



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:13 PM UTC

PDB ID : 1FNU / pdb_00001fnu
Title : STRUCTURE OF STREPTOCOCCAL PYROGENIC EXOTOXIN A
Authors : Earhart, C.A.; Vath, G.M.; Roggiani, M.; Schlievert, P.M.; Ohlendorf, D.H.
Deposited on : 2000-08-23
Resolution : 1.94 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

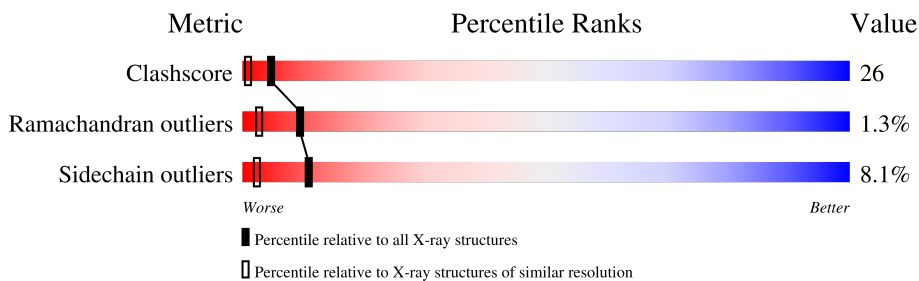
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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))
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	221	
1	B	221	
1	C	221	
1	D	221	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7934 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 EXOTOXIN TYPE A PRECURSOR (ALLELE 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	5	0	0
			1823	1166	293	358	6			
1	B	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			
1	C	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			
1	D	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	THR	LEU	conflict	UNP P62560
A	154	ILE	THR	conflict	UNP P62560
A	209	ASN	SER	conflict	UNP P62560
A	210	LYS	ASN	conflict	UNP P62560
B	453	THR	LEU	conflict	UNP P62560
B	454	ILE	THR	conflict	UNP P62560
B	509	ASN	SER	conflict	UNP P62560
B	510	LYS	ASN	conflict	UNP P62560
C	753	THR	LEU	conflict	UNP P62560
C	754	ILE	THR	conflict	UNP P62560
C	809	ASN	SER	conflict	UNP P62560
C	810	LYS	ASN	conflict	UNP P62560
D	1053	THR	LEU	conflict	UNP P62560
D	1054	ILE	THR	conflict	UNP P62560
D	1109	ASN	SER	conflict	UNP P62560
D	1110	LYS	ASN	conflict	UNP P62560

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	Cd 4	0	0
2	B	4	Total 4	Cd 4	0	0
2	C	4	Total 4	Cd 4	0	0
2	D	3	Total 3	Cd 3	0	0

- Molecule 3 is water.

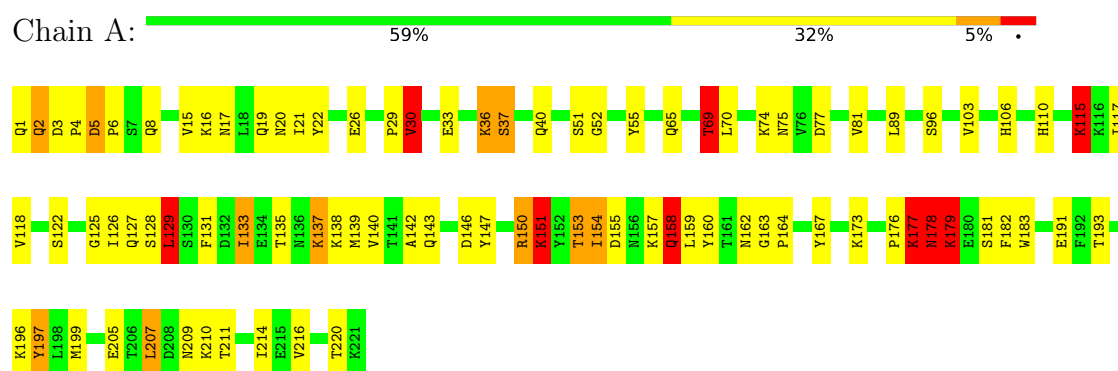
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	156	Total 156	O 156	0	0
3	B	169	Total 169	O 169	0	0
3	C	176	Total 176	O 176	0	0
3	D	126	Total 126	O 126	0	0

