



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:14 PM UTC

PDB ID : 3NND / pdb_00003nnd
Title : The crystal structure of ABC transporter from Rhodopseudomonas palustris
Authors : Zhang, Z.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center
for Structural Genomics (NYSGXRC)
Deposited on : 2010-06-23
Resolution : 2.80 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

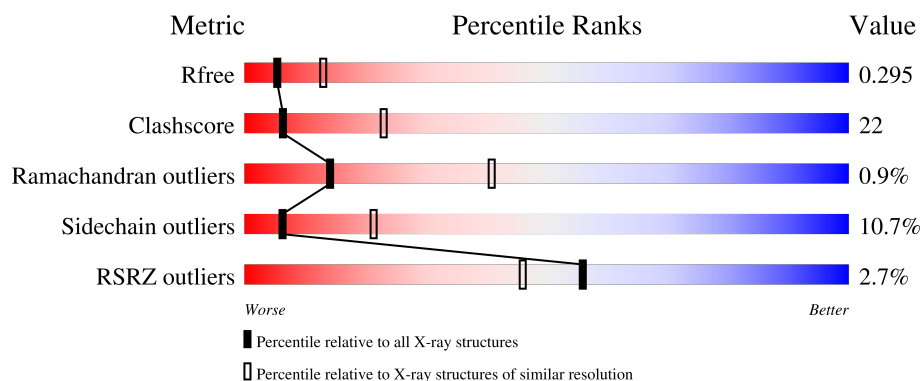
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	366	2% 51% 36% 5% 7%
1	B	366	% 52% 32% 6% 10%
1	C	366	4% 51% 34% 5% 10%
1	D	366	3% 49% 36% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10255 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 Possible substrate binding protein of ABC transporter system.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	330	Total	C	N	O	Se	0	0	0
			2516	1609	415	482	10			
1	A	339	Total	C	N	O	Se	0	0	0
			2592	1656	429	497	10			
1	C	329	Total	C	N	O	Se	0	0	0
			2501	1597	414	480	10			
1	D	328	Total	C	N	O	Se	0	0	0
			2506	1604	415	477	10			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MSE	-	expression tag	UNP Q6N1K8
B	10	SER	-	expression tag	UNP Q6N1K8
B	11	LEU	-	expression tag	UNP Q6N1K8
B	367	GLU	-	expression tag	UNP Q6N1K8
B	368	GLY	-	expression tag	UNP Q6N1K8
B	369	HIS	-	expression tag	UNP Q6N1K8
B	370	HIS	-	expression tag	UNP Q6N1K8
B	371	HIS	-	expression tag	UNP Q6N1K8
B	372	HIS	-	expression tag	UNP Q6N1K8
B	373	HIS	-	expression tag	UNP Q6N1K8
B	374	HIS	-	expression tag	UNP Q6N1K8
A	9	MSE	-	expression tag	UNP Q6N1K8
A	10	SER	-	expression tag	UNP Q6N1K8
A	11	LEU	-	expression tag	UNP Q6N1K8
A	367	GLU	-	expression tag	UNP Q6N1K8
A	368	GLY	-	expression tag	UNP Q6N1K8
A	369	HIS	-	expression tag	UNP Q6N1K8
A	370	HIS	-	expression tag	UNP Q6N1K8
A	371	HIS	-	expression tag	UNP Q6N1K8
A	372	HIS	-	expression tag	UNP Q6N1K8
A	373	HIS	-	expression tag	UNP Q6N1K8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	374	HIS	-	expression tag	UNP Q6N1K8
C	9	MSE	-	expression tag	UNP Q6N1K8
C	10	SER	-	expression tag	UNP Q6N1K8
C	11	LEU	-	expression tag	UNP Q6N1K8
C	367	GLU	-	expression tag	UNP Q6N1K8
C	368	GLY	-	expression tag	UNP Q6N1K8
C	369	HIS	-	expression tag	UNP Q6N1K8
C	370	HIS	-	expression tag	UNP Q6N1K8
C	371	HIS	-	expression tag	UNP Q6N1K8
C	372	HIS	-	expression tag	UNP Q6N1K8
C	373	HIS	-	expression tag	UNP Q6N1K8
C	374	HIS	-	expression tag	UNP Q6N1K8
D	9	MSE	-	expression tag	UNP Q6N1K8
D	10	SER	-	expression tag	UNP Q6N1K8
D	11	LEU	-	expression tag	UNP Q6N1K8
D	367	GLU	-	expression tag	UNP Q6N1K8
D	368	GLY	-	expression tag	UNP Q6N1K8
D	369	HIS	-	expression tag	UNP Q6N1K8
D	370	HIS	-	expression tag	UNP Q6N1K8
D	371	HIS	-	expression tag	UNP Q6N1K8
D	372	HIS	-	expression tag	UNP Q6N1K8
D	373	HIS	-	expression tag	UNP Q6N1K8
D	374	HIS	-	expression tag	UNP Q6N1K8

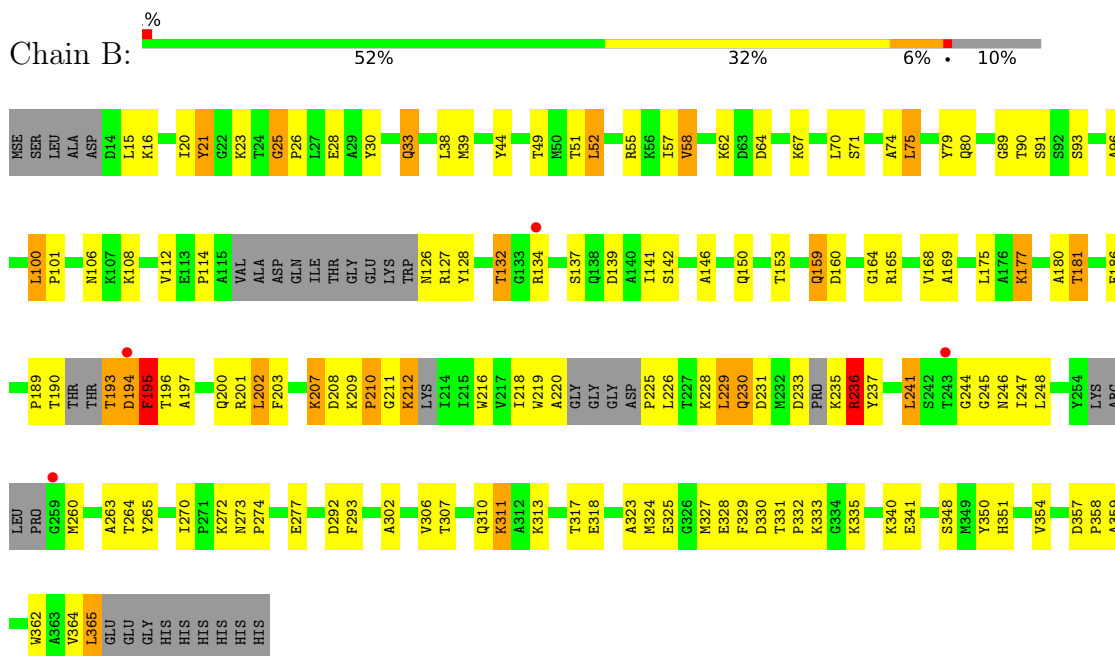
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	30	Total O 30 30	0	0
2	A	54	Total O 54 54	0	0
2	C	29	Total O 29 29	0	0
2	D	27	Total O 27 27	0	0

