Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2025 – 08:08 AM EDT

PDB ID	:	9B48
Title	:	Asp324Glu variant of phosphate transporter PiPT from Piriformospora indica
Authors	:	Gupta, M.; Finer-Moore, J.; Stroud, R.M.
Deposited on	:	2024-03-20
Resolution	:	4.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

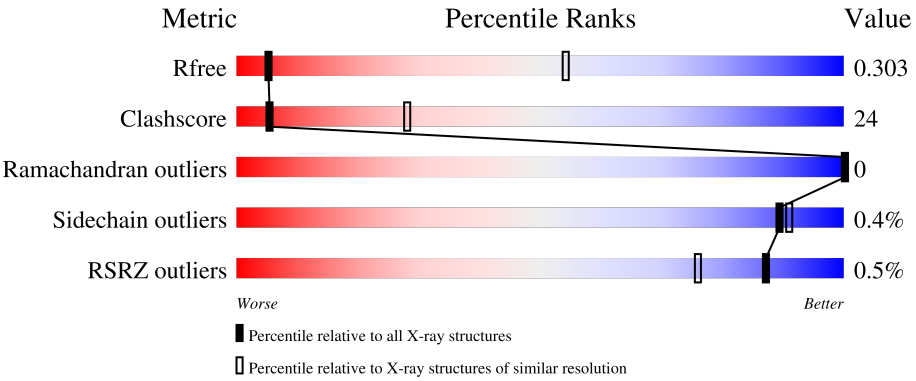
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 4.00 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}	164625	1028 (4.22-3.78)
Clashscore	180529	1055 (4.20-3.80)
Ramachandran outliers	177936	1004 (4.20-3.80)
Sidechain outliers	177891	1027 (4.22-3.78)
RSRZ outliers	164620	1029 (4.22-3.78)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	530	% 51% 30% 19%
1	B	530	48% 33% 19%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 13266 atoms, of which 6648 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	B	429	Total	C	H	N	O	S	0	0	0
			6633	2186	3324	543	564	16			
1	A	429	Total	C	H	N	O	S	0	0	0
			6633	2186	3324	543	564	16			

There are 18 discrepancies between the modelled and reference sequences:

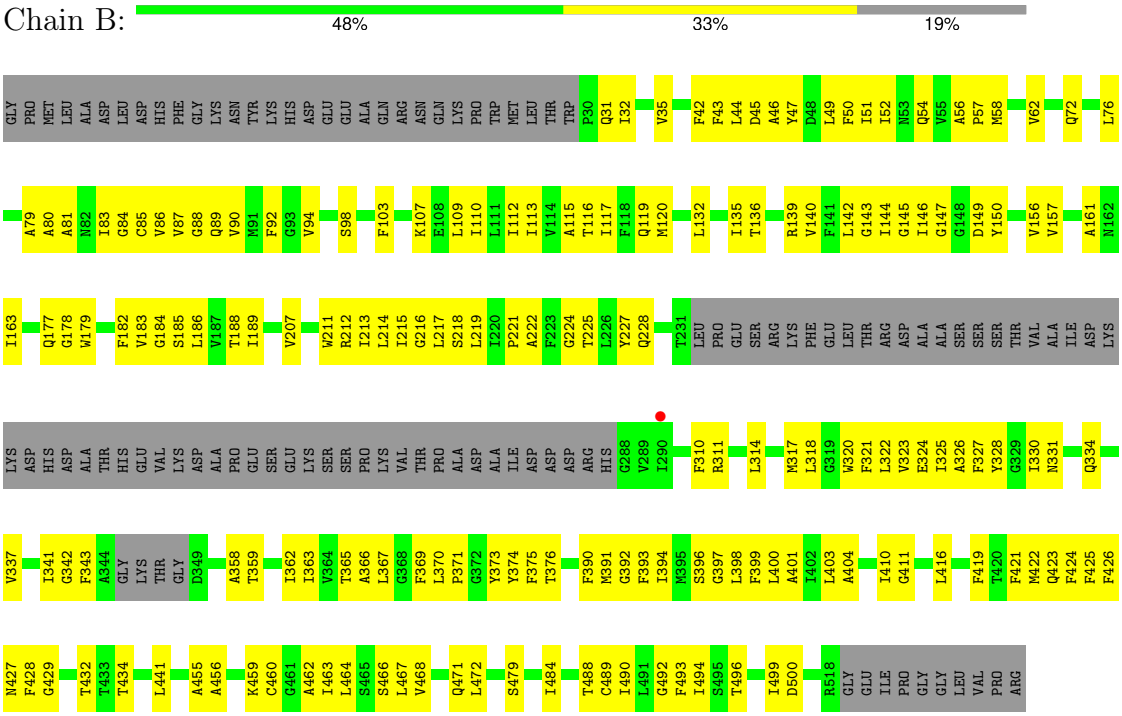
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP A8N031
B	0	PRO	-	expression tag	UNP A8N031
B	324	GLU	ASP	engineered mutation	UNP A8N031
B	523	GLY	-	expression tag	UNP A8N031
B	524	GLY	-	expression tag	UNP A8N031
B	525	LEU	-	expression tag	UNP A8N031
B	526	VAL	-	expression tag	UNP A8N031
B	527	PRO	-	expression tag	UNP A8N031
B	528	ARG	-	expression tag	UNP A8N031
A	-1	GLY	-	expression tag	UNP A8N031
A	0	PRO	-	expression tag	UNP A8N031
A	324	GLU	ASP	engineered mutation	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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

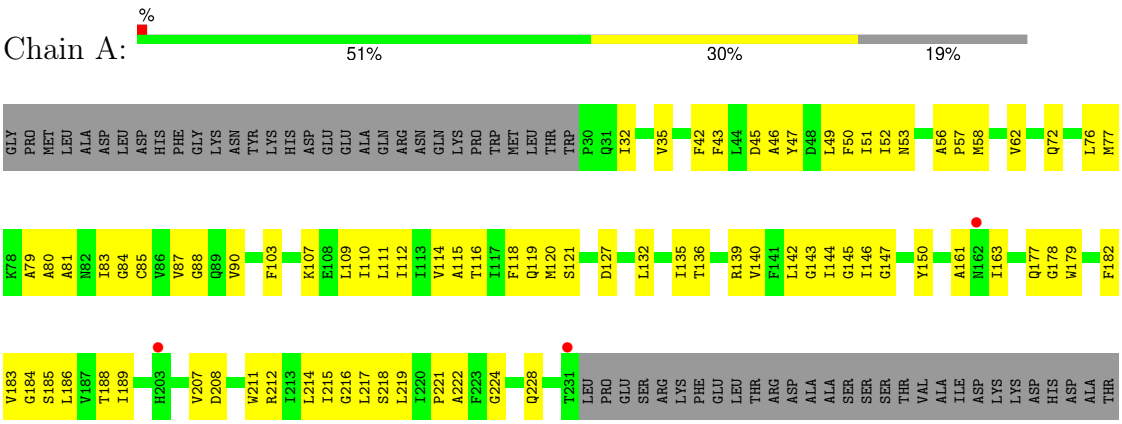
• Molecule 1: Phosphate transporter

