Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:04 PM GMT

PDB ID	:	3SRH
Title	:	Human M2 pyruvate kinase
Authors	:	Morgan, H.P.; O'Reilly, F.; Palmer, R.; McNae, I.W.; Nowicki, M.W.; Wear, M.A.; Fothergill-Gilmore, L.A.; Walkinshaw, M.D.
Deposited on	:	2011-07-07
Resolution	:	2.60 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 ①) were used in the production of this report:

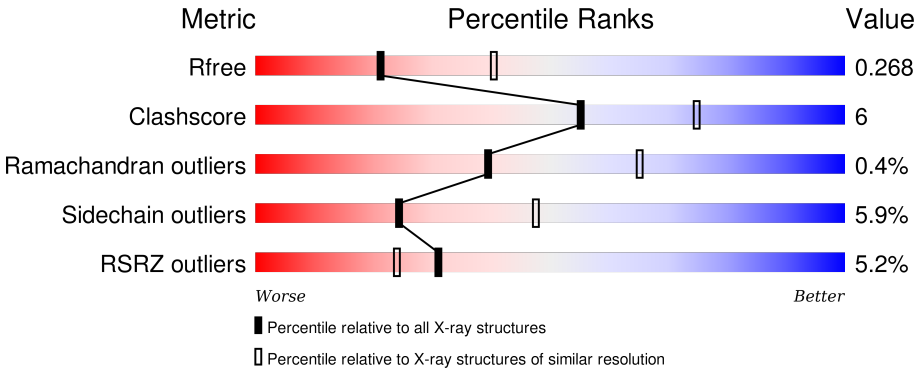
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	551	6% 76% 16% • 6%
1	B	551	9% 76% 16% • 6%
1	C	551	2% 79% 14% • 6%
1	D	551	2% 78% 13% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16232 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	0	0
			3965	2492	704	744	25			
1	C	518	Total	C	N	O	S	0	0	0
			3965	2492	704	744	25			
1	D	518	Total	C	N	O	S	0	0	0
			3965	2492	704	744	25			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP P14618
A	-19	GLY	-	EXPRESSION TAG	UNP P14618
A	-18	SER	-	EXPRESSION TAG	UNP P14618
A	-17	SER	-	EXPRESSION TAG	UNP P14618
A	-16	HIS	-	EXPRESSION TAG	UNP P14618
A	-15	HIS	-	EXPRESSION TAG	UNP P14618
A	-14	HIS	-	EXPRESSION TAG	UNP P14618
A	-13	HIS	-	EXPRESSION TAG	UNP P14618
A	-12	HIS	-	EXPRESSION TAG	UNP P14618
A	-11	HIS	-	EXPRESSION TAG	UNP P14618
A	-10	SER	-	EXPRESSION TAG	UNP P14618
A	-9	SER	-	EXPRESSION TAG	UNP P14618
A	-8	GLY	-	EXPRESSION TAG	UNP P14618
A	-7	LEU	-	EXPRESSION TAG	UNP P14618
A	-6	VAL	-	EXPRESSION TAG	UNP P14618
A	-5	PRO	-	EXPRESSION TAG	UNP P14618
A	-4	ARG	-	EXPRESSION TAG	UNP P14618
A	-3	GLY	-	EXPRESSION TAG	UNP P14618
A	-2	SER	-	EXPRESSION TAG	UNP P14618
A	-1	HIS	-	EXPRESSION TAG	UNP P14618
B	-20	MET	-	EXPRESSION TAG	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	GLY	-	EXPRESSION TAG	UNP P14618
B	-18	SER	-	EXPRESSION TAG	UNP P14618
B	-17	SER	-	EXPRESSION TAG	UNP P14618
B	-16	HIS	-	EXPRESSION TAG	UNP P14618
B	-15	HIS	-	EXPRESSION TAG	UNP P14618
B	-14	HIS	-	EXPRESSION TAG	UNP P14618
B	-13	HIS	-	EXPRESSION TAG	UNP P14618
B	-12	HIS	-	EXPRESSION TAG	UNP P14618
B	-11	HIS	-	EXPRESSION TAG	UNP P14618
B	-10	SER	-	EXPRESSION TAG	UNP P14618
B	-9	SER	-	EXPRESSION TAG	UNP P14618
B	-8	GLY	-	EXPRESSION TAG	UNP P14618
B	-7	LEU	-	EXPRESSION TAG	UNP P14618
B	-6	VAL	-	EXPRESSION TAG	UNP P14618
B	-5	PRO	-	EXPRESSION TAG	UNP P14618
B	-4	ARG	-	EXPRESSION TAG	UNP P14618
B	-3	GLY	-	EXPRESSION TAG	UNP P14618
B	-2	SER	-	EXPRESSION TAG	UNP P14618
B	-1	HIS	-	EXPRESSION TAG	UNP P14618
C	-20	MET	-	EXPRESSION TAG	UNP P14618
C	-19	GLY	-	EXPRESSION TAG	UNP P14618
C	-18	SER	-	EXPRESSION TAG	UNP P14618
C	-17	SER	-	EXPRESSION TAG	UNP P14618
C	-16	HIS	-	EXPRESSION TAG	UNP P14618
C	-15	HIS	-	EXPRESSION TAG	UNP P14618
C	-14	HIS	-	EXPRESSION TAG	UNP P14618
C	-13	HIS	-	EXPRESSION TAG	UNP P14618
C	-12	HIS	-	EXPRESSION TAG	UNP P14618
C	-11	HIS	-	EXPRESSION TAG	UNP P14618
C	-10	SER	-	EXPRESSION TAG	UNP P14618
C	-9	SER	-	EXPRESSION TAG	UNP P14618
C	-8	GLY	-	EXPRESSION TAG	UNP P14618
C	-7	LEU	-	EXPRESSION TAG	UNP P14618
C	-6	VAL	-	EXPRESSION TAG	UNP P14618
C	-5	PRO	-	EXPRESSION TAG	UNP P14618
C	-4	ARG	-	EXPRESSION TAG	UNP P14618
C	-3	GLY	-	EXPRESSION TAG	UNP P14618
C	-2	SER	-	EXPRESSION TAG	UNP P14618
C	-1	HIS	-	EXPRESSION TAG	UNP P14618
D	-20	MET	-	EXPRESSION TAG	UNP P14618
D	-19	GLY	-	EXPRESSION TAG	UNP P14618
D	-18	SER	-	EXPRESSION TAG	UNP P14618