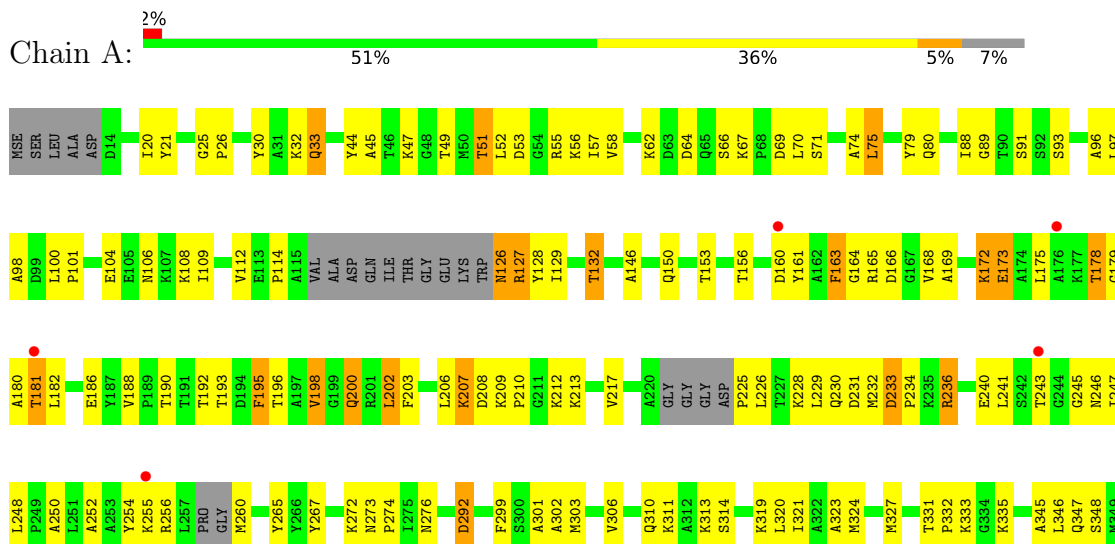
3 Residue-property plots

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: Possible substrate binding protein of ABC transporter system

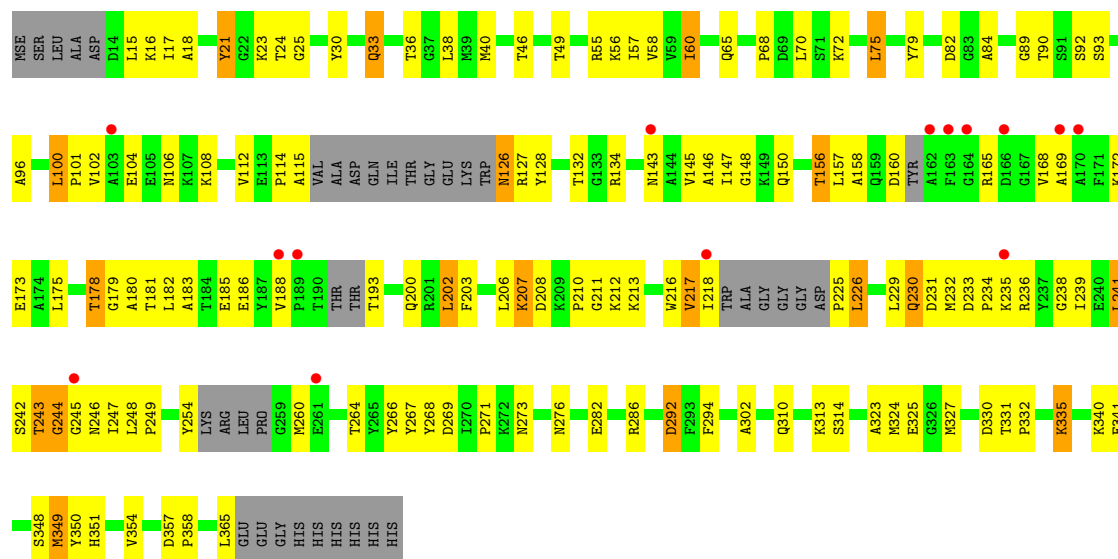


- Molecule 1: Possible substrate binding protein of ABC transporter system

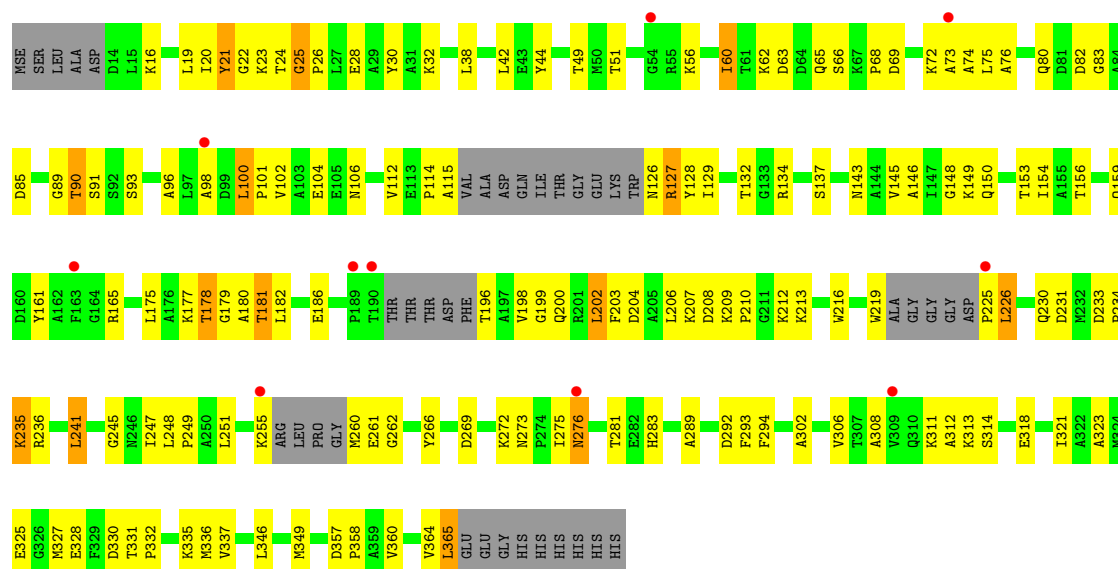




- Molecule 1: Possible substrate binding protein of ABC transporter system



- Molecule 1: Possible substrate binding protein of ABC transporter system



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.74Å 118.43Å 93.46Å 90.00° 106.87° 90.00°	Depositor
Resolution (Å)	51.54 – 2.80 51.54 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (51.54-2.80) 99.3 (51.54-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.244 , 0.296 0.242 , 0.295	Depositor DCC
R_{free} test set	2927 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	10255	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.50% 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	0.51	0/2631	0.85	3/3544 (0.1%)
1	B	0.56	0/2550	0.94	11/3429 (0.3%)
1	C	0.47	0/2534	0.82	3/3407 (0.1%)
1	D	0.47	0/2543	0.89	3/3423 (0.1%)
All	All	0.50	0/10258	0.88	20/13803 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	PHE	N-CA-C	10.05	123.45	109.18
1	B	169	ALA	N-CA-C	-7.51	103.11	112.72
1	B	236	ARG	N-CA-C	-7.46	104.31	113.19
1	D	25	GLY	CA-C-N	6.85	126.81	119.28
1	D	25	GLY	C-N-CA	6.85	126.81	119.28
1	A	25	GLY	CA-C-N	6.51	126.74	119.32
1	A	25	GLY	C-N-CA	6.51	126.74	119.32
1	B	244	GLY	N-CA-C	-6.30	105.71	112.08
1	C	25	GLY	CA-C-N	5.85	125.72	119.28
1	C	25	GLY	C-N-CA	5.85	125.72	119.28
1	B	25	GLY	CA-C-N	5.82	125.95	119.32
1	B	25	GLY	C-N-CA	5.82	125.95	119.32
1	B	270	ILE	N-CA-C	5.49	114.14	107.61
1	D	262	GLY	N-CA-C	5.45	119.07	112.48
1	C	349	MSE	N-CA-C	5.19	117.14	108.99
1	B	201	ARG	N-CA-C	-5.19	105.63	111.28
1	A	226	LEU	N-CA-C	-5.18	104.89	111.11
1	B	200	GLN	N-CA-C	-5.18	106.65	113.12
1	B	195	PHE	CA-C-N	5.01	127.45	120.63
1	B	195	PHE	C-N-CA	5.01	127.45	120.63

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	2592	0	2607	136	0
1	B	2516	0	2521	125	0
1	C	2501	0	2518	128	0
1	D	2506	0	2528	112	0
2	A	54	0	0	2	0
2	B	30	0	0	0	0
2	C	29	0	0	1	0
2	D	27	0	0	1	0
All	All	10255	0	10174	449	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 22.

