYS	3.5
1	C	338	PRO	3.5
1	C	504	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	246	ARG	3.5
1	A	426	GLY	3.5
1	C	278	ARG	3.4
1	D	352	VAL	3.4
1	B	220	ALA	3.4
1	C	117	PRO	3.4
1	A	333	SER	3.4
1	D	336	LYS	3.4
1	B	356	ALA	3.4
1	C	250	ASP	3.4
1	B	337	LYS	3.4
1	B	468	GLY	3.4
1	C	401	LEU	3.4
1	D	98	PHE	3.4
1	C	325	ILE	3.4
1	D	89	LYS	3.3
1	B	531	PRO	3.3
1	D	353	LEU	3.3
1	D	404	ILE	3.3
1	A	373	GLU	3.3
1	B	40	ILE	3.3
1	A	405	THR	3.3
1	B	98	PHE	3.3
1	A	522	THR	3.2
1	B	261	LYS	3.2
1	A	103	ILE	3.2
1	D	47	ILE	3.2
1	D	307	PHE	3.2
1	A	299	ILE	3.2
1	A	484	GLU	3.2
1	B	469	ILE	3.2
1	B	334	MET	3.2
1	C	335	ILE	3.2
1	B	371	PRO	3.1
1	B	477	PRO	3.1
1	A	467	ARG	3.1
1	C	103	ILE	3.1
1	A	500	ARG	3.1
1	D	350	ASN	3.1
1	C	359	ILE	3.1
1	B	467	ARG	3.1
1	B	299	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	323	PRO	3.0
1	B	263	LYS	3.0
1	A	477	PRO	3.0
1	C	273	ASN	3.0
1	C	352	VAL	3.0
1	B	488	LEU	3.0
1	D	93	THR	3.0
1	C	286	ALA	3.0
1	D	359	ILE	3.0
1	B	504	LYS	3.0
1	A	508	VAL	3.0
1	A	401	LEU	3.0
1	A	482	TRP	3.0
1	B	404	ILE	3.0
1	C	282	GLU	2.9
1	B	247	LYS	2.9
1	D	339	ARG	2.9
1	B	45	THR	2.9
1	D	351	ALA	2.9
1	B	32	ARG	2.9
1	C	482	TRP	2.9
1	C	46	GLY	2.9
1	A	404	ILE	2.9
1	A	475	LYS	2.9
1	D	390	TYR	2.8
1	D	360	MET	2.8
1	B	328	THR	2.8
1	D	48	ILE	2.8
1	D	234	GLU	2.8
1	D	347	ASP	2.8
1	D	37	SER	2.8
1	C	486	VAL	2.8
1	C	411	ALA	2.8
1	B	245	ILE	2.8
1	D	465	LEU	2.8
1	A	392	LEU	2.7
1	D	328	THR	2.7
1	C	463	ALA	2.7
1	C	299	ILE	2.7
1	A	357	ASP	2.7
1	D	475	LYS	2.7
1	A	455	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	268	ILE	2.7
1	B	259	GLY	2.7
1	B	370	TYR	2.7
1	A	359	ILE	2.6
1	C	274	HIS	2.6
1	B	224	LYS	2.6
1	C	263	LYS	2.6
1	D	349	ALA	2.6
1	C	444	TYR	2.6
1	C	351	ALA	2.6
1	A	506	GLY	2.6
1	B	114	THR	2.6
1	C	277	VAL	2.6
1	D	329	GLN	2.6
1	B	358	CYS	2.6
1	C	45	THR	2.6
1	C	324	VAL	2.6
1	A	323	PRO	2.6
1	B	339	ARG	2.6
1	D	467	ARG	2.6
1	D	35	ILE	2.6
1	B	342	ARG	2.6
1	A	369	ASP	2.6
1	C	480	GLU	2.5
1	B	301	ILE	2.5
1	B	329	GLN	2.5
1	C	360	MET	2.5
1	D	462	GLN	2.5
1	C	358	CYS	2.5
1	D	36	ASP	2.5
1	A	337	LYS	2.5
1	A	450	ILE	2.5
1	C	354	ASP	2.5
1	D	357	ASP	2.5
1	D	52	GLY	2.5
1	A	406	SER	2.5
1	D	436	ARG	2.5
1	D	45	THR	2.5