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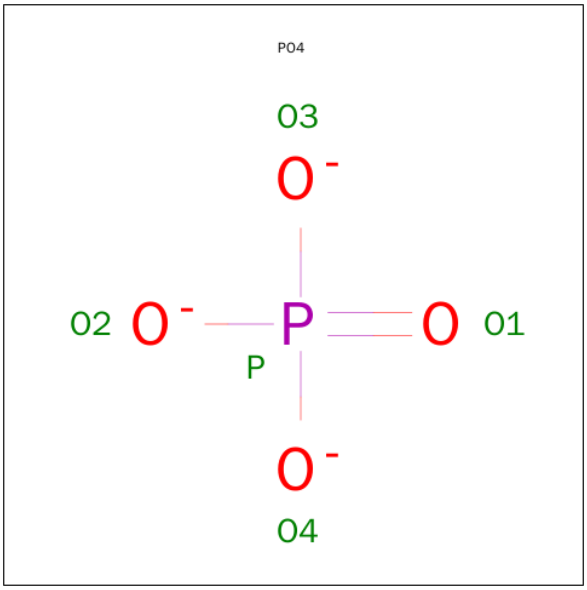
Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	EXPRESSION TAG	UNP P14618
D	-16	HIS	-	EXPRESSION TAG	UNP P14618
D	-15	HIS	-	EXPRESSION TAG	UNP P14618
D	-14	HIS	-	EXPRESSION TAG	UNP P14618
D	-13	HIS	-	EXPRESSION TAG	UNP P14618
D	-12	HIS	-	EXPRESSION TAG	UNP P14618
D	-11	HIS	-	EXPRESSION TAG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

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

- Molecule 3 is water.

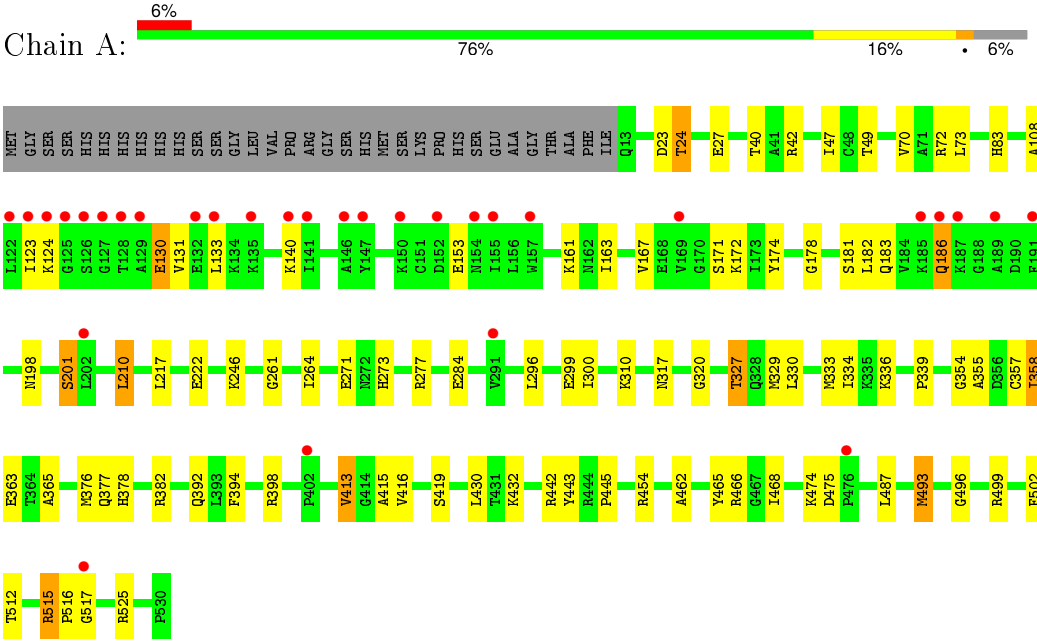
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	126	Total O 126 126	0	0
3	B	57	Total O 57 57	0	0
3	C	60	Total O 60 60	0	0
3	D	114	Total O 114 114	0	0

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.