All (449) 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:212:LYS:HE3	1:B:247:ILE:O	1.40	1.19
1:B:248:LEU:HD12	1:B:260:MSE:HE2	1.41	1.03
1:B:307:THR:HB	1:B:327:MSE:HE1	1.40	1.00
1:B:233:ASP:HB3	1:B:236:ARG:HG2	1.47	0.97
1:D:230:GLN:HE21	1:D:241:LEU:HD22	1.31	0.95
1:C:248:LEU:HD12	1:C:260:MSE:HE2	1.48	0.95
1:B:168:VAL:HG22	1:B:218:ILE:HD12	1.47	0.93
1:C:175:LEU:HD11	1:C:180:ALA:HB3	1.50	0.92
1:A:248:LEU:HD12	1:A:260:MSE:HE2	1.54	0.90
1:B:245:GLY:HA3	1:D:231:ASP:HA	1.54	0.89
1:A:178:THR:HG22	1:A:180:ALA:H	1.39	0.87
1:B:146:ALA:O	1:B:150:GLN:HG3	1.73	0.87
1:D:178:THR:HG22	1:D:180:ALA:H	1.39	0.86
1:A:126:ASN:HD22	1:A:128:TYR:H	1.21	0.85
1:A:203:PHE:O	1:A:207:LYS:HG3	1.76	0.83
1:A:80:GLN:HE21	1:A:106:ASN:HD21	1.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:LEU:HD12	1:D:302:ALA:HB2	1.62	0.81
1:D:175:LEU:O	1:D:178:THR:HB	1.80	0.81
1:C:341:GLU:HB2	2:C:8:HOH:O	1.78	0.81
1:D:175:LEU:HD11	1:D:180:ALA:HB3	1.63	0.80
1:C:146:ALA:O	1:C:150:GLN:HG3	1.81	0.80
1:B:194:ASP:HB2	1:B:228:LYS:HG3	1.63	0.80
1:C:178:THR:HG22	1:C:180:ALA:H	1.46	0.80
1:B:175:LEU:HD11	1:B:180:ALA:HB3	1.62	0.79
1:C:357:ASP:HB3	1:D:255:LYS:HZ2	1.48	0.78
1:D:330:ASP:OD1	1:D:335:LYS:HD2	1.84	0.78
1:D:248:LEU:HD12	1:D:260:MSE:HE2	1.65	0.78
1:A:233:ASP:O	1:A:236:ARG:HG3	1.84	0.77
1:C:335:LYS:HG3	1:C:348:SER:HB3	1.66	0.77
1:A:33:GLN:HG2	1:A:292:ASP:OD2	1.84	0.77
1:B:89:GLY:O	1:B:112:VAL:HA	1.84	0.77
1:D:230:GLN:NE2	1:D:241:LEU:HD22	2.00	0.76
1:B:231:ASP:OD1	1:D:245:GLY:HA2	1.85	0.76
1:B:153:THR:HG23	1:B:181:THR:HG22	1.66	0.76
1:B:75:LEU:HD22	1:B:79:TYR:CE2	2.22	0.75
1:B:186:GLU:HG3	1:B:202:LEU:HD13	1.69	0.75
1:B:245:GLY:HA2	1:D:231:ASP:OD1	1.87	0.74
1:A:245:GLY:HA2	1:C:231:ASP:OD1	1.87	0.74
1:D:153:THR:HG23	1:D:181:THR:HG22	1.70	0.73
1:D:89:GLY:O	1:D:112:VAL:HA	1.90	0.72
1:C:357:ASP:HB3	1:D:255:LYS:NZ	2.05	0.71
1:A:67:LYS:HD2	1:A:70:LEU:HD12	1.70	0.71
1:A:252:ALA:HA	1:A:255:LYS:HG2	1.73	0.70
1:B:324:MSE:HA	1:B:327:MSE:HG2	1.73	0.70
1:B:194:ASP:HB3	1:B:225:PRO:HA	1.71	0.70
1:A:168:VAL:O	1:A:172:LYS:HB2	1.92	0.69
1:A:195:PHE:CE1	1:A:228:LYS:HG3	2.27	0.69
1:D:126:ASN:HB2	1:D:129:ILE:HG12	1.72	0.69
1:C:33:GLN:HG2	1:C:292:ASP:OD2	1.92	0.69
1:D:323:ALA:O	1:D:327:MSE:HE3	1.92	0.69
1:C:175:LEU:O	1:C:178:THR:HB	1.93	0.69
1:B:195:PHE:HD1	1:B:196:THR:H	1.35	0.68
1:A:232:MSE:HA	1:C:267:TYR:CE2	2.29	0.68
1:A:356:VAL:O	1:A:360:VAL:HG23	1.94	0.68
1:D:178:THR:HG22	1:D:180:ALA:N	2.09	0.67
1:B:233:ASP:CB	1:B:236:ARG:HG2	2.23	0.67
1:C:330:ASP:OD1	1:C:335:LYS:HE3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:PRO:HG2	1:A:241:LEU:HD11	1.76	0.67
1:B:330:ASP:OD1	1:B:335:LYS:HE3	1.94	0.66
1:A:80:GLN:HE21	1:A:106:ASN:ND2	1.93	0.66
1:A:209:LYS:O	1:A:213:LYS:HE2	1.95	0.66
1:B:160:ASP:OD1	1:B:165:ARG:NH1	2.29	0.66
1:B:357:ASP:HB2	1:B:358:PRO:HD3	1.78	0.65
1:B:168:VAL:HG12	1:B:168:VAL:O	1.96	0.65
1:B:272:LYS:HE3	1:A:350:TYR:CZ	2.31	0.65
1:D:357:ASP:HB2	1:D:358:PRO:HD3	1.78	0.65
1:B:33:GLN:HG2	1:B:292:ASP:OD2	1.95	0.65
1:B:233:ASP:O	1:B:235:LYS:N	2.30	0.65
1:A:88:ILE:HD13	1:A:301:ALA:HB1	1.79	0.64
1:B:246:ASN:CG	1:B:264:THR:HG23	2.23	0.64
1:A:212:LYS:HE2	1:A:247:ILE:O	1.97	0.64
1:D:28:GLU:O	1:D:32:LYS:HG3	1.97	0.64
1:C:186:GLU:HG3	1:C:202:LEU:CD1	2.28	0.63
1:B:80:GLN:HG3	1:B:106:ASN:HD21	1.62	0.63
1:D:62:LYS:HB3	1:D:74:ALA:HB1	1.80	0.63
1:B:134:ARG:CZ	1:C:210:PRO:HG3	2.28	0.63
1:D:233:ASP:OD1	1:D:235:LYS:HG3	1.99	0.62
1:B:235:LYS:C	1:B:237:TYR:H	2.05	0.62
1:A:52:LEU:HD22	1:A:306:VAL:HG13	1.81	0.62
1:A:126:ASN:ND2	1:A:128:TYR:H	1.95	0.62
1:A:230:GLN:HG2	1:A:241:LEU:HD22	1.80	0.62
1:C:16:LYS:HE3	1:C:60:ILE:HG12	1.80	0.62
1:A:320:LEU:O	1:A:324:MSE:HG3	2.00	0.62
1:B:365:LEU:C	1:B:365:LEU:HD23	2.25	0.61
1:D:364:VAL:HG23	1:D:365:LEU:H	1.65	0.61
1:A:146:ALA:O	1:A:150:GLN:HG3	2.00	0.61
1:C:225:PRO:HG2	1:C:226:LEU:H	1.65	0.61
1:A:89:GLY:O	1:A:112:VAL:HA	2.01	0.61
1:A:195:PHE:HE1	1:A:228:LYS:HG3	1.64	0.61
