



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:59 PM GMT

PDB ID : 4B2D
Title : human PKM2 with L-serine and FBP bound.
Authors : Chaneton, B.; Hillmann, P.; Zheng, L.; Martin, A.C.L.; Maddocks, O.D.K.; Chokkathukalam, A.; Coyle, J.E.; Jankevics, A.; Holding, F.P.; Vousden, K.H.; Frezza, C.; O'Reilly, M.; Gottlieb, E.
Deposited on : 2012-07-13
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 ⓘ 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

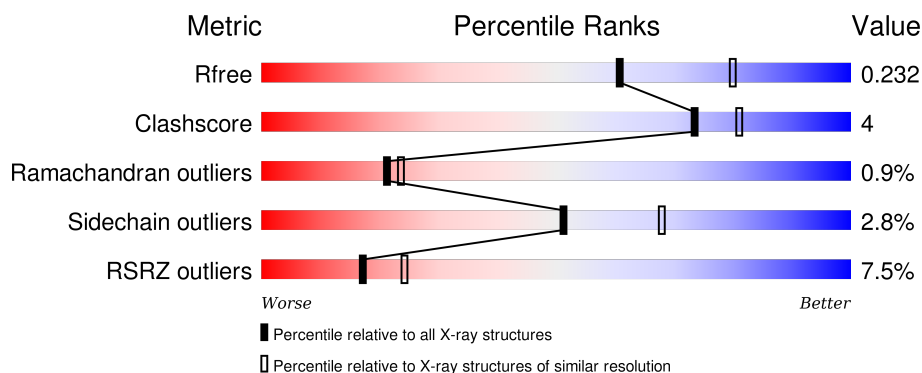
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 $\leq 5\%$. 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	548	<div> <div>83%</div> <div>11% • 5%</div> </div>
1	B	548	<div> <div>12%</div> <div>82%</div> <div>12% 6%</div> </div>
1	C	548	<div> <div>84%</div> <div>11% 5%</div> </div>
2	D	548	<div> <div>15%</div> <div>81%</div> <div>12% • 5%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16980 atoms, of which 28 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
			3906	2453	695	733	25			
1	B	514	Total	C	N	O	S	0	1	0
			3872	2436	691	721	24			
1	C	518	Total	C	N	O	S	0	0	0
			3907	2460	695	728	24			

There are 54 discrepancies between the modelled and reference sequences:

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

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

- Molecule 2 is a protein called PYRUVATE KINASE ISOZYMES M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	518	Total	C	N	O	S	0	0	0
			3914	2462	692	735	25			

There are 19 discrepancies between the modelled and reference sequences:

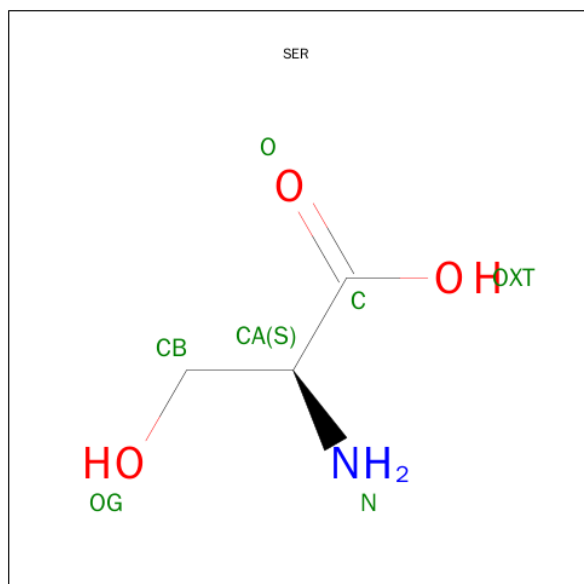
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	MET	-	EXPRESSION TAG	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	GLY	-	EXPRESSION TAG	UNP P14618
D	-14	SER	-	EXPRESSION TAG	UNP P14618
D	-13	SER	-	EXPRESSION TAG	UNP P14618
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	HIS	-	EXPRESSION TAG	UNP P14618
D	-7	HIS	-	EXPRESSION TAG	UNP P14618
D	-6	SER	-	EXPRESSION TAG	UNP P14618
D	-5	SER	-	EXPRESSION TAG	UNP P14618
D	-4	GLY	-	EXPRESSION TAG	UNP P14618
D	-3	LEU	-	EXPRESSION TAG	UNP P14618
D	-2	VAL	-	EXPRESSION TAG	UNP P14618
D	-1	PRO	-	EXPRESSION TAG	UNP P14618
D	0	ARG	-	EXPRESSION TAG	UNP P14618
D	1	GLY	-	EXPRESSION TAG	UNP P14618
D	142	LEU	ILE	CONFLICT	UNP P14618

- Molecule 3 is SERINE (three-letter code: SER) (formula: $\text{C}_3\text{H}_7\text{NO}_3$).