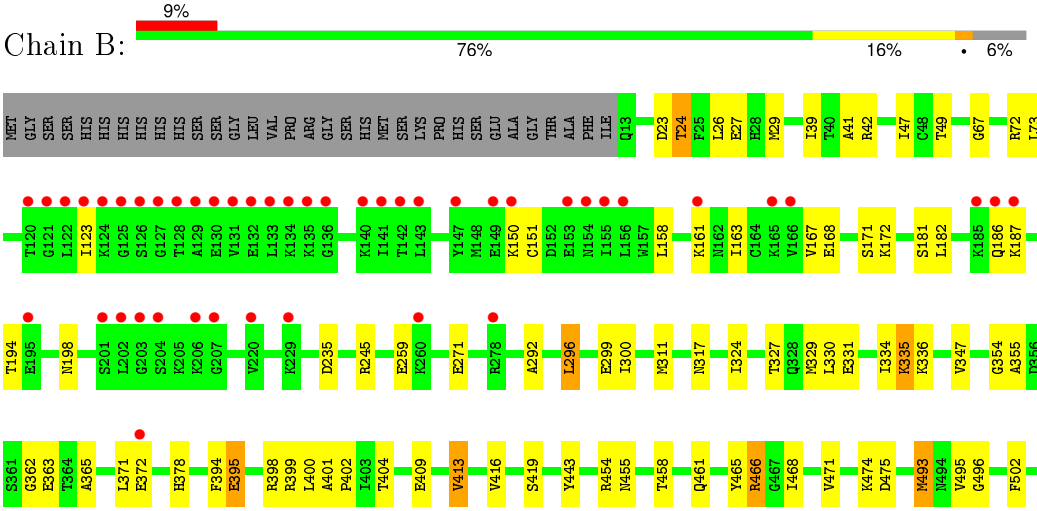
- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain A:



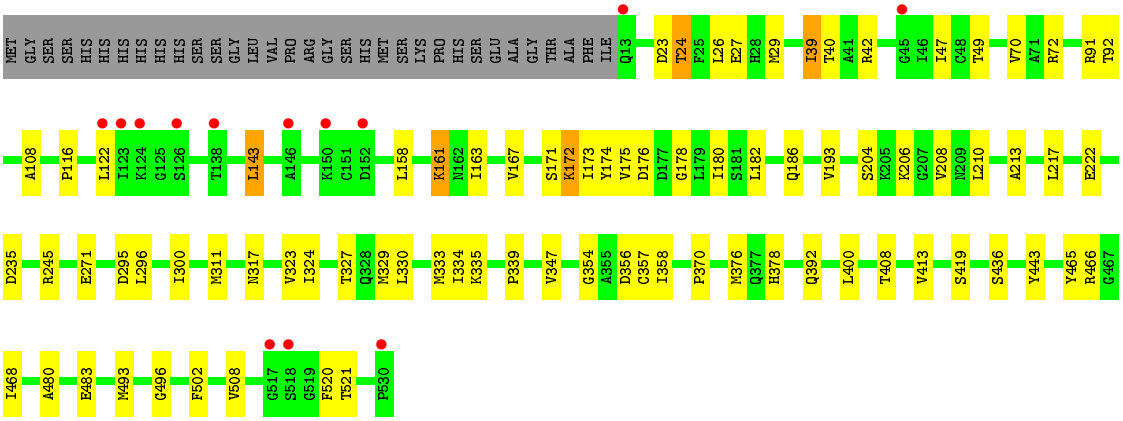
- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain B:



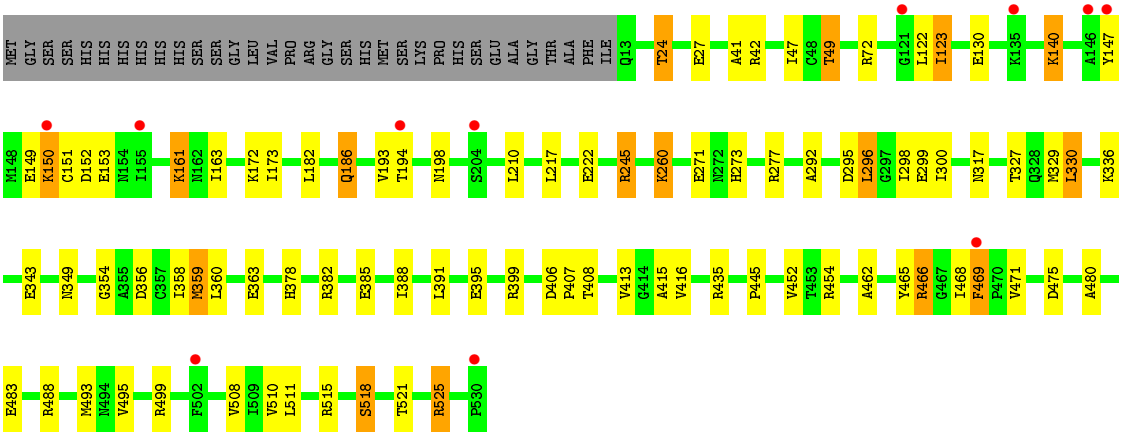
• Molecule 1: Pyruvate kinase isozymes M1/M2

Chain C:



• Molecule 1: Pyruvate kinase isozymes M1/M2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.20Å 154.31Å 98.59Å 90.00° 105.59° 90.00°	Depositor
Resolution (Å)	47.46 – 2.60 44.08 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.46-2.60) 97.9 (44.08-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	5.14 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.270 0.216 , 0.268	Depositor DCC
R_{free} test set	3558 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	55.7	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 70295 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16232	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: PO4

