



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:08 pm GMT

PDB ID : 4J05
Title : Crystal structure of a eukaryotic phosphate transporter
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Deposited on : 2013-01-30
Resolution : 2.90 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

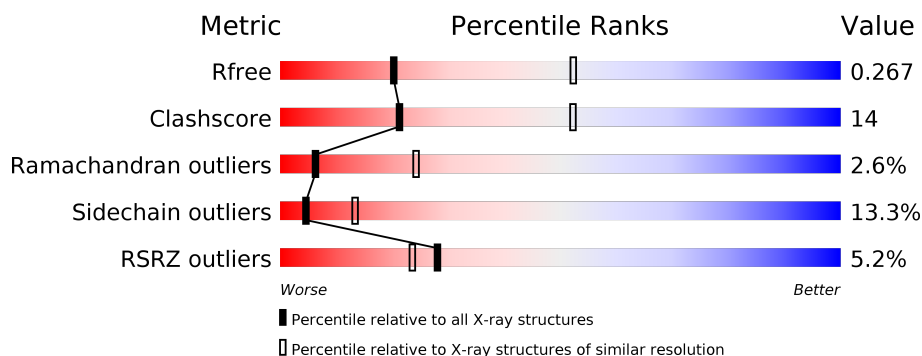
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	530	
1	B	530	

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
2	PO4	A	600	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6590 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.

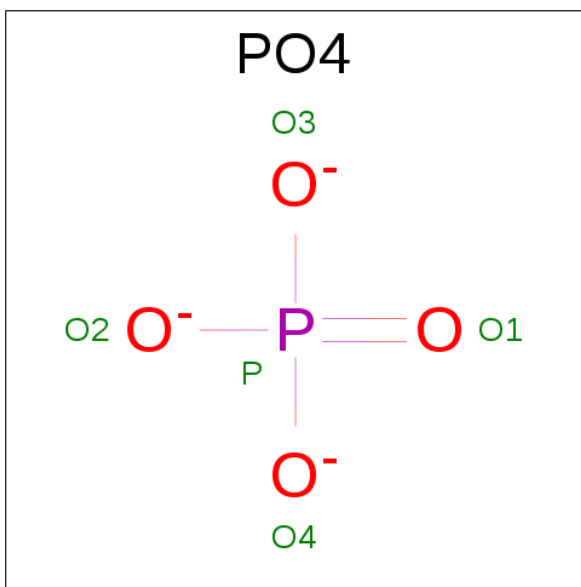
- Molecule 1 is a protein called Phosphate transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3290	2173	543	558	16			
1	B	422	Total	C	N	O	S	0	0	0
			3290	2173	543	558	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP A8N031
A	0	PRO	-	EXPRESSION TAG	UNP A8N031
A	523	GLY	-	EXPRESSION TAG	UNP A8N031
A	524	GLY	-	EXPRESSION TAG	UNP A8N031
A	525	LEU	-	EXPRESSION TAG	UNP A8N031
A	526	VAL	-	EXPRESSION TAG	UNP A8N031
A	527	PRO	-	EXPRESSION TAG	UNP A8N031
A	528	ARG	-	EXPRESSION TAG	UNP A8N031
B	-1	GLY	-	EXPRESSION TAG	UNP A8N031
B	0	PRO	-	EXPRESSION TAG	UNP A8N031
B	523	GLY	-	EXPRESSION TAG	UNP A8N031
B	524	GLY	-	EXPRESSION TAG	UNP A8N031
B	525	LEU	-	EXPRESSION TAG	UNP A8N031
B	526	VAL	-	EXPRESSION TAG	UNP A8N031
B	527	PRO	-	EXPRESSION TAG	UNP A8N031
B	528	ARG	-	EXPRESSION TAG	UNP A8N031