1:C:168:VAL:HG12	1:C:168:VAL:O	2.00	0.61
1:C:21:TYR:OH	1:C:23:LYS:HD2	2.01	0.61
1:B:134:ARG:CG	1:C:208:ASP:HB3	2.31	0.60
1:A:311:LYS:HG2	1:A:323:ALA:HB1	1.82	0.60
1:C:79:TYR:CD1	1:C:108:LYS:HD2	2.37	0.60
1:B:307:THR:CB	1:B:327:MSE:HE1	2.24	0.60
1:D:321:ILE:O	1:D:325:GLU:HG3	2.01	0.60
1:B:52:LEU:O	1:B:55:ARG:HB2	2.01	0.60
1:B:21:TYR:CE2	1:B:23:LYS:HB2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:PHE:HD1	1:B:196:THR:N	1.97	0.60
1:C:158:ALA:HB2	1:C:218:ILE:HB	1.83	0.59
1:C:186:GLU:HG3	1:C:202:LEU:HD13	1.83	0.59
1:C:354:VAL:HG12	1:D:266:TYR:HB3	1.83	0.59
1:A:357:ASP:HB2	1:A:358:PRO:HD3	1.84	0.59
1:B:233:ASP:C	1:B:235:LYS:N	2.61	0.59
1:C:211:GLY:O	1:C:213:LYS:NZ	2.35	0.59
1:D:209:LYS:O	1:D:213:LYS:HE3	2.03	0.59
1:A:91:SER:HA	1:A:114:PRO:HD2	1.85	0.59
1:B:79:TYR:CD1	1:B:108:LYS:HD2	2.39	0.58
1:B:134:ARG:HG2	1:C:208:ASP:HB3	1.84	0.58
1:C:282:GLU:O	1:C:286:ARG:HG3	2.03	0.58
1:C:15:LEU:HD13	1:C:57:ILE:HG12	1.86	0.58
1:D:146:ALA:O	1:D:150:GLN:HG3	2.04	0.58
1:B:208:ASP:O	1:C:134:ARG:HG3	2.03	0.58
1:A:20:ILE:HD11	1:A:75:LEU:HD23	1.84	0.57
1:B:49:THR:O	1:B:51:THR:HG23	2.04	0.57
1:C:269:ASP:HB2	1:D:349:MSE:HE3	1.86	0.57
1:D:96:ALA:O	1:D:100:LEU:HD13	2.05	0.57
1:B:52:LEU:HD22	1:B:306:VAL:HG13	1.87	0.57
1:B:328:GLU:OE2	1:A:272:LYS:NZ	2.38	0.57
1:A:153:THR:HG23	1:A:181:THR:HG22	1.87	0.57
1:A:346:LEU:CD2	1:D:208:ASP:HB2	2.35	0.57
1:D:328:GLU:HG2	1:D:337:VAL:HB	1.86	0.57
1:B:364:VAL:HG23	1:B:365:LEU:N	2.20	0.57
1:D:233:ASP:OD1	1:D:235:LYS:HE2	2.04	0.57
1:A:365:LEU:HD22	1:A:365:LEU:O	2.05	0.56
1:A:314:SER:OG	1:A:319:LYS:HD3	2.04	0.56
1:B:233:ASP:HB3	1:B:236:ARG:CG	2.29	0.56
1:C:269:ASP:CB	1:D:349:MSE:HE3	2.35	0.56
1:B:235:LYS:O	1:B:235:LYS:CG	2.52	0.56
1:C:160:ASP:OD1	1:C:165:ARG:NH1	2.38	0.56
1:C:323:ALA:O	1:C:327:MSE:HE3	2.05	0.56
1:A:245:GLY:HA3	1:C:231:ASP:HA	1.88	0.56
1:A:195:PHE:N	1:A:195:PHE:CD1	2.74	0.55
1:B:38:LEU:HD12	1:B:302:ALA:HB2	1.88	0.55
1:B:195:PHE:CD1	1:B:196:THR:N	2.66	0.55
1:D:273:ASN:H	1:D:276:ASN:HB2	1.72	0.55
1:C:230:GLN:HE21	1:C:241:LEU:HD22	1.72	0.55
1:B:96:ALA:O	1:B:100:LEU:HD13	2.07	0.55
1:A:98:ALA:O	1:A:101:PRO:HD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:GLY:HA2	1:C:249:PRO:HB3	1.87	0.55
1:B:139:ASP:O	1:B:142:SER:HB2	2.06	0.54
1:D:273:ASN:N	1:D:276:ASN:HD22	2.04	0.54
1:B:325:GLU:OE1	1:B:340:LYS:HE3	2.07	0.54
1:B:331:THR:HB	1:B:332:PRO:CD	2.38	0.54
1:D:178:THR:HG22	1:D:179:GLY:N	2.21	0.54
1:B:362:TRP:CZ3	1:A:26:PRO:HG3	2.41	0.54
1:B:91:SER:HA	1:B:114:PRO:HD2	1.89	0.54
1:A:56:LYS:HD2	1:A:57:ILE:H	1.73	0.54
1:C:33:GLN:HG2	1:C:294:PHE:HB2	1.89	0.54
1:A:323:ALA:C	1:A:327:MSE:HE3	2.33	0.53
1:C:156:THR:HG21	1:C:168:VAL:HG11	1.89	0.53
1:D:49:THR:O	1:D:51:THR:HG23	2.08	0.53
1:B:364:VAL:HG23	1:B:365:LEU:H	1.72	0.53
1:A:166:ASP:O	1:A:169:ALA:HB3	2.08	0.53
1:A:206:LEU:HB3	1:A:213:LYS:HB3	1.90	0.53
1:C:178:THR:HG22	1:C:180:ALA:N	2.18	0.53
1:C:213:LYS:HD2	1:C:238:GLY:O	2.08	0.53
1:C:233:ASP:O	1:C:236:ARG:HG2	2.09	0.53
1:A:175:LEU:HD12	1:A:178:THR:HG21	1.90	0.53
1:C:357:ASP:OD2	1:D:255:LYS:CE	2.57	0.53
1:B:241:LEU:O	1:B:247:ILE:HD13	2.09	0.53
1:C:350:TYR:CD2	1:D:272:LYS:HG2	2.44	0.53
1:A:186:GLU:HG3	1:A:202:LEU:HD13	1.90	0.53
1:D:186:GLU:HG3	1:D:202:LEU:HD13	1.90	0.53
1:B:348:SER:OG	1:A:272:LYS:HD2	2.08	0.53
1:B:359:ALA:HB2	1:A:30:TYR:HE2	1.73	0.53
1:C:16:LYS:HZ2	1:C:58:VAL:HG12	1.74	0.53
1:B:210:PRO:HG3	1:C:134:ARG:NH2	2.24	0.53
1:A:347:GLN:HE21	1:A:348:SER:H	1.57	0.53
1:D:302:ALA:O	1:D:306:VAL:HG23	2.08	0.53
1:B:137:SER:HB2	1:B:293:PHE:CE1	2.44	0.52
1:A:80:GLN:NE2	1:A:106:ASN:HD21	2.04	0.52
1:A:225:PRO:O	1:A:229:LEU:HB2	2.10	0.52
1:C:60:ILE:HD13	1:C:82:ASP:HB3	1.91	0.52
1:C:357:ASP:HB2	1:C:358:PRO:HD3	1.91	0.52
1:D:68:PRO:O	1:D:72:LYS:HG3	2.09	0.52
1:B:15:LEU:C	1:B:15:LEU:HD23	2.34	0.52
1:D:127:ARG:NH2	1:D:318:GLU:OE2	2.42	0.52
1:B:15:LEU:HD13	1:B:57:ILE:HG12	1.91	0.52