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	0.34	0/4029	0.51	1/5441 (0.0%)
1	B	0.32	0/4029	0.49	0/5441
1	C	0.32	0/4029	0.48	0/5441
1	D	0.33	0/4029	0.50	0/5441
All	All	0.33	0/16116	0.50	1/21764 (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	A	210	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3965	0	4049	56	0
1	B	3965	0	4049	50	0
1	C	3965	0	4049	48	0
1	D	3965	0	4049	56	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	5	0	0	1	0
3	A	126	0	0	3	0
3	B	57	0	0	0	0
3	C	60	0	0	1	0
3	D	114	0	0	0	0
All	All	16232	0	16196	202	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 (202) 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:B:49:THR:HG22	1:B:72:ARG:HD3	1.32	1.08
1:A:329:MET:HE1	1:A:358:ILE:HB	1.47	0.97
1:C:42:ARG:HE	1:C:378:HIS:HD2	1.18	0.88
1:D:42:ARG:HE	1:D:378:HIS:HD2	1.20	0.88
1:D:525:ARG:HH11	1:D:525:ARG:HG3	1.39	0.87
1:A:329:MET:CE	1:A:358:ILE:HB	2.10	0.81
1:A:49:THR:HG22	1:A:72:ARG:HD3	1.63	0.81
1:A:430:LEU:HD23	1:A:512:THR:HG22	1.65	0.79
1:A:273:HIS:HD2	1:A:277:ARG:HH12	1.30	0.77
1:D:49:THR:HG23	1:D:360:LEU:O	1.86	0.75
1:D:329:MET:HE1	1:D:358:ILE:HB	1.69	0.74
1:C:42:ARG:HE	1:C:378:HIS:CD2	2.04	0.73
1:A:49:THR:HG23	1:A:360:LEU:O	1.88	0.73
1:A:24:THR:HG22	1:A:27:GLU:H	1.54	0.73
1:A:273:HIS:CD2	1:A:277:ARG:HH12	2.07	0.73
1:A:49:THR:HG21	1:A:72:ARG:HH11	1.55	0.72
1:B:42:ARG:HE	1:B:378:HIS:HD2	1.36	0.71
1:A:273:HIS:HD2	1:A:277:ARG:NH1	1.89	0.70
1:D:42:ARG:HE	1:D:378:HIS:CD2	2.08	0.70
1:B:493:MET:HE1	1:B:508:VAL:HG21	1.74	0.69
1:B:49:THR:CG2	1:B:72:ARG:HD3	2.17	0.69
1:C:92:THR:HB	3:C:549:HOH:O	1.93	0.69
1:C:49:THR:CG2	1:C:72:ARG:HH11	2.06	0.67
1:B:181:SER:H	1:B:198:ASN:HB2	1.61	0.65
1:D:49:THR:HG21	1:D:72:ARG:HH11	1.59	0.64
1:C:186:GLN:HB2	1:C:193:VAL:HB	1.80	0.64
1:A:327:THR:HG22	3:A:558:HOH:O	1.99	0.63
1:D:415:ALA:HB2	1:D:511:LEU:HD11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:MET:CE	1:D:358:ILE:HB	2.28	0.62
1:D:161:LYS:H	1:D:161:LYS:HD2	1.62	0.62
1:A:493:MET:HE1	1:A:508:VAL:HG21	1.82	0.62
1:C:47:ILE:HG13	1:C:70:VAL:HB	1.81	0.62
1:A:42:ARG:HE	1:A:378:HIS:HD2	1.47	0.61
1:C:408:THR:HG22	1:C:521:THR:H	1.64	0.61
1:C:330:LEU:HD23	1:C:333:MET:SD	2.40	0.61
1:D:260:LYS:HD3	1:D:260:LYS:H	1.66	0.61
1:C:122:LEU:HA	1:C:204:SER:HB2	1.82	0.60
1:C:339:PRO:HG3	1:C:376:MET:HG2	1.83	0.60
1:B:24:THR:HG22	1:B:27:GLU:H	1.64	0.60
1:B:334:ILE:HG23	1:B:335:LYS:HG2	1.82	0.60
1:A:133:LEU:HD13	1:A:153:GLU:HB2	1.83	0.60
1:A:394:PHE:O	1:A:398:ARG:HG2	2.02	0.59
1:D:182:LEU:HB3	1:D:194:THR:HG21	1.84	0.59
1:B:404:THR:HG21	1:B:409:GLU:HB3	1.84	0.59
1:B:394:PHE:O	1:B:398:ARG:HG2	2.04	0.58
1:D:408:THR:HG22	1:D:521:THR:HB	1.86	0.58
1:C:161:LYS:HD3	1:C:161:LYS:H	1.69	0.57
1:D:292:ALA:O	1:D:296:LEU:HB2	2.03	0.57
1:A:23:ASP:HB3	1:B:399:ARG:HH12	1.70	0.57
1:A:49:THR:CG2	1:A:72:ARG:HH11	2.17	0.57
1:D:493:MET:HE2	1:D:493:MET:HA	1.87	0.56
1:A:273:HIS:CD2	1:A:277:ARG:NH1	2.68	0.56
1:B:292:ALA:O	1:B:296:LEU:HB2	2.05	0.56
1:D:24:THR:CG2	1:D:27:GLU:H	2.19	0.56
1:C:496:GLY:HA3	1:C:502:PHE:CZ	2.41	0.55
1:A:317:ASN:HD21	1:A:354:GLY:HA3	1.71	0.55
1:B:296:LEU:HD22	1:B:300:ILE:HG12	1.89	0.55
1:B:454:ARG:NH1	1:B:475:ASP:O	2.40	0.55
1:D:49:THR:HG22	1:D:72:ARG:HD3	1.88	0.55
1:C:116:PRO:HB2	1:C:217:LEU:HD13	1.89	0.54