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

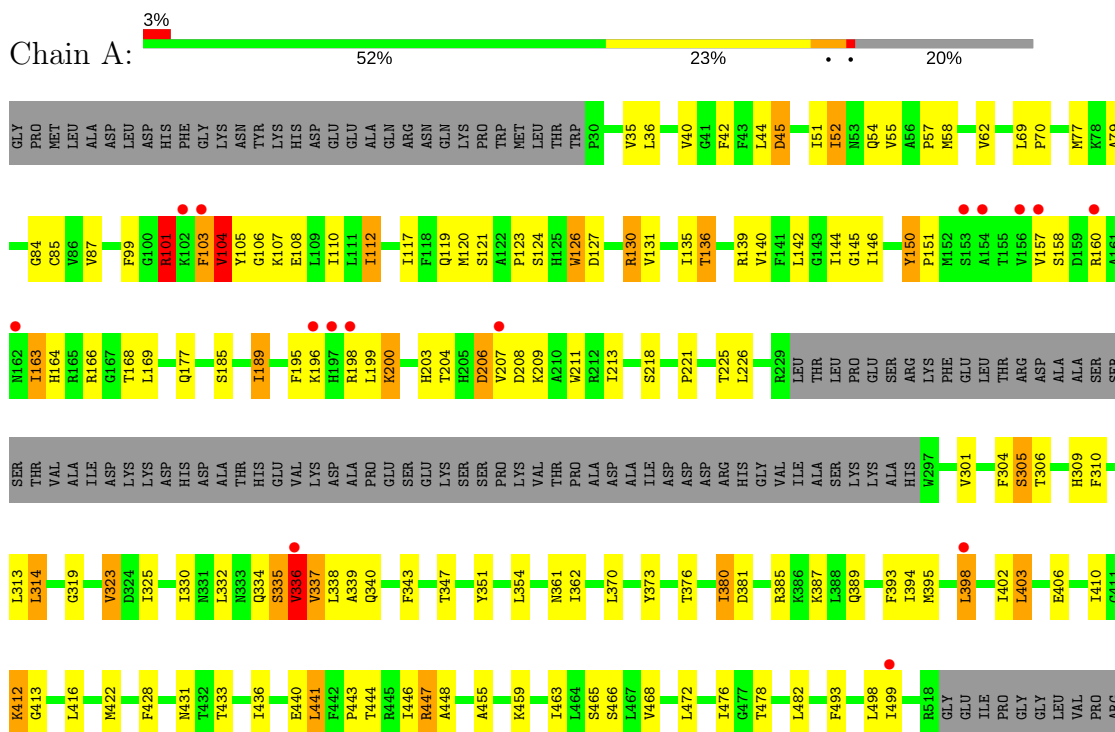


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

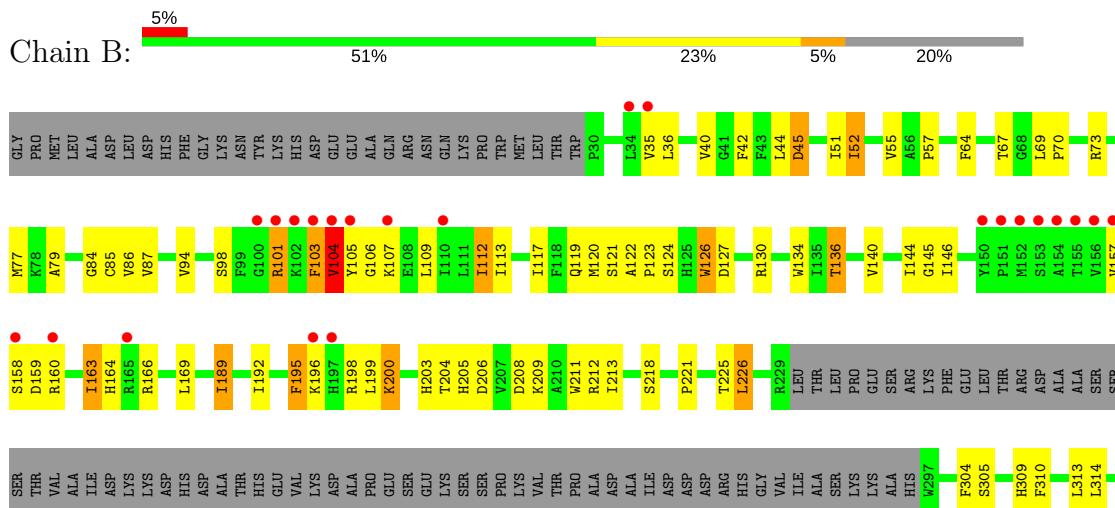
3 Residue-property plots

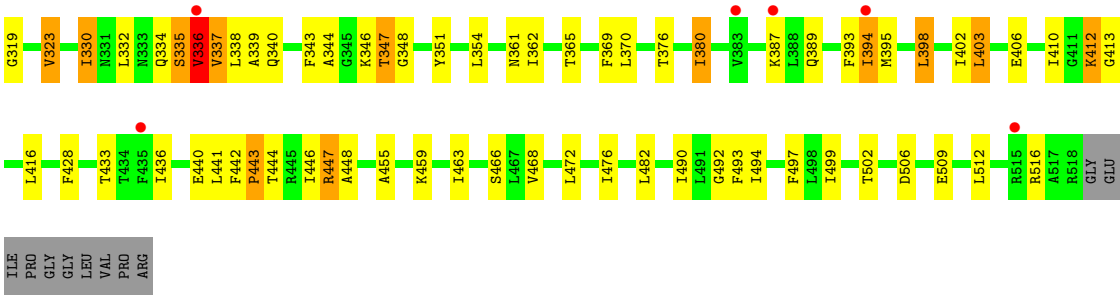
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Phosphate transporter



• Molecule 1: Phosphate transporter





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	174.51Å 174.51Å 173.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	69.00 – 2.90 75.21 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.6 (69.00-2.90) 93.6 (75.21-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.222 , 0.259 0.229 , 0.267	Depositor DCC
R_{free} test set	1980 reflections (4.86%)	DCC
Wilson B-factor (Å ²)	81.2	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 96.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6590	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.57	0/3373	0.70	0/4567
1	B	0.53	0/3373	0.68	0/4567
All	All	0.55	0/6746	0.69	0/9134

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	3290	0	3342	93	0
1	B	3290	0	3342	88	0
2	A	5	0	0	2	0
2	B	5	0	0	0	0
All	All	6590	0	6684	181	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 14.