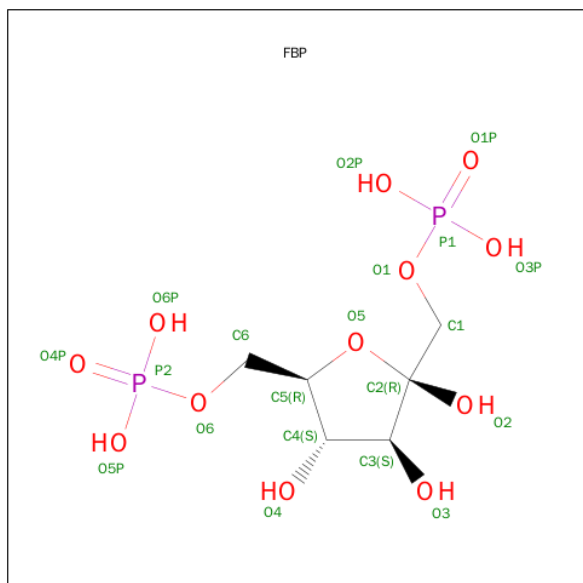
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 14	C 3	H 7	N 1	O 3	0	0
3	B	1	Total 14	C 3	H 7	N 1	O 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	H	N	O	0	0
			14	3	7	1	3		
3	D	1	Total	C	H	N	O	0	0
			14	3	7	1	3		

- Molecule 4 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
4	A	1	Total	C	O	P	0	0
			20	6	12	2		
4	B	1	Total	C	O	P	0	0
			20	6	12	2		
4	C	1	Total	C	O	P	0	0
			20	6	12	2		
4	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

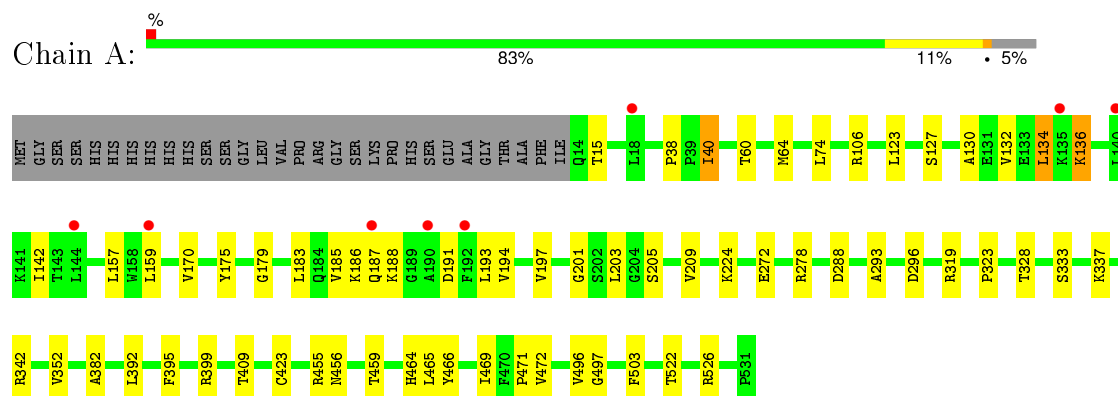
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	395	Total 395	O 395	0	0
6	B	270	Total 270	O 270	0	0
6	C	327	Total 327	O 327	0	0
6	D	251	Total 251	O 251	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 ($\text{RSRZ} > 2$). 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.

