



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:49 PM UTC

PDB ID : 7R0G / pdb_00007r0g
Title : STRUCTURAL BASIS OF ION UPTAKE IN COPPER-TRANSPORTING
P1B-TYPE ATPASES
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Deposited on : 2022-02-02
Resolution : 4.01 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

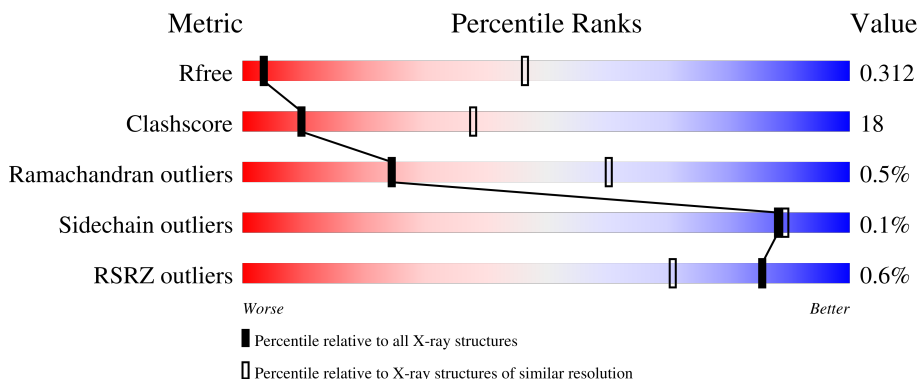
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.01 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}	180053	1095 (4.24-3.80)
Clashscore	190562	1142 (4.24-3.80)
Ramachandran outliers	187476	1074 (4.24-3.80)
Sidechain outliers	187428	1065 (4.24-3.80)
RSRZ outliers	180081	1095 (4.24-3.80)

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 $\leq 5\%$. 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	658	
1	B	658	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9841 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 Putative copper-exporting P-type ATPase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	0	0	0
			4929	3176	829	909	15			
1	B	652	Total	C	N	O	S	0	0	0
			4912	3167	827	903	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	GLY	-	expression tag	UNP A0A117KM49
B	79	GLY	-	expression tag	UNP A0A117KM49

L694	L695	G699	V700	V701	F702	A707	M711	A712	M713	S714	S715	V716	S717	V718	V719	L723	L724	P731	I732	R733	R734	G735	G736																										
W576	S583	L586	V591	E594	V604	Q608	A614	G617	D618	G619	L626	D630	I633	S639	E644	D647	L650	I651	R652	D653	R656	D657	V658	V659	M669	S670	K671	N675	L680	N683	L686	I687	P688	A689	A690	A691	G692	L693											
A465	E466	A467	I468	V469	K470	K471	A472	L473	E474	H475	G476	I477	E481	K484	V485	G492	A495	D496	G497	I498	L499	V500	L505	V511	A512	V513	K529	T530	A531	V534	N537	G542	T543	I544	A545	V546	S547	D548	T549	L550	K551	K555	P556	L561	D574	N575			
A387	L388	P389	T390	L391	T392	T393	M396	K407	D410	A411	L412	E413	V414	A415	V418	V421	D424	K425	T428	L429	T430	K431	P434	E435	V436	T437	D438	L439	V440	P441	L442	N443	G444	D445	E446	R447	E448	L449	L450	R451	L452	A453	A454	E457	R458	R459	H462	P463	I464
V300	L301	I303	R307	V308	L313	I317	V318	X319	L320	V321	E322	M325	P330	L334	A335	V338	I343	P344	T345	V346	V349	F354	I355	Y356	Y357	Y358	F359	L365	L366	F367	T370	T371	L372	V375	L376	V377	V378	A379	C380	P381	C382	A383	F384	G385	L386				

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.19Å 226.06Å 111.11Å 90.00° 134.06° 90.00°	Depositor
Resolution (Å)	48.75 – 4.01 48.75 – 4.01	Depositor EDS
% Data completeness (in resolution range)	94.0 (48.75-4.01) 93.9 (48.75-4.01)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.263 , 0.312 0.267 , 0.312	Depositor DCC
R_{free} test set	1827 reflections (9.59%)	wwPDB-VP
Wilson B-factor (Å ²)	191.1	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 123.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9841	wwPDB-VP
Average B, all atoms (Å ²)	203.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.25	0/5003	0.58	0/6785
1	B	0.27	0/4986	0.62	3/6762 (0.0%)
All	All	0.26	0/9989	0.60	3/13547 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	694	LEU	CB-CG-CD2	-7.16	89.22	110.70
1	B	547	SER	CA-C-N	5.26	131.59	121.54
1	B	547	SER	C-N-CA	5.26	131.59	121.54

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	4929	0	5172	177	0
1	B	4912	0	5162	180	0
All	All	9841	0	10334	357	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 18.