1:B:20:ILE:HD13	1:B:62:LYS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ASP:HB3	1:B:225:PRO:CA	2.37	0.52
1:A:323:ALA:O	1:A:327:MSE:HE3	2.09	0.52
1:C:158:ALA:CB	1:C:218:ILE:HB	2.40	0.52
1:C:217:VAL:HG11	1:C:226:LEU:HG	1.90	0.52
1:D:233:ASP:O	1:D:236:ARG:HG2	2.10	0.52
1:B:26:PRO:HB2	1:A:362:TRP:CD1	2.44	0.52
1:A:364:VAL:C	1:A:366:GLU:H	2.16	0.52
1:D:199:GLY:HA2	1:D:202:LEU:HB2	1.91	0.52
1:A:97:LEU:HD12	1:A:100:LEU:HD22	1.92	0.52
1:B:327:MSE:CE	1:B:329:PHE:HB3	2.40	0.52
1:C:310:GLN:O	1:C:313:LYS:HD2	2.10	0.52
1:D:80:GLN:HG3	1:D:106:ASN:HD21	1.73	0.52
1:B:100:LEU:HB2	1:B:101:PRO:HD3	1.91	0.52
1:A:69:ASP:OD1	1:A:70:LEU:N	2.42	0.52
1:B:134:ARG:HG3	1:C:208:ASP:O	2.09	0.51
1:A:132:THR:O	1:A:345:ALA:HB3	2.10	0.51
1:B:235:LYS:C	1:B:237:TYR:N	2.67	0.51
1:B:64:ASP:HB2	1:B:71:SER:HB2	1.91	0.51
1:A:173:GLU:OE1	1:A:173:GLU:HA	2.08	0.51
1:A:241:LEU:O	1:A:247:ILE:HD13	2.10	0.51
1:C:46:THR:O	1:C:49:THR:HG23	2.11	0.51
1:C:323:ALA:O	1:C:327:MSE:HB2	2.10	0.51
1:D:308:ALA:HA	1:D:327:MSE:HE1	1.91	0.51
1:A:310:GLN:O	1:A:313:LYS:HD3	2.11	0.51
1:B:67:LYS:HD2	1:B:70:LEU:CD1	2.41	0.51
1:A:88:ILE:HD13	1:A:301:ALA:CB	2.41	0.50
1:D:216:TRP:HH2	1:D:260:MSE:CG	2.25	0.50
1:D:311:LYS:HG2	1:D:327:MSE:HE2	1.93	0.50
1:D:331:THR:HB	1:D:332:PRO:HD2	1.93	0.50
1:D:149:LYS:HB2	1:D:149:LYS:HZ2	1.77	0.50
1:C:357:ASP:OD2	1:D:255:LYS:HE3	2.12	0.50
1:D:283:HIS:ND1	1:D:289:ALA:O	2.44	0.50
1:A:33:GLN:HE21	1:A:292:ASP:CG	2.20	0.50
1:A:126:ASN:ND2	1:A:129:ILE:HG12	2.26	0.50
1:B:175:LEU:O	1:B:175:LEU:HG	2.11	0.49
1:B:21:TYR:OH	1:B:23:LYS:HD2	2.12	0.49
1:B:127:ARG:NH2	1:B:318:GLU:OE1	2.44	0.49
1:A:272:LYS:HA	1:A:276:ASN:HD22	1.77	0.49
1:D:90:THR:OG1	1:D:91:SER:N	2.44	0.49
1:C:104:GLU:HG3	1:C:128:TYR:CD2	2.47	0.49
1:C:90:THR:HG22	1:C:96:ALA:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:TRP:HH2	1:B:260:MSE:CG	2.25	0.49
1:B:272:LYS:HE2	2:A:407:HOH:O	2.12	0.49
1:A:56:LYS:HD2	1:A:57:ILE:N	2.28	0.49
1:A:161:TYR:HE1	1:A:163:PHE:HB3	1.77	0.49
1:A:254:TYR:C	1:A:256:ARG:H	2.20	0.49
1:C:172:LYS:HE3	1:C:185:GLU:OE2	2.13	0.49
1:B:64:ASP:OD2	1:B:71:SER:HB2	2.13	0.49
1:D:44:TYR:CD1	1:D:44:TYR:C	2.91	0.49
1:D:177:LYS:O	1:D:177:LYS:CG	2.60	0.49
1:B:194:ASP:OD1	1:B:194:ASP:N	2.46	0.48
1:C:203:PHE:O	1:C:207:LYS:HG3	2.12	0.48
1:B:159:GLN:HG3	1:B:219:TRP:CH2	2.48	0.48
1:A:52:LEU:O	1:A:55:ARG:HB2	2.12	0.48
1:A:267:TYR:CD2	1:C:232:MSE:HA	2.47	0.48
1:A:335:LYS:O	1:A:347:GLN:NE2	2.46	0.48
1:A:208:ASP:O	1:D:134:ARG:HG3	2.14	0.48
1:C:157:LEU:HB2	1:C:202:LEU:HD21	1.95	0.48
1:D:177:LYS:HE3	2:D:394:HOH:O	2.12	0.48
1:D:126:ASN:C	1:D:128:TYR:H	2.22	0.48
1:A:299:PHE:O	1:A:302:ALA:HB3	2.14	0.48
1:C:126:ASN:C	1:C:128:TYR:H	2.21	0.48
1:C:271:PRO:O	1:C:276:ASN:ND2	2.47	0.48
1:C:331:THR:HB	1:C:332:PRO:CD	2.44	0.48
1:A:178:THR:HG22	1:A:179:GLY:N	2.29	0.48
1:C:36:THR:O	1:C:40:MSE:HG3	2.13	0.48
1:C:72:LYS:HB3	1:C:102:VAL:HG21	1.95	0.48
1:C:335:LYS:CG	1:C:348:SER:HB3	2.41	0.48
1:B:273:ASN:HB2	1:B:274:PRO:CD	2.44	0.47
1:C:168:VAL:CG2	1:C:218:ILE:HG13	2.44	0.47
1:A:233:ASP:O	1:A:236:ARG:CG	2.61	0.47
1:C:24:THR:O	1:C:65:GLN:HA	2.15	0.47
1:D:104:GLU:CD	1:D:126:ASN:ND2	2.72	0.47
1:B:137:SER:HB2	1:B:293:PHE:CZ	2.49	0.47
1:D:323:ALA:C	1:D:327:MSE:HE3	2.39	0.47
1:B:203:PHE:O	1:B:207:LYS:HG3	2.14	0.47
1:B:153:THR:HG21	1:B:209:LYS:HD3	1.97	0.47
1:B:177:LYS:O	1:B:177:LYS:CG	2.63	0.47
1:B:216:TRP:HH2	1:B:260:MSE:HG2	1.80	0.47
1:B:310:GLN:O	1:B:313:LYS:HD3	2.14	0.47
1:A:252:ALA:HA	1:A:255:LYS:CG	2.42	0.47
1:D:323:ALA:O	1:D:327:MSE:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ILE:HD11	1:C:84:ALA:HB2	1.96	0.47
1:B:62:LYS:HB3	1:B:74:ALA:HB1	1.97	0.47
1:A:234:PRO:HG2	1:A:241:LEU:CD1	2.45	0.47
1:C:79:TYR:HB2	1:C:106:ASN:HD22	1.79	0.47
1:C:89:GLY:O	1:C:112:VAL:HA	2.15	0.47
1:C:96:ALA:O	1:C:100:LEU:HD13	2.14	0.47
1:B:134:ARG:NH2	1:C:210:PRO:HG3	2.30	0.47
1:B:230:GLN:O	1:D:245:GLY:HA3	2.15	0.47
1:A:347:GLN:HE21	1:A:348:SER:N	2.12	0.46
1:B:219:TRP:CD1	1:B:220:ALA:H	2.33	0.46
