Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2024 – 03:51 PM JST

PDB ID	:	8JKT
Title	:	Crystal structure of feline aminopeptidase N ectodomain
Authors	:	Tan, Y.B.; Shi, Y.J.; Peng, G.Q.
Deposited on	:	2023-06-01
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

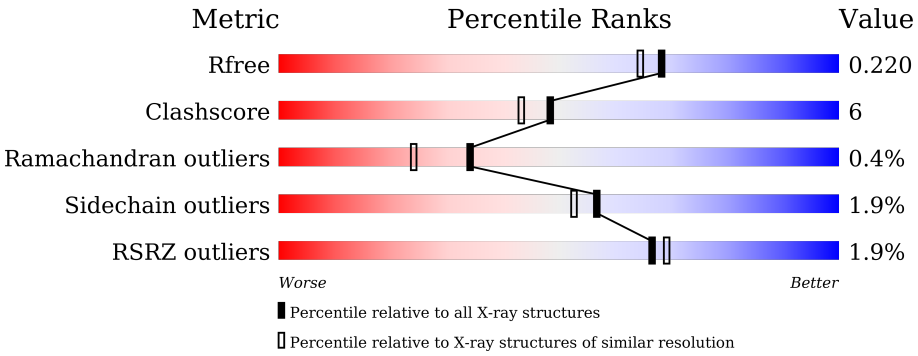
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	979	2% 79% 12% • 8%
1	B	979	% 81% 10% • 8%
1	C	979	2% 79% 12% • 8%
1	D	979	2% 80% 11% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 32894 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	904	Total	C	N	O	S	0	0	0
			7286	4680	1217	1364	25			
1	B	901	Total	C	N	O	S	0	0	0
			7260	4665	1212	1358	25			
1	C	900	Total	C	N	O	S	0	0	0
			7254	4662	1211	1356	25			
1	D	900	Total	C	N	O	S	0	0	0
			7254	4662	1211	1356	25			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	905	SER	-	expression tag	UNP P79171
A	906	GLY	-	expression tag	UNP P79171
A	907	SER	-	expression tag	UNP P79171
A	908	GLY	-	expression tag	UNP P79171
A	909	HIS	-	expression tag	UNP P79171
A	910	HIS	-	expression tag	UNP P79171
A	911	HIS	-	expression tag	UNP P79171
A	912	HIS	-	expression tag	UNP P79171
A	913	HIS	-	expression tag	UNP P79171
A	914	HIS	-	expression tag	UNP P79171
A	915	HIS	-	expression tag	UNP P79171
A	916	HIS	-	expression tag	UNP P79171
B	905	SER	-	expression tag	UNP P79171
B	906	GLY	-	expression tag	UNP P79171
B	907	SER	-	expression tag	UNP P79171
B	908	GLY	-	expression tag	UNP P79171
B	909	HIS	-	expression tag	UNP P79171
B	910	HIS	-	expression tag	UNP P79171
B	911	HIS	-	expression tag	UNP P79171
B	912	HIS	-	expression tag	UNP P79171
B	913	HIS	-	expression tag	UNP P79171

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Chain	Residue	Modelled	Actual	Comment	Reference
B	914	HIS	-	expression tag	UNP P79171
B	915	HIS	-	expression tag	UNP P79171
B	916	HIS	-	expression tag	UNP P79171
C	905	SER	-	expression tag	UNP P79171
C	906	GLY	-	expression tag	UNP P79171
C	907	SER	-	expression tag	UNP P79171
C	908	GLY	-	expression tag	UNP P79171
C	909	HIS	-	expression tag	UNP P79171
C	910	HIS	-	expression tag	UNP P79171
C	911	HIS	-	expression tag	UNP P79171
C	912	HIS	-	expression tag	UNP P79171
C	913	HIS	-	expression tag	UNP P79171
C	914	HIS	-	expression tag	UNP P79171
C	915	HIS	-	expression tag	UNP P79171
C	916	HIS	-	expression tag	UNP P79171
D	905	SER	-	expression tag	UNP P79171
D	906	GLY	-	expression tag	UNP P79171
D	907	SER	-	expression tag	UNP P79171
D	908	GLY	-	expression tag	UNP P79171
D	909	HIS	-	expression tag	UNP P79171
D	910	HIS	-	expression tag	UNP P79171
D	911	HIS	-	expression tag	UNP P79171
D	912	HIS	-	expression tag	UNP P79171
D	913	HIS	-	expression tag	UNP P79171
D	914	HIS	-	expression tag	UNP P79171
D	915	HIS	-	expression tag	UNP P79171
D	916	HIS	-	expression tag	UNP P79171

- Molecule 2 is water.

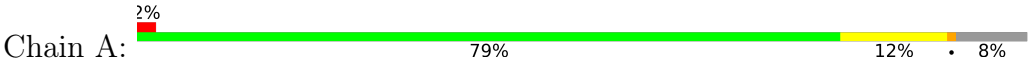
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	868	Total O 868 868	0	0
2	B	1046	Total O 1046 1046	0	0
2	C	937	Total O 937 937	0	0
2	D	989	Total O 989 989	0	0

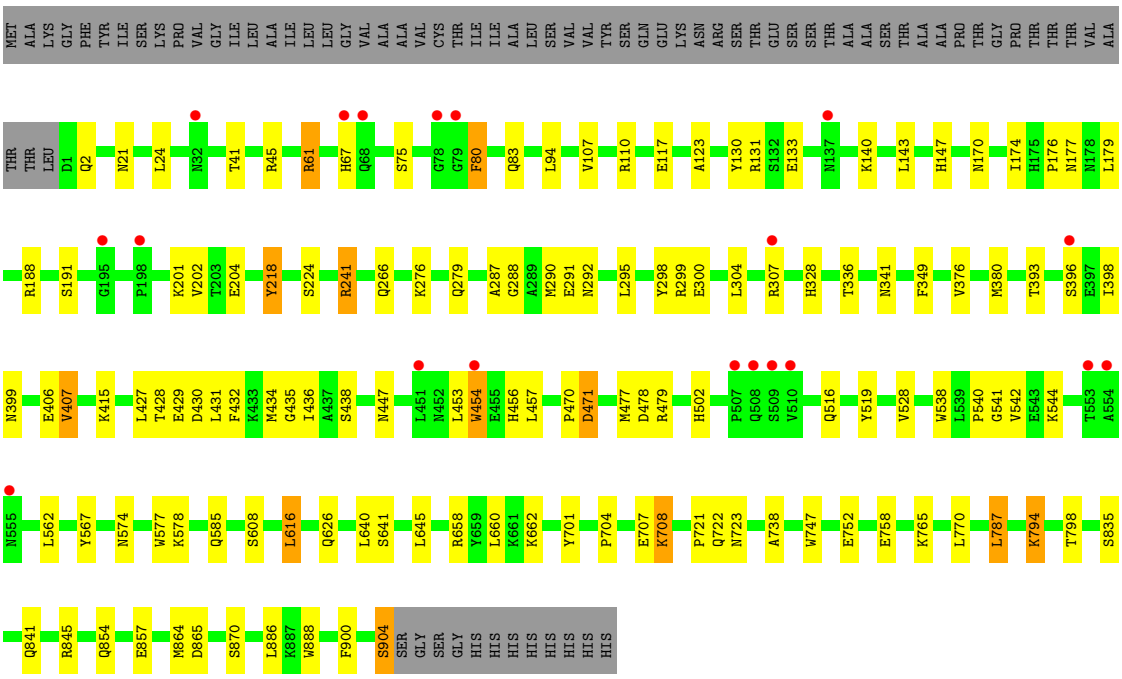
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Aminopeptidase N