1:C:39:ILE:HD13	1:C:40:THR:N	2.22	0.54
1:D:24:THR:HG22	1:D:27:GLU:H	1.73	0.54
1:A:47:ILE:CD1	1:A:357:CYS:HB3	2.37	0.54
1:D:465:TYR:HB2	1:D:468:ILE:HD12	1.90	0.54
3:A:571:HOH:O	1:B:398:ARG:HD3	2.07	0.54
1:B:271:GLU:O	1:B:299:GLU:HG3	2.08	0.54
1:A:415:ALA:HB2	1:A:511:LEU:HD21	1.90	0.54
1:A:42:ARG:HE	1:A:378:HIS:CD2	2.25	0.53
1:C:167:VAL:HG13	1:C:171:SER:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:480:ALA:HB3	1:D:483:GLU:HG3	1.90	0.53
1:B:465:TYR:HB2	1:B:468:ILE:HD12	1.90	0.53
1:A:515:ARG:HB2	1:A:516:PRO:HD2	1.91	0.53
1:D:525:ARG:NH1	1:D:525:ARG:HG3	2.15	0.53
1:B:49:THR:HG21	1:B:72:ARG:HH11	1.74	0.53
1:A:116:PRO:HB2	1:A:217:LEU:HD13	1.91	0.53
1:D:471:VAL:HG11	1:D:495:VAL:HG11	1.91	0.52
1:C:49:THR:HG21	1:C:72:ARG:HH11	1.72	0.52
1:D:173:ILE:HB	1:D:182:LEU:HB2	1.91	0.52
1:A:47:ILE:HD12	1:A:357:CYS:HB3	1.91	0.52
1:A:186:GLN:HB2	1:A:193:VAL:HB	1.91	0.52
1:C:271:GLU:HA	1:C:296:LEU:HG	1.91	0.52
1:B:39:ILE:HD12	1:B:41:ALA:HB3	1.92	0.52
1:B:168:GLU:HA	1:B:187:LYS:HE2	1.91	0.51
1:D:415:ALA:CB	1:D:511:LEU:HD11	2.41	0.51
1:D:273:HIS:CE1	1:D:300:ILE:HG22	2.44	0.51
1:B:167:VAL:HG13	1:B:171:SER:HB2	1.91	0.51
1:A:496:GLY:HA3	1:A:502:PHE:CZ	2.45	0.51
1:D:360:LEU:HB3	1:D:363:GLU:HB2	1.94	0.50
1:A:465:TYR:HB2	1:A:468:ILE:HD12	1.91	0.50
1:C:49:THR:HG22	1:C:72:ARG:HH11	1.74	0.50
1:C:493:MET:HE1	1:C:508:VAL:HG21	1.93	0.50
1:B:47:ILE:CD1	1:B:357:CYS:HB3	2.42	0.50
1:C:42:ARG:NE	1:C:378:HIS:HD2	1.97	0.50
1:C:324:ILE:HG13	1:C:357:CYS:HB2	1.94	0.49
1:C:408:THR:CG2	1:C:521:THR:H	2.26	0.49
1:D:388:ILE:HD11	1:D:466:ARG:HH21	1.77	0.49
1:B:329:MET:HE3	1:B:347:VAL:HG22	1.93	0.49
1:C:317:ASN:HD21	1:C:354:GLY:HA3	1.78	0.49
1:B:400:LEU:HD22	1:C:26:LEU:HD23	1.94	0.49
1:B:73:LEU:HD23	1:B:83:HIS:HB3	1.95	0.49
1:B:515:ARG:HG2	1:B:516:PRO:HD2	1.95	0.49
1:A:454:ARG:NH1	1:A:475:ASP:O	2.46	0.49
1:A:130:GLU:HG2	1:A:201:SER:OG	2.13	0.48
1:A:339:PRO:HG3	1:A:376:MET:HG2	1.95	0.48
1:B:29:MET:O	1:C:311:MET:HA	2.12	0.48
1:D:416:VAL:HG13	1:D:445:PRO:HB3	1.95	0.48
1:B:496:GLY:HA3	1:B:502:PHE:CZ	2.48	0.48
1:D:356:ASP:HA	1:D:466:ARG:HB2	1.94	0.48
1:B:360:LEU:HB3	1:B:363:GLU:HB2	1.94	0.48
1:C:480:ALA:HB3	1:C:483:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ALA:O	1:A:466:ARG:NH1	2.45	0.48
1:C:465:TYR:HB2	1:C:468:ILE:HD12	1.96	0.47
1:A:174:TYR:HB3	1:A:178:GLY:HA2	1.96	0.47
1:B:317:ASN:HD21	1:B:354:GLY:HA3	1.79	0.47
1:D:493:MET:HE3	1:D:508:VAL:HG21	1.96	0.47
1:B:413:VAL:HG13	1:B:443:TYR:CZ	2.49	0.47
1:A:70:VAL:HG22	1:A:108:ALA:HB3	1.96	0.47
1:B:42:ARG:HE	1:B:378:HIS:CD2	2.24	0.47
1:A:273:HIS:CE1	1:A:300:ILE:HG22	2.50	0.47
1:D:49:THR:CG2	1:D:72:ARG:HH11	2.25	0.46
1:B:324:ILE:HG13	1:B:357:CYS:HB2	1.96	0.46
1:C:23:ASP:HB3	1:D:399:ARG:HH12	1.80	0.46
1:C:49:THR:HG22	1:C:72:ARG:HD3	1.97	0.46
1:B:26:LEU:HD23	1:C:400:LEU:HD22	1.98	0.46
1:A:49:THR:HG21	1:A:72:ARG:NH1	2.26	0.46
1:C:24:THR:CG2	1:C:27:GLU:H	2.29	0.46
1:D:182:LEU:HB3	1:D:194:THR:CG2	2.46	0.46
1:C:329:MET:HE3	1:C:347:VAL:HG22	1.98	0.46
1:A:462:ALA:HB1	1:A:468:ILE:HG21	1.98	0.46
1:B:455:ASN:HB3	1:B:458:THR:HB	1.98	0.45
1:B:182:LEU:HB3	1:B:194:THR:HG21	1.97	0.45
1:A:333:MET:HA	1:A:336:LYS:O	2.16	0.45
1:D:140:LYS:N	1:D:140:LYS:HE3	2.31	0.45
1:B:311:MET:HA	1:C:29:MET:O	2.16	0.45
