



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:45 AM UTC

PDB ID : 3ZTT / pdb_00003ztt
Title : Crystal structure of pneumococcal surface antigen PsaA with manganese
Authors : McDevitt, C.A.; Ogunniyi, A.D.; Valkov, E.; Lawrence, M.C.; Kobe, B.; McEwan, A.G.; Paton, J.C.
Deposited on : 2011-07-12
Resolution : 2.70 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

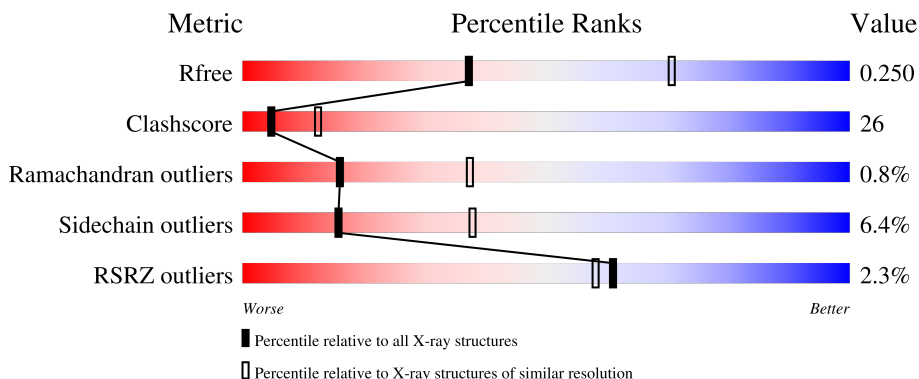
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	303	2% 59% 28% 5% 8%
1	B	303	% 54% 33% 5% 8%
1	C	303	2% 59% 28% • 8%
1	D	303	3% 58% 30% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9024 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 MANGANESE ABC TRANSPORTER SUBSTRATE-BINDING LIPOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2217	1414	355	445	3			
1	B	278	Total	C	N	O	S	0	0	0
			2217	1414	355	445	3			
1	C	278	Total	C	N	O	S	0	0	0
			2216	1414	355	444	3			
1	D	278	Total	C	N	O	S	0	0	0
			2217	1414	355	445	3			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	TRP	-	expression tag	UNP P0A4G3
A	8	ARG	-	expression tag	UNP P0A4G3
A	9	GLY	-	expression tag	UNP P0A4G3
A	10	SER	-	expression tag	UNP P0A4G3
A	11	HIS	-	expression tag	UNP P0A4G3
A	12	HIS	-	expression tag	UNP P0A4G3
A	13	HIS	-	expression tag	UNP P0A4G3
A	14	HIS	-	expression tag	UNP P0A4G3
A	15	HIS	-	expression tag	UNP P0A4G3
A	16	HIS	-	expression tag	UNP P0A4G3
A	17	GLY	-	expression tag	UNP P0A4G3
A	18	SER	-	expression tag	UNP P0A4G3
B	7	TRP	-	expression tag	UNP P0A4G3
B	8	ARG	-	expression tag	UNP P0A4G3
B	9	GLY	-	expression tag	UNP P0A4G3
B	10	SER	-	expression tag	UNP P0A4G3
B	11	HIS	-	expression tag	UNP P0A4G3
B	12	HIS	-	expression tag	UNP P0A4G3
B	13	HIS	-	expression tag	UNP P0A4G3
B	14	HIS	-	expression tag	UNP P0A4G3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	HIS	-	expression tag	UNP P0A4G3
B	16	HIS	-	expression tag	UNP P0A4G3
B	17	GLY	-	expression tag	UNP P0A4G3
B	18	SER	-	expression tag	UNP P0A4G3
C	7	TRP	-	expression tag	UNP P0A4G3
C	8	ARG	-	expression tag	UNP P0A4G3
C	9	GLY	-	expression tag	UNP P0A4G3
C	10	SER	-	expression tag	UNP P0A4G3
C	11	HIS	-	expression tag	UNP P0A4G3
C	12	HIS	-	expression tag	UNP P0A4G3
C	13	HIS	-	expression tag	UNP P0A4G3
C	14	HIS	-	expression tag	UNP P0A4G3
C	15	HIS	-	expression tag	UNP P0A4G3
C	16	HIS	-	expression tag	UNP P0A4G3
C	17	GLY	-	expression tag	UNP P0A4G3
C	18	SER	-	expression tag	UNP P0A4G3
D	7	TRP	-	expression tag	UNP P0A4G3
D	8	ARG	-	expression tag	UNP P0A4G3
D	9	GLY	-	expression tag	UNP P0A4G3
D	10	SER	-	expression tag	UNP P0A4G3
D	11	HIS	-	expression tag	UNP P0A4G3
D	12	HIS	-	expression tag	UNP P0A4G3
D	13	HIS	-	expression tag	UNP P0A4G3
D	14	HIS	-	expression tag	UNP P0A4G3
D	15	HIS	-	expression tag	UNP P0A4G3
D	16	HIS	-	expression tag	UNP P0A4G3
D	17	GLY	-	expression tag	UNP P0A4G3
D	18	SER	-	expression tag	UNP P0A4G3

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0

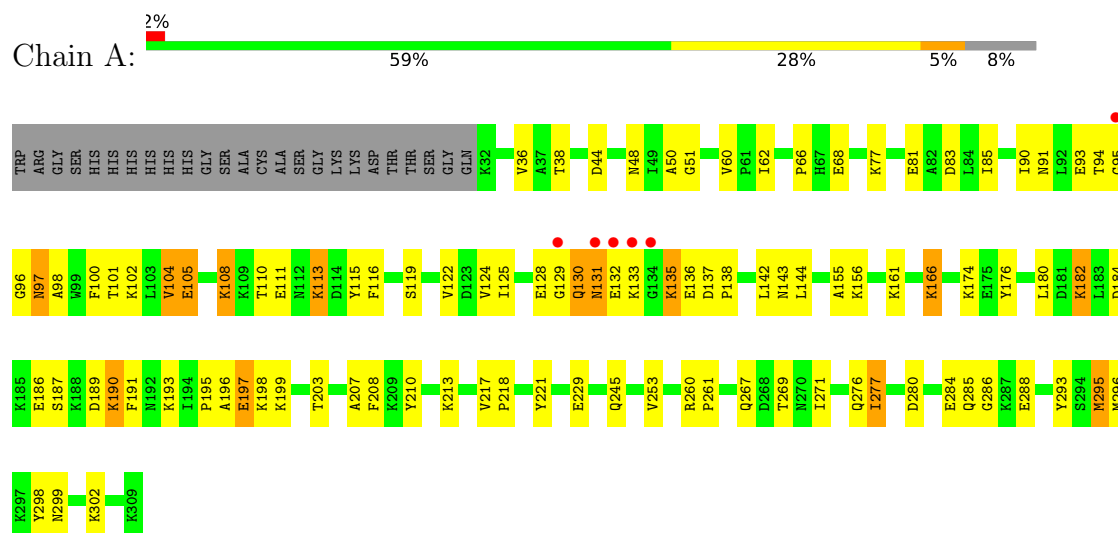
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total 45	O 45	0	0
3	B	37	Total 37	O 37	0	0
3	C	38	Total 38	O 38	0	0
3	D	33	Total 33	O 33	0	0