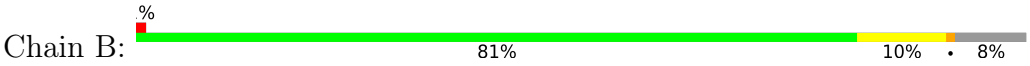
Chain A:

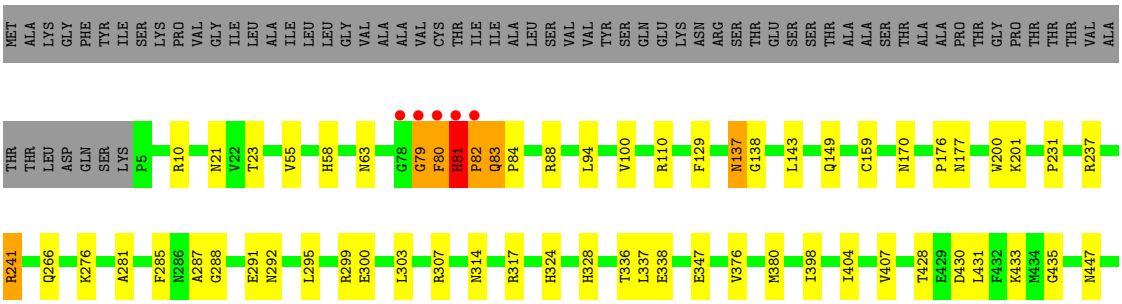


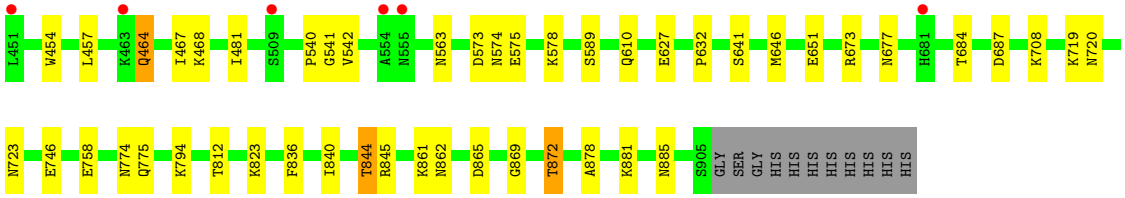


• Molecule 1: Aminopeptidase N

Chain B:

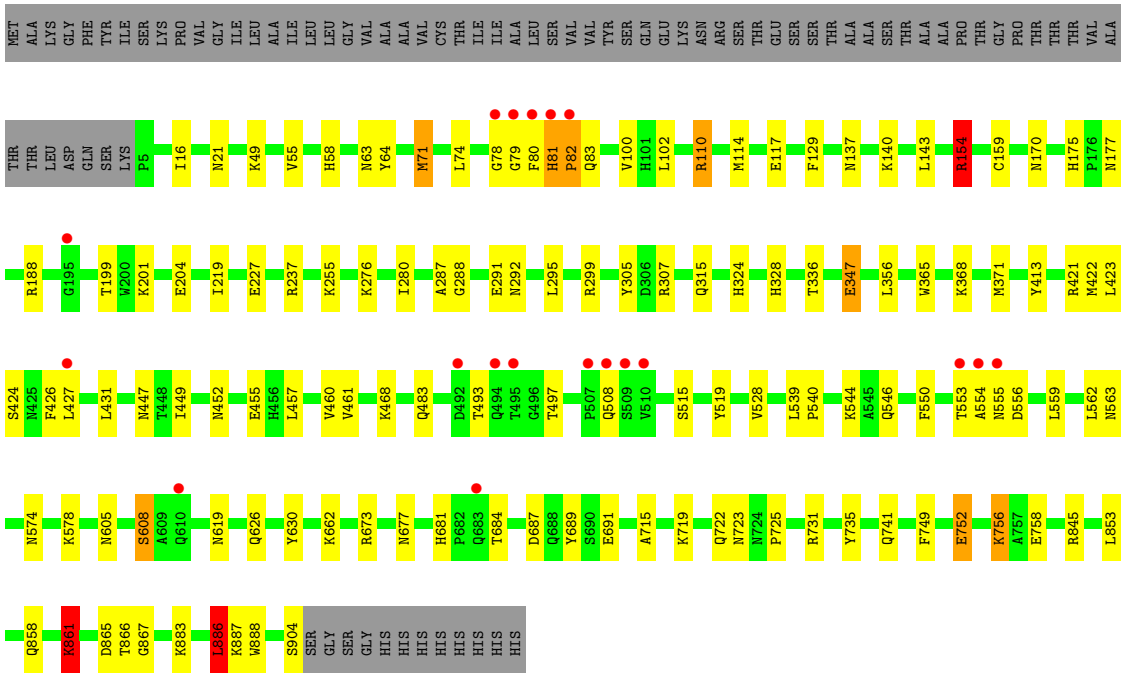






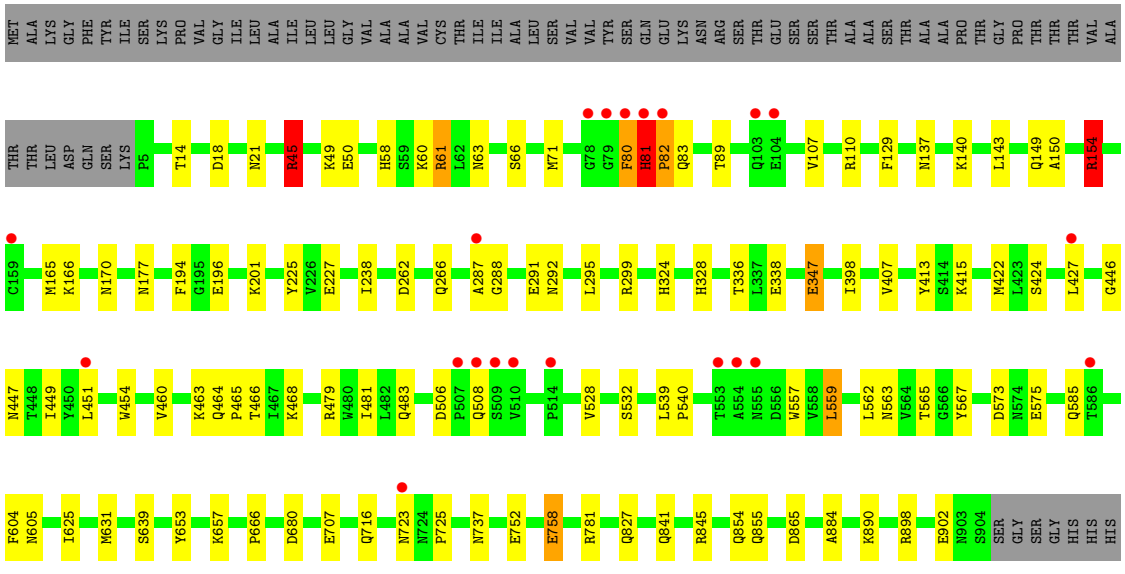
• Molecule 1: Aminopeptidase N

Chain C:



• Molecule 1: Aminopeptidase N

Chain D:




HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	123.20Å 132.59Å 129.36Å 90.00° 101.18° 90.00°	Depositor
Resolution (Å)	35.83 – 1.90 40.74 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.83-1.90) 99.9 (40.74-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 1.91Å)	Xtriage
Refinement program	PHENIX v1.0	Depositor
R, R_{free}	0.178 , 0.221 0.177 , 0.220	Depositor DCC
R_{free} test set	2014 reflections (0.63%)	wwPDB-VP
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	32894	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.42	0/7482	0.68	7/10205 (0.1%)
1	B	0.45	0/7456	0.71	4/10170 (0.0%)
1	C	0.52	5/7450 (0.1%)	0.75	8/10162 (0.1%)
1	D	0.51	2/7450 (0.0%)	0.75	7/10162 (0.1%)
All	All	0.48	7/29838 (0.0%)	0.72	26/40699 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	C	0	2
1	D	0	3
All	All	0	9

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	347	GLU	CD-OE1	18.31	1.45	1.25
1	D	347	GLU	CD-OE1	16.20	1.43	1.25
1	C	455	GLU	CG-CD	-7.70	1.40	1.51
1	C	455	GLU	CD-OE1	6.57	1.32	1.25
1	C	347	GLU	CG-CD	5.97	1.60	1.51
1	D	347	GLU	CG-CD	5.64	1.60	1.51
1	C	756	LYS	CE-NZ	5.54	1.62	1.49

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	347	GLU	CG-CD-OE2	-13.97	90.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	347	GLU	CG-CD-OE2	-13.54	91.23	118.30
1	C	347	GLU	CG-CD-OE1	12.12	142.53	118.30
1	D	347	GLU	CG-CD-OE1	11.02	140.34	118.30
1	B	287	ALA	C-N-CA	-8.83	103.76	122.30
1	C	886	LEU	CA-CB-CG	8.65	135.19	115.30
1	D	287	ALA	C-N-CA	-8.64	104.15	122.30
1	B	137	ASN	C-N-CA	-8.57	104.29	122.30
1	D	559	LEU	CA-CB-CG	8.09	133.92	115.30
1	C	287	ALA	C-N-CA	-8.09	105.32	122.30
1	A	287	ALA	C-N-CA	-7.63	106.28	122.30
1	D	45	ARG	CG-CD-NE	-7.62	95.79	111.80
1	A	471	ASP	CB-CG-OD1	-7.32	111.71	118.30
1	A	471	ASP	CB-CG-OD2	6.98	124.58	118.30
1	D	154	ARG	CB-CG-CD	-6.72	94.12	111.60
1	A	787	LEU	CA-CB-CG	6.46	130.15	115.30
1	C	154	ARG	CB-CG-CD	-6.41	94.94	111.60
1	C	861	LYS	CA-CB-CG	5.98	126.55	113.40
1	C	71	MET	CA-CB-CG	5.56	122.75	113.30
1	D	347	GLU	CB-CG-CD	5.56	129.21	114.20
1	B	430	ASP	CB-CG-OD1	5.48	123.23	118.30
1	C	347	GLU	CB-CG-CD	5.42	128.84	114.20
1	A	454	TRP	CA-CB-CG	-5.32	103.60	113.70
1	B	673	ARG	CA-CB-CG	5.28	125.00	113.40
1	A	407	VAL	CB-CA-C	-5.25	101.43	111.40
1	A	886	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	ARG	Sidechain
1	B	237	ARG	Sidechain
1	B	241	ARG	Sidechain
1	B	81	HIS	Peptide
1	C	154	ARG	Sidechain
1	C	508	GLN	Peptide
1	D	154	ARG	Sidechain
1	D	45	ARG	Sidechain
1	D	81	HIS	Peptide

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	7286	0	7124	89	1
1	B	7260	0	7097	81	0
1	C	7254	0	7092	98	0
1	D	7254	0	7092	79	2
2	A	868	0	0	34	2
2	B	1046	0	0	34	4
2	C	937	0	0	24	1
2	D	989	0	0	26	5
All	All	32894	0	28405	342	8

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 6.