3 Residue-property plots

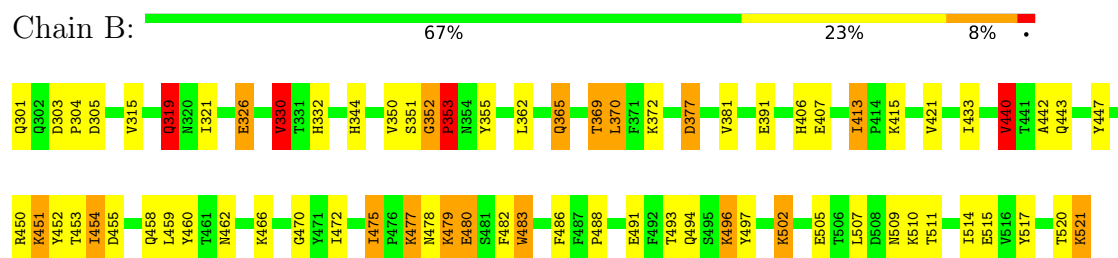
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

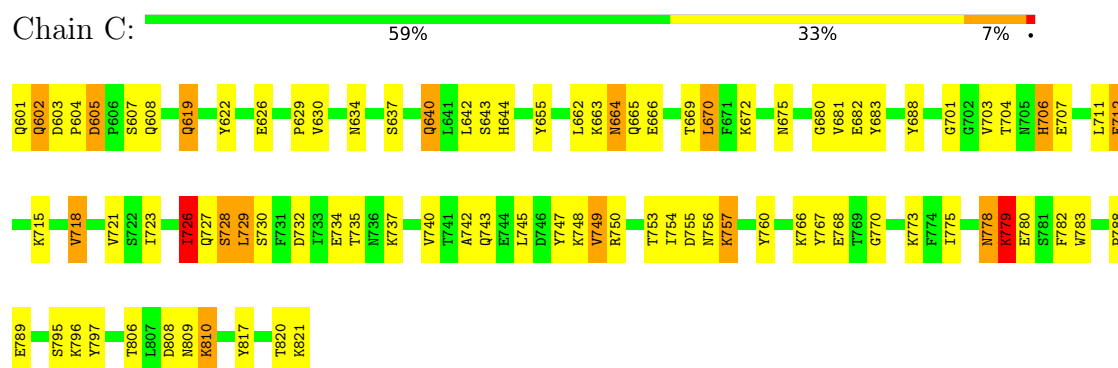
• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)



• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

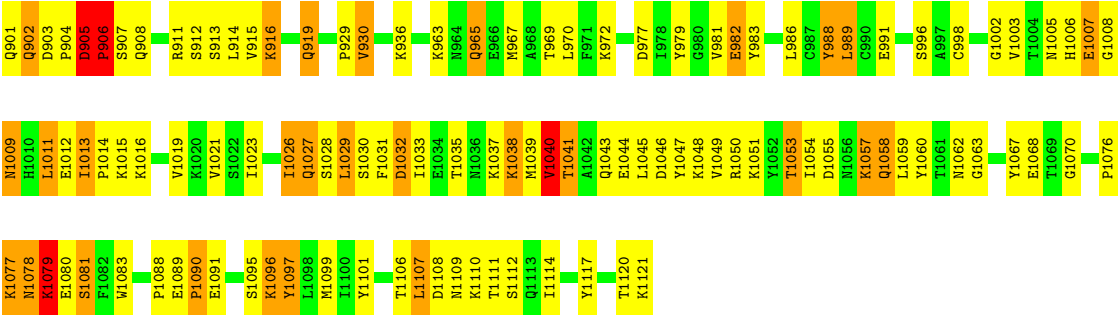


• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)



• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

Chain D: 49% 37% 13% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.30Å 126.80Å 148.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.94	Depositor
% Data completeness (in resolution range)	79.7 (20.00-1.94)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7934	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.40	4/1865 (0.2%)	1.54	32/2522 (1.3%)
1	B	1.43	9/1865 (0.5%)	1.53	29/2522 (1.1%)
1	C	1.40	6/1865 (0.3%)	1.49	22/2522 (0.9%)
1	D	1.29	6/1865 (0.3%)	1.49	23/2522 (0.9%)
All	All	1.38	25/7460 (0.3%)	1.51	106/10088 (1.1%)

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	2
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	THR	CA-CB	8.77	1.68	1.53
1	D	1039	MET	SD-CE	8.75	2.01	1.79
1	A	69	THR	CA-CB	8.36	1.67	1.53
1	A	30	VAL	CA-CB	6.68	1.61	1.54
1	B	421	VAL	CA-CB	6.64	1.62	1.54
1	D	1011	LEU	CA-C	6.49	1.60	1.52
1	B	319	GLN	CB-CG	6.49	1.72	1.52
1	C	704	THR	CA-C	6.34	1.60	1.52
1	C	721	VAL	CA-CB	6.26	1.63	1.54
1	B	491	GLU	CA-C	6.25	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	353	PRO	C-O	5.98	1.31	1.24
1	C	664	ASN	CA-C	5.91	1.60	1.52
1	C	703	VAL	CA-CB	5.77	1.61	1.54
1	D	965	GLN	CA-C	5.57	1.60	1.52
1	A	199	MET	SD-CE	-5.44	1.66	1.79
1	B	319	GLN	CA-C	5.43	1.60	1.52
1	B	319	GLN	CG-CD	-5.41	1.38	1.52
1	D	930	VAL	CA-CB	5.28	1.60	1.54
1	B	502	LYS	CD-CE	5.21	1.68	1.52
1	B	462	ASN	C-O	-5.20	1.18	1.23
1	C	605	ASP	CA-C	5.09	1.59	1.53
1	C	749	VAL	CA-CB	5.08	1.59	1.54
1	D	1041	THR	CA-CB	5.08	1.61	1.53
1	D	1048	LYS	CA-C	5.05	1.59	1.52
1	B	365	GLN	CA-C	5.02	1.59	1.52