All (181) 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:406:GLU:HB3	1:B:410:ILE:HD12	1.50	0.91
1:A:85:CYS:SG	1:A:459:LYS:NZ	2.45	0.89
1:A:335:SER:O	1:A:337:VAL:N	2.12	0.82
1:A:406:GLU:HB3	1:A:410:ILE:HD12	1.62	0.81
1:B:335:SER:O	1:B:337:VAL:N	2.17	0.78
1:B:389:GLN:HB2	1:B:433:THR:HG21	1.65	0.75
1:B:335:SER:OG	1:B:336:VAL:N	2.21	0.74
1:A:101:ARG:HB2	1:A:107:LYS:HZ1	1.55	0.72
1:A:196:LYS:HB2	1:A:351:TYR:CD1	2.24	0.72
1:B:189:ILE:HD11	1:B:362:ILE:HD13	1.72	0.72
1:A:389:GLN:HB2	1:A:433:THR:HG21	1.71	0.71
1:A:196:LYS:HE3	1:A:200:LYS:HD3	1.72	0.71
1:B:157:VAL:HG13	1:B:169:LEU:HD23	1.73	0.71
1:B:376:THR:O	1:B:380:ILE:HG12	1.91	0.70
1:A:117:ILE:O	1:A:121:SER:OG	2.08	0.70
1:B:196:LYS:HE3	1:B:200:LYS:HD3	1.75	0.69
1:A:412:LYS:HD2	1:A:413:GLY:H	1.58	0.69
1:A:196:LYS:HE2	1:A:354:LEU:HD12	1.74	0.69
1:A:335:SER:OG	1:A:336:VAL:N	2.22	0.68
1:B:103:PHE:O	1:B:105:TYR:N	2.27	0.68
1:A:209:LYS:O	1:A:213:ILE:HG13	1.95	0.67
1:A:77:MET:HA	1:A:136:THR:HB	1.78	0.66
1:B:209:LYS:O	1:B:213:ILE:HG13	1.96	0.66
1:B:412:LYS:HD2	1:B:413:GLY:H	1.61	0.66
1:A:44:LEU:HD21	1:A:112:ILE:HD11	1.79	0.65
1:B:376:THR:OG1	1:B:428:PHE:O	2.14	0.65
1:B:159:ASP:OD2	1:B:444:THR:OG1	2.10	0.64
1:B:79:ALA:HB2	1:B:466:SER:HB3	1.79	0.64
1:A:158:SER:OG	1:A:447:ARG:NH1	2.32	0.63
1:A:103:PHE:O	1:A:105:TYR:N	2.30	0.63
1:A:431:ASN:ND2	2:A:600:PO4:O1	2.31	0.63
1:B:196:LYS:HA	1:B:200:LYS:HB2	1.81	0.63
1:A:101:ARG:HB2	1:A:107:LYS:NZ	2.14	0.63
1:B:117:ILE:O	1:B:121:SER:OG	2.15	0.62
1:A:200:LYS:HE2	1:A:204:THR:HA	1.82	0.62
1:B:196:LYS:HB2	1:B:351:TYR:CD1	2.35	0.62
1:B:94:VAL:O	1:B:98:SER:N	2.27	0.61
1:A:200:LYS:HZ1	1:A:206:ASP:N	1.98	0.61
1:B:196:LYS:HE2	1:B:354:LEU:HD12	1.82	0.61
1:A:200:LYS:NZ	1:A:207:VAL:HG12	2.16	0.61
1:A:189:ILE:HD11	1:A:362:ILE:HD13	1.81	0.61
1:B:105:TYR:O	1:B:107:LYS:N	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:SER:O	1:B:221:PRO:HD2	2.02	0.60
1:B:45:ASP:HB3	1:B:146:ILE:HG12	1.83	0.60
1:A:36:LEU:O	1:A:40:VAL:HG23	2.02	0.59