All (342) 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:307:ARG:NH1	2:A:1002:HOH:O	1.92	1.01
1:A:67:HIS:ND1	2:A:1003:HOH:O	1.93	1.01
1:C:662:LYS:NZ	2:C:1003:HOH:O	1.93	0.98
1:C:554:ALA:O	2:C:1001:HOH:O	1.85	0.95
1:D:508:GLN:OE1	2:D:1001:HOH:O	1.85	0.94
1:A:479:ARG:NH1	2:A:1005:HOH:O	2.04	0.91
1:A:429:GLU:OE2	2:A:1001:HOH:O	1.85	0.91
1:C:619:ASN:ND2	2:C:1004:HOH:O	2.00	0.91
1:C:137:ASN:O	2:C:1002:HOH:O	1.87	0.91
1:B:574:ASN:OD1	1:B:578:LYS:NZ	2.04	0.89
1:D:137:ASN:O	2:D:1002:HOH:O	1.90	0.88
1:D:758:GLU:OE2	2:D:1003:HOH:O	1.91	0.87
1:B:862:ASN:OD1	2:B:1001:HOH:O	1.92	0.87
1:B:723:ASN:OD1	2:B:1002:HOH:O	1.93	0.86
1:C:177:ASN:HA	1:C:201:LYS:HD3	1.60	0.83
1:A:304:LEU:O	2:A:1004:HOH:O	1.95	0.83
1:D:716:GLN:HG2	1:D:725:PRO:HG3	1.59	0.83
1:C:328:HIS:NE2	1:C:347:GLU:OE1	2.11	0.81
1:B:137:ASN:O	2:B:1003:HOH:O	1.99	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ASN:ND2	2:D:1010:HOH:O	2.11	0.79
1:B:347:GLU:OE1	2:B:1004:HOH:O	2.00	0.79
1:C:883:LYS:HA	1:C:886:LEU:HD12	1.64	0.79
1:C:21:ASN:ND2	2:C:1009:HOH:O	2.07	0.79
1:A:428:THR:HG21	2:A:1733:HOH:O	1.81	0.79
1:B:241:ARG:NH2	2:B:1008:HOH:O	2.14	0.78
1:D:58:HIS:HB3	1:D:154:ARG:HD3	1.66	0.78
1:C:117:GLU:OE1	2:C:1006:HOH:O	2.02	0.77
1:C:722:GLN:OE1	2:C:1005:HOH:O	2.01	0.77
1:C:673:ARG:NH1	2:C:1013:HOH:O	2.12	0.77
1:B:324:HIS:NE2	2:B:1004:HOH:O	2.18	0.76
1:D:855:GLN:HG2	2:D:1773:HOH:O	1.84	0.76
1:C:546:GLN:O	2:C:1007:HOH:O	2.05	0.75
1:D:170:ASN:ND2	2:D:1006:HOH:O	2.09	0.75
1:A:61:ARG:NH2	2:A:1008:HOH:O	2.20	0.73
1:B:775:GLN:OE1	2:B:1005:HOH:O	2.05	0.73
1:A:516:GLN:OE1	2:A:1006:HOH:O	2.07	0.72
1:B:338:GLU:OE2	2:B:1007:HOH:O	2.07	0.71
1:C:756:LYS:NZ	2:C:1008:HOH:O	2.06	0.71
1:B:266:GLN:HG2	2:B:1389:HOH:O	1.91	0.71
1:D:680:ASP:OD1	2:D:1004:HOH:O	2.08	0.71
1:A:857:GLU:HG3	2:A:1720:HOH:O	1.89	0.71
1:C:528:VAL:HG13	1:C:562:LEU:HD21	1.73	0.71
1:B:177:ASN:HB3	1:B:201:LYS:HD3	1.73	0.70
1:B:684:THR:HG22	1:B:687:ASP:H	1.56	0.70
1:C:904:SER:HB3	2:C:1751:HOH:O	1.90	0.70
1:D:398:ILE:HD12	1:D:407:VAL:HG11	1.71	0.70
1:C:78:GLY:HA2	1:C:80:PHE:CZ	2.26	0.70
1:D:465:PRO:O	1:D:468:LYS:NZ	2.25	0.70
1:C:758:GLU:OE2	2:C:1011:HOH:O	2.10	0.69
1:D:716:GLN:OE1	2:D:1008:HOH:O	2.10	0.69
1:A:427:LEU:O	1:A:428:THR:HB	1.92	0.69
1:A:752:GLU:OE2	1:B:719:LYS:HE3	1.93	0.69
1:D:707:GLU:HG2	2:D:1018:HOH:O	1.91	0.69
1:C:887:LYS:NZ	2:C:1018:HOH:O	2.25	0.69
1:D:81:HIS:HB3	1:D:110:ARG:HH12	1.56	0.68
1:D:227:GLU:OE1	2:D:1007:HOH:O	2.10	0.68
1:D:324:HIS:NE2	1:D:347:GLU:OE1	2.24	0.68
1:C:305:TYR:CE2	1:C:307:ARG:HD3	2.29	0.68
1:C:684:THR:HG22	1:C:687:ASP:H	1.58	0.68
1:D:898:ARG:O	1:D:902:GLU:HG3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:ASN:ND2	2:B:1012:HOH:O	2.22	0.67
1:A:864:MET:HB2	2:A:1165:HOH:O	1.93	0.67
1:C:305:TYR:HE2	1:C:307:ARG:HD3	1.59	0.66
1:D:854:GLN:OE1	2:D:1011:HOH:O	2.13	0.66
1:C:81:HIS:HB3	1:C:82:PRO:HD3	1.76	0.66
1:C:227:GLU:OE1	2:C:1012:HOH:O	2.12	0.66
1:A:75:SER:HB2	1:A:83:GLN:HE22	1.62	0.64
1:B:758:GLU:HB2	2:B:1141:HOH:O	1.98	0.64
1:D:758:GLU:HB2	2:D:1168:HOH:O	1.98	0.64
1:B:869:GLY:O	1:B:872:THR:HG23	1.98	0.63
1:D:328:HIS:NE2	1:D:347:GLU:OE1	2.18	0.63
1:C:188:ARG:HD2	1:C:204:GLU:HG2	1.79	0.63
1:D:81:HIS:HB3	1:D:110:ARG:NH1	2.14	0.63
1:B:288:GLY:HA2	1:B:299:ARG:HG3	1.81	0.63
1:B:94:LEU:HD12	1:B:94:LEU:H	1.63	0.63
1:C:324:HIS:NE2	1:C:347:GLU:OE1	2.21	0.63
1:A:640:LEU:HD13	1:A:660:LEU:HD21	1.79	0.63
1:C:328:HIS:HE2	1:C:347:GLU:CD	2.03	0.62
1:A:24:LEU:HD13	1:A:218:TYR:CE2	2.34	0.62
1:B:646:MET:SD	1:B:885:ASN:HB3	2.40	0.62
1:D:177:ASN:HA	1:D:201:LYS:HG3	1.82	0.62
1:C:426:PHE:O	2:C:1015:HOH:O	2.16	0.62
1:D:21:ASN:ND2	2:D:1014:HOH:O	2.25	0.61
1:D:328:HIS:HE2	1:D:347:GLU:CD	2.03	0.61
1:C:866:THR:HG22	1:C:867:GLY:O	1.99	0.61
1:A:758:GLU:HB3	2:A:1630:HOH:O	1.99	0.61
1:B:177:ASN:CB	1:B:201:LYS:HD3	2.31	0.60
1:C:756:LYS:HG3	2:C:1154:HOH:O	2.01	0.60
1:D:557:TRP:HZ3	1:D:559:LEU:HD12	1.65	0.60
1:A:723:ASN:ND2	2:A:1014:HOH:O	2.25	0.60
1:B:746:GLU:OE1	2:B:1009:HOH:O	2.16	0.60
1:D:201:LYS:NZ	2:D:1023:HOH:O	2.32	0.60
1:A:147:HIS:CE1	1:A:290:MET:HG2	2.36	0.60
1:D:80:PHE:O	1:D:81:HIS:HB2	2.02	0.60
1:A:131:ARG:NH1	1:A:133:GLU:OE2	2.34	0.60
1:A:188:ARG:HD2	1:A:204:GLU:HG2	1.83	0.60
1:A:454:TRP:HZ3	1:A:478:ASP:OD1	1.84	0.60
1:C:170:ASN:ND2	2:C:1010:HOH:O	2.09	0.60
1:C:715:ALA:O	1:C:719:LYS:HD2	2.01	0.59
1:B:878:ALA:HA	1:B:881:LYS:HE3	1.84	0.59
1:C:553:THR:HG22	1:C:554:ALA:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:NH2	2:A:1022:HOH:O	2.33	0.59
1:A:406:GLU:HG2	1:A:870:SER:HA	1.85	0.59
1:D:347:GLU:HG3	1:D:413:TYR:CZ	2.37	0.58
1:C:497:THR:HG21	1:C:544:LYS:HE2	1.85	0.58
1:B:21:ASN:ND2	2:B:1017:HOH:O	2.26	0.58
1:C:424:SER:O	1:C:427:LEU:O	2.21	0.58
1:B:774:ASN:OD1	2:B:1010:HOH:O	2.17	0.58
1:C:457:LEU:O	1:C:461:VAL:HG23	2.03	0.58
1:C:853:LEU:HD22	1:C:886:LEU:HD11	1.85	0.57
1:D:737:ASN:ND2	2:D:1018:HOH:O	2.31	0.57
1:B:845:ARG:NH2	2:B:1035:HOH:O	2.38	0.57
1:D:454:TRP:HZ2	1:D:481:ILE:HG13	1.69	0.56
