



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 02:39 AM EDT

PDB ID : 3NND  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

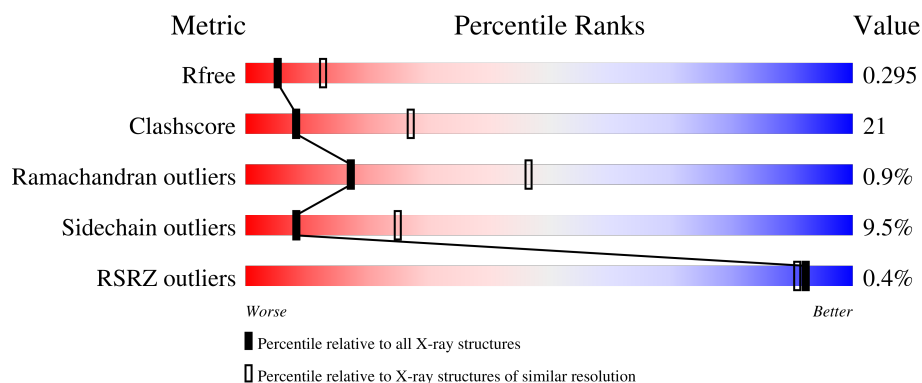
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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  $\geq 3$ , 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	
1	B	366	
1	C	366	
1	D	366	

## 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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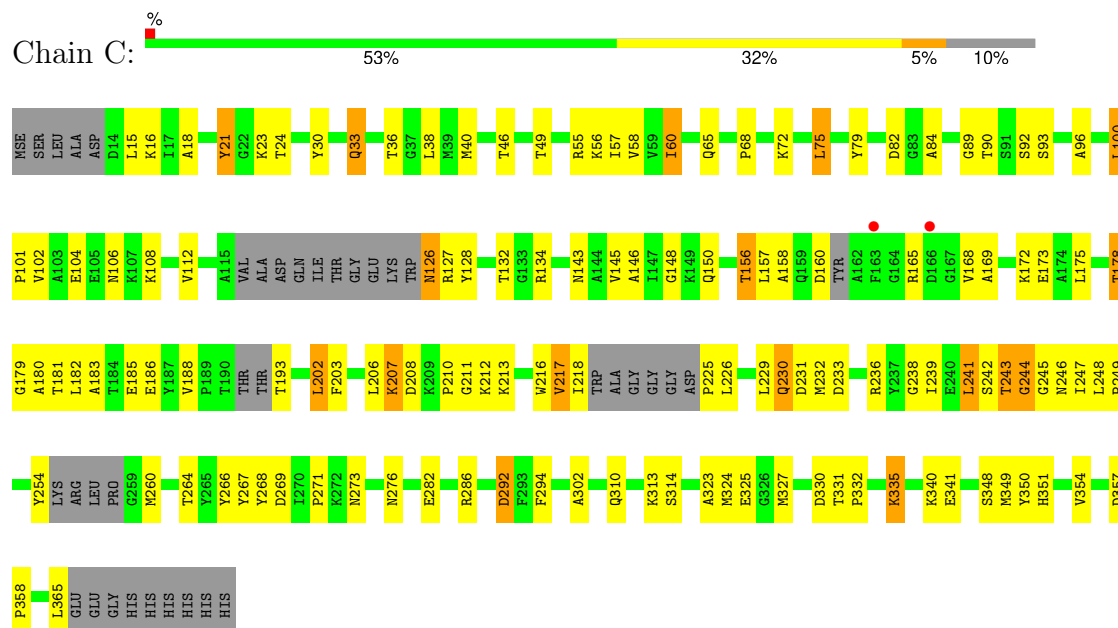
Chain	Residue	Modelled	Actual	Comment	Reference
A	374	HIS	-	expression tag	UNP Q6N1K8
C	9	MSE	-	expression tag	UNP Q6N1K8
C	10	SER	-	expression tag	UNP Q6N1K8
C	11	LEU	-	expression tag	UNP Q6N1K8
C	367	GLU	-	expression tag	UNP Q6N1K8
C	368	GLY	-	expression tag	UNP Q6N1K8
C	369	HIS	-	expression tag	UNP 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.