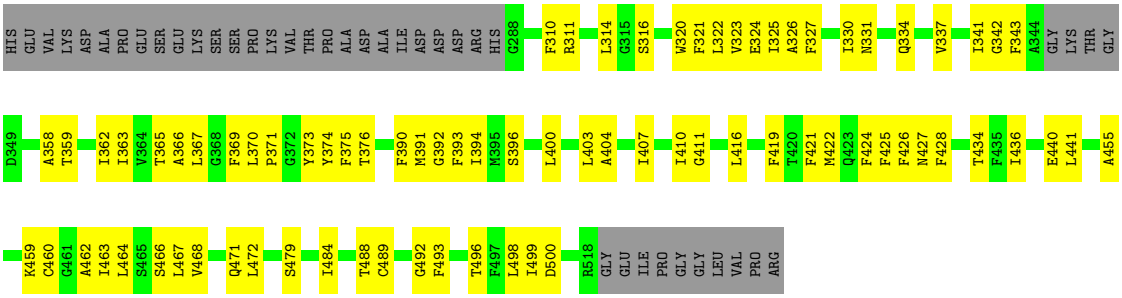
Chain B:



• Molecule 1: Phosphate transporter

Chain A:




HIS GLU VAL LYS ASP ALA PRO GLU SER GLU LYS SER SER PRO LYS VAL THR PRO ALA ASP ALA ILE ASP ASP ASP ARG HIS G288 F310 R311 L314 G315 S316 W320 F321 L322 V323 E324 I325 A326 F327 I330 N331 Q334 V337 I341 G342 F343 A344 GLY LYS THR GLY
D349 A358 T359 I362 I363 V364 T365 A366 L367 G368 F369 L370 P371 G372 Y373 Y374 F375 T376 F390 M391 G392 F393 I394 M395 S396 L400 L403 A404 I407 I410 G411 L416 F419 T420 F421 M422 Q423 F424 F425 F426 M427 F428 T434 F435 I436 E440 L441 A455
K459 C460 G461 A462 I463 L464 S465 S466 L467 V468 Q471 L472 S479 I484 T488 C489 G492 F493 T496 F497 L498 I499 D500 R518 GLY GLU ILE PRO GLY GLY LEU VAL PRO ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	173.39Å 173.39Å 169.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	86.69 – 4.00 86.69 – 4.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (86.69-4.00) 86.1 (86.69-4.00)	Depositor EDS
R_{merge}	0.53	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.61 (at 4.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.261 , 0.266 0.289 , 0.303	Depositor DCC
R_{free} test set	1372 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å^2)	115.0	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 176.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.277 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13266	wwPDB-VP
Average B, all atoms (Å^2)	187.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.32	0/3391	0.52	0/4595
1	B	0.32	0/3391	0.53	0/4595
All	All	0.32	0/6782	0.53	0/9190

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	3309	3324	3324	152	0
1	B	3309	3324	3324	162	0
All	All	6618	6648	6648	312	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 24.