1:D:462:ALA:HB1	1:D:468:ILE:HG21	1.98	0.45
1:D:123:ILE:HA	1:D:151:CYS:HB2	1.98	0.45
1:C:323:VAL:H	1:C:356:ASP:HB2	1.82	0.45
1:D:510:VAL:HB	1:D:525:ARG:HB2	1.98	0.45
1:D:518:SER:HB2	2:D:531:PO4:O1	2.16	0.45
1:C:329:MET:HE2	1:C:358:ILE:HB	1.98	0.45
1:B:416:VAL:O	1:B:419:SER:HB3	2.17	0.44
1:D:186:GLN:HB2	1:D:193:VAL:HB	2.00	0.44
1:A:261:GLY:HA2	1:A:264:ILE:HD13	1.98	0.44
1:C:176:ASP:HB2	1:C:206:LYS:HG2	2.00	0.44
1:B:395:GLU:O	1:B:399:ARG:HG2	2.17	0.43
1:B:123:ILE:HG13	1:B:151:CYS:HB2	2.00	0.43
1:D:41:ALA:O	1:D:382:ARG:HG2	2.19	0.43
1:A:49:THR:CG2	1:A:72:ARG:HD3	2.41	0.43
1:D:295:ASP:HA	1:D:298:ILE:HD12	2.00	0.43
1:C:210:LEU:HB3	1:C:213:ALA:HB3	1.99	0.43
1:B:362:GLY:HA2	1:B:365:ALA:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:ALA:HA	1:B:402:PRO:HD3	1.87	0.43
1:A:310:LYS:NZ	1:D:349:ASN:HD21	2.16	0.43
1:B:471:VAL:HG11	1:B:495:VAL:HG11	2.01	0.43
1:D:47:ILE:HB	1:D:359:MET:HB2	2.00	0.43
1:D:385:GLU:HA	1:D:388:ILE:HD12	2.01	0.43
1:A:182:LEU:HB3	1:A:194:THR:HG21	2.00	0.43
1:C:413:VAL:HG22	1:C:443:TYR:CE2	2.53	0.43
1:A:416:VAL:O	1:A:419:SER:HB3	2.18	0.43
1:B:355:ALA:O	1:B:466:ARG:NH1	2.51	0.43
1:D:271:GLU:O	1:D:299:GLU:HG3	2.19	0.43
1:D:317:ASN:HD21	1:D:354:GLY:HA3	1.84	0.43
1:B:329:MET:CE	1:B:358:ILE:HB	2.48	0.42
1:B:515:ARG:HD3	1:B:520:PHE:CE1	2.55	0.42
1:D:122:LEU:HD12	1:D:149:GLU:HG2	2.00	0.42
1:A:182:LEU:HB3	1:A:194:THR:CG2	2.49	0.42
1:D:330:LEU:HD12	1:D:343:GLU:HB3	2.02	0.42
1:C:91:ARG:NH2	1:C:235:ASP:O	2.53	0.42
1:A:320:GLY:HA2	3:A:594:HOH:O	2.19	0.42
1:B:529:VAL:HA	1:B:530:PRO:HD3	1.94	0.42
1:D:24:THR:HG22	1:D:27:GLU:HB3	2.01	0.42
1:C:143:LEU:HG	1:C:161:LYS:HA	2.02	0.42
1:C:296:LEU:O	1:C:300:ILE:HG12	2.20	0.42
1:B:515:ARG:O	1:B:517:GLY:N	2.50	0.42
1:C:174:TYR:HB3	1:C:178:GLY:HA2	2.01	0.42
1:D:469:PHE:HE2	1:D:499:ARG:HH21	1.67	0.42
1:A:181:SER:H	1:A:198:ASN:HB2	1.83	0.42
1:D:217:LEU:O	1:D:245:ARG:NH2	2.51	0.41
1:A:23:ASP:OD2	1:A:23:ASP:N	2.49	0.41
1:A:271:GLU:O	1:A:299:GLU:HG3	2.20	0.41
1:C:175:VAL:HB	1:C:180:ILE:HB	2.03	0.41
1:A:416:VAL:HG13	1:A:445:PRO:HB3	2.01	0.41
1:A:167:VAL:HG13	1:A:171:SER:HB2	2.03	0.41
1:A:413:VAL:HG13	1:A:443:TYR:CZ	2.55	0.41
1:C:70:VAL:HG22	1:C:108:ALA:HB3	2.01	0.41
1:C:158:LEU:HD22	1:C:208:VAL:HG21	2.03	0.41
1:D:406:ASP:HA	1:D:407:PRO:HD2	1.89	0.41
1:D:24:THR:HG22	1:D:27:GLU:CB	2.51	0.41
1:D:452:VAL:HG11	1:D:488:ARG:HB3	2.01	0.41
1:A:49:THR:OG1	1:A:365:ALA:HB2	2.20	0.41
1:D:147:TYR:HA	1:D:150:LYS:HG3	2.03	0.41
1:B:186:GLN:HB3	1:B:193:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:ASP:OD2	1:D:153:GLU:HG2	2.21	0.41
1:A:73:LEU:HD23	1:A:83:HIS:ND1	2.35	0.41
1:D:454:ARG:NH1	1:D:475:ASP:O	2.44	0.41
1:B:91:ARG:HH22	1:B:235:ASP:HB3	1.84	0.41
1:C:271:GLU:HB2	1:C:295:ASP:HB2	2.02	0.41
1:C:172:LYS:HE3	1:C:172:LYS:HB2	1.96	0.40
1:A:123:ILE:HG21	1:A:131:VAL:HG23	2.03	0.40
1:A:360:LEU:HB3	1:A:363:GLU:HB2	2.04	0.40
1:A:525:ARG:HD2	1:B:523:THR:HG22	2.03	0.40
1:C:173:ILE:HB	1:C:182:LEU:HB2	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	516/551 (94%)	500 (97%)	14 (3%)	2 (0%)	39	65
1	B	516/551 (94%)	491 (95%)	23 (4%)	2 (0%)	39	65
1	C	516/551 (94%)	498 (96%)	15 (3%)	3 (1%)	30	56
1	D	516/551 (94%)	500 (97%)	15 (3%)	1 (0%)	52	77
All	All	2064/2204 (94%)	1989 (96%)	67 (3%)	8 (0%)	39	65