1:A:441:LEU:HD11	1:A:499:ILE:HD12	1.84	0.59
1:A:45:ASP:HB3	1:A:146:ILE:HG12	1.84	0.59
1:A:459:LYS:O	1:A:463:ILE:HG23	2.03	0.59
1:B:57:PRO:HD3	1:B:336:VAL:HG22	1.84	0.59
1:A:57:PRO:HD3	1:A:336:VAL:HG22	1.84	0.58
1:A:306:THR:HB	1:A:309:HIS:HB2	1.86	0.58
1:B:338:LEU:C	1:B:340:GLN:H	2.07	0.58
1:B:117:ILE:HA	1:B:120:MET:HE3	1.87	0.57
1:A:79:ALA:HB2	1:A:466:SER:HB3	1.86	0.56
1:A:140:VAL:O	1:A:144:ILE:HG13	2.06	0.56
1:B:338:LEU:O	1:B:340:GLN:N	2.38	0.56
1:A:335:SER:C	1:A:337:VAL:H	2.09	0.56
1:A:110:ILE:HG22	1:A:226:LEU:HD11	1.87	0.56
1:A:126:TRP:HB3	1:A:131:VAL:HG23	1.88	0.56
1:A:304:PHE:HA	1:A:309:HIS:O	2.06	0.55
1:B:77:MET:HA	1:B:136:THR:HB	1.89	0.55
1:B:158:SER:OG	1:B:447:ARG:NH1	2.41	0.54
1:B:44:LEU:HD21	1:B:112:ILE:HD11	1.88	0.54
1:A:168:THR:OG1	1:A:381:ASP:OD2	2.23	0.54
1:B:163:ILE:HG23	1:B:164:HIS:O	2.07	0.54
1:A:218:SER:O	1:A:221:PRO:HD2	2.08	0.54
1:A:177:GLN:OE1	1:A:373:TYR:OH	2.17	0.54
1:A:335:SER:HB2	1:A:361:ASN:HD21	1.73	0.54
1:B:335:SER:C	1:B:337:VAL:H	2.12	0.54
1:B:412:LYS:HD2	1:B:413:GLY:N	2.23	0.54
1:A:104:VAL:HG12	1:A:107:LYS:HD2	1.89	0.53
1:A:177:GLN:NE2	2:A:600:PO4:O4	2.37	0.53
1:A:319:GLY:O	1:A:323:VAL:HG22	2.08	0.53
1:B:36:LEU:O	1:B:40:VAL:HG23	2.09	0.53
1:B:444:THR:HA	1:B:447:ARG:HB3	1.90	0.53
1:A:338:LEU:O	1:A:340:GLN:N	2.42	0.52
1:A:108:GLU:N	1:A:108:GLU:OE1	2.39	0.52
1:A:150:TYR:HB3	1:A:151:PRO:HD3	1.92	0.52
1:A:335:SER:C	1:A:337:VAL:N	2.64	0.52
1:A:376:THR:OG1	1:A:428:PHE:O	2.24	0.52
1:B:459:LYS:O	1:B:463:ILE:HG23	2.10	0.52
1:A:338:LEU:C	1:A:340:GLN:H	2.12	0.52
1:B:455:ALA:O	1:B:459:LYS:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:TYR:O	1:A:107:LYS:N	2.36	0.51
1:A:200:LYS:HE3	1:A:206:ASP:HB2	1.91	0.51
1:B:122:ALA:HB2	1:B:134:TRP:CD1	2.45	0.50
1:A:447:ARG:HG3	1:A:448:ALA:N	2.27	0.50
1:B:104:VAL:HG12	1:B:107:LYS:HD2	1.93	0.50
1:A:112:ILE:HB	1:A:142:LEU:HD12	1.92	0.50
1:A:412:LYS:HD2	1:A:413:GLY:N	2.27	0.50
1:A:376:THR:O	1:A:380:ILE:HG12	2.11	0.50
1:B:208:ASP:OD1	1:B:211:TRP:NE1	2.40	0.50