1:D:460:VAL:O	1:D:463:LYS:HB3	2.06	0.56
1:B:110:ARG:HD2	2:B:1403:HOH:O	2.06	0.56
1:B:398:ILE:HD12	1:B:407:VAL:CG1	2.35	0.56
1:C:626:GLN:OE1	2:C:1016:HOH:O	2.17	0.56
1:C:741:GLN:NE2	2:C:1017:HOH:O	2.17	0.56
1:B:376:VAL:O	1:B:380:MET:HG3	2.06	0.55
1:C:80:PHE:H	1:C:83:GLN:HE21	1.53	0.55
1:C:177:ASN:CA	1:C:201:LYS:HD3	2.34	0.55
1:B:398:ILE:HD12	1:B:407:VAL:HG11	1.88	0.55
1:C:63:ASN:ND2	2:C:1025:HOH:O	2.33	0.55
1:B:840:ILE:O	1:B:844:THR:HB	2.06	0.55
1:C:219:ILE:HD13	1:C:280:ILE:HD13	1.89	0.55
1:C:752:GLU:O	1:C:756:LYS:HG2	2.07	0.55
1:A:544:LYS:NZ	2:A:1033:HOH:O	2.40	0.54
1:B:454:TRP:HZ2	1:B:481:ILE:HG13	1.72	0.54
1:A:288:GLY:HA2	1:A:299:ARG:HG3	1.89	0.54
1:C:315:GLN:HG2	1:C:365:TRP:HH2	1.73	0.54
1:C:449:ILE:HG12	1:C:452:ASN:OD1	2.08	0.54
1:A:396:SER:HB2	2:A:1141:HOH:O	2.08	0.54
1:C:78:GLY:HA2	1:C:80:PHE:CE2	2.42	0.54
1:C:347:GLU:HG3	1:C:413:TYR:CZ	2.42	0.54
1:D:841:GLN:NE2	2:D:1033:HOH:O	2.40	0.54
1:B:138:GLY:HA3	1:C:626:GLN:NE2	2.23	0.54
1:C:81:HIS:HB3	1:C:82:PRO:CD	2.38	0.54
1:D:291:GLU:HG3	1:D:328:HIS:HB3	1.90	0.53
1:A:574:ASN:ND2	2:A:1036:HOH:O	2.41	0.53
1:B:794:LYS:NZ	2:B:1018:HOH:O	2.28	0.53
1:B:435:GLY:HA3	1:B:457:LEU:HD23	1.91	0.53
1:A:454:TRP:CZ3	1:A:478:ASP:OD1	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:PHE:HB2	1:B:82:PRO:O	2.08	0.53
1:B:241:ARG:HD3	1:B:300:GLU:OE2	2.08	0.53
1:A:177:ASN:HB2	1:A:201:LYS:HE3	1.91	0.52
1:A:435:GLY:HA3	1:A:457:LEU:HD23	1.91	0.52
1:A:585:GLN:HE21	1:A:626:GLN:HE21	1.57	0.52
1:B:467:ILE:O	1:B:468:LYS:HE2	2.09	0.52
1:A:140:LYS:HE3	2:A:1682:HOH:O	2.10	0.52
1:C:16:ILE:HG12	1:C:49:LYS:HG3	1.92	0.52
1:A:658:ARG:NH2	2:A:1026:HOH:O	2.33	0.52
1:C:858:GLN:HE22	1:C:861:LYS:HE3	1.75	0.52
1:D:398:ILE:HD12	1:D:407:VAL:CG1	2.39	0.52
1:A:61:ARG:NH2	2:A:1011:HOH:O	2.22	0.51
1:B:338:GLU:HB3	2:B:1552:HOH:O	2.11	0.51
1:C:749:PHE:O	1:C:752:GLU:HG3	2.10	0.51
1:B:758:GLU:HB3	2:B:1758:HOH:O	2.09	0.51
1:D:557:TRP:CZ3	1:D:559:LEU:HD12	2.45	0.51
1:D:563:ASN:ND2	2:D:1038:HOH:O	2.41	0.51
1:C:305:TYR:CE1	1:C:315:GLN:HB2	2.45	0.51
1:B:862:ASN:HA	2:B:1001:HOH:O	2.11	0.51
1:A:707:GLU:HG2	2:A:1035:HOH:O	2.10	0.51
1:C:605:ASN:ND2	2:C:1040:HOH:O	2.44	0.50
1:D:506:ASP:O	1:D:508:GLN:N	2.43	0.50
1:A:398:ILE:HD12	1:A:407:VAL:HG13	1.93	0.50
1:B:21:ASN:ND2	2:B:1043:HOH:O	2.44	0.50
1:D:449:ILE:HD11	1:D:451:LEU:HD12	1.93	0.50
1:B:79:GLY:O	1:B:80:PHE:HB3	2.12	0.50
1:B:314:ASN:HB3	2:B:1397:HOH:O	2.11	0.49
1:D:262:ASP:O	1:D:266:GLN:HG3	2.13	0.49
1:A:41:THR:HG22	1:A:117:GLU:HG3	1.94	0.49
1:A:170:ASN:ND2	2:A:1047:HOH:O	2.45	0.49
1:D:506:ASP:C	1:D:508:GLN:H	2.16	0.49
1:A:291:GLU:HG3	1:A:328:HIS:HB3	1.95	0.49
1:C:493:THR:HA	1:C:550:PHE:O	2.13	0.49
1:A:241:ARG:NH2	2:A:1027:HOH:O	2.34	0.49
1:A:738:ALA:HB2	2:A:1367:HOH:O	2.11	0.49
1:D:827:GLN:HG3	2:D:1515:HOH:O	2.12	0.49
1:B:288:GLY:CA	1:B:299:ARG:HG3	2.43	0.49
1:C:858:GLN:NE2	1:C:861:LYS:HE3	2.27	0.49
1:A:430:ASP:O	1:A:434:MET:HG2	2.13	0.49
1:D:528:VAL:HG13	1:D:562:LEU:HD11	1.94	0.48
1:C:58:HIS:HB2	1:C:159:CYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:865:ASP:OD1	1:D:865:ASP:N	2.46	0.48
1:A:174:ILE:HG12	1:A:202:VAL:HG22	1.96	0.48
1:C:539:LEU:HD12	1:C:540:PRO:HD2	1.94	0.48
1:C:845:ARG:HG3	1:C:845:ARG:HH11	1.79	0.48
1:D:631:MET:HG3	2:D:1627:HOH:O	2.12	0.48
1:D:66:SER:HA	1:D:71:MET:HA	1.95	0.48
1:C:55:VAL:HG11	1:C:114:MET:HE3	1.96	0.48
1:B:170:ASN:ND2	2:B:1016:HOH:O	2.25	0.48
1:D:464:GLN:HG3	1:D:466:THR:H	1.78	0.48
1:C:175:HIS:HE1	1:C:201:LYS:HE2	1.79	0.47
1:C:431:LEU:HD22	1:C:460:VAL:CG1	2.45	0.47
1:C:288:GLY:HA2	1:C:299:ARG:HG3	1.96	0.47
1:A:722:GLN:OE1	1:B:708:LYS:NZ	2.35	0.47
1:B:336:THR:O	1:B:447:ASN:HA	2.14	0.47
1:A:349:PHE:CZ	1:A:453:LEU:HD11	2.50	0.47
1:A:658:ARG:NE	2:A:1026:HOH:O	2.45	0.47
1:D:424:SER:O	1:D:427:LEU:O	2.32	0.47
1:A:660:LEU:HD13	1:A:701:TYR:CZ	2.49	0.47
1:B:540:PRO:O	1:B:542:VAL:N	2.45	0.47
1:D:479:ARG:O	1:D:483:GLN:HG2	2.15	0.47
1:A:540:PRO:O	1:A:542:VAL:N	2.44	0.47
1:B:573:ASP:OD2	1:B:575:GLU:HB2	2.14	0.47
1:D:336:THR:O	1:D:447:ASN:HA	2.14	0.47
1:A:470:PRO:HG3	1:A:538:TRP:CG	2.50	0.47
1:B:844:THR:HG21	1:B:878:ALA:HB1	1.96	0.47
1:B:80:PHE:CD2	1:B:81:HIS:N	2.78	0.47
1:A:704:PRO:O	1:A:708:LYS:HD3	2.14	0.46
1:C:328:HIS:NE2	1:C:347:GLU:CD	2.67	0.46
2:A:1014:HOH:O	1:B:677:ASN:ND2	2.48	0.46
1:B:63:ASN:ND2	2:B:1054:HOH:O	2.48	0.46
1:C:555:ASN:HA	2:C:1001:HOH:O	2.15	0.46
1:A:747:TRP:CE2	1:A:770:LEU:HD22	2.51	0.46
1:B:431:LEU:HD12	1:B:431:LEU:HA	1.75	0.46
1:B:651:GLU:HB3	1:D:781:ARG:HG3	1.97	0.46
1:C:553:THR:HG22	1:C:554:ALA:N	2.31	0.46
1:C:227:GLU:HG3	1:C:237:ARG:HG2	1.97	0.46
1:C:291:GLU:HG3	1:C:328:HIS:HB3	1.97	0.46
1:D:625:ILE:HG12	1:D:666:PRO:HG2	1.96	0.46
1:A:170:ASN:ND2	2:A:1021:HOH:O	2.32	0.46
1:C:681:HIS:ND1	1:C:691:GLU:OE2	2.42	0.46
1:C:177:ASN:ND2	1:C:199:THR:HA	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:GLN:HE21	1:A:626:GLN:NE2	2.13	0.46
1:D:194:PHE:CE2	1:D:196:GLU:HB3	2.51	0.46
1:A:266:GLN:NE2	2:A:1015:HOH:O	2.28	0.45