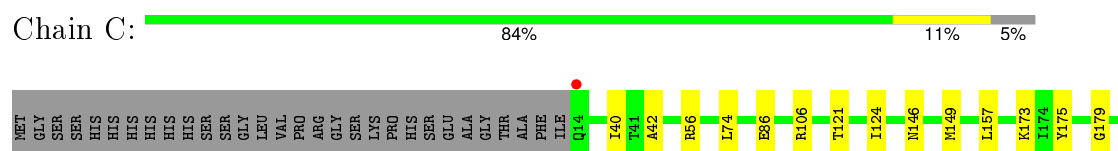
• Molecule 1: PYRUVATE KINASE ISOZYMES M1/M2



• Molecule 1: PYRUVATE KINASE ISOZYMES M1/M2

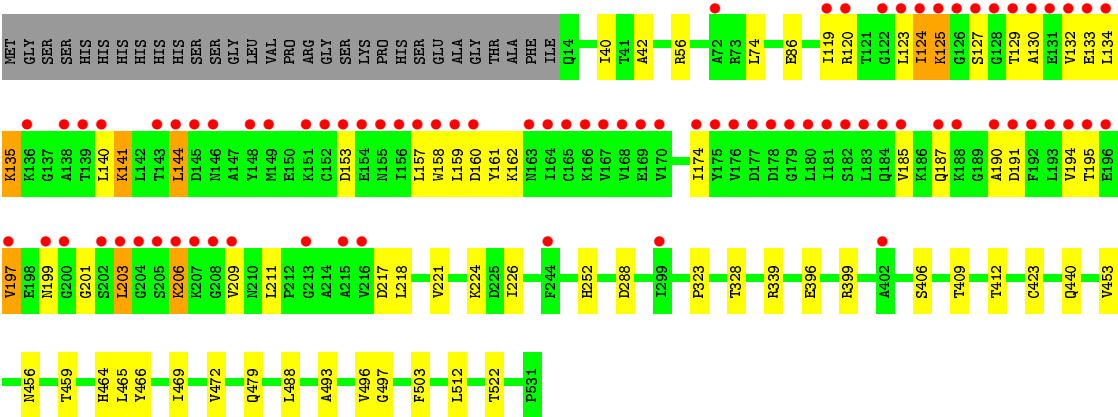
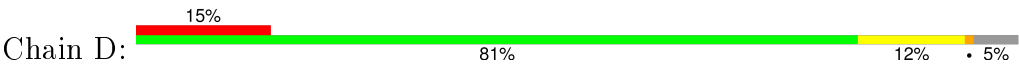


• Molecule 1: PYRUVATE KINASE ISOZYMES M1/M2





● Molecule 2: 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	80.61Å 151.10Å 91.79Å 90.00° 102.01° 90.00°	Depositor
Resolution (Å)	78.85 – 2.30 78.85 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (78.85-2.30) 97.9 (78.85-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.173 , 0.226 0.179 , 0.232	Depositor DCC
R_{free} test set	4702 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 57.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 93185 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16980	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.60	0/3970	0.65	0/5370
1	B	0.59	0/3937	0.65	0/5326
1	C	0.56	0/3971	0.63	0/5370
2	D	0.55	0/3978	0.66	0/5379
All	All	0.57	0/15856	0.65	0/21445

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3906	0	3924	34	0
1	B	3872	0	3889	34	0
1	C	3907	0	3944	31	0
2	D	3914	0	3946	37	0
3	A	7	7	4	1	0
3	B	7	7	4	1	0
3	C	7	7	4	1	0
3	D	7	7	4	1	0
4	A	20	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	20	0	10	0	0
4	C	20	0	10	0	0
4	D	20	0	10	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	395	0	0	1	0
6	B	270	0	0	5	0
6	C	327	0	0	1	0
6	D	251	0	0	2	0
All	All	16952	28	15759	129	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 4.