All (357) 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:529:LYS:HG2	1:A:547:SER:HB2	1.51	0.92
1:B:438:ASP:HB2	1:B:545:ALA:HB3	1.52	0.89
1:A:313:LEU:HD12	1:A:639:SER:HA	1.58	0.83
1:B:457:GLU:HB2	1:B:468:ILE:HD11	1.60	0.83
1:B:692:GLY:O	1:B:694:LEU:N	2.12	0.82
1:B:424:ASP:O	1:B:428:THR:OG1	1.97	0.81
1:B:176:SER:HB2	1:B:185:TYR:HB2	1.63	0.81
1:A:267:GLU:HG3	1:A:285:SER:HB3	1.68	0.76
1:A:560:GLU:HG3	1:A:732:ILE:HD13	1.65	0.75
1:B:357:TRP:HZ2	1:B:692:GLY:HA2	1.52	0.75
1:B:355:ILE:O	1:B:359:PHE:HB2	1.87	0.74
1:B:212:THR:HG22	1:B:393:THR:HG21	1.71	0.73
1:A:525:GLU:OE2	1:A:575:ASN:ND2	2.23	0.72
1:A:459:ARG:NH1	1:A:483:GLU:OE2	2.23	0.72
1:A:101:LYS:HG2	1:A:139:SER:HA	1.72	0.71
1:B:158:MET:HA	1:B:380:CYS:SG	2.30	0.71
1:B:320:LEU:HD11	1:B:407:LYS:HG2	1.73	0.70
1:B:143:ILE:HG21	1:B:198:LEU:HD21	1.72	0.70
1:A:158:MET:HA	1:A:380:CYS:SG	2.31	0.70
1:A:212:THR:HG22	1:A:393:THR:HG21	1.72	0.70
1:A:159:ASP:O	1:A:163:SER:OG	2.05	0.70
1:B:450:LEU:HD21	1:B:472:ALA:HA	1.73	0.69
1:B:452:LEU:HD22	1:B:498:ILE:HG12	1.72	0.69
1:A:143:ILE:HG21	1:A:198:LEU:HD21	1.76	0.68
1:B:161:MET:HE1	1:B:376:LEU:HD22	1.75	0.68
1:B:191:SER:HA	1:B:194:LEU:HB2	1.76	0.68
1:B:731:PRO:HA	1:B:734:ARG:HE	1.59	0.68
1:B:425:LYS:NZ	1:B:574:ASP:OD2	2.21	0.67
1:A:329:PRO:HD2	1:A:332:GLN:HB2	1.77	0.67
1:A:429:LEU:HD12	1:A:570:MET:HG3	1.76	0.67
1:B:136:ILE:HD11	1:B:192:VAL:HG22	1.76	0.67
1:A:96:SER:HA	1:A:99:LYS:HZ2	1.59	0.66
1:A:251:VAL:HG21	1:A:257:ILE:HG12	1.76	0.66
1:B:296:ASN:ND2	1:B:299:GLY:O	2.27	0.66
1:B:357:TRP:CD2	1:B:367:PHE:HE1	2.13	0.66
1:B:381:PRO:HA	1:B:711:MET:HE3	1.78	0.66
1:A:366:LEU:O	1:A:370:THR:HG23	1.95	0.66
1:B:366:LEU:O	1:B:370:THR:HG23	1.95	0.66
1:B:688:PRO:HB2	1:B:693:LEU:HD22	1.77	0.66
1:A:734:ARG:NE	1:A:735:GLY:H	1.96	0.64
1:B:550:LEU:HD11	1:B:586:LEU:HD21	1.78	0.64
1:B:583:SER:HB2	1:B:591:VAL:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ASP:HB2	1:A:545:ALA:HB3	1.80	0.64
1:B:101:LYS:NZ	1:B:138:TYR:O	2.31	0.64
1:A:136:ILE:HD11	1:A:192:VAL:HG22	1.78	0.64
1:B:439:LEU:HD13	1:B:446:GLU:HB3	1.80	0.63
1:B:499:LEU:HD22	1:B:505:LEU:HD11	1.80	0.63
1:A:176:SER:OG	1:A:183:ARG:NH2	2.30	0.63
1:A:482:PRO:HB3	1:A:496:ASP:HB2	1.79	0.63
1:A:187:PHE:HZ	1:A:370:THR:HG22	1.64	0.63
1:B:225:LYS:O	1:B:240:VAL:N	2.31	0.63
1:B:434:PRO:HA	1:B:548:ASP:OD1	1.99	0.63
1:A:250:ILE:HG22	1:A:302:LYS:HG2	1.81	0.62
1:A:355:ILE:O	1:A:359:PHE:HB2	1.99	0.62