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	517	GLY
1	C	327	THR
1	B	327	THR
1	C	520	PHE
1	D	327	THR

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Mol	Chain	Res	Type
1	A	327	THR
1	C	370	PRO
1	B	67	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	426/453 (94%)	394 (92%)	32 (8%)	17	33
1	B	426/453 (94%)	401 (94%)	25 (6%)	24	47
1	C	426/453 (94%)	412 (97%)	14 (3%)	45	73
1	D	426/453 (94%)	397 (93%)	29 (7%)	20	39
All	All	1704/1812 (94%)	1604 (94%)	100 (6%)	24	47

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	40	THR
1	A	124	LYS
1	A	130	GLU
1	A	140	LYS
1	A	161	LYS
1	A	163	ILE
1	A	172	LYS
1	A	183	GLN
1	A	186	GLN
1	A	194	THR
1	A	201	SER
1	A	210	LEU
1	A	222	GLU
1	A	246	LYS
1	A	284	GLU
1	A	296	LEU
1	A	330	LEU

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Mol	Chain	Res	Type
1	A	334	ILE
1	A	358	ILE
1	A	361	SER
1	A	377	GLN
1	A	382	ARG
1	A	392	GLN
1	A	413	VAL
1	A	432	LYS
1	A	442	ARG
1	A	474	LYS
1	A	487	LEU
1	A	493	MET
1	A	499	ARG
1	A	515	ARG
1	B	23	ASP
1	B	24	THR
1	B	150	LYS
1	B	158	LEU
1	B	161	LYS
1	B	163	ILE
1	B	172	LYS
1	B	245	ARG
1	B	259	GLU
1	B	296	LEU
1	B	330	LEU
1	B	331	GLU
1	B	335	LYS
1	B	336	LYS
1	B	358	ILE
1	B	371	LEU
1	B	372	GLU
1	B	395	GLU
1	B	413	VAL
1	B	461	GLN
1	B	466	ARG
1	B	474	LYS
1	B	493	MET
1	B	515	ARG
1	B	520	PHE
1	C	24	THR
1	C	39	ILE
1	C	143	LEU

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Mol	Chain	Res	Type
1	C	161	LYS
1	C	163	ILE
1	C	172	LYS
1	C	222	GLU
1	C	245	ARG
1	C	334	ILE
1	C	335	LYS
1	C	392	GLN
1	C	419	SER
1	C	436	SER
1	C	466	ARG
1	D	24	THR
1	D	49	THR
1	D	123	ILE
1	D	130	GLU
1	D	140	LYS
1	D	150	LYS
1	D	161	LYS
1	D	163	ILE
1	D	172	LYS
1	D	186	GLN
1	D	198	ASN
1	D	210	LEU
1	D	222	GLU
1	D	245	ARG
1	D	260	LYS
1	D	277	ARG
1	D	296	LEU
1	D	330	LEU
1	D	336	LYS
1	D	359	MET
1	D	391	LEU
1	D	395	GLU
1	D	413	VAL
1	D	435	ARG
1	D	466	ARG
1	D	469	PHE
1	D	515	ARG
1	D	518	SER
1	D	525	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	186	GLN
1	A	209	ASN
1	A	273	HIS
1	A	317	ASN
1	A	349	ASN
1	A	377	GLN
1	A	378	HIS
1	B	154	ASN
1	B	198	ASN
1	B	263	ASN
1	B	317	ASN
1	B	349	ASN
1	B	378	HIS
1	B	392	GLN
1	C	263	ASN
1	C	317	ASN
1	C	349	ASN
1	C	378	HIS
1	C	392	GLN
1	D	183	GLN
1	D	209	ASN
1	D	263	ASN
1	D	273	HIS
1	D	317	ASN
1	D	349	ASN
1	D	378	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)