All (129) 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:187:GLN:HB2	1:A:194:VAL:HB	1.58	0.85
1:C:518:GLY:O	1:C:519:SER:HB2	1.79	0.80
2:D:134:LEU:HA	2:D:135:LYS:HB2	1.65	0.76
1:A:106:ARG:NH2	1:A:471:PRO:O	2.18	0.75
1:C:464:HIS:HD1	3:C:1532:SER:N	1.88	0.71
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.71	0.70
1:B:175:TYR:HB3	1:B:179:GLY:HA2	1.74	0.70
1:C:410:GLU:HG2	1:C:440:GLN:HE21	1.57	0.69
1:C:187:GLN:HB3	1:C:194:VAL:HB	1.74	0.67
2:D:140:LEU:HD13	2:D:197:VAL:HG21	1.79	0.65
1:B:410:GLU:HG3	1:B:440:GLN:HE21	1.60	0.65
2:D:464:HIS:HD1	3:D:1532:SER:N	1.96	0.64
1:B:440:GLN:HG2	6:B:2211:HOH:O	1.98	0.63
1:C:146:ASN:O	1:C:149:MET:HB2	1.99	0.62
1:C:175:TYR:HB3	1:C:179:GLY:HA2	1.82	0.61
2:D:124:ILE:HD13	2:D:130:ALA:HB3	1.83	0.60
1:B:336:LYS:HG2	6:B:2186:HOH:O	2.01	0.59
2:D:56:ARG:NH2	2:D:86:GLU:HB3	2.19	0.58
1:A:319:ARG:HD2	6:B:2016:HOH:O	2.03	0.58
1:B:122:GLY:HA3	6:B:2097:HOH:O	2.03	0.57
1:B:121:THR:HB	1:B:157:LEU:HD11	1.86	0.57
1:A:142:ILE:HA	1:A:157:LEU:O	2.04	0.57
1:B:464:HIS:HD1	3:B:1532:SER:N	2.02	0.56
1:B:134:LEU:CD1	1:B:181:ILE:HG12	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:TYR:HB3	1:A:179:GLY:HA2	1.86	0.56
1:B:175:TYR:HB2	1:B:210:ASN:HB2	1.88	0.56
2:D:174:ILE:HG23	2:D:209:VAL:HG22	1.87	0.56
2:D:125:LYS:HA	2:D:129:THR:HG22	1.88	0.55
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.88	0.54
2:D:141:LYS:HB2	2:D:195:THR:HG21	1.89	0.54
2:D:409:THR:HG23	2:D:522:THR:HB	1.89	0.54
1:B:56:ARG:NH2	1:B:86:GLU:HB3	2.21	0.54
2:D:412:THR:HG22	2:D:512:LEU:HD22	1.90	0.54
2:D:409:THR:HG21	2:D:440:GLN:HE22	1.73	0.53
1:B:410:GLU:HG2	6:B:2229:HOH:O	2.07	0.53
2:D:174:ILE:HD12	2:D:185:VAL:HG21	1.91	0.53
2:D:409:THR:CG2	2:D:440:GLN:NE2	2.72	0.53
2:D:466:TYR:HB2	2:D:469:ILE:HD12	1.91	0.52
2:D:472:VAL:HG11	2:D:496:VAL:HG11	1.92	0.52
1:C:395:PHE:CE2	1:C:399:ARG:HD2	2.45	0.52
1:C:412:THR:HG22	1:C:512:LEU:HD22	1.92	0.52
1:B:288:ASP:O	1:B:323:PRO:HD2	2.10	0.52
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.92	0.51
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.92	0.51
2:D:409:THR:CG2	2:D:440:GLN:HE22	2.23	0.51
1:B:399:ARG:HH12	2:D:399:ARG:CD	2.23	0.51
1:A:132:VAL:HG23	1:A:203:LEU:HB3	1.92	0.50
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.46	0.50
1:A:423:CYS:HA	1:C:405:THR:O	2.11	0.50
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.47	0.50
1:C:121:THR:O	1:C:206:LYS:HA	2.12	0.49
2:D:120:ARG:HD2	2:D:206:LYS:HB3	1.94	0.49
1:A:123:LEU:HA	1:A:205:SER:HB3	1.93	0.49
2:D:288:ASP:O	2:D:323:PRO:HD2	2.12	0.49
1:C:466:TYR:HB2	1:C:469:ILE:HD12	1.94	0.49
1:C:352:VAL:HG21	1:C:382:ALA:HA	1.95	0.49
1:A:409:THR:HG23	1:A:522:THR:HB	1.94	0.48
1:A:342:ARG:HE	1:B:298:GLY:HA3	1.78	0.48
2:D:497:GLY:HA3	2:D:503:PHE:CZ	2.48	0.48
1:A:60:THR:O	1:A:64:MET:HG2	2.14	0.48
1:B:182:SER:HB3	1:B:198:GLU:HB2	1.96	0.48
1:C:272:GLU:HB3	1:C:293:ALA:HB3	1.95	0.48
1:A:288:ASP:O	1:A:323:PRO:HD2	2.13	0.47
1:B:134:LEU:HD13	1:B:181:ILE:HG12	1.95	0.47
1:A:395:PHE:CE2	1:A:399:ARG:HD2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:THR:HG22	1:A:38:PRO:HG2	1.95	0.47