1:A:662:LYS:NZ	2:A:1019:HOH:O	2.30	0.45
1:D:60:LYS:O	1:D:61:ARG:HB2	2.16	0.45
1:D:110:ARG:NE	2:D:1054:HOH:O	2.49	0.45
1:A:288:GLY:CA	1:A:299:ARG:HG3	2.46	0.45
1:C:79:GLY:O	1:C:110:ARG:NH2	2.49	0.45
1:D:653:TYR:CE2	1:D:657:LYS:HE2	2.51	0.45
1:C:681:HIS:HD1	1:C:691:GLU:CD	2.19	0.45
1:B:878:ALA:HA	1:B:881:LYS:CE	2.46	0.45
1:D:81:HIS:O	1:D:82:PRO:C	2.54	0.45
1:A:279:GLN:HB3	1:A:298:TYR:CE2	2.51	0.45
1:A:900:PHE:O	1:A:904:SER:HB2	2.17	0.45
1:C:100:VAL:HG21	1:C:114:MET:HE2	1.99	0.45
1:D:107:VAL:HG21	2:D:1196:HOH:O	2.17	0.45
1:A:61:ARG:HD3	2:A:1117:HOH:O	2.17	0.44
1:A:794:LYS:NZ	2:A:1052:HOH:O	2.48	0.44
1:B:80:PHE:CG	1:B:81:HIS:N	2.84	0.44
1:C:356:LEU:HD23	1:C:368:LYS:HE2	1.99	0.44
1:A:21:ASN:ND2	2:A:1062:HOH:O	2.49	0.44
1:D:288:GLY:HA2	1:D:299:ARG:HD2	1.98	0.44
1:B:149:GLN:OE1	2:B:1011:HOH:O	2.21	0.44
1:D:80:PHE:HA	1:D:83:GLN:HG2	1.99	0.44
1:D:422:MET:HB2	1:D:565:THR:O	2.16	0.44
1:A:585:GLN:NE2	1:A:626:GLN:HE21	2.16	0.44
1:B:10:ARG:NH1	2:B:1032:HOH:O	2.36	0.44
1:D:45:ARG:NH2	2:D:1056:HOH:O	2.50	0.44
1:D:292:ASN:HB2	1:D:295:LEU:O	2.18	0.44
1:A:528:VAL:HG13	1:A:562:LEU:HD21	1.99	0.44
1:B:80:PHE:O	1:B:81:HIS:HB2	2.17	0.44
1:D:723:ASN:O	1:D:725:PRO:HD3	2.17	0.44
1:B:464:GLN:HE21	1:B:464:GLN:HB3	1.63	0.44
1:C:431:LEU:HD22	1:C:460:VAL:HG12	1.98	0.44
1:D:14:THR:HG22	1:D:50:GLU:HG2	2.00	0.44
1:B:83:GLN:HG3	1:B:84:PRO:HD2	1.99	0.44
1:B:823:LYS:HE2	2:B:1071:HOH:O	2.17	0.44
1:D:166:LYS:HE3	1:D:446:GLY:O	2.18	0.44
1:A:415:LYS:HE3	1:A:567:TYR:CE2	2.52	0.43
1:A:721:PRO:HG2	2:B:1260:HOH:O	2.18	0.43
1:A:502:HIS:HB2	1:A:519:TYR:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:528:VAL:HG13	1:D:562:LEU:HD21	2.00	0.43
1:A:454:TRP:CZ2	1:A:477:MET:HB3	2.53	0.43
1:B:138:GLY:HA3	1:C:626:GLN:HE22	1.83	0.43
1:B:292:ASN:HB2	1:B:295:LEU:O	2.18	0.43
1:C:292:ASN:HB2	1:C:295:LEU:O	2.18	0.43
1:A:376:VAL:O	1:A:380:MET:HG3	2.19	0.43
1:D:140:LYS:HE3	2:D:1399:HOH:O	2.17	0.43
1:A:432:PHE:O	1:A:436:ILE:HG12	2.19	0.43
1:B:404:ILE:O	1:B:407:VAL:HG22	2.18	0.43
1:C:288:GLY:CA	1:C:299:ARG:HG3	2.49	0.43
1:C:608:SER:HA	1:C:888:TRP:HE1	1.83	0.43
1:A:45:ARG:NH2	2:A:1012:HOH:O	2.24	0.43
1:A:292:ASN:HB2	1:A:295:LEU:O	2.19	0.43
1:C:574:ASN:O	1:C:578:LYS:HG3	2.19	0.43
1:A:608:SER:HA	1:A:888:TRP:NE1	2.34	0.42
1:B:80:PHE:HD2	1:B:82:PRO:O	2.02	0.42
1:C:371:MET:SD	1:C:421:ARG:HD3	2.59	0.42
1:C:608:SER:HA	1:C:888:TRP:NE1	2.34	0.42
1:A:176:PRO:HG2	1:A:179:LEU:HD12	2.01	0.42
1:A:765:LYS:HE2	2:A:1243:HOH:O	2.19	0.42
1:C:64:TYR:CB	1:C:71:MET:HG2	2.48	0.42
1:A:438:SER:OG	1:A:456:HIS:HD2	2.01	0.42
1:C:497:THR:CG2	1:C:544:LYS:HE2	2.50	0.42
1:D:415:LYS:HE3	1:D:567:TYR:CE2	2.54	0.42
1:D:845:ARG:NH1	2:D:1062:HOH:O	2.51	0.42
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.70	0.42
1:C:731:ARG:HD3	1:C:735:TYR:OH	2.19	0.42
1:A:854:GLN:NE2	2:A:1063:HOH:O	2.50	0.42
1:B:58:HIS:HB2	1:B:159:CYS:O	2.19	0.42
1:B:291:GLU:HG3	1:B:328:HIS:HB3	2.01	0.42
1:D:149:GLN:HA	1:D:150:ALA:HA	1.79	0.42
1:B:23:THR:HG22	2:B:1765:HOH:O	2.19	0.42
1:B:63:ASN:ND2	2:B:1024:HOH:O	2.33	0.42
1:C:630:TYR:CD1	1:C:689:TYR:HB3	2.55	0.42
1:B:337:LEU:O	1:B:337:LEU:HD12	2.19	0.42
1:C:422:MET:HB3	1:C:422:MET:HE2	1.94	0.42
1:A:241:ARG:HD3	1:A:300:GLU:OE1	2.19	0.42
1:B:231:PRO:HG2	2:B:1671:HOH:O	2.20	0.42
1:B:720:ASN:HB3	2:B:1608:HOH:O	2.19	0.42
1:D:49:LYS:HA	1:D:49:LYS:HD3	1.86	0.42
1:D:506:ASP:HB2	1:D:884:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:TRP:CG	1:A:616:LEU:HD11	2.55	0.42
1:B:281:ALA:HB2	1:B:303:LEU:HD23	2.02	0.42
1:C:64:TYR:HB2	1:C:71:MET:HG2	2.02	0.41
1:C:305:TYR:HE2	1:C:307:ARG:CD	2.30	0.41
1:D:605:ASN:ND2	2:D:1068:HOH:O	2.53	0.41
1:A:349:PHE:HZ	1:A:453:LEU:HD11	1.84	0.41
1:A:431:LEU:HD12	1:A:431:LEU:HA	1.72	0.41
1:B:55:VAL:HB	1:B:100:VAL:HB	2.02	0.41
1:B:610:GLN:HG3	2:B:1225:HOH:O	2.20	0.41
1:B:176:PRO:HD3	1:B:200:TRP:CZ3	2.55	0.41
1:C:81:HIS:CB	1:C:82:PRO:HD3	2.48	0.41
1:C:483:GLN:OE1	1:C:519:TYR:HA	2.21	0.41
1:A:107:VAL:HB	1:A:110:ARG:HG3	2.01	0.41
1:C:563:ASN:ND2	2:C:1049:HOH:O	2.48	0.41
1:D:338:GLU:HB3	2:D:1179:HOH:O	2.19	0.41
1:D:328:HIS:NE2	1:D:347:GLU:CD	2.71	0.41
1:B:285:PHE:HB3	1:B:299:ARG:HG2	2.02	0.41
1:C:677:ASN:ND2	2:C:1014:HOH:O	2.14	0.41
1:C:58:HIS:HB3	1:C:154:ARG:HD3	2.03	0.41
1:A:341:ASN:HB2	1:A:393:THR:O	2.21	0.41
1:A:398:ILE:HD12	1:A:407:VAL:CG1	2.51	0.41
1:C:74:LEU:HD12	1:C:102:LEU:HD21	2.02	0.41
1:D:539:LEU:HA	1:D:540:PRO:HD3	1.79	0.41
1:D:604:PHE:CG	1:D:639:SER:HB3	2.56	0.41
1:A:336:THR:O	1:A:447:ASN:HA	2.20	0.41
1:B:684:THR:HG23	2:B:1484:HOH:O	2.20	0.41
1:C:723:ASN:O	1:C:725:PRO:HD3	2.21	0.41
1:D:573:ASP:OD2	1:D:575:GLU:HB2	2.20	0.41
1:A:574:ASN:O	1:A:578:LYS:HE2	2.21	0.41
1:B:627:GLU:OE2	1:B:632:PRO:HG2	2.21	0.41
1:C:423:LEU:HA	1:C:426:PHE:CE2	2.56	0.41
1:A:841:GLN:O	1:A:845:ARG:HG3	2.20	0.40
1:C:336:THR:O	1:C:447:ASN:HA	2.21	0.40
1:D:225:TYR:HA	1:D:238:ILE:O	2.21	0.40
1:A:123:ALA:O	1:A:130:TYR:HB2	2.22	0.40
1:A:645:LEU:HD13	1:A:845:ARG:HB3	2.03	0.40