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	779	LYS	N-CA-C	14.71	126.98	108.45
1	D	1079	LYS	N-CA-C	11.12	126.19	109.63
1	B	440	VAL	CB-CA-C	-10.68	95.19	111.31
1	B	479	LYS	N-CA-C	9.48	124.94	109.96
1	A	21	ILE	N-CA-C	-9.07	101.97	111.58
1	B	315	VAL	N-CA-C	8.91	120.44	109.30
1	C	605	ASP	N-CA-C	-8.74	98.01	110.08
1	B	303	ASP	CA-C-N	8.49	128.50	119.76
1	B	303	ASP	C-N-CA	8.49	128.50	119.76
1	A	52	GLY	CA-C-N	-8.25	111.51	119.76
1	A	52	GLY	C-N-CA	-8.25	111.51	119.76
1	B	319	GLN	CB-CG-CD	-7.82	99.30	112.60
1	A	133	ILE	N-CA-C	-7.76	97.94	108.96
1	D	905	ASP	N-CA-C	-7.74	100.33	110.39
1	C	808	ASP	N-CA-C	-7.62	97.60	109.25
1	D	1081	SER	N-CA-C	-7.38	101.04	110.19
1	D	903	ASP	N-CA-C	7.33	126.01	109.81
1	A	2	GLN	N-CA-C	-7.27	99.68	110.23
1	B	514	ILE	N-CA-C	7.13	118.09	108.11
1	B	466	LYS	N-CA-C	-7.04	104.16	112.89
1	D	1063	GLY	CA-C-N	7.01	127.00	119.78
1	D	1063	GLY	C-N-CA	7.01	127.00	119.78
1	C	706	HIS	N-CA-C	6.95	118.74	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	963	LYS	N-CA-C	6.95	118.93	111.36
1	B	477	LYS	CA-C-N	6.91	129.77	120.65
1	B	477	LYS	C-N-CA	6.91	129.77	120.65
1	D	1040	VAL	CB-CA-C	-6.82	99.97	110.95
1	A	51	SER	N-CA-C	6.72	120.09	109.81
1	B	377	ASP	N-CA-C	-6.71	99.29	109.95
1	A	30	VAL	CB-CA-C	6.66	120.11	110.98
1	C	728	SER	N-CA-C	6.64	121.39	113.28
1	A	5	ASP	N-CA-C	-6.61	101.74	109.93
1	D	1062	ASN	N-CA-C	-6.55	97.12	108.52
1	D	982	GLU	N-CA-C	6.50	120.14	110.52
1	C	742	ALA	N-CA-C	-6.50	103.47	111.33
1	A	211	THR	N-CA-C	6.50	121.03	111.87
1	C	766	LYS	CB-CA-C	-6.48	98.64	110.63
1	A	220	THR	N-CA-C	-6.28	100.91	110.14
1	C	726	ILE	N-CA-C	6.27	116.94	108.17
1	D	988	TYR	CB-CA-C	-6.21	100.20	110.14
1	B	442	ALA	N-CA-C	-6.15	104.58	111.28
1	A	30	VAL	N-CA-CB	-6.06	104.12	111.21
1	B	483	TRP	N-CA-C	6.06	118.39	109.24
1	A	150	ARG	N-CA-C	6.00	117.90	111.36
1	B	352	GLY	CA-C-N	6.00	127.33	119.84
1	B	352	GLY	C-N-CA	6.00	127.33	119.84
1	A	151	LYS	CB-CG-CD	5.96	125.00	111.30
1	C	607	SER	N-CA-C	-5.92	106.04	113.20
1	C	682	GLU	N-CA-C	5.88	119.54	110.42
1	B	451	LYS	CD-CE-NZ	-5.83	93.26	111.90
1	A	15	VAL	N-CA-C	5.82	117.23	109.37
1	B	447	TYR	N-CA-C	-5.82	104.84	111.07
1	D	1009	ASN	N-CA-C	5.80	119.97	113.01
1	B	494	GLN	N-CA-C	-5.78	104.89	111.07
1	B	433	ILE	N-CA-C	-5.78	99.41	108.95
1	A	142	ALA	N-CA-C	-5.77	104.99	111.28
1	B	452	TYR	CA-C-N	-5.77	111.04	121.14
1	B	452	TYR	C-N-CA	-5.77	111.04	121.14
1	C	663	LYS	N-CA-C	5.76	118.02	111.11
1	B	511	THR	N-CA-C	5.75	121.19	113.72
1	B	305	ASP	N-CA-C	-5.71	102.42	110.29
1	D	1114	ILE	N-CA-C	5.61	116.08	107.77
1	A	179	LYS	N-CA-C	5.61	122.74	110.80
1	C	775	ILE	CA-C-N	-5.60	114.82	120.31