1:C:409:THR:HG23	1:C:522:THR:HB	1.97	0.47
1:B:399:ARG:HH21	2:D:396:GLU:HG2	1.79	0.47
2:D:144:LEU:HD12	2:D:187:GLN:HE22	1.80	0.47
1:C:157:LEU:HD13	1:C:203:LEU:HD21	1.96	0.47
1:B:132:VAL:HG22	1:B:203:LEU:HB3	1.97	0.47
2:D:323:PRO:HB3	2:D:465:LEU:O	2.14	0.46
1:C:323:PRO:HB3	1:C:465:LEU:O	2.15	0.46
1:A:464:HIS:HD1	3:A:1532:SER:N	2.13	0.46
1:A:456:ASN:HB3	1:A:459:THR:HB	1.98	0.46
1:A:455:ARG:HD2	6:A:2359:HOH:O	2.16	0.46
1:B:176:VAL:HB	1:B:181:ILE:HB	1.98	0.46
2:D:134:LEU:HA	2:D:135:LYS:CB	2.40	0.46
2:D:479:GLN:HG2	2:D:488:LEU:HD22	1.97	0.46
1:A:159:LEU:HD22	1:A:209:VAL:HG21	1.97	0.45
2:D:409:THR:HG22	2:D:440:GLN:NE2	2.31	0.45
1:C:288:ASP:O	1:C:323:PRO:HD2	2.17	0.45
2:D:453:VAL:CG2	2:D:493:ALA:HB2	2.47	0.45
2:D:40:ILE:HD12	2:D:42:ALA:HB3	1.98	0.45
1:B:159:LEU:HD11	1:B:209:VAL:HG21	1.99	0.45
1:A:272:GLU:HB3	1:A:293:ALA:HB3	1.98	0.45
1:C:472:VAL:HG11	1:C:496:VAL:HG11	1.99	0.45
2:D:132:VAL:O	2:D:134:LEU:N	2.49	0.45
1:B:405:THR:O	2:D:423:CYS:HA	2.17	0.44
1:A:188:LYS:HA	1:A:193:LEU:HD23	1.99	0.44
2:D:456:ASN:HB3	2:D:459:THR:HB	1.98	0.44
2:D:339:ARG:NH1	6:D:2171:HOH:O	2.49	0.44
1:B:323:PRO:HB3	1:B:465:LEU:O	2.17	0.44
1:C:272:GLU:HB2	1:C:296:ASP:HB2	1.98	0.44
1:A:136:LYS:H	1:A:136:LYS:HD3	1.83	0.44
1:A:526:ARG:HA	1:C:523:ASN:O	2.17	0.44
1:A:127:SER:HB3	1:A:130:ALA:HB2	1.99	0.44
1:B:268:ILE:HG21	1:B:325:ILE:HD12	2.00	0.44
1:C:106:ARG:NH2	1:C:471:PRO:O	2.38	0.44
1:C:221:VAL:HG12	1:C:226:ILE:HG13	1.99	0.44
1:C:526:ARG:HD3	6:C:2320:HOH:O	2.18	0.43
1:C:124:ILE:HD11	1:C:203:LEU:HG	2.00	0.43
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.53	0.43
1:A:323:PRO:HB3	1:A:465:LEU:O	2.19	0.43
1:B:456:ASN:HB3	1:B:459:THR:HB	2.01	0.43
1:A:134:LEU:HB2	1:A:201:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ILE:HD12	1:C:42:ALA:HB3	2.01	0.43
1:B:174:ILE:HG12	1:B:211:LEU:HD22	2.01	0.43
1:B:122:GLY:O	1:B:206:LYS:N	2.51	0.43
1:A:272:GLU:HB2	1:A:296:ASP:HB2	2.01	0.43
1:B:117:PRO:HG3	1:B:246:ARG:NH2	2.34	0.43
1:C:56:ARG:NH2	1:C:86:GLU:HB2	2.34	0.43
1:C:416:ALA:HB2	1:C:512:LEU:HD21	2.00	0.42
1:A:134:LEU:HD22	1:A:203:LEU:HB2	2.01	0.42
1:B:407:ASP:OD1	1:B:409[B]:THR:OG1	2.23	0.42
1:B:40:ILE:HD12	1:B:42:ALA:HB3	2.02	0.42
2:D:161:TYR:CD1	2:D:218:LEU:HD21	2.54	0.42
1:C:456:ASN:HB3	1:C:459:THR:HB	2.01	0.42
2:D:119:ILE:HG12	2:D:161:TYR:HB3	2.01	0.42
2:D:221:VAL:HG12	2:D:226:ILE:HG13	2.01	0.42
1:B:124:ILE:HG21	1:B:130:ALA:HA	2.02	0.41
1:A:352:VAL:HG21	1:A:382:ALA:HA	2.03	0.41
2:D:129:THR:OG1	2:D:203:LEU:HB3	2.21	0.41
1:A:183:LEU:HD23	1:A:197:VAL:HA	2.03	0.40
1:A:399:ARG:HH12	1:C:399:ARG:CZ	2.33	0.40
2:D:252:HIS:HE1	6:D:2127:HOH:O	2.04	0.40
1:A:333:SER:HB2	1:A:337:LYS:HE3	2.04	0.40
1:C:173:LYS:HA	1:C:183:LEU:O	2.22	0.40
1:B:221:VAL:HG12	1:B:226:ILE:HG13	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	516/548 (94%)	499 (97%)	14 (3%)	3 (1%)	30 36
1	B	511/548 (93%)	489 (96%)	16 (3%)	6 (1%)	16 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	516/548 (94%)	502 (97%)	12 (2%)	2 (0%)	39	48
2	D	516/548 (94%)	461 (89%)	47 (9%)	8 (2%)	12	11
All	All	2059/2192 (94%)	1951 (95%)	89 (4%)	19 (1%)	21	24