All (312) 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:85:CYS:SG	1:A:459:LYS:NZ	2.52	0.81
1:B:392:GLY:O	1:B:396:SER:OG	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:GLY:O	1:B:147:GLY:N	2.15	0.79
1:A:376:THR:OG1	1:A:427:ASN:O	2.03	0.77
1:B:119:GLN:HE22	1:B:142:LEU:HD22	1.51	0.75
1:A:365:THR:HA	1:A:369:PHE:HB3	1.68	0.75
1:B:365:THR:HA	1:B:369:PHE:HB3	1.69	0.75
1:B:462:ALA:O	1:B:466:SER:OG	2.05	0.74
1:A:143:GLY:O	1:A:147:GLY:N	2.20	0.74
1:B:139:ARG:HA	1:B:142:LEU:HB3	1.71	0.73
1:A:219:LEU:HA	1:A:222:ALA:HB3	1.69	0.73
1:A:139:ARG:HA	1:A:142:LEU:HB3	1.69	0.71
1:B:219:LEU:HA	1:B:222:ALA:HB3	1.71	0.71
1:A:45:ASP:O	1:A:49:LEU:N	2.20	0.71
1:B:72:GLN:O	1:B:76:LEU:HD13	1.91	0.70
1:A:140:VAL:O	1:A:144:ILE:N	2.21	0.70
1:A:334:GLN:HE22	1:A:365:THR:HG23	1.57	0.70
1:B:320:TRP:HD1	1:B:324:GLU:HG2	1.56	0.70
1:A:330:ILE:O	1:A:334:GLN:N	2.26	0.69
1:A:462:ALA:O	1:A:466:SER:OG	2.11	0.69
1:A:119:GLN:HE22	1:A:142:LEU:HD22	1.57	0.68
1:B:334:GLN:HE22	1:B:365:THR:HG23	1.58	0.68
1:B:464:LEU:O	1:B:468:VAL:HG12	1.92	0.68
1:B:376:THR:OG1	1:B:427:ASN:O	2.08	0.68
1:B:132:LEU:O	1:B:136:THR:HG23	1.95	0.67
1:A:132:LEU:O	1:A:136:THR:HG23	1.95	0.67
1:B:112:ILE:HG23	1:B:145:GLY:HA3	1.78	0.66
1:A:112:ILE:O	1:A:116:THR:N	2.29	0.66
1:B:45:ASP:O	1:B:49:LEU:N	2.23	0.66
1:B:334:GLN:OE1	1:B:423:GLN:NE2	2.29	0.66
1:B:376:THR:OG1	1:B:428:PHE:HA	1.96	0.66
1:B:422:MET:O	1:B:426:PHE:N	2.29	0.66
1:A:489:CYS:O	1:A:493:PHE:N	2.28	0.65
1:A:178:GLY:O	1:A:182:PHE:N	2.26	0.65
1:B:489:CYS:O	1:B:493:PHE:N	2.26	0.64
1:B:330:ILE:O	1:B:334:GLN:N	2.30	0.64
1:B:140:VAL:O	1:B:144:ILE:N	2.24	0.64
1:A:109:LEU:HD12	1:A:112:ILE:HD11	1.79	0.64
1:B:178:GLY:O	1:B:182:PHE:N	2.28	0.63
1:A:464:LEU:O	1:A:468:VAL:HG12	1.98	0.63
1:A:182:PHE:CE1	1:A:362:ILE:HD11	2.33	0.63
1:A:62:VAL:HG22	1:A:207:VAL:HG13	1.81	0.63
1:B:492:GLY:O	1:B:496:THR:OG1	2.10	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLY:O	1:A:396:SER:OG	2.12	0.62
1:A:331:ASN:OD1	1:A:369:PHE:CE1	2.53	0.62
1:A:391:MET:HA	1:A:394:ILE:HG22	1.82	0.61
1:B:182:PHE:CE1	1:B:362:ILE:HD11	2.36	0.61
1:A:376:THR:OG1	1:A:428:PHE:HA	2.01	0.61
1:B:320:TRP:CD1	1:B:324:GLU:HG2	2.36	0.61
1:A:49:LEU:O	1:A:52:ILE:HG22	2.01	0.61
1:B:81:ALA:O	1:B:85:CYS:HB2	2.01	0.60
1:A:50:PHE:HE2	1:A:177:GLN:HG3	1.66	0.60
1:A:460:CYS:HA	1:A:463:ILE:HG12	1.82	0.60
1:A:81:ALA:O	1:A:85:CYS:HB2	2.02	0.60