All (8) 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)
2:A:1492:HOH:O	2:D:1152:HOH:O[1_455]	1.75	0.45
1:D:463:LYS:NZ	1:D:752:GLU:OE2[2_755]	1.83	0.37
2:B:2043:HOH:O	2:C:1935:HOH:O[2_646]	1.84	0.36
2:B:2000:HOH:O	2:D:1836:HOH:O[2_745]	1.95	0.25
2:B:2017:HOH:O	2:D:1943:HOH:O[2_746]	2.07	0.13
2:B:1988:HOH:O	2:D:1845:HOH:O[2_746]	2.14	0.06
2:A:1484:HOH:O	2:D:1386:HOH:O[2_645]	2.15	0.05
1:A:865:ASP:OD1	1:D:89:THR:OG1[1_455]	2.17	0.03

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	902/979 (92%)	873 (97%)	27 (3%)	2 (0%)	47	38
1	B	899/979 (92%)	867 (96%)	26 (3%)	6 (1%)	22	12
1	C	898/979 (92%)	866 (96%)	30 (3%)	2 (0%)	47	38
1	D	898/979 (92%)	872 (97%)	23 (3%)	3 (0%)	41	31
All	All	3597/3916 (92%)	3478 (97%)	106 (3%)	13 (0%)	34	24