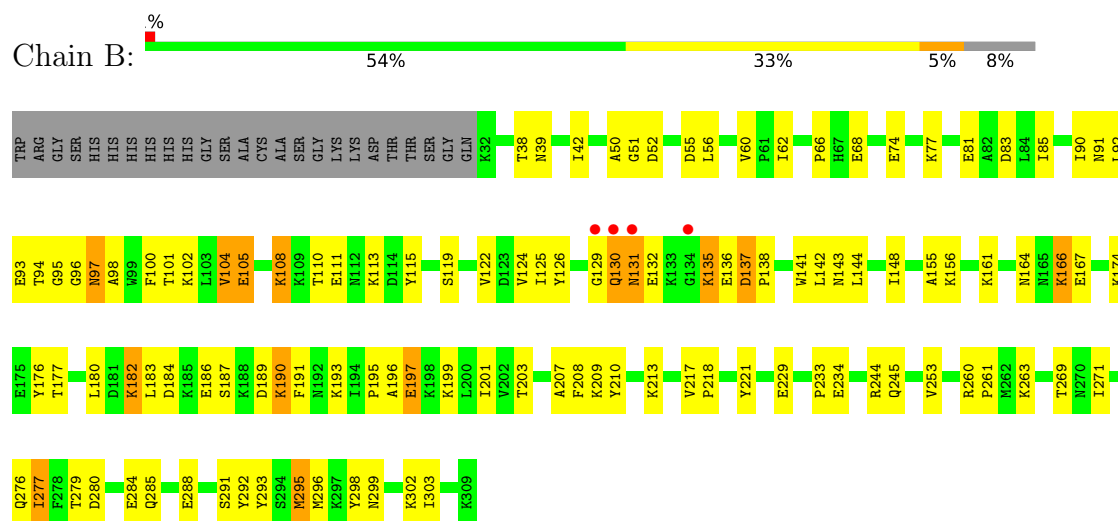
3 Residue-property plots

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: MANGANESE ABC TRANSPORTER SUBSTRATE-BINDING LIPOPROTEIN

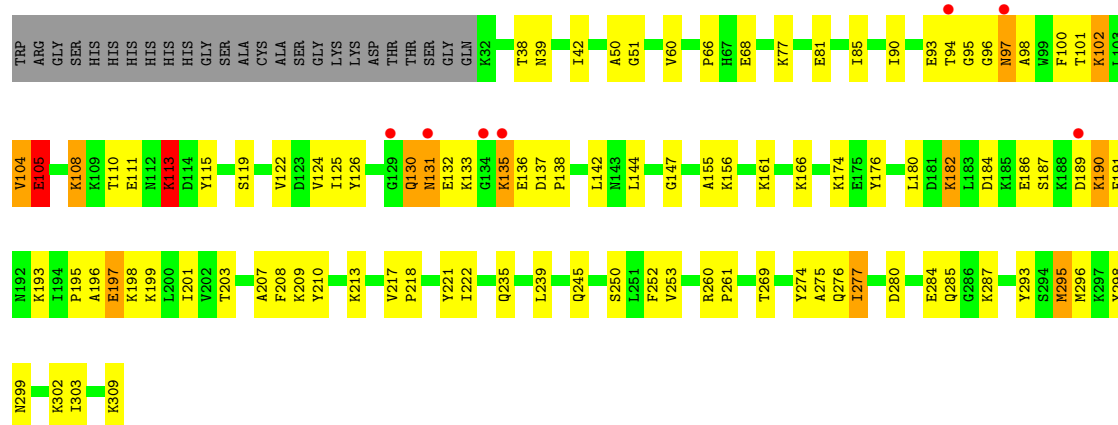


• Molecule 1: MANGANESE ABC TRANSPORTER SUBSTRATE-BINDING LIPOPROTEIN

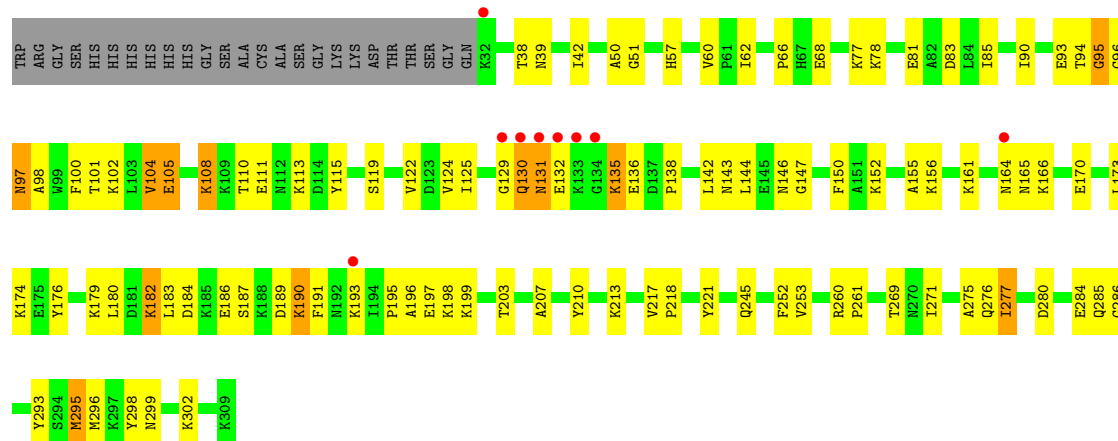


• Molecule 1: MANGANESE ABC TRANSPORTER SUBSTRATE-BINDING LIPOPROTEIN





● Molecule 1: MANGANESE ABC TRANSPORTER SUBSTRATE-BINDING LIPOPROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.33Å 107.69Å 77.94Å 90.00° 95.67° 90.00°	Depositor
Resolution (Å)	19.73 – 2.70 19.73 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.73-2.70) 98.9 (19.73-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.215 , 0.246 0.220 , 0.250	Depositor DCC
R_{free} test set	1547 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9024	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	1.08	1/2260 (0.0%)	1.08	5/3050 (0.2%)
1	B	1.02	1/2260 (0.0%)	1.09	8/3050 (0.3%)
1	C	1.04	1/2259 (0.0%)	1.07	8/3050 (0.3%)
1	D	1.00	1/2260 (0.0%)	1.06	7/3050 (0.2%)
All	All	1.04	4/9039 (0.0%)	1.08	28/12200 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	303	ILE	CA-CB	-6.33	1.46	1.54
1	B	279	THR	N-CA	-5.44	1.41	1.46
1	D	275	ALA	CA-CB	-5.40	1.44	1.53
1	A	36	VAL	CA-CB	-5.21	1.48	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	135	LYS	N-CA-C	-10.64	98.42	114.16
1	B	135	LYS	N-CA-C	-10.62	98.44	114.16
1	D	95	GLY	N-CA-C	-6.80	101.75	111.20
1	D	269	THR	N-CA-C	-6.23	105.62	113.72
1	A	269	THR	N-CA-C	-6.16	105.72	113.72
1	D	147	GLY	N-CA-C	-5.99	105.55	112.73
1	D	271	ILE	CA-C-N	-5.95	113.84	119.85
1	D	271	ILE	C-N-CA	-5.95	113.84	119.85
1	A	135	LYS	N-CA-C	-5.80	98.44	110.80
1	A	271	ILE	CA-C-N	-5.80	113.99	119.85
1	A	271	ILE	C-N-CA	-5.80	113.99	119.85
1	B	271	ILE	CA-C-N	-5.73	114.06	119.85
1	B	271	ILE	C-N-CA	-5.73	114.06	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	THR	N-CA-C	-5.69	106.32	113.72
1	C	198	LYS	N-CA-C	-5.59	106.46	113.72
1	D	135	LYS	N-CA-C	-5.57	98.94	110.80
1	C	269	THR	N-CA-C	-5.49	106.58	113.72
1	B	137	ASP	CA-C-N	5.42	125.03	119.56
1	B	137	ASP	C-N-CA	5.42	125.03	119.56
1	A	198	LYS	N-CA-C	-5.40	106.61	114.12
1	B	201	ILE	CB-CA-C	-5.38	104.78	111.08
1	C	137	ASP	CA-C-N	5.26	125.72	120.04
1	C	137	ASP	C-N-CA	5.26	125.72	120.04
1	B	263	LYS	N-CA-C	-5.25	105.56	111.28
1	C	147	GLY	N-CA-C	-5.24	106.44	112.73
1	C	113	LYS	N-CA-C	-5.21	106.06	112.72
1	D	198	LYS	N-CA-C	-5.11	107.08	113.72
1	C	201	ILE	CB-CA-C	-5.07	105.15	111.08

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	2217	0	2202	114	4
1	B	2217	0	2202	137	9
1	C	2216	0	2202	127	20
1	D	2217	0	2202	116	21
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	45	0	0	12	0
3	B	37	0	0	10	0
3	C	38	0	0	16	0
3	D	33	0	0	12	0
All	All	9024	0	8808	454	27

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 26.