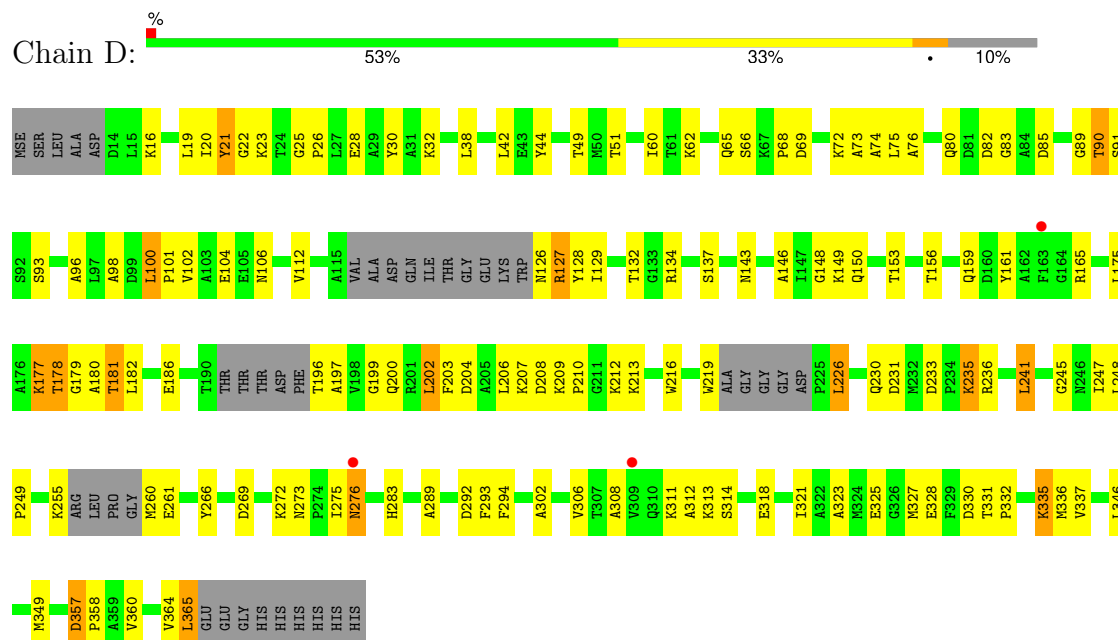
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	30	Total O 30 30	0	0
2	A	54	Total O 54 54	0	0
2	C	29	Total O 29 29	0	0
2	D	27	Total O 27 27	0	0



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



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.74Å 118.43Å 93.46Å 90.00° 106.87° 90.00°	Depositor
Resolution (Å)	51.54 – 2.80 118.43 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.1 (51.54-2.80) 99.1 (118.43-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.244 , 0.296 0.241 , 0.295	Depositor DCC
$R_{free}$ test set	2927 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	10255	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.39	0/2631	0.56	0/3544
1	B	0.42	0/2550	0.63	0/3429
1	C	0.36	0/2534	0.54	0/3407
1	D	0.35	0/2543	0.56	0/3423
All	All	0.38	0/10258	0.57	0/13803

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 [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	2592	0	2607	128	0
1	B	2516	0	2521	121	0
1	C	2501	0	2518	121	0
1	D	2506	0	2528	107	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	426	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 21.

All (426) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:195:PHE:HD1	1:B:196:THR:N	1.97	0.60
1:B:246:ASN:CG	1:B:264:THR:HG23	2.23	0.59
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: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:B:235:LYS:C	1:B:237:TYR:H	2.05	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:B:365:LEU:C	1:B:365:LEU:HD23	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:233:ASP:C	1:B:235:LYS:N	2.61	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:173:GLU:OE1	1:A:173:GLU:HA	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:64:ASP:HB2	1:B:71:SER:HB2	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:THR:HB	1:D:332:PRO:HD2	1.93	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: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
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:323:ALA:C	1:A:327:MSE:HE3	2.33	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: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:B:235:LYS:C	1:B:237:TYR:N	2.67	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:A:299:PHE:O	1:A:302:ALA:HB3	2.14	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:15:LEU:C	1:B:15:LEU:HD23	2.34	0.47
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:364:VAL:C	1:A:366:GLU:H	2.16	0.47
1:A:233:ASP:O	1:A:236:ARG:CG	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:THR:O	1:C:65:GLN:HA	2.15	0.47
1:B:137:SER:HB2	1:B:293:PHE:CZ	2.49	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:CG	1:B:177:LYS:O	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
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: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: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:149:LYS:HB2	1:D:149:LYS:HZ2	1.80	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:HD11	1:A:180:ALA:HB3	1.96	0.46
1:A:175:LEU:O	1:A:178:THR:HB	2.16	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:VAL:HG11	1:A:198:VAL:HG21	1.97	0.45
1:A:33:GLN:HE21	1:A:292:ASP:CG	2.20	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
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: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:49:THR:O	1:A:51:THR:HG23	2.17	0.44
1:A:254:TYR:C	1:A:256:ARG:H	2.20	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: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:D:44:TYR:CD1	1:D:44:TYR:C	2.91	0.44
1:C:79:TYR:HB2	1:C:106:ASN:ND2	2.32	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:A:331:THR:HB	1:A:332:PRO:HD2	1.99	0.44
1:C:126:ASN:C	1:C:128:TYR:H	2.21	0.44
1:D:126:ASN:C	1:D:128:TYR:H	2.22	0.43
1:B:132:THR:HG23	1:B:132:THR:O	2.18	0.43
1:D:364:VAL:HG23	1:D:365:LEU:N	2.32	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:C:351:HIS:ND1	1:D:269:ASP:OD1	2.41	0.43
1:D:104:GLU:CD	1:D:126:ASN:ND2	2.72	0.43
1:B:67:LYS:HD2	1:B:70:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:137:SER:O	1:B:141:ILE:HD12	2.19	0.42
1:B:196:THR:HG22	1:B:197:ALA:N	2.34	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:D:323:ALA:C	1:D:327:MSE:HE3	2.39	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: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: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:C:216:TRP:HA	1:C:242:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:44:TYR:CD1	1:B:44:TYR:C	2.93	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: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: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:C:246:ASN:CG	1:C:264:THR:HG23	2.41	0.41
1:C:350:TYR:CE2	1:D:272:LYS:HG2	2.56	0.41
1:D:159:GLN:HG3	1:D:219:TRP:CH2	2.55	0.41
1:D:275:ILE:O	1:D:276:ASN:C	2.58	0.41
1:C:18:ALA:HA	1:C:60:ILE:HG13	2.03	0.41
1:D:196:THR:HG22	1:D:197:ALA:N	2.35	0.41
1:B:357:ASP:HA	1:A:250:ALA:HB1	2.03	0.40
1:C:266:TYR:CE2	1:C:268:TYR:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:364:VAL:C	1:A:366:GLU:N	2.75	0.40
1:C:21:TYR:N	1:C:21:TYR:HD2	2.19	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:B:15:LEU:C	1:B:15:LEU:CD2	2.90	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