1:A:314:LEU:HD22	1:A:498:LEU:HD13	1.83	0.59
1:A:84:GLY:O	1:A:88:GLY:N	2.30	0.59
1:B:331:ASN:OD1	1:B:369:PHE:CE1	2.55	0.59
1:B:391:MET:HA	1:B:394:ILE:HG22	1.84	0.58
1:A:323:VAL:O	1:A:327:PHE:N	2.24	0.58
1:B:330:ILE:HD13	1:B:426:PHE:CE2	2.39	0.58
1:A:224:GLY:O	1:A:228:GLN:HG2	2.04	0.58
1:B:50:PHE:HE2	1:B:177:GLN:HG3	1.67	0.58
1:B:460:CYS:HA	1:B:463:ILE:HG12	1.86	0.58
1:A:322:LEU:HA	1:A:325:ILE:HD12	1.86	0.58
1:B:112:ILE:O	1:B:116:THR:OG1	2.13	0.56
1:A:103:PHE:O	1:A:107:LYS:HD3	2.06	0.56
1:A:179:TRP:O	1:A:183:VAL:N	2.32	0.56
1:A:182:PHE:O	1:A:186:LEU:N	2.34	0.56
1:B:343:PHE:HE2	1:B:416:LEU:HD13	1.70	0.56
1:B:87:VAL:HA	1:B:90:VAL:HG12	1.87	0.56
1:A:212:ARG:O	1:A:216:GLY:N	2.32	0.56
1:A:326:ALA:O	1:A:330:ILE:HD12	2.06	0.56
1:A:467:LEU:O	1:A:471:GLN:NE2	2.39	0.56
1:B:363:ILE:HG23	1:B:367:LEU:HD12	1.87	0.56
1:B:424:PHE:O	1:B:428:PHE:N	2.33	0.56
1:B:330:ILE:HD13	1:B:426:PHE:HE2	1.70	0.55
1:B:49:LEU:O	1:B:52:ILE:HG22	2.07	0.55
1:B:459:LYS:HA	1:B:462:ALA:HB3	1.88	0.55
1:A:50:PHE:HE2	1:A:177:GLN:CG	2.19	0.55
1:A:321:PHE:O	1:A:325:ILE:HG13	2.06	0.55
1:A:363:ILE:HG23	1:A:367:LEU:HD12	1.87	0.55
1:A:72:GLN:O	1:A:76:LEU:HD13	2.07	0.55
1:B:490:ILE:O	1:B:494:ILE:N	2.28	0.55
1:A:139:ARG:O	1:A:143:GLY:N	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:LYS:O	1:A:463:ILE:HG12	2.07	0.54
1:A:310:PHE:CE2	1:A:314:LEU:HD12	2.43	0.54
1:A:43:PHE:O	1:A:47:TYR:N	2.28	0.54
1:A:488:THR:O	1:A:492:GLY:N	2.38	0.54
1:A:321:PHE:CE1	1:A:464:LEU:HD12	2.42	0.53
1:A:47:TYR:O	1:A:51:ILE:HB	2.09	0.53
1:B:161:ALA:HB1	1:B:163:ILE:HG22	1.88	0.53
1:B:179:TRP:O	1:B:183:VAL:N	2.34	0.53
1:B:337:VAL:HG11	1:B:419:PHE:CE1	2.43	0.53
1:A:422:MET:O	1:A:426:PHE:N	2.41	0.53
1:B:459:LYS:O	1:B:463:ILE:HG12	2.09	0.53
1:A:46:ALA:CB	1:A:177:GLN:HA	2.39	0.53
1:B:182:PHE:O	1:B:186:LEU:N	2.35	0.52
1:A:215:ILE:O	1:A:218:SER:OG	2.22	0.52
1:A:337:VAL:HG11	1:A:419:PHE:CE1	2.45	0.52
1:B:112:ILE:O	1:B:116:THR:N	2.35	0.52
1:A:184:GLY:O	1:A:188:THR:OG1	2.15	0.52
1:B:43:PHE:HZ	1:B:183:VAL:HG11	1.75	0.52
1:B:221:PRO:O	1:B:225:THR:N	2.39	0.52
1:B:441:LEU:HD11	1:B:499:ILE:HD12	1.92	0.52
1:A:463:ILE:O	1:A:467:LEU:HB2	2.10	0.52
1:B:76:LEU:O	1:B:80:ALA:N	2.43	0.51
1:A:50:PHE:CE1	1:A:331:ASN:HB3	2.45	0.51
1:A:43:PHE:HZ	1:A:183:VAL:HG11	1.75	0.51
1:A:62:VAL:CG2	1:A:207:VAL:HG13	2.41	0.51
1:A:211:TRP:CE3	1:A:215:ILE:HD12	2.46	0.51
1:B:393:PHE:CD1	1:B:489:CYS:HA	2.46	0.51