All (454) 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:130:GLN:C	1:A:135:LYS:HD2	1.39	1.45
1:B:130:GLN:C	1:B:135:LYS:HD2	1.35	1.45
1:D:130:GLN:C	1:D:135:LYS:HD2	1.36	1.45
1:C:130:GLN:C	1:C:135:LYS:HD2	1.45	1.42
1:C:131:ASN:N	1:C:135:LYS:HD2	1.16	1.41
1:B:130:GLN:CB	1:B:135:LYS:HZ2	1.36	1.38
1:B:131:ASN:N	1:B:135:LYS:CD	1.87	1.35
1:A:97:ASN:HB3	1:D:78:LYS:NZ	1.37	1.34
1:D:131:ASN:N	1:D:135:LYS:CD	1.87	1.34
1:A:131:ASN:N	1:A:135:LYS:HD2	1.03	1.33
1:D:132:GLU:N	1:D:135:LYS:HG3	1.47	1.29
1:A:131:ASN:N	1:A:135:LYS:CD	1.95	1.29
1:B:131:ASN:N	1:B:135:LYS:HD2	0.97	1.28
1:D:131:ASN:N	1:D:135:LYS:HD2	0.94	1.26
1:B:132:GLU:N	1:B:135:LYS:HG3	1.48	1.26
1:C:132:GLU:N	1:C:135:LYS:HG3	1.51	1.23
1:A:97:ASN:CB	1:D:78:LYS:NZ	2.01	1.23
1:B:130:GLN:CA	1:B:135:LYS:HZ2	1.52	1.23
1:A:132:GLU:N	1:A:135:LYS:HG3	1.53	1.22
1:A:97:ASN:CG	1:D:78:LYS:HZ2	1.49	1.21
1:C:130:GLN:CB	1:C:135:LYS:HZ3	1.53	1.20
1:B:130:GLN:HB2	1:B:135:LYS:NZ	1.56	1.20
1:C:131:ASN:N	1:C:135:LYS:CD	2.05	1.20
1:A:97:ASN:CB	1:D:78:LYS:HZ1	1.54	1.19
1:B:130:GLN:C	1:B:135:LYS:CD	2.12	1.19
1:B:130:GLN:CB	1:B:135:LYS:NZ	2.05	1.19
1:A:130:GLN:HB2	1:A:135:LYS:NZ	1.56	1.18
1:A:130:GLN:CB	1:A:135:LYS:HZ3	1.57	1.17
1:A:267:GLN:HG2	3:A:2034:HOH:O	1.00	1.17
1:A:130:GLN:C	1:A:135:LYS:CD	2.17	1.17
1:B:74:GLU:HG2	3:B:2005:HOH:O	1.43	1.16
1:A:130:GLN:CB	1:A:135:LYS:NZ	2.09	1.15
1:D:130:GLN:HB2	1:D:135:LYS:NZ	1.60	1.15
1:C:130:GLN:HB2	1:C:135:LYS:NZ	1.61	1.14
1:D:130:GLN:C	1:D:135:LYS:CD	2.12	1.14
1:D:130:GLN:CB	1:D:135:LYS:NZ	2.12	1.12
1:C:130:GLN:CB	1:C:135:LYS:NZ	2.14	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:GLN:HB2	1:D:135:LYS:CE	1.85	1.07
1:D:130:GLN:CB	1:D:135:LYS:HZ3	1.68	1.07
1:C:132:GLU:H	1:C:135:LYS:CG	1.68	1.06
1:B:130:GLN:HB2	1:B:135:LYS:CE	1.84	1.05
1:A:130:GLN:HB2	1:A:135:LYS:CD	1.87	1.05
1:B:132:GLU:H	1:B:135:LYS:CG	1.69	1.05
1:B:233:PRO:HG2	1:C:302:LYS:HD2	1.36	1.04
1:D:132:GLU:H	1:D:135:LYS:CG	1.69	1.04
1:C:130:GLN:C	1:C:135:LYS:CD	2.29	1.04
1:D:130:GLN:OE1	3:D:2009:HOH:O	1.76	1.04
1:D:130:GLN:HB2	1:D:135:LYS:CD	1.88	1.04
1:B:166:LYS:HB2	3:B:2020:HOH:O	1.57	1.04
1:A:130:GLN:HB2	1:A:135:LYS:CE	1.86	1.03
1:C:130:GLN:HB2	1:C:135:LYS:HZ3	1.13	1.03
1:C:130:GLN:HB2	1:C:135:LYS:CD	1.88	1.02
1:A:97:ASN:CG	1:D:78:LYS:NZ	2.16	1.02
1:B:130:GLN:HB2	1:B:135:LYS:CD	1.89	1.02
1:A:132:GLU:H	1:A:135:LYS:HG3	1.13	1.00
1:C:132:GLU:H	1:C:135:LYS:HG3	1.07	1.00
1:A:132:GLU:H	1:A:135:LYS:CG	1.73	1.00
1:C:130:GLN:HB2	1:C:135:LYS:CE	1.93	0.99
1:D:130:GLN:HA	1:D:135:LYS:HZ2	1.28	0.98
1:B:131:ASN:H	1:B:135:LYS:HD2	1.28	0.98
1:A:130:GLN:HB2	1:A:135:LYS:HD3	1.43	0.98
1:C:130:GLN:HB2	1:C:135:LYS:HD3	1.44	0.97
1:A:97:ASN:ND2	1:D:78:LYS:HE3	1.79	0.97
1:B:132:GLU:H	1:B:135:LYS:HG3	1.09	0.97
1:B:229:GLU:HG2	1:C:309:LYS:HE3	1.46	0.97
1:D:130:GLN:HB2	1:D:135:LYS:HD3	1.45	0.96
1:D:38:THR:O	1:D:60:VAL:HG23	1.65	0.96
1:A:130:GLN:CB	1:A:135:LYS:HD3	1.96	0.96
1:D:130:GLN:CB	1:D:135:LYS:HD3	1.97	0.95
1:B:130:GLN:HB2	1:B:135:LYS:HD3	1.46	0.95
1:D:131:ASN:H	1:D:135:LYS:HD2	1.24	0.94
1:A:128:GLU:O	3:A:2014:HOH:O	1.86	0.94
1:D:130:GLN:CA	1:D:135:LYS:HZ2	1.80	0.94
1:B:130:GLN:CB	1:B:135:LYS:HD3	1.98	0.93
1:D:97:ASN:HB2	3:D:2003:HOH:O	1.69	0.93
1:A:131:ASN:H	1:A:135:LYS:HD2	1.32	0.93
1:A:130:GLN:HA	1:A:135:LYS:HZ2	1.30	0.92
1:A:130:GLN:CA	1:A:135:LYS:HZ2	1.82	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:GLN:CG	3:C:2015:HOH:O	2.18	0.91
1:A:166:LYS:HE3	3:A:2018:HOH:O	1.70	0.91
1:A:166:LYS:CE	3:A:2018:HOH:O	2.17	0.90
1:A:130:GLN:HB2	1:A:135:LYS:HZ3	1.16	0.90
1:D:132:GLU:H	1:D:135:LYS:HG3	1.09	0.89
1:C:130:GLN:HG3	3:C:2015:HOH:O	1.71	0.89
1:C:38:THR:O	1:C:60:VAL:HG23	1.72	0.89
1:D:132:GLU:N	1:D:135:LYS:CG	2.32	0.89
1:B:130:GLN:HA	1:B:135:LYS:HZ2	1.35	0.89
1:B:132:GLU:N	1:B:135:LYS:CG	2.32	0.88
1:D:131:ASN:CA	1:D:135:LYS:HD2	2.03	0.88
1:B:131:ASN:CA	1:B:135:LYS:HD2	2.04	0.88
1:C:95:GLY:HA2	3:C:2011:HOH:O	1.72	0.87
1:C:130:GLN:HA	1:C:135:LYS:HZ2	1.38	0.87
1:C:130:GLN:CB	1:C:135:LYS:HD3	2.04	0.87
1:B:38:THR:O	1:B:60:VAL:HG23	1.76	0.86
1:C:130:GLN:NE2	3:C:2016:HOH:O	2.09	0.86
1:B:129:GLY:HA3	3:B:2015:HOH:O	1.74	0.85
1:D:132:GLU:H	1:D:135:LYS:CB	1.90	0.85
1:B:97:ASN:HA	3:B:2008:HOH:O	1.74	0.85
1:C:131:ASN:H	1:C:135:LYS:HD2	1.43	0.84
1:A:166:LYS:NZ	3:A:2018:HOH:O	2.10	0.84
1:B:132:GLU:H	1:B:135:LYS:CB	1.89	0.84
1:B:229:GLU:HG2	1:C:309:LYS:CE	2.07	0.84
1:B:130:GLN:CA	1:B:135:LYS:NZ	2.38	0.84
1:C:130:GLN:HB3	1:C:135:LYS:HZ3	1.43	0.83
1:B:130:GLN:CB	1:B:135:LYS:CD	2.56	0.83
1:C:132:GLU:H	1:C:135:LYS:CB	1.93	0.82
1:D:129:GLY:HA3	3:D:2006:HOH:O	1.79	0.82
1:A:130:GLN:HB3	1:A:135:LYS:HZ3	1.44	0.81
1:A:132:GLU:H	1:A:135:LYS:CB	1.93	0.81
1:B:131:ASN:H	1:B:135:LYS:CE	1.93	0.81
1:B:131:ASN:H	1:B:135:LYS:CD	1.84	0.80
1:C:130:GLN:CB	1:C:135:LYS:CD	2.59	0.80