1:B:125:ASP:OD2	1:B:183:ARG:NH2	2.25	0.62
1:B:230:ILE:HG12	1:B:235:GLU:HG2	1.80	0.62
1:A:456:ALA:HA	1:A:495:ALA:HB3	1.81	0.62
1:A:171:LEU:HA	1:A:174:VAL:HG12	1.81	0.61
1:A:289:GLU:OE2	1:A:307:ARG:NH2	2.30	0.61
1:A:205:GLU:HA	1:A:386:LEU:HD21	1.82	0.61
1:A:561:LEU:HG	1:A:659:VAL:HG22	1.83	0.61
1:B:267:GLU:HG2	1:B:283:LEU:HD11	1.82	0.61
1:A:96:SER:HA	1:A:99:LYS:NZ	2.15	0.61
1:B:731:PRO:HG3	1:B:734:ARG:HH21	1.66	0.60
1:B:267:GLU:HG3	1:B:285:SER:HB3	1.82	0.60
1:A:687:ILE:HG23	1:A:688:PRO:HD3	1.82	0.60
1:B:313:LEU:HD13	1:B:639:SER:HA	1.83	0.60
1:A:583:SER:HB2	1:A:591:VAL:HG21	1.84	0.59
1:A:500:VAL:HG22	1:A:534:VAL:HG12	1.84	0.59
1:A:191:SER:H	1:A:194:LEU:HD23	1.67	0.59
1:A:452:LEU:HD13	1:A:536:ARG:HB2	1.85	0.59
1:B:159:ASP:O	1:B:163:SER:OG	2.16	0.59
1:B:263:VAL:HG12	1:B:288:ASP:O	2.02	0.59
1:B:551:LYS:NZ	1:B:653:ASP:HB3	2.17	0.59
1:A:484:LYS:HB3	1:A:496:ASP:H	1.66	0.59
1:B:230:ILE:HD11	1:B:250:ILE:HB	1.84	0.59
1:B:284:LYS:HE3	1:B:290:VAL:HG12	1.85	0.59
1:A:212:THR:O	1:A:216:ILE:HD12	2.03	0.59
1:B:313:LEU:O	1:B:317:ILE:HG12	2.03	0.59
1:B:392:LEU:O	1:B:396:MET:HG3	2.02	0.59
1:A:191:SER:HA	1:A:194:LEU:HB2	1.84	0.58
1:A:263:VAL:HG11	1:A:285:SER:O	2.03	0.58
1:B:98:MET:HB3	1:B:203:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ALA:HB2	1:B:256:LYS:HD2	1.83	0.58
1:A:156:LEU:HD23	1:A:343:ILE:HG22	1.87	0.57
1:B:434:PRO:HG2	1:B:463:PRO:O	2.03	0.57
1:A:346:VAL:HA	1:A:349:VAL:HG22	1.85	0.57
1:A:671:LYS:HE3	1:A:724:LEU:HD22	1.85	0.57
1:B:551:LYS:HZ2	1:B:653:ASP:HB3	1.69	0.57
1:B:561:LEU:HG	1:B:659:VAL:HG22	1.87	0.57
1:B:604:VAL:O	1:B:608:GLN:HG3	2.04	0.57
1:B:367:PHE:HE2	1:B:695:TYR:CE1	2.23	0.57
1:B:212:THR:O	1:B:216:ILE:HD12	2.05	0.56
1:A:230:ILE:HD11	1:A:250:ILE:HG23	1.87	0.56
1:A:604:VAL:O	1:A:608:GLN:HG3	2.05	0.56
1:B:459:ARG:HD2	1:B:485:VAL:HG21	1.87	0.56
1:B:199:LEU:O	1:B:203:THR:HG23	2.05	0.56
1:B:381:PRO:HB3	1:B:683:ASN:HD21	1.71	0.56
1:B:555:LYS:HB2	1:B:556:PRO:HD3	1.87	0.56
1:A:436:VAL:HA	1:A:546:VAL:HG12	1.87	0.56
1:B:457:GLU:HB2	1:B:468:ILE:CD1	2.34	0.56
1:B:389:PRO:O	1:B:393:THR:HG23	2.06	0.56
1:B:438:ASP:OD2	1:B:529:LYS:NZ	2.39	0.55
1:A:85:GLN:H	1:A:85:GLN:CD	2.15	0.55
1:A:433:LYS:NZ	1:A:466:GLU:OE1	2.40	0.55
1:A:424:ASP:O	1:A:428:THR:HB	2.07	0.55
1:B:260:ASP:HB2	1:B:307:ARG:HB2	1.89	0.55
1:A:407:LYS:NZ	1:A:644:GLU:O	2.38	0.55
1:A:413:GLU:HG3	1:A:669:MET:HE2	1.88	0.55
1:A:504:ARG:O	1:A:508:ASP:HB2	2.07	0.55