1:B:47:TYR:O	1:B:51:ILE:HB	2.11	0.51
1:B:463:ILE:O	1:B:467:LEU:HB2	2.11	0.51
1:A:424:PHE:O	1:A:428:PHE:N	2.31	0.51
1:B:484:ILE:O	1:B:488:THR:HG23	2.10	0.51
1:B:321:PHE:O	1:B:325:ILE:HG13	2.12	0.50
1:B:365:THR:O	1:B:370:LEU:HB2	2.11	0.50
1:B:404:ALA:O	1:B:479:SER:OG	2.20	0.50
1:B:468:VAL:HG22	1:B:472:LEU:HG	1.93	0.50
1:B:467:LEU:O	1:B:471:GLN:NE2	2.44	0.50
1:B:463:ILE:O	1:B:467:LEU:N	2.33	0.50
1:A:404:ALA:O	1:A:479:SER:OG	2.23	0.50
1:B:84:GLY:O	1:B:88:GLY:N	2.35	0.50
1:A:217:LEU:O	1:A:221:PRO:HD2	2.11	0.50
1:A:146:ILE:O	1:A:150:TYR:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:PHE:CZ	1:A:314:LEU:HD12	2.46	0.50
1:B:45:ASP:OD2	1:B:149:ASP:OD2	2.30	0.50
1:A:208:ASP:HA	1:A:211:TRP:CD1	2.47	0.50
1:A:459:LYS:O	1:A:463:ILE:N	2.30	0.50
1:A:189:ILE:HG23	1:A:358:ALA:HB1	1.93	0.49
1:A:110:ILE:O	1:A:114:VAL:HG23	2.12	0.49
1:B:146:ILE:O	1:B:150:TYR:HB2	2.13	0.49
1:B:396:SER:O	1:B:400:LEU:N	2.42	0.49
1:B:488:THR:O	1:B:492:GLY:N	2.38	0.49
1:A:83:ILE:HD11	1:A:467:LEU:HD21	1.95	0.49
1:A:87:VAL:HA	1:A:90:VAL:HG12	1.94	0.49
1:B:370:LEU:HD21	1:B:374:TYR:HE2	1.76	0.49
1:A:459:LYS:HA	1:A:462:ALA:HB3	1.95	0.49
1:B:50:PHE:HE2	1:B:177:GLN:CG	2.25	0.49
1:A:370:LEU:C	1:A:370:LEU:HD23	2.33	0.49
1:A:403:LEU:O	1:A:407:ILE:HB	2.13	0.48
1:B:227:TYR:HB2	1:A:118:PHE:CE2	2.48	0.48
1:B:139:ARG:O	1:B:143:GLY:N	2.36	0.48
1:B:178:GLY:HA2	1:B:369:PHE:CE2	2.48	0.48
1:B:394:ILE:O	1:B:398:LEU:HG	2.12	0.48
1:A:88:GLY:HA2	1:A:144:ILE:HG23	1.94	0.48
1:B:212:ARG:O	1:B:216:GLY:N	2.37	0.48
1:B:320:TRP:CD1	1:B:324:GLU:CG	2.97	0.48
1:A:109:LEU:CD1	1:A:112:ILE:HD11	2.43	0.48
1:B:85:CYS:SG	1:B:459:LYS:NZ	2.63	0.48
1:B:322:LEU:HA	1:B:325:ILE:HD12	1.96	0.47
1:A:76:LEU:O	1:A:80:ALA:N	2.46	0.47
1:A:369:PHE:O	1:A:427:ASN:ND2	2.38	0.47
1:A:463:ILE:O	1:A:467:LEU:N	2.41	0.47
1:B:211:TRP:CE3	1:B:215:ILE:HD12	2.50	0.47
1:B:392:GLY:HA3	1:B:429:GLY:HA3	1.97	0.47
1:B:224:GLY:O	1:B:228:GLN:HG2	2.15	0.47
1:B:317:MET:O	1:B:321:PHE:CB	2.62	0.47
1:A:330:ILE:HD13	1:A:426:PHE:CE2	2.49	0.47
1:B:86:VAL:HA	1:B:89:GLN:HG2	1.97	0.47
1:B:103:PHE:O	1:B:107:LYS:HD3	2.14	0.47
1:B:362:ILE:O	1:B:366:ALA:N	2.36	0.47
1:B:341:ILE:HG22	1:B:342:GLY:H	1.79	0.47
1:B:311:ARG:NH1	1:B:500:ASP:OD1	2.45	0.47
1:A:119:GLN:HG3	1:A:135:ILE:HG23	1.96	0.47
1:B:359:THR:HA	1:B:362:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ILE:HA	1:A:466:SER:HB2	1.97	0.47