1:B:285:GLN:OE1	1:B:285:GLN:HA	1.80	0.80
1:A:38:THR:O	1:A:60:VAL:HG23	1.79	0.80
1:A:131:ASN:CA	1:A:135:LYS:HD2	2.09	0.80
1:B:229:GLU:CG	1:C:309:LYS:HE3	2.12	0.79
1:D:130:GLN:CB	1:D:135:LYS:CD	2.55	0.79
1:A:285:GLN:HA	1:A:285:GLN:OE1	1.82	0.78
1:A:130:GLN:CB	1:A:135:LYS:CD	2.55	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:GLN:CA	1:C:135:LYS:HZ2	1.96	0.77
1:D:130:GLN:HB3	1:D:135:LYS:HZ3	1.49	0.77
1:A:130:GLN:CA	1:A:135:LYS:NZ	2.46	0.76
1:B:95:GLY:HA2	3:B:2007:HOH:O	1.84	0.76
1:C:285:GLN:OE1	1:C:285:GLN:HA	1.84	0.76
1:A:131:ASN:H	1:A:135:LYS:CD	1.93	0.75
1:C:189:ASP:HB2	3:C:2018:HOH:O	1.86	0.75
1:C:130:GLN:OE1	3:C:2014:HOH:O	2.03	0.75
1:A:97:ASN:HD22	1:D:78:LYS:HE3	1.51	0.75
1:D:285:GLN:HA	1:D:285:GLN:OE1	1.86	0.75
1:A:90:ILE:HG13	1:A:138:PRO:HA	1.69	0.74
1:B:125:ILE:HD12	1:B:210:TYR:CD2	2.23	0.74
1:C:90:ILE:HG13	1:C:138:PRO:HA	1.67	0.74
1:A:97:ASN:HB3	1:D:78:LYS:HZ1	0.66	0.73
1:D:131:ASN:H	1:D:135:LYS:CE	2.00	0.73
1:B:229:GLU:HG2	1:C:309:LYS:HZ1	1.53	0.73
1:D:179:LYS:HE3	3:D:2019:HOH:O	1.88	0.73
1:D:125:ILE:HD12	1:D:210:TYR:CD2	2.23	0.72
1:C:130:GLN:CA	1:C:135:LYS:NZ	2.52	0.72
1:A:124:VAL:HG11	1:A:136:GLU:HG2	1.70	0.72
1:D:124:VAL:HG11	1:D:136:GLU:HG2	1.71	0.71
1:D:130:GLN:HB2	1:D:135:LYS:HZ3	1.27	0.71
1:A:132:GLU:N	1:A:135:LYS:CG	2.37	0.71
1:C:124:VAL:HG11	1:C:136:GLU:HG2	1.73	0.71
1:A:97:ASN:ND2	1:D:78:LYS:CE	2.54	0.70
1:A:125:ILE:HD12	1:A:210:TYR:CD2	2.26	0.70
1:B:90:ILE:HG13	1:B:138:PRO:HA	1.73	0.70
1:B:131:ASN:N	1:B:135:LYS:CE	2.53	0.70
1:C:125:ILE:HD12	1:C:210:TYR:CD2	2.26	0.70
1:C:132:GLU:O	1:C:135:LYS:HB2	1.92	0.70
1:C:131:ASN:H	1:C:135:LYS:CE	2.05	0.70
1:A:131:ASN:H	1:A:135:LYS:CE	2.04	0.70
1:B:132:GLU:O	1:B:135:LYS:HB2	1.91	0.70
1:C:132:GLU:N	1:C:135:LYS:CG	2.35	0.70
1:D:132:GLU:H	1:D:135:LYS:HB2	1.57	0.69
1:A:129:GLY:HA3	3:A:2014:HOH:O	1.91	0.69
1:B:130:GLN:HA	1:B:135:LYS:NZ	2.04	0.69
1:D:90:ILE:HG13	1:D:138:PRO:HA	1.73	0.69
1:C:131:ASN:CA	1:C:135:LYS:HD2	2.19	0.69
1:B:124:VAL:HG11	1:B:136:GLU:HG2	1.73	0.69
1:B:132:GLU:H	1:B:135:LYS:HB2	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:GLU:O	1:D:135:LYS:HB2	1.94	0.68
1:B:244:ARG:HH12	1:C:287:LYS:NZ	1.92	0.68
1:B:229:GLU:HG2	1:C:309:LYS:NZ	2.08	0.67
1:B:166:LYS:CB	3:B:2020:HOH:O	2.25	0.67
1:C:182:LYS:O	1:C:186:GLU:HG3	1.93	0.67
1:C:130:GLN:CD	3:C:2015:HOH:O	2.37	0.67
3:A:2009:HOH:O	1:D:57:HIS:HB2	1.95	0.67
1:A:130:GLN:CG	1:A:135:LYS:HD3	2.25	0.67
1:C:97:ASN:HA	3:C:2011:HOH:O	1.93	0.67
1:A:132:GLU:O	1:A:135:LYS:HB2	1.95	0.67
1:D:130:GLN:CA	1:D:135:LYS:NZ	2.48	0.67
1:B:130:GLN:C	1:B:135:LYS:HD3	2.17	0.66
1:B:288:GLU:HB2	1:D:286:GLY:O	1.95	0.66
1:D:170:GLU:O	3:D:2018:HOH:O	2.13	0.66
1:D:130:GLN:CG	1:D:135:LYS:HD3	2.25	0.66
1:B:229:GLU:CG	1:C:309:LYS:CE	2.72	0.65
1:A:132:GLU:H	1:A:135:LYS:HB2	1.60	0.65
1:B:244:ARG:HH12	1:C:287:LYS:HZ3	1.44	0.65
1:D:131:ASN:H	1:D:135:LYS:CD	1.83	0.65
1:B:130:GLN:CG	1:B:135:LYS:HD3	2.26	0.65
1:A:97:ASN:CB	1:D:78:LYS:HZ2	1.85	0.65
1:B:229:GLU:CB	1:C:309:LYS:NZ	2.61	0.64
1:C:95:GLY:O	1:C:98:ALA:N	2.31	0.64
1:B:130:GLN:CA	1:B:135:LYS:CD	2.76	0.63
1:B:233:PRO:CG	1:C:302:LYS:HD2	2.21	0.63
1:A:97:ASN:CG	1:D:78:LYS:CE	2.71	0.63
1:D:130:GLN:CA	1:D:135:LYS:CD	2.75	0.63
1:A:182:LYS:O	1:A:186:GLU:HG3	1.98	0.63
1:B:166:LYS:CG	3:B:2020:HOH:O	2.43	0.63
1:C:132:GLU:H	1:C:135:LYS:HB2	1.63	0.63
1:A:77:LYS:HE2	1:B:276:GLN:NE2	2.13	0.63
1:A:130:GLN:C	1:A:135:LYS:HD3	2.21	0.63
1:B:233:PRO:HG2	1:C:302:LYS:CD	2.21	0.62
1:B:166:LYS:HG3	3:B:2020:HOH:O	1.99	0.62
1:A:131:ASN:N	1:A:135:LYS:CE	2.61	0.62
1:B:229:GLU:HB3	1:C:309:LYS:CE	2.30	0.62
1:B:229:GLU:CG	1:C:309:LYS:HZ1	2.12	0.62
1:D:130:GLN:C	1:D:135:LYS:HD3	2.15	0.61
1:A:130:GLN:CA	1:A:135:LYS:CD	2.78	0.61
1:A:95:GLY:O	1:A:98:ALA:N	2.35	0.60
1:C:130:GLN:CG	1:C:135:LYS:HD3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ASN:H	1:C:135:LYS:CD	2.00	0.59
1:A:142:LEU:HD12	1:A:207:ALA:O	2.03	0.58
1:C:95:GLY:CA	3:C:2011:HOH:O	2.40	0.58
1:D:165:ASN:HA	3:D:2017:HOH:O	2.02	0.58
1:C:142:LEU:HD12	1:C:207:ALA:O	2.03	0.58
1:C:119:SER:O	1:C:122:VAL:HG13	2.03	0.58
1:D:142:LEU:HD12	1:D:207:ALA:O	2.03	0.58
1:A:101:THR:O	1:A:104:VAL:HG12	2.03	0.58
1:C:97:ASN:N	3:C:2011:HOH:O	2.36	0.57
1:D:179:LYS:CE	3:D:2019:HOH:O	2.48	0.57
1:B:142:LEU:HD12	1:B:207:ALA:O	2.04	0.57
1:C:130:GLN:HB3	3:C:2014:HOH:O	2.05	0.57
1:A:105:GLU:O	1:A:108:LYS:N	2.33	0.57
1:B:125:ILE:HD11	1:B:213:LYS:HD3	1.87	0.57
1:B:234:GLU:HB2	1:C:275:ALA:HA	1.86	0.57
1:D:152:LYS:HE2	3:D:2016:HOH:O	2.05	0.56
1:B:130:GLN:HB3	1:B:135:LYS:NZ	2.12	0.56
1:C:97:ASN:CA	3:C:2011:HOH:O	2.52	0.56
1:B:52:ASP:HB3	3:B:2001:HOH:O	2.05	0.56
1:C:105:GLU:O	1:C:108:LYS:N	2.34	0.56
1:A:285:GLN:OE1	1:A:285:GLN:CA	2.50	0.56
1:B:229:GLU:HB3	1:C:309:LYS:NZ	2.21	0.56
1:C:130:GLN:HA	3:C:2013:HOH:O	2.06	0.56
1:B:208:PHE:HB2	3:B:2024:HOH:O	2.06	0.56