1:B:411:ALA:HB2	1:B:647:ASP:HB3	1.88	0.55
1:A:330:PRO:HD3	1:A:410:ASP:OD1	2.07	0.54
1:A:468:ILE:HD12	1:A:469:VAL:N	2.23	0.54
1:B:204:LEU:HD11	1:B:716:VAL:HG12	1.89	0.54
1:A:619:GLY:HA2	1:A:626:LEU:CD1	2.38	0.54
1:B:712:ALA:O	1:B:716:VAL:HG13	2.08	0.54
1:B:156:LEU:HD23	1:B:343:ILE:HG22	1.90	0.54
1:A:162:TYR:HE1	1:A:380:CYS:HB3	1.73	0.54
1:A:466:GLU:O	1:A:470:LYS:HB2	2.08	0.54
1:A:471:LYS:NZ	1:A:474:GLU:OE2	2.33	0.53
1:A:430:THR:HB	1:A:548:ASP:OD2	2.08	0.53
1:B:173:SER:HA	1:B:185:TYR:O	2.08	0.53
1:B:112:LEU:HD11	1:B:131:ILE:HB	1.90	0.53
1:A:462:HIS:CG	1:A:463:PRO:HD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:VAL:HG11	1:B:630:ASP:O	2.08	0.53
1:B:450:LEU:HD22	1:B:477:ILE:HG13	1.90	0.53
1:A:484:LYS:HB3	1:A:495:ALA:HA	1.91	0.53
1:A:458:ARG:HA	1:A:469:VAL:HG11	1.91	0.53
1:B:407:LYS:NZ	1:B:644:GLU:O	2.31	0.53
1:B:413:GLU:HG3	1:B:669:MET:HE2	1.91	0.53
1:A:433:LYS:HE2	1:A:433:LYS:HA	1.90	0.52
1:A:449:LEU:HD13	1:A:542:GLY:HA3	1.91	0.52
1:B:576:TRP:HD1	1:B:594:GLU:OE2	1.93	0.52
1:A:263:VAL:HG12	1:A:288:ASP:O	2.10	0.52
1:B:434:PRO:HG3	1:B:463:PRO:HB2	1.91	0.52
1:B:330:PRO:HD3	1:B:410:ASP:OD1	2.11	0.51
1:B:447:ARG:NH2	1:B:476:GLY:O	2.43	0.51
1:B:686:LEU:HA	1:B:689:ALA:HB3	1.93	0.51
1:B:689:ALA:O	1:B:694:LEU:HD21	2.10	0.51
1:A:521:LEU:O	1:A:525:GLU:HG3	2.11	0.51
1:B:471:LYS:HD2	1:B:475:HIS:ND1	2.25	0.51
1:B:694:LEU:HD22	1:B:702:PHE:CE1	2.44	0.51
1:A:187:PHE:HB3	1:A:190:THR:OG1	2.10	0.51
1:A:211:ARG:HD2	1:A:390:THR:HG23	1.93	0.51
1:A:230:ILE:HD11	1:A:250:ILE:CG2	2.41	0.51
1:B:245:VAL:HG23	1:B:308:VAL:HG12	1.92	0.51
1:B:449:LEU:HD13	1:B:542:GLY:HA3	1.93	0.51
1:A:127:VAL:O	1:A:131:ILE:HG13	2.11	0.50
1:B:367:PHE:HE2	1:B:695:TYR:HE1	1.59	0.50
1:A:712:ALA:O	1:A:716:VAL:HG13	2.10	0.50
1:A:464:ILE:O	1:A:468:ILE:HG13	2.09	0.50
1:B:633:ILE:HG23	1:B:650:LEU:HD23	1.93	0.50
1:B:171:LEU:HA	1:B:174:VAL:HG12	1.93	0.50
1:B:431:LYS:HG2	1:B:549:THR:O	2.12	0.50
1:B:652:ARG:HD3	1:B:657:ASP:OD2	2.11	0.50
1:B:492:GLY:HA3	1:B:505:LEU:HG	1.93	0.50
1:A:211:ARG:HA	1:A:214:GLU:CD	2.37	0.50
1:B:211:ARG:HD2	1:B:390:THR:HG23	1.93	0.49
1:B:325:MET:HE3	1:B:393:THR:HA	1.94	0.49
1:A:100:ARG:O	1:A:104:VAL:HG23	2.12	0.49
1:A:416:GLU:OE1	1:A:673:LYS:NZ	2.29	0.49
1:B:434:PRO:HG3	1:B:463:PRO:CB	2.42	0.49
1:B:671:LYS:HE3	1:B:724:LEU:HD22	1.93	0.49
1:B:172:ALA:HB1	1:B:185:TYR:HD2	1.78	0.49