1:B:326:ALA:O	1:B:330:ILE:HD12	2.14	0.46
1:B:217:LEU:O	1:B:221:PRO:HD2	2.16	0.46
1:B:324:GLU:OE1	1:B:328:TYR:CD2	2.68	0.46
1:B:369:PHE:O	1:B:427:ASN:ND2	2.38	0.46
1:B:327:PHE:CE1	1:B:331:ASN:ND2	2.83	0.46
1:A:421:PHE:O	1:A:425:PHE:CD2	2.69	0.46
1:A:462:ALA:O	1:A:466:SER:N	2.37	0.46
1:B:318:LEU:O	1:B:322:LEU:N	2.37	0.46
1:A:311:ARG:NH2	1:A:500:ASP:OD1	2.40	0.46
1:A:324:GLU:HA	1:A:327:PHE:HB3	1.97	0.46
1:A:499:ILE:HG22	1:A:500:ASP:O	2.15	0.46
1:B:310:PHE:CZ	1:B:314:LEU:HD12	2.51	0.46
1:B:320:TRP:O	1:B:324:GLU:HG2	2.16	0.46
1:B:359:THR:O	1:B:362:ILE:HG22	2.15	0.46
1:A:370:LEU:HD21	1:A:374:TYR:HE2	1.79	0.46
1:B:362:ILE:O	1:B:366:ALA:CB	2.64	0.46
1:A:43:PHE:O	1:A:47:TYR:CB	2.64	0.46
1:B:43:PHE:O	1:B:47:TYR:N	2.34	0.45
1:A:32:ILE:O	1:A:35:VAL:HG22	2.17	0.45
1:A:365:THR:O	1:A:370:LEU:CB	2.65	0.45
1:B:88:GLY:HA3	1:B:144:ILE:HA	1.97	0.45
1:B:390:PHE:HD1	1:B:493:PHE:CD1	2.34	0.45
1:B:462:ALA:O	1:B:466:SER:CB	2.64	0.45
1:A:47:TYR:O	1:A:51:ILE:N	2.41	0.45
1:A:84:GLY:O	1:A:144:ILE:HA	2.16	0.45
1:B:109:LEU:HA	1:B:112:ILE:HG12	1.99	0.45
1:A:359:THR:HA	1:A:362:ILE:HG22	1.98	0.45
1:B:115:ALA:O	1:B:119:GLN:HB2	2.16	0.45
1:B:323:VAL:HG11	1:B:434:THR:OG1	2.17	0.45
1:A:468:VAL:HG22	1:A:472:LEU:HG	1.99	0.45
1:B:216:GLY:O	1:B:219:LEU:HB2	2.16	0.45
1:A:366:ALA:O	1:A:371:PRO:HD3	2.17	0.45
1:B:83:ILE:HD11	1:B:467:LEU:HD21	1.98	0.45
1:A:115:ALA:O	1:A:119:GLN:HB2	2.17	0.45
1:B:213:ILE:O	1:B:217:LEU:HG	2.17	0.45
1:B:393:PHE:O	1:B:397:GLY:N	2.46	0.45
1:B:455:ALA:O	1:B:459:LYS:HG3	2.17	0.45
1:A:343:PHE:HE2	1:A:416:LEU:HD13	1.82	0.45
1:A:373:TYR:CE2	1:A:427:ASN:ND2	2.85	0.44
1:A:393:PHE:CD1	1:A:489:CYS:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ALA:O	1:B:83:ILE:N	2.37	0.44
1:B:116:THR:O	1:B:120:MET:N	2.40	0.44
1:B:375:PHE:CD1	1:B:424:PHE:CE1	3.05	0.44
1:A:327:PHE:CE1	1:A:331:ASN:ND2	2.85	0.44
1:B:112:ILE:HB	1:B:142:LEU:HD12	1.99	0.44
1:B:112:ILE:HG22	1:B:142:LEU:HD12	1.99	0.44
1:A:492:GLY:O	1:A:496:THR:OG1	2.23	0.44
1:B:463:ILE:HA	1:B:466:SER:HB2	1.98	0.44
1:A:462:ALA:O	1:A:466:SER:CB	2.65	0.44
1:B:310:PHE:CE2	1:B:314:LEU:HD12	2.53	0.44
1:B:365:THR:O	1:B:370:LEU:CB	2.66	0.44
1:B:317:MET:O	1:B:321:PHE:HB3	2.17	0.43
1:A:359:THR:O	1:A:362:ILE:HG22	2.18	0.43
1:A:410:ILE:HG13	1:A:411:GLY:H	1.82	0.43
1:B:47:TYR:O	1:B:51:ILE:N	2.38	0.43
1:B:50:PHE:CE1	1:B:331:ASN:HB3	2.54	0.43
1:B:321:PHE:CE1	1:B:464:LEU:HD12	2.53	0.43