1	A	46	GLY	2.5
1	C	275	GLU	2.5
1	C	296	ASP	2.4
1	B	255	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	292	VAL	2.4
1	C	307	PHE	2.4
1	A	491	ASN	2.4
1	B	103	ILE	2.4
1	C	74	LEU	2.4
1	B	80	THR	2.4
1	B	369	ASP	2.4
1	B	405	THR	2.4
1	C	390	TYR	2.4
1	D	434	SER	2.4
1	C	483	ALA	2.4
1	D	101	ASP	2.3
1	D	63	GLU	2.3
1	A	325	ILE	2.3
1	C	295	GLY	2.3
1	C	243	SER	2.3
1	C	252	HIS	2.3
1	C	476	ASP	2.3
1	C	246	ARG	2.3
1	B	357	ASP	2.3
1	C	357	ASP	2.3
1	D	299	ILE	2.3
1	D	32	ARG	2.3
1	B	373	GLU	2.3
1	D	31	CYS	2.3
1	A	469	ILE	2.3
1	C	356	ALA	2.3
1	C	445	ARG	2.3
1	A	367	LYS	2.3
1	C	247	LYS	2.3
1	A	430	VAL	2.3
1	B	446	PRO	2.3
1	B	99	ALA	2.2
1	B	366	ALA	2.2
1	C	305	LYS	2.2
1	D	90	ASN	2.2
1	A	52	GLY	2.2
1	D	435	GLY	2.2
1	D	338	PRO	2.2
1	B	343	ALA	2.2
1	D	356	ALA	2.2
1	D	385	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	325	ILE	2.2
1	D	469	ILE	2.2
1	B	46	GLY	2.2
1	B	289	GLY	2.2
1	D	115	LYS	2.2
1	C	314	ILE	2.2
1	A	464	HIS	2.2
1	D	231	PHE	2.2
1	C	221	VAL	2.2
1	C	306	VAL	2.2
1	B	476	ASP	2.2
1	D	67	SER	2.2
1	C	492	PHE	2.2
1	D	28	GLU	2.2
1	A	466	TYR	2.2
1	D	466	TYR	2.2
1	D	106	ARG	2.2
1	D	100	SER	2.2
1	A	329	GLN	2.2
1	B	465	LEU	2.2
1	C	405	THR	2.2
1	D	376	ARG	2.2
1	B	352	VAL	2.1
1	A	226	ILE	2.1
1	C	99	ALA	2.1
1	D	377	MET	2.1
1	C	485	ASP	2.1
1	D	369	ASP	2.1
1	D	275	GLU	2.1
1	B	367	LYS	2.1
1	D	463	ALA	2.1
1	C	370	TYR	2.1
1	B	223	GLU	2.1
1	B	492	PHE	2.1
1	C	425	SER	2.1
1	C	301	ILE	2.1
1	A	97	SER	2.1
1	B	36	ASP	2.1
1	B	359	ILE	2.1
1	A	274	HIS	2.1
1	D	24	ASP	2.1
1	B	414	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	330	MET	2.1
1	A	474	CYS	2.1
1	B	79	GLY	2.1
1	B	353	LEU	2.1
1	C	366	ALA	2.0
1	B	279	ARG	2.0
1	C	530	VAL	2.0
1	C	446	PRO	2.0
1	B	427	ALA	2.0
1	C	42	ALA	2.0
1	C	349	ALA	2.0
1	C	481	ALA	2.0
1	D	451	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, 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
2	FBP	D	600	20/20	0.95	0.19	-0.03	54,66,83,89	0
2	FBP	C	600	20/20	0.88	0.22	-0.12	78,86,103,112	0
2	FBP	B	600	20/20	0.94	0.19	-0.19	59,74,94,99	0
2	FBP	A	600	20/20	0.94	0.17	-0.71	70,90,100,102	0

6.5 Other polymers (i)

There are no such residues in this entry.