1:C:79:TYR:HD1	1:C:108:LYS:HD2	1.80	0.46
1:B:354:VAL:O	1:A:265:TYR:HA	2.15	0.46
1:C:100:LEU:HB2	1:C:101:PRO:HD3	1.97	0.46
1:C:331:THR:HB	1:C:332:PRO:HD2	1.97	0.46
1:D:100:LEU:HG	1:D:129:ILE:HG13	1.97	0.46
1:B:44:TYR:CD1	1:B:44:TYR:C	2.93	0.46
1:B:263:ALA:CB	1:A:355:LYS:HE3	2.45	0.46
1:B:350:TYR:CE2	1:A:272:LYS:HG2	2.51	0.46
1:D:161:TYR:O	1:D:165:ARG:HG3	2.16	0.46
1:D:16:LYS:HE2	1:D:83:GLY:O	2.15	0.46
1:A:96:ALA:O	1:A:100:LEU:HD13	2.16	0.46
1:A:161:TYR:CE1	1:A:163:PHE:HB3	2.50	0.46
1:A:175:LEU:O	1:A:178:THR:HB	2.16	0.46
1:A:175:LEU:HD11	1:A:180:ALA:HB3	1.96	0.46
1:C:75:LEU:HD23	1:C:75:LEU:HA	1.77	0.46
1:A:104:GLU:HA	1:A:128:TYR:CD2	2.52	0.45
1:B:126:ASN:HD22	1:B:128:TYR:HD2	1.64	0.45
1:C:246:ASN:CG	1:C:264:THR:HG23	2.41	0.45
1:B:362:TRP:CE3	1:A:26:PRO:CB	2.99	0.45
1:D:360:VAL:O	1:D:364:VAL:HG22	2.16	0.45
1:B:164:GLY:O	1:B:168:VAL:HG23	2.15	0.45
1:A:243:THR:HG21	1:C:243:THR:HG21	1.98	0.45
1:C:16:LYS:HZ3	1:C:58:VAL:HG11	1.81	0.45
1:C:325:GLU:OE1	1:C:340:LYS:HE3	2.16	0.45
1:A:188:VAL:HG11	1:A:198:VAL:HG21	1.97	0.45
1:D:275:ILE:O	1:D:276:ASN:C	2.58	0.45
1:A:208:ASP:HB2	1:D:346:LEU:HD22	1.98	0.45
1:C:178:THR:HG23	1:C:254:TYR:CE1	2.52	0.45
1:D:149:LYS:HB2	1:D:149:LYS:NZ	2.32	0.45
1:C:169:ALA:O	1:C:173:GLU:HB2	2.17	0.45
1:D:60:ILE:HD13	1:D:82:ASP:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LEU:C	1:B:15:LEU:CD2	2.90	0.45
1:A:160:ASP:OD1	1:A:165:ARG:NH1	2.50	0.45
1:C:273:ASN:H	1:C:276:ASN:HB2	1.80	0.45
1:D:75:LEU:HD23	1:D:102:VAL:HB	1.98	0.45
1:D:114:PRO:O	1:D:115:ALA:C	2.60	0.44
1:A:212:LYS:CE	1:A:247:ILE:O	2.63	0.44
1:A:333:LYS:HB3	1:A:333:LYS:HE2	1.88	0.44
1:A:364:VAL:C	1:A:366:GLU:N	2.75	0.44
1:A:49:THR:O	1:A:51:THR:HG23	2.17	0.44
1:C:55:ARG:HH22	1:C:314:SER:HA	1.82	0.44
1:B:333:LYS:O	1:B:333:LYS:HG2	2.17	0.44
1:A:44:TYR:CD1	1:A:44:TYR:C	2.96	0.44
1:A:75:LEU:HD13	1:A:79:TYR:CE2	2.52	0.44
1:A:127:ARG:CB	1:A:127:ARG:HH11	2.30	0.44
1:C:79:TYR:HB2	1:C:106:ASN:ND2	2.32	0.44
1:C:348:SER:C	1:C:349:MSE:HG2	2.43	0.44
1:D:212:LYS:HE2	1:D:247:ILE:O	2.17	0.44
1:C:145:VAL:HG22	1:D:360:VAL:HA	1.99	0.44
1:C:324:MSE:HA	1:C:327:MSE:HB3	1.99	0.44
1:D:98:ALA:O	1:D:101:PRO:HD2	2.18	0.44
1:A:62:LYS:HB3	1:A:74:ALA:HB1	1.99	0.44
1:A:153:THR:HG23	1:A:181:THR:CG2	2.47	0.44
1:A:231:ASP:OD1	1:C:246:ASN:N	2.50	0.44
1:A:246:ASN:HA	2:A:418:HOH:O	2.17	0.44
1:D:204:ASP:HA	1:D:207:LYS:CG	2.48	0.44
1:D:225:PRO:O	1:D:226:LEU:C	2.60	0.44
1:A:132:THR:C	1:A:345:ALA:HB3	2.43	0.44
1:A:331:THR:HB	1:A:332:PRO:HD2	1.99	0.44
1:D:364:VAL:HG23	1:D:365:LEU:N	2.32	0.43
1:A:64:ASP:C	1:A:66:SER:H	2.26	0.43
1:C:248:LEU:HD13	1:C:254:TYR:HB3	2.00	0.43
1:D:127:ARG:NH2	1:D:318:GLU:OE1	2.48	0.43
1:C:16:LYS:NZ	1:C:58:VAL:CG1	2.81	0.43
1:C:30:TYR:CZ	1:D:358:PRO:HB2	2.54	0.43
1:A:53:ASP:C	1:A:55:ARG:H	2.27	0.43
1:C:234:PRO:O	1:C:235:LYS:C	2.61	0.43
1:C:351:HIS:ND1	1:D:269:ASP:OD1	2.41	0.43
1:B:67:LYS:HD2	1:B:70:LEU:HD12	2.00	0.43
1:A:127:ARG:CB	1:A:127:ARG:NH1	2.82	0.43
1:A:127:ARG:NH1	1:A:127:ARG:HB2	2.33	0.43
1:C:212:LYS:HD3	1:C:247:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:ASP:CB	1:D:255:LYS:NZ	2.77	0.43
1:D:204:ASP:HA	1:D:207:LYS:HD2	1.99	0.43
1:B:132:THR:O	1:B:132:THR:HG23	2.18	0.43
1:A:45:ALA:HB2	1:A:303:MSE:SE	2.69	0.43
1:A:75:LEU:CD1	1:A:79:TYR:CE2	3.02	0.43
1:C:354:VAL:HG23	1:D:293:PHE:HB3	1.99	0.43
1:B:30:TYR:CZ	1:A:358:PRO:HB2	2.53	0.43
1:A:311:LYS:CG	1:A:323:ALA:HB1	2.47	0.43
1:A:88:ILE:CD1	1:A:301:ALA:HB1	2.48	0.43
1:D:127:ARG:NH2	1:D:318:GLU:CD	2.77	0.43
1:B:137:SER:O	1:B:141:ILE:HD12	2.19	0.42
1:C:75:LEU:HD22	1:C:79:TYR:CE2	2.53	0.42
1:C:324:MSE:O	1:C:327:MSE:HB3	2.19	0.42
1:D:312:ALA:O	1:D:313:LYS:HB2	2.18	0.42
1:B:341:GLU:HG3	1:C:183:ALA:O	2.19	0.42
1:D:148:GLY:HA2	1:D:249:PRO:HB3	2.00	0.42
1:B:351:HIS:CD2	1:C:200:GLN:CD	2.98	0.42
1:D:38:LEU:O	1:D:42:LEU:HG	2.19	0.42
1:D:65:GLN:O	1:D:66:SER:HB2	2.19	0.42
1:D:327:MSE:O	1:D:337:VAL:HA	2.19	0.42
1:D:328:GLU:HA	1:D:336:MSE:O	2.20	0.42