1:A:130:GLN:HG3	1:A:135:LYS:HD3	1.88	0.55
1:C:189:ASP:O	1:C:191:PHE:N	2.39	0.55
1:B:119:SER:O	1:B:122:VAL:HG13	2.06	0.55
1:D:101:THR:O	1:D:104:VAL:HG12	2.06	0.55
1:D:182:LYS:O	1:D:186:GLU:HG3	2.06	0.55
1:A:66:PRO:CD	1:A:280:ASP:HB3	2.37	0.55
1:A:68:GLU:HG2	1:A:96:GLY:H	1.71	0.55
1:A:119:SER:O	1:A:122:VAL:HG13	2.06	0.54
1:B:285:GLN:OE1	1:B:285:GLN:CA	2.49	0.54
1:B:39:ASN:ND2	1:B:42:ILE:HD12	2.22	0.54
1:D:130:GLN:HG3	1:D:135:LYS:HD3	1.89	0.54
1:C:95:GLY:C	1:C:97:ASN:N	2.63	0.54
1:C:285:GLN:OE1	1:C:285:GLN:CA	2.53	0.54
1:A:189:ASP:O	1:A:191:PHE:N	2.41	0.54
1:C:95:GLY:C	3:C:2011:HOH:O	2.51	0.54
1:C:66:PRO:CD	1:C:280:ASP:HB3	2.39	0.53
1:A:97:ASN:CB	1:D:78:LYS:CE	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:GLN:CA	1:C:135:LYS:CD	2.87	0.53
1:C:125:ILE:HD11	1:C:213:LYS:HD3	1.89	0.53
1:A:298:TYR:CE1	1:A:302:LYS:HE2	2.43	0.53
1:C:130:GLN:HG3	1:C:135:LYS:HD3	1.90	0.53
1:A:277:ILE:HB	1:A:299:ASN:OD1	2.08	0.53
1:B:130:GLN:HG3	1:B:135:LYS:HD3	1.91	0.53
1:C:132:GLU:CA	1:C:135:LYS:HG3	2.36	0.53
1:B:182:LYS:O	1:B:186:GLU:HG3	2.08	0.53
1:C:101:THR:O	1:C:104:VAL:HG12	2.09	0.53
1:D:119:SER:O	1:D:122:VAL:HG13	2.08	0.53
3:A:2009:HOH:O	1:D:78:LYS:HE2	2.09	0.52
1:D:66:PRO:CD	1:D:280:ASP:HB3	2.39	0.52
1:B:155:ALA:O	1:B:156:LYS:C	2.52	0.52
1:B:85:ILE:HB	1:B:115:TYR:HB3	1.92	0.52
1:B:101:THR:O	1:B:104:VAL:HG12	2.10	0.52
1:C:155:ALA:O	1:C:156:LYS:C	2.53	0.52
1:B:113:LYS:O	1:B:161:LYS:NZ	2.41	0.52
1:B:229:GLU:CG	1:C:309:LYS:NZ	2.72	0.52
1:D:170:GLU:CA	3:D:2018:HOH:O	2.58	0.52
1:B:229:GLU:CB	1:C:309:LYS:HZ1	2.24	0.51
1:D:85:ILE:HB	1:D:115:TYR:HB3	1.90	0.51
1:C:68:GLU:HG2	1:C:96:GLY:H	1.75	0.51
1:A:77:LYS:NZ	1:A:81:GLU:OE2	2.44	0.51
1:B:229:GLU:HB3	1:C:309:LYS:HE2	1.93	0.51
1:B:244:ARG:NH1	1:C:287:LYS:NZ	2.59	0.51
1:D:176:TYR:CE2	1:D:180:LEU:HD11	2.46	0.51
1:D:183:LEU:O	1:D:187:SER:OG	2.19	0.51
1:B:189:ASP:O	1:B:191:PHE:N	2.43	0.51
1:B:66:PRO:CD	1:B:280:ASP:HB3	2.40	0.51
1:C:132:GLU:CG	1:C:135:LYS:HG3	2.40	0.51
1:C:144:LEU:HB2	1:C:184:ASP:HB2	1.93	0.51
1:D:95:GLY:O	1:D:98:ALA:N	2.44	0.50
1:B:141:TRP:C	1:B:143:ASN:H	2.20	0.50
1:B:144:LEU:HB2	1:B:184:ASP:HB2	1.93	0.50
1:C:113:LYS:O	1:C:161:LYS:NZ	2.40	0.50
1:C:199:LYS:O	1:C:218:PRO:HG2	2.12	0.50
1:A:125:ILE:HD11	1:A:213:LYS:HD3	1.94	0.50
1:C:131:ASN:N	1:C:135:LYS:CE	2.63	0.50
1:D:95:GLY:C	1:D:97:ASN:N	2.68	0.50
1:D:93:GLU:HB3	1:D:100:PHE:HB2	1.93	0.50
1:D:97:ASN:OD1	3:D:2004:HOH:O	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:LYS:O	1:D:218:PRO:HG2	2.12	0.50
1:A:50:ALA:O	1:A:51:GLY:C	2.54	0.49
1:A:132:GLU:CG	1:A:135:LYS:HG3	2.42	0.49
1:D:170:GLU:HA	3:D:2018:HOH:O	2.12	0.49
1:A:85:ILE:HB	1:A:115:TYR:HB3	1.93	0.49
1:A:166:LYS:NZ	3:A:2019:HOH:O	2.32	0.49
1:C:94:THR:HA	1:C:98:ALA:HA	1.93	0.49
1:A:94:THR:HA	1:A:98:ALA:HA	1.95	0.49
1:B:277:ILE:HB	1:B:299:ASN:OD1	2.12	0.49
1:B:229:GLU:HA	1:C:309:LYS:NZ	2.28	0.49
1:D:144:LEU:HB2	1:D:184:ASP:HB2	1.95	0.49
1:B:110:THR:HG22	1:B:111:GLU:O	2.12	0.49
1:B:229:GLU:CB	1:C:309:LYS:CE	2.91	0.49
1:C:50:ALA:O	1:C:51:GLY:C	2.55	0.49
1:C:277:ILE:HB	1:C:299:ASN:OD1	2.13	0.49
1:D:277:ILE:HB	1:D:299:ASN:OD1	2.13	0.49
1:A:144:LEU:HB2	1:A:184:ASP:HB2	1.95	0.49
1:D:110:THR:HG22	1:D:111:GLU:O	2.13	0.49
1:A:95:GLY:C	1:A:97:ASN:N	2.68	0.48
1:A:155:ALA:O	1:A:156:LYS:C	2.54	0.48
1:C:85:ILE:HB	1:C:115:TYR:HB3	1.94	0.48
1:D:285:GLN:OE1	1:D:285:GLN:CA	2.54	0.48
1:B:93:GLU:HB3	1:B:100:PHE:HB2	1.94	0.48
1:D:155:ALA:O	1:D:156:LYS:C	2.56	0.48
1:A:110:THR:HG22	1:A:111:GLU:O	2.14	0.48
1:B:83:ASP:O	1:B:161:LYS:HE2	2.13	0.48
1:C:110:THR:HG22	1:C:111:GLU:O	2.13	0.48
1:C:298:TYR:CE1	1:C:302:LYS:HE2	2.48	0.48
1:D:132:GLU:CA	1:D:135:LYS:HG3	2.37	0.48
1:C:39:ASN:ND2	1:C:42:ILE:HD12	2.29	0.48
1:D:105:GLU:O	1:D:108:LYS:N	2.39	0.48
1:A:288:GLU:HB2	3:A:2043:HOH:O	2.14	0.48
1:B:183:LEU:O	1:B:187:SER:OG	2.20	0.48
1:A:93:GLU:HB3	1:A:100:PHE:HB2	1.96	0.48
1:B:95:GLY:C	1:B:97:ASN:N	2.71	0.47
1:B:293:TYR:CD1	1:B:293:TYR:C	2.92	0.47
1:C:187:SER:C	1:C:189:ASP:H	2.22	0.47
1:A:176:TYR:CE2	1:A:180:LEU:HD11	2.49	0.47
1:B:98:ALA:HB1	1:B:101:THR:HB	1.95	0.47
1:B:105:GLU:O	1:B:108:LYS:N	2.37	0.47
1:D:125:ILE:HD11	1:D:213:LYS:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LYS:O	1:A:161:LYS:NZ	2.42	0.47
1:B:50:ALA:O	1:B:51:GLY:C	2.57	0.47
1:A:143:ASN:OD1	1:A:143:ASN:C	2.58	0.47
1:C:189:ASP:O	1:C:190:LYS:C	2.58	0.47
1:A:199:LYS:O	1:A:218:PRO:HG2	2.15	0.47
1:B:195:PRO:O	1:B:196:ALA:C	2.58	0.47
1:D:298:TYR:CE1	1:D:302:LYS:HE2	2.50	0.47
1:B:68:GLU:HG2	1:B:96:GLY:H	1.79	0.47
1:A:253:VAL:O	1:A:276:GLN:HA	2.15	0.46
1:B:131:ASN:H	1:B:135:LYS:HE3	1.79	0.46
1:D:68:GLU:HG2	1:D:96:GLY:H	1.80	0.46
1:B:189:ASP:O	1:B:190:LYS:C	2.58	0.46
1:B:182:LYS:HD3	1:D:186:GLU:OE2	2.16	0.46
1:B:77:LYS:NZ	1:B:81:GLU:OE2	2.48	0.46
1:A:203:THR:O	1:A:221:TYR:HA	2.15	0.46