1:B:490:ILE:HA	1:B:493:PHE:HB3	2.00	0.43
1:A:365:THR:O	1:A:370:LEU:HB2	2.18	0.43
1:A:396:SER:O	1:A:400:LEU:N	2.43	0.43
1:B:46:ALA:CB	1:B:177:GLN:HA	2.48	0.43
1:A:455:ALA:O	1:A:459:LYS:HG3	2.18	0.43
1:B:44:LEU:HD12	1:B:218:SER:HB2	2.01	0.43
1:A:341:ILE:HG22	1:A:342:GLY:H	1.83	0.43
1:B:366:ALA:O	1:B:371:PRO:HD3	2.19	0.43
1:B:456:ALA:O	1:B:460:CYS:N	2.40	0.43
1:A:424:PHE:O	1:A:428:PHE:CB	2.67	0.43
1:A:424:PHE:O	1:A:428:PHE:HB3	2.18	0.43
1:B:424:PHE:O	1:B:428:PHE:CB	2.66	0.43
1:A:58:MET:SD	1:A:214:LEU:HD11	2.59	0.43
1:A:375:PHE:CD1	1:A:424:PHE:CE1	3.06	0.43
1:A:390:PHE:O	1:A:394:ILE:HG22	2.19	0.43
1:B:112:ILE:O	1:B:116:THR:CB	2.67	0.43
1:B:227:TYR:OH	1:A:121:SER:O	2.22	0.43
1:A:316:SER:N	1:A:499:ILE:HD11	2.34	0.43
1:A:161:ALA:HB1	1:A:163:ILE:HG22	2.01	0.43
1:A:182:PHE:O	1:A:185:SER:N	2.52	0.43
1:B:113:ILE:O	1:B:117:ILE:N	2.39	0.42
1:B:94:VAL:O	1:B:98:SER:N	2.49	0.42
1:B:184:GLY:O	1:B:188:THR:OG1	2.25	0.42
1:A:109:LEU:HA	1:A:112:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ILE:HG23	1:A:145:GLY:HA3	2.01	0.42
1:A:116:THR:O	1:A:120:MET:N	2.40	0.42
1:B:390:PHE:CE1	1:B:496:THR:HB	2.54	0.42
1:B:393:PHE:HD1	1:B:489:CYS:HA	1.84	0.42
1:B:459:LYS:O	1:B:463:ILE:N	2.30	0.42
1:B:56:ALA:N	1:B:57:PRO:HD2	2.35	0.42
1:A:330:ILE:HD13	1:A:426:PHE:HE2	1.85	0.42
1:B:43:PHE:O	1:B:47:TYR:CB	2.68	0.42
1:A:88:GLY:HA3	1:A:144:ILE:HA	2.00	0.42
1:B:410:ILE:HG13	1:B:411:GLY:H	1.84	0.42
1:B:424:PHE:O	1:B:428:PHE:HB3	2.19	0.42
1:A:140:VAL:O	1:A:144:ILE:HG13	2.20	0.42
1:A:211:TRP:HE3	1:A:215:ILE:HD12	1.84	0.42
1:A:323:VAL:HG13	1:A:324:GLU:N	2.35	0.42
1:B:58:MET:SD	1:B:214:LEU:HD11	2.60	0.42
1:B:422:MET:O	1:B:425:PHE:N	2.53	0.42
1:A:50:PHE:O	1:A:53:ASN:HB3	2.20	0.42
1:A:323:VAL:HG11	1:A:434:THR:OG1	2.20	0.42
1:B:178:GLY:HA2	1:B:369:PHE:HE2	1.85	0.41
1:B:460:CYS:O	1:B:464:LEU:HG	2.20	0.41
1:B:54:GLN:NE2	1:B:185:SER:HA	2.35	0.41
1:A:112:ILE:HB	1:A:142:LEU:HD12	2.02	0.41
1:A:321:PHE:CZ	1:A:464:LEU:HD12	2.54	0.41
1:B:399:PHE:O	1:B:403:LEU:HB2	2.20	0.41
1:A:362:ILE:O	1:A:366:ALA:CB	2.69	0.41
1:A:179:TRP:HA	1:A:182:PHE:HB3	2.02	0.41
1:A:484:ILE:O	1:A:488:THR:HG23	2.20	0.41
1:B:50:PHE:CE2	1:B:177:GLN:CG	3.03	0.41
1:B:89:GLN:OE1	1:B:459:LYS:HE3	2.21	0.41
1:B:156:VAL:HG23	1:B:157:VAL:HG13	2.03	0.41
1:B:373:TYR:CE2	1:B:427:ASN:ND2	2.89	0.41
1:A:56:ALA:N	1:A:57:PRO:HD2	2.36	0.41
1:A:112:ILE:O	1:A:116:THR:CB	2.69	0.41