### 5.3.1 Protein backbone

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%)	13	39
1	B	316/366 (86%)	298 (94%)	16 (5%)	2 (1%)	25	56
1	C	317/366 (87%)	296 (93%)	19 (6%)	2 (1%)	25	56
1	D	318/366 (87%)	294 (92%)	21 (7%)	3 (1%)	17	46
All	All	1282/1464 (88%)	1198 (93%)	73 (6%)	11 (1%)	17	46

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%)	241 (91%)	24 (9%)	9	27
1	B	256/275 (93%)	233 (91%)	23 (9%)	9	28
1	C	256/275 (93%)	229 (90%)	27 (10%)	7	20
1	D	256/275 (93%)	232 (91%)	24 (9%)	8	26
All	All	1033/1100 (94%)	935 (90%)	98 (10%)	8	25

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	21	TYR
1	B	33	GLN
1	B	39	MSE
1	B	75	LEU
1	B	81	ASP
1	B	93	SER
1	B	100	LEU
1	B	132	THR
1	B	177	LYS
1	B	181	THR
1	B	190	THR

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Mol	Chain	Res	Type
1	B	193	THR
1	B	194	ASP
1	B	195	PHE
1	B	200	GLN
1	B	202	LEU
1	B	226	LEU
1	B	229	LEU
1	B	230	GLN
1	B	236	ARG
1	B	241	LEU
1	B	357	ASP
1	B	365	LEU
1	A	21	TYR
1	A	47	LYS
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	178	THR
1	A	181	THR
1	A	182	LEU
1	A	190	THR
1	A	193	THR
1	A	195	PHE
1	A	200	GLN
1	A	202	LEU
1	A	217	VAL
1	A	236	ARG
1	A	292	ASP
1	A	335	LYS
1	A	365	LEU
1	C	21	TYR
1	C	33	GLN
1	C	56	LYS
1	C	60	ILE
1	C	75	LEU
1	C	92	SER

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Mol	Chain	Res	Type
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	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	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
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	156	THR
1	D	177	LYS
1	D	178	THR
1	D	181	THR
1	D	182	LEU
1	D	202	LEU
1	D	226	LEU
1	D	235	LYS
1	D	241	LEU
1	D	292	ASP
1	D	314	SER

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Mol	Chain	Res	Type
1	D	335	LYS
1	D	357	ASP
1	D	365	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	33	GLN
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
1	C	80	GLN
1	C	106	ASN
1	C	230	GLN
1	C	276	ASN
1	C	284	GLN
1	D	33	GLN
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 ⓘ

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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	329/366 (89%)	-0.18	0	100 100	21, 29, 44, 64	0
1	B	320/366 (87%)	-0.29	0	100 100	19, 27, 38, 48	0
1	C	319/366 (87%)	-0.18	2 (0%)	89 86	23, 34, 46, 76	0
1	D	318/366 (86%)	-0.13	3 (0%)	84 80	23, 34, 47, 61	0
All	All	1286/1464 (87%)	-0.20	5 (0%)	92 91	19, 31, 45, 76	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	166	ASP	3.4
1	D	163	PHE	3.3
1	C	163	PHE	2.9
1	D	309	VAL	2.6
1	D	276	ASN	2.6

### 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 monosaccharides 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.