1:B:132:GLU:CA	1:B:135:LYS:HG3	2.38	0.46
1:C:98:ALA:HB1	1:C:101:THR:HB	1.98	0.46
1:A:195:PRO:O	1:A:196:ALA:C	2.59	0.46
1:B:199:LYS:O	1:B:218:PRO:HG2	2.16	0.46
1:C:260:ARG:O	1:C:261:PRO:C	2.58	0.45
1:B:132:GLU:CG	1:B:135:LYS:HG3	2.45	0.45
1:C:187:SER:C	1:C:189:ASP:N	2.73	0.45
1:A:298:TYR:CZ	1:A:302:LYS:HG3	2.52	0.45
1:D:260:ARG:O	1:D:261:PRO:C	2.59	0.45
1:C:189:ASP:CB	3:C:2018:HOH:O	2.55	0.45
1:D:98:ALA:HB1	1:D:101:THR:HB	1.99	0.45
1:A:295:MET:CG	1:A:296:MET:N	2.79	0.45
1:B:176:TYR:CE2	1:B:180:LEU:HD11	2.50	0.45
1:A:98:ALA:HB1	1:A:101:THR:HB	1.98	0.45
1:B:244:ARG:NH1	1:C:287:LYS:HZ1	2.15	0.45
1:A:44:ASP:O	1:A:48:ASN:ND2	2.42	0.45
1:B:130:GLN:CB	1:B:135:LYS:HZ3	2.20	0.45
1:A:189:ASP:O	1:A:190:LYS:C	2.59	0.45
1:D:94:THR:HA	1:D:98:ALA:HA	1.98	0.45
1:A:293:TYR:CD1	1:A:293:TYR:C	2.95	0.45
1:B:94:THR:HA	1:B:98:ALA:HA	1.99	0.45
1:D:131:ASN:C	1:D:135:LYS:HG3	2.30	0.45
1:B:197:GLU:H	1:B:197:GLU:HG3	1.25	0.44
1:D:189:ASP:O	1:D:191:PHE:N	2.50	0.44
1:A:187:SER:C	1:A:189:ASP:H	2.24	0.44
1:B:62:ILE:HG21	1:B:284:GLU:HA	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.78	0.44
1:D:50:ALA:O	1:D:51:GLY:C	2.59	0.44
1:C:252:PHE:HB3	1:C:277:ILE:HD13	1.99	0.44
1:A:132:GLU:CA	1:A:135:LYS:HG3	2.40	0.44
1:A:137:ASP:HA	1:A:138:PRO:HD3	1.83	0.44
1:C:293:TYR:CD1	1:C:293:TYR:C	2.95	0.44
1:A:83:ASP:O	1:A:161:LYS:HE2	2.18	0.44
1:B:182:LYS:CD	1:D:186:GLU:OE2	2.66	0.44
1:B:203:THR:O	1:B:221:TYR:HA	2.18	0.44
1:D:83:ASP:O	1:D:161:LYS:HE2	2.18	0.44
1:B:141:TRP:C	1:B:143:ASN:N	2.76	0.44
1:B:95:GLY:O	1:B:98:ALA:N	2.51	0.43
1:C:126:TYR:CE2	1:C:136:GLU:HG3	2.53	0.43
1:D:143:ASN:OD1	1:D:143:ASN:C	2.60	0.43
1:B:39:ASN:OD1	1:B:39:ASN:C	2.61	0.43
1:D:113:LYS:O	1:D:161:LYS:NZ	2.41	0.43
1:A:182:LYS:HE3	1:A:182:LYS:HB2	1.72	0.43
1:A:187:SER:C	1:A:189:ASP:N	2.73	0.43
1:A:298:TYR:CE2	1:A:302:LYS:HG3	2.53	0.43
1:C:298:TYR:CZ	1:C:302:LYS:HG3	2.54	0.43
1:C:302:LYS:HD3	1:C:302:LYS:HA	1.78	0.43
1:B:208:PHE:O	1:B:209:LYS:C	2.60	0.43
1:D:105:GLU:O	1:D:108:LYS:HE3	2.18	0.43
1:D:252:PHE:HB3	1:D:277:ILE:HD13	2.00	0.43
1:A:62:ILE:HG21	1:A:284:GLU:HA	2.01	0.43
1:A:197:GLU:H	1:A:197:GLU:HG3	1.21	0.43
1:A:260:ARG:O	1:A:261:PRO:C	2.59	0.43
1:B:91:ASN:O	1:B:138:PRO:HG3	2.18	0.43
1:C:222:ILE:O	1:C:235:GLN:HB3	2.19	0.43
1:C:93:GLU:HB3	1:C:100:PHE:HB2	2.00	0.43
1:D:77:LYS:NZ	1:D:81:GLU:OE2	2.51	0.43
1:B:229:GLU:HA	1:C:309:LYS:HZ1	1.84	0.43
1:C:208:PHE:O	1:C:209:LYS:C	2.62	0.43
1:A:229:GLU:HA	3:A:2029:HOH:O	2.18	0.42
1:B:182:LYS:HE3	1:B:182:LYS:HB2	1.70	0.42
1:D:39:ASN:ND2	1:D:42:ILE:HD12	2.33	0.42
1:C:77:LYS:NZ	1:C:81:GLU:OE2	2.50	0.42
1:D:195:PRO:O	1:D:196:ALA:C	2.60	0.42
1:D:62:ILE:HG21	1:D:284:GLU:HA	2.01	0.42
1:D:293:TYR:CD1	1:D:293:TYR:C	2.97	0.42
1:B:187:SER:C	1:B:189:ASP:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ILE:HD12	1:D:210:TYR:CE2	2.55	0.42
1:D:131:ASN:HA	1:D:135:LYS:HB3	2.01	0.42
1:D:253:VAL:O	1:D:276:GLN:HA	2.20	0.42
1:C:250:SER:HB3	1:C:274:TYR:HB2	2.02	0.42
1:D:132:GLU:CG	1:D:135:LYS:HG3	2.50	0.42
1:D:203:THR:O	1:D:221:TYR:HA	2.20	0.42
1:B:105:GLU:O	1:B:108:LYS:HE3	2.19	0.42
1:B:302:LYS:HD3	1:B:302:LYS:HA	1.84	0.42
1:A:221:TYR:CD1	1:A:221:TYR:C	2.98	0.42
1:A:116:PHE:CD1	1:A:116:PHE:N	2.86	0.41
1:B:92:LEU:HD13	1:B:138:PRO:HB2	2.03	0.41
1:B:137:ASP:HA	1:B:138:PRO:HD3	1.89	0.41
1:C:239:LEU:HD12	1:C:239:LEU:HA	1.81	0.41
1:C:195:PRO:O	1:C:196:ALA:C	2.63	0.41
1:D:173:LEU:HA	1:D:173:LEU:HD12	1.87	0.41
1:C:132:GLU:HG2	1:C:135:LYS:HG3	2.02	0.41
1:C:284:GLU:O	1:C:285:GLN:C	2.63	0.41
1:B:298:TYR:CE1	1:B:302:LYS:HE2	2.55	0.41
1:D:173:LEU:HB3	3:D:2018:HOH:O	2.20	0.41
1:B:291:SER:O	1:B:292:TYR:C	2.63	0.41
1:A:110:THR:O	1:A:111:GLU:C	2.64	0.41
1:B:148:ILE:HG23	1:B:177:THR:CG2	2.51	0.41
1:C:203:THR:O	1:C:221:TYR:HA	2.20	0.41
1:C:253:VAL:O	1:C:276:GLN:HA	2.20	0.41
1:D:187:SER:C	1:D:189:ASP:N	2.78	0.41
1:D:295:MET:CG	1:D:296:MET:N	2.81	0.41
1:A:132:GLU:HG2	1:A:135:LYS:HG3	2.03	0.41
1:A:286:GLY:HA3	3:A:2040:HOH:O	2.20	0.41
1:C:132:GLU:HG2	1:C:135:LYS:CE	2.51	0.41
1:D:189:ASP:O	1:D:190:LYS:C	2.63	0.41
1:B:125:ILE:HD12	1:B:210:TYR:CE2	2.56	0.41
1:C:176:TYR:CE2	1:C:180:LEU:HD11	2.56	0.41
1:B:156:LYS:HE2	1:B:156:LYS:HB2	1.77	0.40
1:B:187:SER:C	1:B:189:ASP:H	2.28	0.40
1:C:295:MET:CG	1:C:296:MET:N	2.84	0.40
1:B:131:ASN:C	1:B:135:LYS:HG3	2.33	0.40
1:B:253:VAL:O	1:B:276:GLN:HA	2.21	0.40
1:B:295:MET:CG	1:B:296:MET:N	2.83	0.40
1:D:182:LYS:HE3	1:D:182:LYS:HB2	1.75	0.40
1:A:130:GLN:HA	1:A:135:LYS:NZ	2.13	0.40
1:A:203:THR:HG21	1:A:208:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:PHE:HE1	1:B:303:ILE:HG22	1.85	0.40
1:C:189:ASP:C	1:C:191:PHE:N	2.79	0.40
1:A:91:ASN:O	1:A:138:PRO:HG3	2.22	0.40
1:B:260:ARG:O	1:B:261:PRO:C	2.63	0.40
1:C:130:GLN:CB	3:C:2015:HOH:O	2.63	0.40
1:D:146:ASN:O	1:D:150:PHE:CD1	2.75	0.40
1:D:187:SER:C	1:D:189:ASP:H	2.29	0.40