1:A:128:GLN:HB3	1:A:188:TYR:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:GLU:O	1:B:128:GLN:HG2	2.12	0.49
1:B:162:TYR:CD2	1:B:198:LEU:HB2	2.48	0.49
1:B:290:VAL:HG21	1:B:303:ILE:HG12	1.95	0.49
1:B:367:PHE:CE2	1:B:701:VAL:HG21	2.48	0.49
1:A:734:ARG:HE	1:A:735:GLY:H	1.58	0.48
1:B:465:ALA:O	1:B:468:ILE:HG13	2.12	0.48
1:A:389:PRO:O	1:A:393:THR:HG23	2.12	0.48
1:A:335:ALA:HA	1:A:338:VAL:HG22	1.96	0.48
1:A:378:VAL:HG23	1:A:707:ALA:HB1	1.95	0.48
1:A:392:LEU:O	1:A:396:MET:HG3	2.12	0.48
1:A:190:THR:HG22	1:A:705:GLU:OE1	2.14	0.48
1:A:652:ARG:HD3	1:A:657:ASP:OD2	2.13	0.48
1:B:439:LEU:HD23	1:B:439:LEU:HA	1.73	0.48
1:B:289:GLU:OE2	1:B:307:ARG:NH2	2.45	0.48
1:A:199:LEU:O	1:A:203:THR:HG23	2.13	0.48
1:A:343:ILE:HA	1:A:346:VAL:HG22	1.96	0.48
1:A:482:PRO:CB	1:A:496:ASP:HB2	2.44	0.48
1:A:633:ILE:HG23	1:A:650:LEU:HD23	1.95	0.48
1:A:705:GLU:CD	1:A:705:GLU:H	2.21	0.48
1:B:112:LEU:HD21	1:B:132:ALA:HB2	1.96	0.48
1:B:530:THR:HB	1:B:546:VAL:CG1	2.44	0.47
1:A:334:LEU:O	1:A:338:VAL:HG13	2.13	0.47
1:A:224:ALA:HB2	1:A:256:LYS:CD	2.44	0.47
1:A:230:ILE:HB	1:A:248:ILE:HB	1.96	0.47
1:A:387:ALA:HB1	1:A:675:ASN:HB3	1.95	0.47
1:A:450:LEU:HD21	1:A:472:ALA:HA	1.95	0.47
1:A:681:ILE:HA	1:A:684:VAL:HG22	1.94	0.47
1:B:260:ASP:OD1	1:B:292:GLY:N	2.39	0.47
1:B:434:PRO:HG2	1:B:467:ALA:HB2	1.96	0.47
1:B:458:ARG:NH1	1:B:481:GLU:OE2	2.47	0.47
1:A:190:THR:C	1:A:192:VAL:H	2.21	0.47
1:A:459:ARG:HD2	1:A:485:VAL:HG21	1.96	0.47
1:B:216:ILE:O	1:B:220:VAL:HG23	2.14	0.47
1:B:386:LEU:HD12	1:B:715:SER:HB3	1.97	0.47
1:A:671:LYS:CE	1:A:724:LEU:HD22	2.44	0.47
1:B:367:PHE:CE2	1:B:695:TYR:HE1	2.32	0.47
1:B:421:VAL:HG22	1:B:614:ALA:HB3	1.96	0.47
1:B:714:SER:O	1:B:718:VAL:HG13	2.14	0.47
1:B:260:ASP:OD2	1:B:313:LEU:N	2.48	0.47
1:B:439:LEU:CD1	1:B:446:GLU:HB3	2.44	0.47
1:B:434:PRO:HA	1:B:548:ASP:CG	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:ALA:HA	1:B:468:ILE:CD1	2.45	0.47
1:A:453:ALA:HB2	1:A:534:VAL:HG11	1.97	0.47
1:B:537:ASN:OD1	1:B:537:ASN:N	2.48	0.47
1:A:176:SER:HB2	1:A:185:TYR:HB2	1.97	0.46
1:B:367:PHE:CE2	1:B:695:TYR:CE1	3.02	0.46
1:B:499:LEU:HD23	1:B:499:LEU:HA	1.78	0.46
1:A:97:ARG:O	1:A:101:LYS:HB2	2.16	0.46
1:A:451:ARG:HG2	1:A:477:ILE:HG23	1.97	0.46
1:A:367:PHE:CE2	1:A:695:TYR:HE1	2.34	0.46
1:A:455:ILE:HD12	1:A:480:GLY:H	1.79	0.46
1:B:217:LYS:NZ	1:B:220:VAL:HG21	2.30	0.46
1:A:357:TRP:CE2	1:A:367:PHE:HE1	2.33	0.46
1:A:224:ALA:HB2	1:A:256:LYS:HD2	1.97	0.46
1:B:231:ARG:O	1:B:234:LYS:HG2	2.16	0.46