1:B:394:ILE:HD12	1:B:493:PHE:CE1	2.47	0.50
1:B:472:LEU:O	1:B:476:ILE:HG22	2.11	0.50
1:B:335:SER:HB2	1:B:361:ASN:HD21	1.77	0.49
1:A:108:GLU:O	1:A:112:ILE:HG23	2.12	0.49
1:B:64:PHE:HB3	1:B:67:THR:O	2.13	0.49
1:B:200:LYS:HE3	1:B:206:ASP:HB2	1.94	0.49
1:A:394:ILE:HD12	1:A:493:PHE:CE1	2.48	0.49
1:B:494:ILE:O	1:B:497:PHE:HB2	2.12	0.49
1:B:196:LYS:HD2	1:B:351:TYR:HD1	1.77	0.48
1:A:398:LEU:O	1:A:402:ILE:HG13	2.13	0.48
1:A:58:MET:O	1:A:62:VAL:HG23	2.13	0.48
1:B:335:SER:C	1:B:337:VAL:N	2.67	0.48
1:B:200:LYS:HE2	1:B:204:THR:HA	1.93	0.48
1:B:199:LEU:HD12	1:B:203:HIS:ND1	2.29	0.48
1:B:330:ILE:O	1:B:334:GLN:N	2.47	0.48
1:B:319:GLY:O	1:B:323:VAL:HG22	2.13	0.47
1:B:490:ILE:O	1:B:493:PHE:HB3	2.14	0.47
1:B:440:GLU:OE1	1:B:502:THR:OG1	2.19	0.47
1:A:112:ILE:HG22	1:A:145:GLY:HA3	1.95	0.47
1:A:455:ALA:O	1:A:459:LYS:HG2	2.15	0.47
1:A:314:LEU:HB3	1:A:498:LEU:HD13	1.96	0.47
1:A:52:ILE:HD11	1:A:332:LEU:HD22	1.95	0.47
1:B:304:PHE:HA	1:B:309:HIS:O	2.14	0.47
1:B:52:ILE:HD11	1:B:332:LEU:HD22	1.95	0.47
1:B:87:VAL:HG13	1:B:144:ILE:HG12	1.96	0.47
1:B:109:LEU:HD23	1:B:226:LEU:HD23	1.95	0.47
1:A:330:ILE:O	1:A:334:GLN:N	2.47	0.47
1:A:301:VAL:O	1:A:305:SER:OG	2.12	0.47
1:A:325:ILE:HG23	1:A:465:SER:HB3	1.97	0.47
1:B:123:PRO:HG2	1:B:126:TRP:CE2	2.50	0.46
1:B:136:THR:O	1:B:140:VAL:HG23	2.15	0.46
1:A:157:VAL:HG13	1:A:169:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ARG:NH2	1:A:440:GLU:OE2	2.49	0.46
1:B:442:PHE:HA	1:B:443:PRO:HD3	1.69	0.45
1:A:84:GLY:HA2	1:A:87:VAL:HG12	1.98	0.45
1:A:226:LEU:HA	1:A:226:LEU:HD23	1.64	0.45
1:B:330:ILE:HG12	1:B:338:LEU:HD11	1.99	0.45
1:B:398:LEU:O	1:B:402:ILE:HG13	2.16	0.45
1:A:472:LEU:O	1:A:476:ILE:HG22	2.17	0.45
1:A:87:VAL:HG13	1:A:144:ILE:HG12	1.99	0.45
1:A:314:LEU:HA	1:A:314:LEU:HD23	1.70	0.44
1:A:323:VAL:HG13	1:A:393:PHE:CZ	2.52	0.44
1:A:444:THR:HA	1:A:447:ARG:HB3	2.00	0.44
1:B:192:ILE:O	1:B:196:LYS:HG3	2.18	0.44
1:B:52:ILE:H	1:B:52:ILE:HG13	1.43	0.44
1:B:112:ILE:HG22	1:B:145:GLY:HA3	2.00	0.44
1:A:196:LYS:HA	1:A:200:LYS:HB2	1.99	0.43