All (27) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:GLU:OE2	1:D:164:ASN:CB[1_455]	1.13	1.07
1:C:132:GLU:N	1:D:131:ASN:ND2[1_456]	1.30	0.90
1:C:197:GLU:OE2	1:D:164:ASN:CA[1_455]	1.34	0.86
1:C:132:GLU:CA	1:D:131:ASN:ND2[1_456]	1.63	0.57
1:A:132:GLU:OE2	1:B:164:ASN:O[2_454]	1.93	0.27
1:B:56:LEU:O	1:C:102:LYS:NZ[1_554]	1.94	0.26
1:C:131:ASN:C	1:D:131:ASN:OD1[1_456]	1.95	0.25
1:B:55:ASP:CB	1:C:97:ASN:ND2[1_554]	1.96	0.24
1:C:126:TYR:CE2	1:D:131:ASN:O[1_456]	1.96	0.24
1:C:131:ASN:O	1:D:131:ASN:OD1[1_456]	1.96	0.24
1:A:197:GLU:OE2	1:B:126:TYR:N[2_455]	1.97	0.23
1:C:131:ASN:ND2	1:D:131:ASN:OD1[1_456]	2.02	0.18
1:C:197:GLU:OE2	1:D:164:ASN:CG[1_455]	2.04	0.16
1:C:197:GLU:OE2	1:D:164:ASN:C[1_455]	2.06	0.14
1:C:131:ASN:C	1:D:131:ASN:ND2[1_456]	2.07	0.13
1:A:133:LYS:O	1:B:167:GLU:CB[2_454]	2.08	0.12
1:B:166:LYS:CE	1:D:77:LYS:CD[2_444]	2.11	0.09
1:C:132:GLU:C	1:D:131:ASN:ND2[1_456]	2.14	0.06
1:C:133:LYS:CE	1:D:132:GLU:CB[1_456]	2.14	0.06
1:C:197:GLU:CD	1:D:164:ASN:CA[1_455]	2.14	0.06
1:C:197:GLU:CD	1:D:164:ASN:CB[1_455]	2.14	0.06
1:C:197:GLU:CD	1:D:164:ASN:OD1[1_455]	2.16	0.04
1:B:166:LYS:NZ	1:D:77:LYS:CB[2_444]	2.17	0.03
1:C:197:GLU:CD	1:D:164:ASN:CG[1_455]	2.17	0.03
1:A:189:ASP:OD2	1:B:196:ALA:CB[2_455]	2.18	0.02
1:B:166:LYS:NZ	1:D:77:LYS:CD[2_444]	2.18	0.02
1:C:132:GLU:O	1:D:131:ASN:ND2[1_456]	2.19	0.01