1:A:121:LEU:HB3	1:A:122:PRO:HD2	1.98	0.46
1:A:458:ARG:HD3	1:A:481:GLU:OE1	2.16	0.46
1:A:243:VAL:O	1:A:308:VAL:HG21	2.16	0.46
1:B:354:PHE:HB2	1:B:372:LEU:HB2	1.97	0.46
1:A:431:LYS:HG3	1:A:549:THR:O	2.16	0.46
1:A:617:GLY:O	1:A:634:ALA:HA	2.16	0.46
1:A:732:ILE:HG13	1:A:732:ILE:O	2.15	0.46
1:B:263:VAL:HG13	1:B:285:SER:O	2.17	0.45
1:B:694:LEU:HD22	1:B:702:PHE:CD1	2.52	0.45
1:A:151:LEU:HD11	1:A:160:VAL:HG13	1.99	0.45
1:A:189:GLU:O	1:A:193:LEU:HG	2.16	0.45
1:A:687:ILE:HG23	1:A:688:PRO:CD	2.47	0.45
1:B:346:VAL:HG23	1:B:379:ALA:HB1	1.99	0.45
1:B:381:PRO:C	1:B:383:ALA:H	2.23	0.45
1:A:484:LYS:CB	1:A:496:ASP:H	2.28	0.45
1:A:698:PHE:HE1	1:A:701:VAL:HG22	1.82	0.45
1:A:169:ALA:HB3	1:A:191:SER:HB3	1.98	0.45
1:A:415:ALA:HA	1:A:418:VAL:HG23	1.98	0.45
1:B:484:LYS:HB3	1:B:496:ASP:H	1.81	0.45
1:A:692:GLY:C	1:A:694:LEU:H	2.25	0.45
1:B:184:GLU:C	1:B:186:SER:H	2.25	0.45
1:B:436:VAL:HG21	1:B:471:LYS:HG2	1.99	0.45
1:A:328:LYS:HG2	1:A:332:GLN:OE1	2.16	0.45
1:A:465:ALA:O	1:A:469:VAL:HG22	2.17	0.45
1:B:357:TRP:CG	1:B:367:PHE:HE1	2.34	0.45
1:B:529:LYS:HD3	1:B:547:SER:HB2	1.98	0.45
1:A:163:SER:HA	1:A:166:VAL:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:ASN:OD1	1:A:537:ASN:N	2.48	0.44
1:A:613:VAL:O	1:A:630:ASP:HB2	2.17	0.44
1:A:222:LEU:HB3	1:A:293:ALA:HB1	1.99	0.44
1:B:211:ARG:HA	1:B:214:GLU:CD	2.42	0.44
1:A:685:ILE:HD13	1:A:685:ILE:HA	1.83	0.44
1:B:97:ARG:NH2	1:B:142:SER:OG	2.50	0.44
1:B:357:TRP:CD2	1:B:367:PHE:CE1	2.99	0.44
1:A:459:ARG:CD	1:A:485:VAL:HG21	2.47	0.44
1:B:334:LEU:O	1:B:338:VAL:HG13	2.17	0.44
1:A:697:ILE:HG13	1:A:697:ILE:O	2.17	0.44
1:B:345:THR:O	1:B:349:VAL:HG13	2.17	0.44
1:A:210:SER:O	1:A:214:GLU:HG3	2.18	0.44
1:A:528:ALA:HB1	1:A:582:ILE:HD11	1.99	0.44
1:B:428:THR:HG21	1:B:617:GLY:HA2	2.00	0.44
1:A:307:ARG:HD2	1:A:311:GLU:O	2.18	0.44
1:B:500:VAL:HG22	1:B:534:VAL:HG12	1.99	0.44
1:B:687:ILE:HG13	1:B:688:PRO:HD3	2.00	0.44
1:A:230:ILE:HD13	1:A:230:ILE:HG21	1.74	0.44
1:B:216:ILE:HG23	1:B:318:VAL:HG13	1.98	0.43
1:A:207:ARG:HH11	1:A:211:ARG:HH22	1.66	0.43
1:A:375:VAL:HG21	1:A:691:ALA:HB2	1.99	0.43
1:B:462:HIS:CG	1:B:463:PRO:HD2	2.53	0.43
1:B:484:LYS:HB3	1:B:495:ALA:HA	2.00	0.43
1:A:162:TYR:CE1	1:A:380:CYS:HB3	2.53	0.43
1:A:217:LYS:HA	1:A:217:LYS:HD3	1.77	0.43
1:B:387:ALA:HB1	1:B:675:ASN:HB3	1.99	0.43
1:B:443:ASN:OD1	1:B:444:GLY:N	2.51	0.43
1:A:324:ALA:O	1:A:396:MET:HE1	2.17	0.43