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	B	138	ALA
1	C	519	SER
1	B	154	GLU
2	D	135	LYS
1	A	328	THR
1	B	155	ASN
2	D	162	LYS
2	D	190	ALA
2	D	206	LYS
2	D	328	THR
1	B	136	LYS
1	B	328	THR
1	C	328	THR
2	D	133	GLU
1	A	185	VAL
1	B	146	ASN
2	D	127	SER
2	D	201	GLY

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	409/450 (91%)	399 (98%)	10 (2%)	57	74
1	B	402/450 (89%)	393 (98%)	9 (2%)	60	77
1	C	408/450 (91%)	401 (98%)	7 (2%)	68	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	411/450 (91%)	391 (95%)	20 (5%)	31	41
All	All	1630/1800 (91%)	1584 (97%)	46 (3%)	51	68

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	A	74	LEU
1	A	134	LEU
1	A	136	LYS
1	A	170	VAL
1	A	186	LYS
1	A	191	ASP
1	A	224	LYS
1	A	278	ARG
1	A	392	LEU
1	B	74	LEU
1	B	140	LEU
1	B	143	THR
1	B	158	TRP
1	B	224	LYS
1	B	244	PHE
1	B	392	LEU
1	B	406	SER
1	B	424	CYS
1	C	74	LEU
1	C	224	LYS
1	C	261	LYS
1	C	275	GLU
1	C	339	ARG
1	C	519	SER
1	C	525	MET
2	D	74	LEU
2	D	123	LEU
2	D	124	ILE
2	D	125	LYS
2	D	141	LYS
2	D	144	LEU
2	D	153	ASP
2	D	157	LEU
2	D	158	TRP
2	D	159	LEU