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	276/303 (91%)	252 (91%)	22 (8%)	2 (1%)	18	41
1	B	276/303 (91%)	250 (91%)	24 (9%)	2 (1%)	18	41
1	C	276/303 (91%)	254 (92%)	19 (7%)	3 (1%)	11	29
1	D	276/303 (91%)	253 (92%)	21 (8%)	2 (1%)	18	41
All	All	1104/1212 (91%)	1009 (91%)	86 (8%)	9 (1%)	16	37

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	190	LYS
1	B	97	ASN
1	B	190	LYS
1	C	97	ASN
1	C	190	LYS
1	D	97	ASN
1	D	190	LYS
1	C	105	GLU

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	244/263 (93%)	228 (93%)	16 (7%)	15	36
1	B	244/263 (93%)	229 (94%)	15 (6%)	17	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	244/263 (93%)	228 (93%)	16 (7%)	15	36
1	D	244/263 (93%)	229 (94%)	15 (6%)	17	40
All	All	976/1052 (93%)	914 (94%)	62 (6%)	16	38

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LYS
1	A	104	VAL
1	A	105	GLU
1	A	108	LYS
1	A	113	LYS
1	A	130	GLN
1	A	131	ASN
1	A	166	LYS
1	A	174	LYS
1	A	182	LYS
1	A	193	LYS
1	A	197	GLU
1	A	217	VAL
1	A	245	GLN
1	A	277	ILE
1	A	295	MET
1	B	102	LYS
1	B	104	VAL
1	B	105	GLU
1	B	108	LYS
1	B	130	GLN
1	B	131	ASN
1	B	166	LYS
1	B	174	LYS
1	B	182	LYS
1	B	193	LYS
1	B	197	GLU
1	B	217	VAL
1	B	245	GLN
1	B	277	ILE
1	B	295	MET
1	C	102	LYS
1	C	104	VAL
1	C	105	GLU

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Mol	Chain	Res	Type
1	C	108	LYS
1	C	113	LYS
1	C	130	GLN
1	C	131	ASN
1	C	166	LYS
1	C	174	LYS
1	C	182	LYS
1	C	193	LYS
1	C	197	GLU
1	C	217	VAL
1	C	245	GLN
1	C	277	ILE
1	C	295	MET
1	D	102	LYS
1	D	104	VAL
1	D	105	GLU
1	D	108	LYS
1	D	130	GLN
1	D	131	ASN
1	D	166	LYS
1	D	174	LYS
1	D	182	LYS
1	D	193	LYS
1	D	197	GLU
1	D	217	VAL
1	D	245	GLN
1	D	277	ILE
1	D	295	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	A	267	GLN
1	B	165	ASN
1	B	276	GLN
1	C	165	ASN
1	D	165	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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	278/303 (91%)	-0.17	6 (2%) 62 59	25, 45, 70, 90	0
1	B	278/303 (91%)	-0.12	4 (1%) 73 72	29, 47, 73, 85	0
1	C	278/303 (91%)	-0.01	7 (2%) 58 55	29, 48, 70, 92	0
1	D	278/303 (91%)	0.09	9 (3%) 50 46	27, 51, 91, 109	0
All	All	1112/1212 (91%)	-0.05	26 (2%) 61 58	25, 48, 78, 109	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	134	GLY	5.1
1	D	131	ASN	5.0
1	A	132	GLU	4.8
1	B	134	GLY	4.4
1	B	129	GLY	4.3
1	D	129	GLY	3.7
1	C	129	GLY	3.6
1	A	133	LYS	3.6
1	D	132	GLU	3.4
1	A	134	GLY	3.3
1	D	133	LYS	3.3
1	D	164	ASN	3.0
1	C	94	THR	3.0
1	C	97	ASN	2.7
1	A	129	GLY	2.6
1	A	95	GLY	2.5
1	D	130	GLN	2.5
1	C	135	LYS	2.4
1	C	131	ASN	2.4
1	B	131	ASN	2.4
1	C	189	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	193	LYS	2.3
1	B	130	GLN	2.3
1	D	32	LYS	2.2
1	C	134	GLY	2.2
1	A	131	ASN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	B	1000	1/1	0.98	0.02	41,41,41,41	0
2	MN	A	1000	1/1	0.99	0.02	31,31,31,31	0
2	MN	C	1000	1/1	0.99	0.01	42,42,42,42	0
2	MN	D	1000	1/1	0.99	0.02	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.