1:B:32:ILE:O	1:B:35:VAL:HG22	2.21	0.41
1:B:83:ILE:O	1:B:86:VAL:HG12	2.20	0.41
1:A:42:PHE:O	1:A:46:ALA:N	2.31	0.41
1:B:43:PHE:O	1:B:47:TYR:HB2	2.21	0.41
1:B:375:PHE:CD1	1:B:424:PHE:HE1	2.38	0.41
1:A:43:PHE:O	1:A:47:TYR:HB2	2.21	0.41
1:A:77:MET:CB	1:A:136:THR:HG22	2.51	0.41
1:A:107:LYS:HA	1:A:110:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:TRP:HE1	1:A:324:GLU:CD	2.24	0.41
1:A:369:PHE:CZ	1:A:373:TYR:OH	2.73	0.41
1:A:422:MET:O	1:A:425:PHE:N	2.54	0.41
1:A:436:ILE:HG22	1:A:440:GLU:OE1	2.20	0.41
1:B:88:GLY:CA	1:B:144:ILE:HA	2.50	0.41
1:B:421:PHE:O	1:B:425:PHE:CD2	2.74	0.41
1:A:77:MET:HB2	1:A:136:THR:HG22	2.03	0.41
1:A:441:LEU:HD11	1:A:499:ILE:HD12	2.02	0.41
1:B:88:GLY:O	1:B:92:PHE:HB2	2.21	0.40
1:B:376:THR:HG21	1:B:432:THR:HG21	2.03	0.40
1:A:79:ALA:O	1:A:83:ILE:N	2.40	0.40
1:B:107:LYS:HA	1:B:110:ILE:HG12	2.02	0.40
1:B:135:ILE:O	1:B:139:ARG:HG3	2.20	0.40
1:A:370:LEU:HD21	1:A:374:TYR:CE2	2.55	0.40
1:B:62:VAL:CG2	1:B:207:VAL:HG13	2.52	0.40
1:B:189:ILE:HG23	1:B:358:ALA:HB1	2.03	0.40
1:A:314:LEU:HD23	1:A:314:LEU:C	2.42	0.40
1:B:140:VAL:O	1:B:144:ILE:HG13	2.22	0.40
1:B:370:LEU:CD2	1:B:374:TYR:HE2	2.35	0.40
1:B:397:GLY:O	1:B:401:ALA:N	2.42	0.40
1:A:58:MET:CE	1:A:214:LEU:HD11	2.52	0.40
1:A:111:LEU:O	1:A:115:ALA:CB	2.70	0.40
1:A:112:ILE:HB	1:A:142:LEU:CD1	2.52	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	423/530 (80%)	411 (97%)	12 (3%)	0	100	100
1	B	423/530 (80%)	413 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	846/1060 (80%)	824 (97%)	22 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	338/433 (78%)	337 (100%)	1 (0%)	91 92
1	B	338/433 (78%)	336 (99%)	2 (1%)	84 88
All	All	676/866 (78%)	673 (100%)	3 (0%)	89 91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	31	GLN
1	B	42	PHE
1	A	127	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	177	GLN
1	B	331	ASN
1	B	334	GLN
1	B	423	GLN
1	B	431	ASN
1	A	177	GLN
1	A	331	ASN
1	A	334	GLN
1	A	423	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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	429/530 (80%)	-0.63	3 (0%)	84	71	127, 174, 284, 372	0
1	B	429/530 (80%)	-0.69	1 (0%)	92	85	124, 177, 284, 374	0
All	All	858/1060 (80%)	-0.66	4 (0%)	87	76	124, 175, 284, 374	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	HIS	3.8
1	B	290	ILE	2.8
1	A	231	THR	2.2
1	A	162	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.