1:B:506:ASP:HB3	1:B:509:GLU:HB2	1.99	0.43
1:B:347:THR:HG22	1:B:348:GLY:H	1.84	0.43
1:B:365:THR:HA	1:B:369:PHE:HB3	2.01	0.43
1:B:472:LEU:HA	1:B:472:LEU:HD23	1.66	0.43
1:B:69:LEU:HA	1:B:70:PRO:HD2	1.86	0.43
1:A:117:ILE:HA	1:A:120:MET:HE3	2.01	0.43
1:B:122:ALA:O	1:B:212:ARG:NH1	2.47	0.43
1:B:344:ALA:HB1	1:B:346:LYS:HG2	2.01	0.43
1:A:403:LEU:HB3	1:A:482:LEU:HD13	2.00	0.43
1:B:122:ALA:HA	1:B:123:PRO:HD3	1.89	0.43
1:A:135:ILE:O	1:A:139:ARG:HG3	2.19	0.43
1:B:512:LEU:HD13	1:B:516:ARG:NH2	2.34	0.42
1:B:52:ILE:HA	1:B:55:VAL:HB	2.01	0.42
1:B:84:GLY:HA2	1:B:87:VAL:HG12	2.01	0.42
1:A:69:LEU:HA	1:A:70:PRO:HD2	1.86	0.42
1:A:208:ASP:HA	1:A:211:TRP:CD1	2.55	0.42
1:B:447:ARG:HG3	1:B:448:ALA:N	2.33	0.42
1:A:447:ARG:O	1:A:448:ALA:HB3	2.19	0.42
1:A:163:ILE:HG23	1:A:164:HIS:O	2.19	0.42
1:A:323:VAL:HG13	1:A:393:PHE:CE2	2.54	0.42
1:B:163:ILE:HD13	1:B:164:HIS:H	1.85	0.42
1:A:478:THR:O	1:A:482:LEU:HG	2.20	0.41
1:A:52:ILE:HG13	1:A:52:ILE:H	1.45	0.41
1:B:195:PHE:HE1	1:B:213:ILE:HD12	1.85	0.41
1:A:406:GLU:CB	1:A:410:ILE:HD12	2.42	0.41
1:B:113:ILE:O	1:B:117:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:HD13	1:A:422:MET:HE1	2.01	0.41
1:A:185:SER:O	1:A:189:ILE:HG12	2.20	0.41
1:B:393:PHE:CE2	1:B:492:GLY:HA3	2.55	0.41
1:A:52:ILE:HA	1:A:55:VAL:HB	2.01	0.41
1:A:160:ARG:HG3	1:A:160:ARG:O	2.21	0.41
1:B:123:PRO:HB2	1:B:126:TRP:CD2	2.56	0.41
1:B:85:CYS:SG	1:B:459:LYS:NZ	2.77	0.41
1:B:192:ILE:HG23	1:B:196:LYS:NZ	2.35	0.41
1:B:403:LEU:HB3	1:B:482:LEU:HD13	2.03	0.41
1:A:199:LEU:HD12	1:A:203:HIS:ND1	2.36	0.40
1:A:112:ILE:HD13	1:A:112:ILE:HG21	1.90	0.40
1:B:323:VAL:HG13	1:B:393:PHE:CZ	2.56	0.40
1:A:123:PRO:HG2	1:A:126:TRP:CE2	2.56	0.40
1:B:200:LYS:HZ1	1:B:206:ASP:N	2.20	0.40
1:A:126:TRP:CD1	1:A:130:ARG:HD3	2.57	0.40
1:B:499:ILE:HD13	1:B:499:ILE:HA	1.87	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	418/530 (79%)	374 (90%)	33 (8%)	11 (3%)	6	24
1	B	418/530 (79%)	374 (90%)	33 (8%)	11 (3%)	6	24
All	All	836/1060 (79%)	748 (90%)	66 (8%)	22 (3%)	6	24