1:B:108:LYS:HA	1:B:317:THR:OG1	2.19	0.42
1:A:231:ASP:OD1	1:C:245:GLY:HA2	2.19	0.42
1:C:16:LYS:NZ	1:C:58:VAL:HG12	2.34	0.42
1:D:145:VAL:O	1:D:146:ALA:C	2.63	0.42
1:B:159:GLN:HG3	1:B:219:TRP:CZ3	2.54	0.42
1:A:64:ASP:OD2	1:A:71:SER:HB2	2.19	0.42
1:A:163:PHE:CD2	1:A:163:PHE:C	2.97	0.42
1:C:243:THR:O	1:C:244:GLY:O	2.38	0.42
1:C:350:TYR:CZ	1:D:272:LYS:HE2	2.54	0.42
1:B:80:GLN:HG3	1:B:106:ASN:ND2	2.32	0.42
1:B:311:LYS:HG2	1:B:323:ALA:HB1	2.01	0.42
1:A:20:ILE:CD1	1:A:75:LEU:HD23	2.50	0.42
1:C:75:LEU:HB3	1:C:102:VAL:HG11	2.02	0.42
1:C:178:THR:HG22	1:C:179:GLY:N	2.34	0.42
1:D:73:ALA:O	1:D:76:ALA:HB3	2.19	0.42
1:D:206:LEU:HB3	1:D:213:LYS:HB3	2.02	0.42
1:B:51:THR:HA	1:B:55:ARG:O	2.20	0.42
1:A:196:THR:O	1:A:200:GLN:HB2	2.20	0.42
1:B:265:TYR:CD1	1:A:353:LYS:HD2	2.55	0.42
1:A:64:ASP:C	1:A:66:SER:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ASN:HD22	1:A:126:ASN:C	2.27	0.42
1:C:216:TRP:HA	1:C:242:SER:HB2	2.02	0.42
1:D:21:TYR:OH	1:D:23:LYS:HD2	2.19	0.42
1:B:359:ALA:O	1:B:362:TRP:HB3	2.19	0.42
1:A:252:ALA:HA	1:A:255:LYS:CD	2.50	0.42
1:C:126:ASN:HB2	1:C:128:TYR:H	1.85	0.42
1:C:175:LEU:O	1:C:175:LEU:HG	2.20	0.42
1:C:266:TYR:CD2	1:C:266:TYR:C	2.97	0.42
1:A:127:ARG:HH11	1:A:127:ARG:HB3	1.85	0.42
1:A:347:GLN:NE2	1:A:348:SER:H	2.17	0.42
1:C:323:ALA:C	1:C:327:MSE:HE3	2.44	0.42
1:D:19:LEU:HD13	1:D:38:LEU:HD22	2.02	0.42
1:A:252:ALA:HA	1:A:255:LYS:HD3	2.01	0.41
1:C:126:ASN:OD1	1:C:126:ASN:N	2.53	0.41
1:D:30:TYR:CD1	1:D:294:PHE:CE1	3.08	0.41
1:C:21:TYR:N	1:C:21:TYR:CD2	2.88	0.41
1:D:199:GLY:O	1:D:203:PHE:CD2	2.74	0.41
1:B:313:LYS:HD2	1:B:313:LYS:HA	1.76	0.41
1:A:192:THR:O	1:A:195:PHE:CZ	2.73	0.41
1:C:16:LYS:HE3	1:C:60:ILE:CG1	2.48	0.41
1:C:79:TYR:CB	1:C:106:ASN:HD22	2.34	0.41
1:B:189:PRO:O	1:B:193:THR:OG1	2.32	0.41
1:D:196:THR:O	1:D:200:GLN:HB2	2.20	0.41
1:D:226:LEU:HD12	1:D:226:LEU:HA	1.92	0.41
1:B:273:ASN:O	1:B:277:GLU:HG3	2.21	0.41
1:A:79:TYR:CD1	1:A:108:LYS:HD2	2.56	0.41
1:C:126:ASN:C	1:C:128:TYR:N	2.78	0.41
1:D:22:GLY:H	1:D:91:SER:HB2	1.85	0.41
1:D:80:GLN:CG	1:D:106:ASN:HD21	2.33	0.41
1:B:89:GLY:HA2	1:B:90:THR:HA	1.81	0.41
1:C:38:LEU:HD12	1:C:302:ALA:HB2	2.01	0.41
1:C:72:LYS:HB3	1:C:102:VAL:CG2	2.50	0.41
1:B:16:LYS:HG2	1:B:58:VAL:HG22	2.02	0.41
1:B:196:THR:HG22	1:B:197:ALA:N	2.34	0.41
1:B:210:PRO:HA	1:B:211:GLY:HA2	1.81	0.41
1:A:109:ILE:HD11	1:A:321:ILE:HG13	2.01	0.41
1:A:163:PHE:CD2	1:A:164:GLY:N	2.89	0.41
1:A:273:ASN:H	1:A:276:ASN:HB2	1.85	0.41
1:A:357:ASP:O	1:A:358:PRO:C	2.64	0.41
1:C:114:PRO:O	1:C:115:ALA:C	2.63	0.41
1:C:350:TYR:CE2	1:D:272:LYS:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:GLN:HG3	1:D:219:TRP:CH2	2.55	0.41
1:D:234:PRO:C	1:D:236:ARG:N	2.79	0.41
1:B:292:ASP:OD2	1:B:292:ASP:C	2.64	0.41
1:C:18:ALA:HA	1:C:60:ILE:HG13	2.03	0.41
1:B:357:ASP:HA	1:A:250:ALA:HB1	2.03	0.40
1:B:357:ASP:O	1:B:358:PRO:C	2.64	0.40
1:C:266:TYR:CE2	1:C:268:TYR:HB3	2.56	0.40
1:B:225:PRO:O	1:B:229:LEU:HB2	2.22	0.40
1:C:68:PRO:O	1:C:72:LYS:HG3	2.21	0.40
1:C:206:LEU:HB2	1:C:239:ILE:HD11	2.03	0.40
1:D:25:GLY:HA3	1:D:26:PRO:HD2	1.87	0.40
1:D:273:ASN:H	1:D:276:ASN:HD22	1.70	0.40
1:B:263:ALA:HB2	1:A:355:LYS:HE3	2.03	0.40
1:A:45:ALA:HB1	1:A:306:VAL:HG11	2.02	0.40
1:A:273:ASN:HB2	1:A:274:PRO:HD2	2.03	0.40
1:A:310:GLN:O	1:A:313:LYS:CD	2.69	0.40
1:C:21:TYR:N	1:C:21:TYR:HD2	2.19	0.40
1:D:24:THR:OG1	1:D:63:ASP:OD2	2.35	0.40
1:B:25:GLY:O	1:B:28:GLU:HB3	2.21	0.40
1:A:212:LYS:HE3	1:A:240:GLU:OE2	2.22	0.40
1:C:348:SER:O	1:C:349:MSE:HG2	2.21	0.40
1:D:313:LYS:HA	1:D:313:LYS:HD2	1.79	0.40
1:D:20:ILE:HD13	1:D:62:LYS:HB2	2.04	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	331/366 (90%)	310 (94%)	17 (5%)	4 (1%)	10 34
1	B	316/366 (86%)	298 (94%)	16 (5%)	2 (1%)	21 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	317/366 (87%)	296 (93%)	19 (6%)	2 (1%)	21	51
1	D	318/366 (87%)	294 (92%)	21 (7%)	3 (1%)	14	41
All	All	1282/1464 (88%)	1198 (93%)	73 (6%)	11 (1%)	14	41