3 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	PO4	A	531	-	4,4,4	0.52	0	6,6,6	0.27	0
2	PO4	B	531	-	4,4,4	0.50	0	6,6,6	0.27	0
2	PO4	D	531	-	4,4,4	0.55	0	6,6,6	0.27	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	PO4	A	531	-	-	0/0/0/0	0/0/0/0
2	PO4	B	531	-	-	0/0/0/0	0/0/0/0
2	PO4	D	531	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	531	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	518/551 (94%)	0.15	34 (6%)	22	16	34, 53, 117, 128	0
1	B	518/551 (94%)	0.49	49 (9%)	10	6	44, 82, 149, 171	0
1	C	518/551 (94%)	0.16	13 (2%)	61	54	47, 76, 115, 129	0
1	D	518/551 (94%)	-0.12	11 (2%)	67	61	36, 59, 108, 117	0
All	All	2072/2204 (94%)	0.17	107 (5%)	31	24	34, 67, 122, 171	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	121	GLY	7.3
1	B	124	LYS	7.0
1	B	123	ILE	6.9
1	C	150	LYS	6.7
1	B	125	GLY	6.5
1	B	126	SER	5.4
1	B	130	GLU	5.4
1	B	202	LEU	5.1
1	A	133	LEU	5.0
1	B	131	VAL	5.0
1	A	147	TYR	4.9
1	D	530	PRO	4.9
1	B	122	LEU	4.7
1	B	133	LEU	4.7
1	D	146	ALA	4.6
1	B	129	ALA	4.6
1	A	169	VAL	4.5
1	B	120	THR	4.4
1	B	128	THR	4.4
1	A	126	SER	4.2
1	B	134	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	191	PHE	4.0
1	A	517	GLY	4.0
1	B	142	THR	3.9
1	B	186	GLN	3.9
1	B	166	VAL	3.9
1	A	193	VAL	3.9
1	B	127	GLY	3.9
1	B	150	LYS	3.8
1	B	201	SER	3.7
1	B	204	SER	3.7
1	B	207	GLY	3.7
1	A	122	LEU	3.7
1	B	206	LYS	3.6
1	C	518	SER	3.6
1	A	202	LEU	3.5
1	C	517	GLY	3.5
1	A	123	ILE	3.5
1	A	189	ALA	3.4
1	A	155	ILE	3.4
1	B	185	LYS	3.4
1	C	146	ALA	3.2
1	A	127	GLY	3.2
1	B	141	ILE	3.2
1	B	187	LYS	3.2
1	B	190	ASP	3.0
1	D	147	TYR	3.0
1	A	124	LYS	2.9
1	B	260	LYS	2.9
1	B	195	GLU	2.9
1	A	129	ALA	2.8
1	A	152	ASP	2.8
1	A	150	LYS	2.7
1	D	155	ILE	2.7
1	A	140	LYS	2.7
1	B	147	TYR	2.7
1	A	195	GLU	2.7
1	B	372	GLU	2.7
1	A	121	GLY	2.6
1	A	128	THR	2.6
1	B	140	LYS	2.6
1	B	161	LYS	2.5
1	A	186	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	126	SER	2.5
1	A	125	GLY	2.5
1	A	185	LYS	2.4
1	B	143	LEU	2.4
1	B	136	GLY	2.4
1	B	155	ILE	2.4
1	B	220	VAL	2.4
1	B	156	LEU	2.4
1	B	132	GLU	2.4
1	C	122	LEU	2.4
1	C	530	PRO	2.4
1	C	124	LYS	2.4
1	A	191	PHE	2.3
1	C	123	ILE	2.3
1	D	194	THR	2.3
1	B	135	LYS	2.3
1	B	203	GLY	2.3
1	C	152	ASP	2.3
1	A	132	GLU	2.3
1	C	138	THR	2.3
1	A	187	LYS	2.3
1	A	157	TRP	2.2
1	B	153	GLU	2.2
1	B	192	LEU	2.2
1	B	154	ASN	2.2
1	B	149	GLU	2.2
1	D	204	SER	2.2
1	D	502	PHE	2.2
1	A	402	PRO	2.2
1	A	476	PRO	2.2
1	A	141	ILE	2.2
1	A	154	ASN	2.2
1	B	165	LYS	2.1
1	A	146	ALA	2.1
1	B	229	LYS	2.1
1	A	291	VAL	2.1
1	D	150	LYS	2.1
1	D	121	GLY	2.1
1	B	278	ARG	2.1
1	D	135	LYS	2.1
1	C	45	GLY	2.0
1	A	135	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	469	PHE	2.0
1	C	13	GLN	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	PO4	D	531	5/5	0.97	0.16	0.42	50,51,51,51	0
2	PO4	A	531	5/5	0.98	0.14	-0.55	65,65,65,65	0
2	PO4	B	531	5/5	0.93	0.14	-1.11	116,116,117,117	0

6.5 Other polymers (i)

There are no such residues in this entry.