1:B:715:SER:O	1:B:719:VAL:HG23	2.19	0.43
1:A:205:GLU:CA	1:A:386:LEU:HD21	2.48	0.43
1:A:715:SER:O	1:A:719:VAL:HG23	2.19	0.43
1:B:346:VAL:HA	1:B:349:VAL:HG22	2.00	0.43
1:B:425:LYS:O	1:B:430:THR:HG23	2.18	0.43
1:A:133:LEU:HB3	1:A:134:PRO:HD3	2.01	0.43
1:A:124:GLU:O	1:A:128:GLN:HG3	2.18	0.43
1:B:325:MET:HE1	1:B:396:MET:HB2	2.01	0.43
1:A:159:ASP:OD2	1:A:202:ARG:NH2	2.52	0.43
1:A:457:GLU:HB2	1:A:468:ILE:HD11	2.01	0.43
1:A:714:SER:O	1:A:718:VAL:HG13	2.18	0.43
1:B:123:TYR:HE1	1:B:126:PHE:HB2	1.83	0.43
1:B:439:LEU:HD23	1:B:544:ILE:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:700:VAL:HG12	1:B:700:VAL:O	2.19	0.43
1:A:329:PRO:HD2	1:A:332:GLN:CB	2.48	0.42
1:B:378:VAL:HG23	1:B:707:ALA:HB1	2.01	0.42
1:A:446:GLU:N	1:A:446:GLU:OE1	2.52	0.42
1:B:216:ILE:HG12	1:B:322:GLU:HG2	2.01	0.42
1:B:245:VAL:HG23	1:B:308:VAL:CG1	2.49	0.42
1:A:284:LYS:HE3	1:A:290:VAL:HG12	2.02	0.42
1:B:263:VAL:HG21	1:B:301:LEU:HD22	2.00	0.42
1:A:439:LEU:HD13	1:A:446:GLU:HB3	2.01	0.42
1:B:415:ALA:HA	1:B:418:VAL:HG23	2.02	0.42
1:B:151:LEU:HD11	1:B:160:VAL:HG13	2.02	0.42
1:B:204:LEU:HD23	1:B:204:LEU:HA	1.83	0.42
1:A:161:MET:HE1	1:A:376:LEU:HD22	2.02	0.42
1:B:236:ILE:HG12	1:B:238:VAL:HG12	2.02	0.42
1:B:499:LEU:HD12	1:B:511:VAL:HG21	2.01	0.42
1:B:335:ALA:HA	1:B:338:VAL:HG22	2.02	0.42
1:A:236:ILE:HG12	1:A:238:VAL:HG12	2.02	0.42
1:A:308:VAL:H	1:A:311:GLU:HB2	1.85	0.42
1:A:471:LYS:HD2	1:A:475:HIS:ND1	2.34	0.42
1:A:699:GLY:O	1:A:701:VAL:N	2.53	0.42
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.76	0.41
1:B:513:VAL:O	1:B:513:VAL:HG13	2.20	0.41
1:B:699:GLY:C	1:B:701:VAL:N	2.77	0.41
1:A:513:VAL:O	1:A:513:VAL:HG13	2.20	0.41
1:A:576:TRP:HD1	1:A:594:GLU:OE2	2.03	0.41
1:A:715:SER:O	1:A:718:VAL:HG22	2.20	0.41
1:B:343:ILE:HA	1:B:346:VAL:HG22	2.02	0.41
1:B:687:ILE:N	1:B:688:PRO:HD2	2.35	0.41
1:A:158:MET:HB3	1:A:202:ARG:NH1	2.34	0.41
1:B:441:PRO:HB2	1:B:443:ASN:OD1	2.20	0.41
1:A:190:THR:O	1:A:192:VAL:N	2.52	0.41
1:A:451:ARG:O	1:A:455:ILE:HG12	2.21	0.41
1:B:367:PHE:O	1:B:371:THR:HG23	2.20	0.41
1:B:384:PHE:HE2	1:B:680:LEU:HG	1.85	0.41
1:B:428:THR:CG2	1:B:617:GLY:HA2	2.51	0.41
1:A:120:SER:O	1:A:121:LEU:HD23	2.20	0.41
1:B:470:LYS:HD3	1:B:470:LYS:C	2.45	0.41
1:B:652:ARG:NH1	1:B:657:ASP:OD2	2.48	0.41
1:A:98:MET:HB3	1:A:203:THR:HG22	2.03	0.41
1:A:204:LEU:HA	1:A:204:LEU:HD23	1.75	0.41
1:A:468:ILE:HD12	1:A:469:VAL:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:VAL:O	1:B:131:ILE:HG13	2.20	0.41