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	VAL
1	A	336	VAL

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Mol	Chain	Res	Type
1	A	343	PHE
1	B	104	VAL
1	B	336	VAL
1	A	101	ARG
1	A	443	PRO
1	B	343	PHE
1	B	443	PRO
1	A	103	PHE
1	A	335	SER
1	A	339	ALA
1	B	101	ARG
1	B	335	SER
1	B	339	ALA
1	A	310	PHE
1	B	103	PHE
1	B	106	GLY
1	B	310	PHE
1	A	106	GLY
1	B	205	HIS
1	A	150	TYR

5.3.2 Protein sidechains ⓘ

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	342/433 (79%)	298 (87%)	44 (13%)	5	15
1	B	342/433 (79%)	295 (86%)	47 (14%)	4	12
All	All	684/866 (79%)	593 (87%)	91 (13%)	4	13

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	42	PHE
1	A	45	ASP

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Mol	Chain	Res	Type
1	A	51	ILE
1	A	52	ILE
1	A	54	GLN
1	A	99	PHE
1	A	101	ARG
1	A	104	VAL
1	A	112	ILE
1	A	119	GLN
1	A	124	SER
1	A	126	TRP
1	A	127	ASP
1	A	130	ARG
1	A	136	THR
1	A	163	ILE
1	A	166	ARG
1	A	189	ILE
1	A	195	PHE
1	A	198	ARG
1	A	200	LYS
1	A	206	ASP
1	A	225	THR
1	A	305	SER
1	A	313	LEU
1	A	314	LEU
1	A	323	VAL
1	A	336	VAL
1	A	337	VAL
1	A	347	THR
1	A	370	LEU
1	A	380	ILE
1	A	387	LYS
1	A	395	MET
1	A	398	LEU
1	A	403	LEU
1	A	412	LYS
1	A	416	LEU
1	A	436	ILE
1	A	441	LEU
1	A	446	ILE
1	A	447	ARG
1	A	468	VAL
1	B	35	VAL