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Mol	Chain	Res	Type
2	D	160	ASP
2	D	191	ASP
2	D	194	VAL
2	D	197	VAL
2	D	199	ASN
2	D	203	LEU
2	D	211	LEU
2	D	217	ASP
2	D	224	LYS
2	D	406	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	ASN
1	A	274	HIS
1	B	440	GLN
1	C	199	ASN
1	C	440	GLN
2	D	187	GLN
2	D	199	ASN
2	D	440	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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
3	SER	A	1532	-	3,6,6	0.10	0	1,7,7	0.19	0
4	FBP	A	600	-	18,20,20	0.88	1 (5%)	21,32,32	0.69	0
3	SER	B	1532	-	3,6,6	0.19	0	1,7,7	0.67	0
4	FBP	B	600	-	18,20,20	1.07	2 (11%)	21,32,32	0.67	0
3	SER	C	1532	-	3,6,6	0.22	0	1,7,7	0.02	0
4	FBP	C	600	-	18,20,20	0.89	1 (5%)	21,32,32	0.60	0
3	SER	D	1532	-	3,6,6	0.14	0	1,7,7	0.45	0
4	FBP	D	600	-	18,20,20	0.75	0	21,32,32	0.72	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
3	SER	A	1532	-	-	0/2/6/6	0/0/0/0
4	FBP	A	600	-	-	0/13/32/32	0/1/1/1
3	SER	B	1532	-	-	0/2/6/6	0/0/0/0
4	FBP	B	600	-	-	0/13/32/32	0/1/1/1
3	SER	C	1532	-	-	0/2/6/6	0/0/0/0
4	FBP	C	600	-	-	0/13/32/32	0/1/1/1
3	SER	D	1532	-	-	0/2/6/6	0/0/0/0
4	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)
4	A	600	FBP	P2-O6P	2.03	1.62	1.54
4	B	600	FBP	O2-C2	2.22	1.44	1.41
4	C	600	FBP	O5-C2	2.71	1.47	1.43
4	B	600	FBP	O5-C2	3.15	1.48	1.43

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1532	SER	1	0
3	B	1532	SER	1	0
3	C	1532	SER	1	0
3	D	1532	SER	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	518/548 (94%)	-0.04	8 (1%) 76 81	33, 45, 83, 110	0
1	B	514/548 (93%)	0.42	64 (12%) 5 8	34, 50, 145, 173	0
1	C	518/548 (94%)	-0.11	2 (0%) 93 95	37, 47, 66, 90	0
2	D	518/548 (94%)	0.83	82 (15%) 3 4	39, 54, 161, 173	0
All	All	2068/2192 (94%)	0.28	156 (7%) 17 24	33, 50, 140, 173	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	194	VAL	16.8
2	D	192	PHE	13.9
2	D	193	LEU	12.2
2	D	152	CYS	11.1
1	B	147	ALA	10.3
2	D	180	LEU	9.8
2	D	140	LEU	9.7
2	D	204	GLY	9.2
2	D	157	LEU	8.7
2	D	123	LEU	8.5
2	D	167	VAL	8.2
2	D	190	ALA	8.1
1	B	132	VAL	7.8
2	D	185	VAL	7.7
2	D	197	VAL	7.6
2	D	153	ASP	7.5
2	D	144	LEU	7.5
2	D	132	VAL	7.4
1	B	124	ILE	7.3
2	D	196	GLU	7.2
2	D	128	GLY	6.6