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	207	LYS
1	A	207	LYS
1	C	207	LYS
1	C	244	GLY
1	D	261	GLU
1	A	365	LEU
1	A	210	PRO
1	D	276	ASN
1	A	233	ASP
1	B	210	PRO
1	D	210	PRO

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	265/275 (96%)	237 (89%)	28 (11%)	6	22
1	B	256/275 (93%)	231 (90%)	25 (10%)	7	25
1	C	256/275 (93%)	225 (88%)	31 (12%)	5	16
1	D	256/275 (93%)	229 (90%)	27 (10%)	6	22
All	All	1033/1100 (94%)	922 (89%)	111 (11%)	6	21

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	21	TYR

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Mol	Chain	Res	Type
1	B	33	GLN
1	B	39	MSE
1	B	52	LEU
1	B	58	VAL
1	B	75	LEU
1	B	93	SER
1	B	100	LEU
1	B	132	THR
1	B	159	GLN
1	B	177	LYS
1	B	181	THR
1	B	190	THR
1	B	193	THR
1	B	194	ASP
1	B	195	PHE
1	B	202	LEU
1	B	212	LYS
1	B	226	LEU
1	B	229	LEU
1	B	230	GLN
1	B	236	ARG
1	B	241	LEU
1	B	311	LYS
1	B	365	LEU
1	A	21	TYR
1	A	32	LYS
1	A	33	GLN
1	A	47	LYS
1	A	51	THR
1	A	58	VAL
1	A	75	LEU
1	A	93	SER
1	A	126	ASN
1	A	127	ARG
1	A	132	THR
1	A	156	THR
1	A	163	PHE
1	A	172	LYS
1	A	173	GLU
1	A	178	THR
1	A	181	THR
1	A	182	LEU

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Mol	Chain	Res	Type
1	A	190	THR
1	A	193	THR
1	A	195	PHE
1	A	198	VAL
1	A	200	GLN
1	A	202	LEU
1	A	217	VAL
1	A	236	ARG
1	A	292	ASP
1	A	365	LEU
1	C	17	ILE
1	C	21	TYR
1	C	33	GLN
1	C	56	LYS
1	C	60	ILE
1	C	70	LEU
1	C	75	LEU
1	C	92	SER
1	C	93	SER
1	C	100	LEU
1	C	126	ASN
1	C	127	ARG
1	C	132	THR
1	C	143	ASN
1	C	147	ILE
1	C	156	THR
1	C	178	THR
1	C	181	THR
1	C	182	LEU
1	C	188	VAL
1	C	193	THR
1	C	202	LEU
1	C	217	VAL
1	C	226	LEU
1	C	229	LEU
1	C	230	GLN
1	C	241	LEU
1	C	243	THR
1	C	292	ASP
1	C	335	LYS
1	C	365	LEU
1	D	21	TYR

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Mol	Chain	Res	Type
1	D	56	LYS
1	D	60	ILE
1	D	69	ASP
1	D	85	ASP
1	D	90	THR
1	D	93	SER
1	D	100	LEU
1	D	127	ARG
1	D	132	THR
1	D	137	SER
1	D	143	ASN
1	D	154	ILE
1	D	156	THR
1	D	178	THR
1	D	181	THR
1	D	182	LEU
1	D	198	VAL
1	D	202	LEU
1	D	226	LEU
1	D	235	LYS
1	D	241	LEU
1	D	251	LEU
1	D	281	THR
1	D	292	ASP
1	D	314	SER
1	D	365	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	80	GLN
1	B	106	ASN
1	B	126	ASN
1	A	33	GLN
1	A	80	GLN
1	A	106	ASN
1	A	126	ASN
1	A	135	ASN
1	A	138	GLN
1	A	276	ASN
1	A	284	GLN
1	A	347	GLN

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Mol	Chain	Res	Type
1	C	106	ASN
1	C	230	GLN
1	C	246	ASN
1	D	106	ASN
1	D	126	ASN
1	D	138	GLN
1	D	230	GLN
1	D	246	ASN
1	D	276	ASN
1	D	347	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no 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 ⓘ

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	329/366 (89%)	0.27	7 (2%) 63 54	21, 29, 44, 64	0
1	B	320/366 (87%)	0.03	4 (1%) 75 66	19, 27, 38, 48	0
1	C	319/366 (87%)	0.40	14 (4%) 39 31	23, 34, 46, 76	0
1	D	318/366 (86%)	0.37	10 (3%) 51 41	23, 34, 47, 61	0
All	All	1286/1464 (87%)	0.27	35 (2%) 56 46	19, 31, 45, 76	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	GLY	4.3
1	C	162	ALA	4.0
1	C	166	ASP	4.0
1	D	190	THR	3.8
1	C	163	PHE	3.6
1	B	194	ASP	3.4
1	D	163	PHE	3.3
1	A	255	LYS	3.3
1	C	261	GLU	3.0
1	D	73	ALA	2.9
1	C	235	LYS	2.9
1	D	54	GLY	2.8
1	D	98	ALA	2.7
1	C	169	ALA	2.6
1	C	245	GLY	2.6
1	C	164	GLY	2.6
1	D	189	PRO	2.6
1	C	103	ALA	2.6
1	C	170	ALA	2.4
1	A	176	ALA	2.4
1	A	160	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	218	ILE	2.4
1	A	243	THR	2.3
1	B	243	THR	2.3
1	C	188	VAL	2.2
1	D	225	PRO	2.2
1	D	309	VAL	2.2
1	C	143	ASN	2.1
1	C	189	PRO	2.1
1	D	255	LYS	2.1
1	D	276	ASN	2.1
1	B	259	GLY	2.1
1	A	181	THR	2.1
1	A	365	LEU	2.0
1	B	134	ARG	2.0

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 oligosaccharides 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.