1:B:529:LYS:HG2	1:B:547:SER:HA	2.03	0.41
1:A:161:MET:HE2	1:A:379:ALA:HB3	2.03	0.41
1:A:471:LYS:HD2	1:A:475:HIS:CE1	2.55	0.41
1:B:531:ALA:HA	1:B:544:ILE:O	2.21	0.41
1:A:199:LEU:HA	1:A:199:LEU:HD23	1.84	0.41
1:A:375:VAL:CG2	1:A:691:ALA:HB2	2.51	0.41
1:A:553:SER:C	1:A:556:PRO:HD2	2.46	0.41
1:A:156:LEU:HB3	1:A:343:ILE:HG21	2.03	0.41
1:A:169:ALA:HB1	1:A:187:PHE:HB3	2.03	0.41
1:A:384:PHE:HE2	1:A:680:LEU:HG	1.86	0.41
1:B:375:VAL:HG22	1:B:690:ALA:HB3	2.02	0.41
1:B:656:ARG:HG2	1:B:732:ILE:CG1	2.50	0.41
1:B:689:ALA:HA	1:B:694:LEU:CD2	2.51	0.41
1:A:325:MET:SD	1:A:396:MET:HE3	2.61	0.41
1:B:365:LEU:HD12	1:B:365:LEU:O	2.21	0.41
1:B:470:LYS:NZ	1:B:474:GLU:OE1	2.35	0.41
1:A:260:ASP:OD1	1:A:292:GLY:N	2.32	0.40
1:A:443:ASN:OD1	1:A:444:GLY:N	2.54	0.40
1:A:700:VAL:O	1:A:700:VAL:HG12	2.21	0.40
1:B:692:GLY:O	1:B:694:LEU:HG	2.21	0.40
1:A:357:TRP:HZ2	1:A:692:GLY:HA3	1.87	0.40
1:B:619:GLY:HA2	1:B:626:LEU:CD1	2.52	0.40
1:A:414:VAL:O	1:A:418:VAL:HG23	2.21	0.40
1:B:126:PHE:O	1:B:129:LEU:HG	2.22	0.40
1:B:184:GLU:O	1:B:186:SER:N	2.53	0.40
1:B:701:VAL:O	1:B:701:VAL:HG12	2.21	0.40
1:A:238:VAL:HG23	1:A:239:PRO:O	2.21	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	652/658 (99%)	618 (95%)	32 (5%)	2 (0%)	36	70
1	B	650/658 (99%)	610 (94%)	35 (5%)	5 (1%)	16	51
All	All	1302/1316 (99%)	1228 (94%)	67 (5%)	7 (0%)	24	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	693	LEU
1	A	700	VAL
1	B	434	PRO
1	B	702	PHE
1	A	434	PRO
1	B	224	ALA
1	B	701	VAL

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	521/523 (100%)	521 (100%)	0	100	100
1	B	519/523 (99%)	518 (100%)	1 (0%)	87	87
All	All	1040/1046 (99%)	1039 (100%)	1 (0%)	88	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	195	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	GLN
1	A	598	HIS
1	B	675	ASN

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Mol	Chain	Res	Type
1	B	683	ASN
1	B	721	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	654/658 (99%)	-0.31	4 (0%)	85 71	134, 192, 275, 295	0
1	B	652/658 (99%)	-0.31	4 (0%)	85 71	139, 196, 273, 295	0
All	All	1306/1316 (99%)	-0.31	8 (0%)	85 71	134, 195, 274, 295	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	87	ALA	5.2
1	A	544	ILE	4.4
1	A	545	ALA	3.5
1	B	233	GLY	3.4
1	A	531	ALA	2.8
1	B	86	ALA	2.4
1	B	723	LEU	2.3
1	A	153	ARG	2.2

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.