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Mol	Chain	Res	Type	RSRZ
2	D	126	GLY	6.6
2	D	139	THR	6.5
2	D	203	LEU	6.4
2	D	129	THR	6.3
1	B	135	LYS	6.3
2	D	177	ASP	6.2
2	D	151	LYS	6.2
1	B	185	VAL	6.2
1	B	134	LEU	6.1
1	B	140	LEU	6.0
2	D	130	ALA	6.0
2	D	154	GLU	5.9
1	B	193	LEU	5.7
1	B	170	VAL	5.5
2	D	138	ALA	5.4
2	D	125	LYS	5.4
2	D	199	ASN	5.4
2	D	215	ALA	5.4
1	B	167	VAL	5.3
1	B	130	ALA	5.3
2	D	205	SER	5.2
2	D	191	ASP	5.2
2	D	164	ILE	5.2
2	D	209	VAL	5.1
1	B	142	ILE	5.1
1	B	122	GLY	5.1
2	D	174	ILE	5.0
1	B	123	LEU	4.8
2	D	181	ILE	4.8
2	D	120	ARG	4.7
1	B	150	GLU	4.7
2	D	216	VAL	4.6
2	D	208	GLY	4.6
1	B	183	LEU	4.6
1	B	181	ILE	4.5
1	B	141	LYS	4.5
1	B	133	GLU	4.4
2	D	202	SER	4.4
2	D	160	ASP	4.4
2	D	148	TYR	4.4
2	D	124	ILE	4.3
2	D	179	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	159	LEU	4.2
2	D	163	ASN	4.1
1	B	125	LYS	4.0
1	A	190	ALA	4.0
1	B	158	TRP	3.9
1	B	143	THR	3.9
2	D	176	VAL	3.9
2	D	122	GLY	3.8
1	B	152	CYS	3.8
1	B	200	GLY	3.7
2	D	146	ASN	3.7
1	B	214	ALA	3.7
1	B	203	LEU	3.7
1	B	164	ILE	3.7
1	B	215	ALA	3.6
1	A	144	LEU	3.6
2	D	158	TRP	3.6
1	B	157	LEU	3.6
1	B	159	LEU	3.6
2	D	207	LYS	3.6
1	B	197	VAL	3.5
2	D	200	GLY	3.5
2	D	195	THR	3.5
2	D	188	LYS	3.4
1	A	192	PHE	3.4
2	D	169	GLU	3.4
2	D	168	VAL	3.4
1	B	161	TYR	3.3
2	D	244	PHE	3.2
2	D	166	LYS	3.2
2	D	183	LEU	3.1
1	B	184	GLN	3.1
2	D	175	TYR	3.0
1	B	148	TYR	3.0
1	B	144	LEU	3.0
1	B	211	LEU	3.0
2	D	127	SER	3.0
1	B	131	GLU	2.9
1	A	18	LEU	2.9
2	D	184	GLN	2.9
1	B	180	LEU	2.9
2	D	136	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	172	SER	2.8
2	D	182	SER	2.8
2	D	178	ASP	2.7
1	B	218	LEU	2.7
1	B	166	LYS	2.7
2	D	149	MET	2.7
2	D	299	ILE	2.7
1	B	191	ASP	2.6
1	C	404	ILE	2.6
2	D	402	ALA	2.6
1	B	121	THR	2.6
2	D	165	CYS	2.6
2	D	134	LEU	2.5
1	B	173	LYS	2.5
2	D	119	ILE	2.5
1	B	177	ASP	2.5
1	C	14	GLN	2.5
2	D	131	GLU	2.5
1	B	221	VAL	2.4
1	A	135	LYS	2.4
1	A	140	LEU	2.4
1	A	187	GLN	2.4
2	D	133	GLU	2.4
1	B	174	ILE	2.3
1	B	136	LYS	2.3
1	B	182	SER	2.3
2	D	156	ILE	2.3
1	B	244	PHE	2.3
2	D	170	VAL	2.3
2	D	187	GLN	2.3
1	B	205	SER	2.3
1	B	18	LEU	2.3
1	B	162	LYS	2.3
1	B	169	GLU	2.3
1	B	190	ALA	2.2
1	B	154	GLU	2.2
1	B	188	LYS	2.2
1	B	118	GLU	2.2
2	D	213	GLY	2.2
1	B	199	ASN	2.1
1	A	159	LEU	2.1
1	B	196	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	143	THR	2.1
2	D	145	ASP	2.1
1	B	171	GLY	2.1
1	B	137	GLY	2.1
1	B	175	TYR	2.1
2	D	155	ASN	2.0
2	D	72	ALA	2.0
2	D	206	LYS	2.0
1	B	139	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SER	C	1532	7/7	0.98	0.15	1.38	27,36,44,44	0
3	SER	D	1532	7/7	0.94	0.17	0.91	36,45,47,47	14
3	SER	A	1532	7/7	0.97	0.12	-0.28	26,36,43,43	14
3	SER	B	1532	7/7	0.98	0.11	-0.52	39,41,43,44	0
4	FBP	C	600	20/20	0.98	0.11	-0.69	38,44,47,48	0
4	FBP	A	600	20/20	0.99	0.10	-0.70	35,40,48,48	0
4	FBP	D	600	20/20	0.99	0.10	-1.16	41,46,49,49	0
4	FBP	B	600	20/20	0.99	0.09	-1.30	33,38,45,45	0
5	MG	A	700	1/1	0.89	0.27	-	53,53,53,53	0
5	MG	C	700	1/1	0.55	0.19	-	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.