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	PHE
1	B	81	HIS
1	B	82	PRO
1	B	428	THR
1	D	82	PRO
1	B	79	GLY
1	B	80	PHE
1	D	80	PHE
1	B	541	GLY
1	C	81	HIS

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Mol	Chain	Res	Type
1	D	81	HIS
1	A	541	GLY
1	C	82	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	806/865 (93%)	788 (98%)	18 (2%)	52	47
1	B	803/865 (93%)	786 (98%)	17 (2%)	53	48
1	C	802/865 (93%)	787 (98%)	15 (2%)	57	53
1	D	802/865 (93%)	791 (99%)	11 (1%)	67	65
All	All	3213/3460 (93%)	3152 (98%)	61 (2%)	57	53

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	61	ARG
1	A	80	PHE
1	A	143	LEU
1	A	191	SER
1	A	218	TYR
1	A	224	SER
1	A	276	LYS
1	A	399	ASN
1	A	471	ASP
1	A	616	LEU
1	A	641	SER
1	A	708	LYS
1	A	787	LEU
1	A	794	LYS
1	A	798	THR
1	A	835	SER
1	A	904	SER

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Mol	Chain	Res	Type
1	B	83	GLN
1	B	88	ARG
1	B	129	PHE
1	B	143	LEU
1	B	276	LYS
1	B	307	ARG
1	B	317	ARG
1	B	433	LYS
1	B	464	GLN
1	B	589	SER
1	B	641	SER
1	B	812	THR
1	B	836	PHE
1	B	844	THR
1	B	861	LYS
1	B	865	ASP
1	B	872	THR
1	C	110	ARG
1	C	129	PHE
1	C	140	LYS
1	C	143	LEU
1	C	255	LYS
1	C	276	LYS
1	C	468	LYS
1	C	515	SER
1	C	556	ASP
1	C	559	LEU
1	C	608	SER
1	C	752	GLU
1	C	861	LYS
1	C	865	ASP
1	C	886	LEU
1	D	18	ASP
1	D	45	ARG
1	D	61	ARG
1	D	81	HIS
1	D	129	PHE
1	D	143	LEU
1	D	165	MET
1	D	532	SER
1	D	585	GLN
1	D	758	GLU

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Mol	Chain	Res	Type
1	D	890	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	149	GLN
1	A	516	GLN
1	A	585	GLN
1	A	775	GLN
1	A	892	ASN
1	B	149	GLN
1	B	425	ASN
1	B	626	GLN
1	B	677	ASN
1	B	720	ASN
1	B	775	GLN
1	B	819	GLN
1	B	858	GLN
1	C	605	ASN
1	C	610	GLN
1	C	723	ASN
1	D	119	GLN
1	D	266	GLN
1	D	308	GLN
1	D	494	GLN
1	D	605	ASN
1	D	626	GLN
1	D	669	ASN
1	D	827	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 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	904/979 (92%)	-0.14	19 (2%)	63	66	13, 22, 36, 51	0
1	B	901/979 (92%)	-0.31	11 (1%)	79	81	10, 18, 33, 56	0
1	C	900/979 (91%)	-0.17	19 (2%)	63	66	10, 20, 37, 57	0
1	D	900/979 (91%)	-0.17	21 (2%)	60	63	11, 20, 36, 60	0
All	All	3605/3916 (92%)	-0.20	70 (1%)	66	69	10, 20, 36, 60	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	78	GLY	10.6
1	D	81	HIS	9.7
1	C	80	PHE	8.5
1	D	80	PHE	7.5
1	B	81	HIS	7.1
1	D	554	ALA	7.0
1	C	81	HIS	6.3
1	C	554	ALA	5.6
1	C	79	GLY	5.4
1	C	508	GLN	5.2
1	B	82	PRO	4.8
1	B	80	PHE	4.4
1	D	82	PRO	4.3
1	C	509	SER	4.2
1	A	555	ASN	4.2
1	C	553	THR	4.0
1	C	82	PRO	4.0
1	A	510	VAL	4.0
1	A	508	GLN	3.9
1	A	509	SER	3.9
1	A	79	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	451	LEU	3.9
1	D	555	ASN	3.8
1	C	555	ASN	3.7
1	B	681	HIS	3.7
1	D	508	GLN	3.7
1	B	555	ASN	3.6
1	B	79	GLY	3.6
1	D	510	VAL	3.6
1	C	494	GLN	3.5
1	A	32	ASN	3.5
1	C	610	GLN	3.4
1	C	510	VAL	3.3
1	A	553	THR	3.2
1	A	554	ALA	3.1
1	D	507	PRO	3.1
1	D	723	ASN	3.0
1	C	683	GLN	3.0
1	A	78	GLY	3.0
1	A	454	TRP	2.9
1	A	507	PRO	2.9
1	C	507	PRO	2.8
1	A	198	PRO	2.8
1	A	307	ARG	2.7
1	B	554	ALA	2.7
1	C	427	LEU	2.7
1	D	514	PRO	2.7
1	A	67	HIS	2.7
1	D	553	THR	2.6
1	D	509	SER	2.5
1	D	79	GLY	2.5
1	A	68	GLN	2.4
1	C	492	ASP	2.4
1	D	104	GLU	2.4
1	D	586	THR	2.4
1	C	195	GLY	2.4
1	D	159	CYS	2.3
1	B	509	SER	2.3
1	C	495	THR	2.3
1	B	463	LYS	2.3
1	A	195	GLY	2.2
1	D	78	GLY	2.2
1	D	287	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	396	SER	2.1
1	D	427	LEU	2.1
1	B	451	LEU	2.0
1	A	137	ASN	2.0
1	B	78	GLY	2.0
1	D	103	GLN	2.0
1	D	451	LEU	2.0

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.