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Mol	Chain	Res	Type
1	B	42	PHE
1	B	45	ASP
1	B	51	ILE
1	B	52	ILE
1	B	73	ARG
1	B	86	VAL
1	B	101	ARG
1	B	104	VAL
1	B	112	ILE
1	B	119	GLN
1	B	124	SER
1	B	126	TRP
1	B	127	ASP
1	B	130	ARG
1	B	136	THR
1	B	160	ARG
1	B	163	ILE
1	B	166	ARG
1	B	189	ILE
1	B	195	PHE
1	B	198	ARG
1	B	200	LYS
1	B	225	THR
1	B	226	LEU
1	B	305	SER
1	B	313	LEU
1	B	314	LEU
1	B	323	VAL
1	B	330	ILE
1	B	336	VAL
1	B	337	VAL
1	B	347	THR
1	B	370	LEU
1	B	380	ILE
1	B	387	LYS
1	B	394	ILE
1	B	395	MET
1	B	398	LEU
1	B	403	LEU
1	B	412	LYS
1	B	416	LEU
1	B	436	ILE

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Mol	Chain	Res	Type
1	B	441	LEU
1	B	446	ILE
1	B	447	ARG
1	B	468	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

2 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	600	-	4,4,4	0.74	0	6,6,6	0.42	0
2	PO4	B	600	-	4,4,4	0.76	0	6,6,6	0.40	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	600	-	-	0/0/0/0	0/0/0/0
2	PO4	B	600	-	-	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	PO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	422/530 (79%)	0.44	15 (3%)	43 37	67, 97, 178, 212	0
1	B	422/530 (79%)	0.57	29 (6%)	18 13	71, 102, 190, 236	0
All	All	844/1060 (79%)	0.51	44 (5%)	28 23	67, 100, 183, 236	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	LYS	10.0
1	A	197	HIS	8.0
1	A	336	VAL	7.5
1	B	104	VAL	7.3
1	B	150	TYR	7.0
1	B	152	MET	7.0
1	B	336	VAL	6.8
1	B	155	THR	6.8
1	B	103	PHE	6.7
1	B	154	ALA	6.0
1	A	196	LYS	5.4
1	B	153	SER	5.3
1	B	101	ARG	5.2
1	B	196	LYS	5.2
1	B	197	HIS	5.1
1	B	156	VAL	5.0
1	B	157	VAL	4.9
1	B	105	TYR	4.9
1	B	100	GLY	4.8
1	B	107	LYS	4.4
1	B	35	VAL	4.3
1	A	103	PHE	4.3
1	A	154	ALA	3.7
1	A	102	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	151	PRO	3.5
1	B	160	ARG	3.5
1	A	198	ARG	3.4
1	B	110	ILE	3.3
1	A	162	ASN	3.2
1	A	160	ARG	3.2
1	A	157	VAL	3.0
1	B	383	VAL	2.8
1	B	34	LEU	2.8
1	B	158	SER	2.7
1	A	156	VAL	2.7
1	A	153	SER	2.5
1	B	165	ARG	2.5
1	B	387	LYS	2.5
1	B	515	ARG	2.4
1	A	207	VAL	2.2
1	B	435	PHE	2.2
1	A	398	LEU	2.2
1	B	394	ILE	2.2
1	A	499	ILE	2.1

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
2	PO4	A	600	5/5	0.94	0.23	0.53	116,124,128,128	0
2	PO4	B	600	5/5	0.94	0.28	-0.08	101,111,115,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.