1	C	775	ILE	C-N-CA	-5.60	114.82	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	GLY	CA-C-N	-5.59	112.85	119.84
1	A	163	GLY	C-N-CA	-5.59	112.85	119.84
1	A	75	ASN	N-CA-C	-5.58	100.88	109.76
1	C	766	LYS	N-CA-C	-5.57	105.30	111.71
1	B	321	ILE	N-CA-C	-5.56	104.94	111.00
1	B	330	VAL	N-CA-CB	-5.53	103.73	111.25
1	D	1003	VAL	N-CA-C	5.53	115.91	108.17
1	A	129	LEU	N-CA-C	5.52	117.49	108.76
1	D	1038	LYS	N-CA-C	-5.52	105.18	111.14
1	A	151	LYS	N-CA-C	-5.49	105.39	111.71
1	B	351	SER	N-CA-C	5.49	118.51	109.72
1	A	115	LYS	N-CA-C	-5.49	101.03	109.76
1	D	1078	ASN	CA-C-N	-5.48	111.21	122.82
1	D	1078	ASN	C-N-CA	-5.48	111.21	122.82
1	C	789	GLU	N-CA-C	-5.47	102.32	110.20
1	C	718	VAL	CA-C-N	-5.42	115.89	123.10
1	C	718	VAL	C-N-CA	-5.42	115.89	123.10
1	D	1033	ILE	N-CA-C	-5.38	99.96	108.90
1	A	181	SER	N-CA-C	-5.37	103.44	110.53
1	D	1077	LYS	N-CA-C	-5.31	105.40	111.14
1	C	680	GLY	N-CA-C	5.29	118.84	110.96
1	A	74	LYS	N-CA-C	5.28	118.71	110.32
1	B	372	LYS	N-CA-C	5.18	117.33	111.11
1	C	640	GLN	CA-CB-CG	5.18	124.45	114.10
1	A	26	GLU	N-CA-C	-5.17	105.71	112.23
1	A	158	GLN	N-CA-C	5.16	118.85	112.24
1	C	712	GLU	CB-CG-CD	5.15	121.36	112.60
1	C	675	ASN	N-CA-C	-5.15	100.78	108.96
1	A	162	ASN	N-CA-C	-5.13	99.60	108.52
1	B	480	GLU	N-CA-C	5.12	121.72	110.80
1	B	326	GLU	N-CA-C	-5.12	106.20	112.90
1	A	125	GLY	CA-C-N	-5.09	116.88	123.19
1	A	125	GLY	C-N-CA	-5.09	116.88	123.19
1	A	137	LYS	N-CA-C	5.08	118.09	109.76
1	C	767	TYR	N-CA-C	5.08	118.09	109.76
1	D	1096	LYS	CG-CD-CE	-5.08	99.62	111.30
1	D	1008	GLY	N-CA-C	5.03	121.07	115.08
1	D	1107	LEU	N-CA-C	5.03	117.35	108.75
1	A	103	VAL	N-CA-C	5.03	115.21	108.17
1	A	216	VAL	N-CA-C	5.03	115.21	108.17
1	D	1058	GLN	N-CA-C	5.01	118.31	111.39

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	TYR	Sidechain
1	A	197	TYR	Sidechain
1	B	497	TYR	Sidechain
1	C	688	TYR	Sidechain
1	C	797	TYR	Sidechain
1	D	1097	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1823	0	1778	94	0
1	B	1823	0	1775	58	1
1	C	1823	0	1775	93	0
1	D	1823	0	1775	127	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
3	A	156	0	0	5	1
3	B	169	0	0	10	0
3	C	176	0	0	7	1
3	D	126	0	0	6	0
All	All	7934	0	7103	371	2

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 (371) 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:C:605:ASP:H	1:C:608:GLN:NE2	1.35	1.22
1:B:450:ARG:O	1:B:454:ILE:HD13	1.40	1.21
1:A:1:GLN:HB2	1:A:182:PHE:HA	1.25	1.10
1:A:150:ARG:O	1:A:154:ILE:HD13	1.48	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:723:ILE:O	1:C:726:ILE:HD13	1.56	1.05
1:D:1120:THR:HG22	1:D:1121:LYS:H	1.22	1.05
1:D:916:LYS:HE2	3:D:1151:HOH:O	1.57	1.04
1:A:177:LYS:HB2	1:A:177:LYS:HZ2	1.21	1.02
1:C:750:ARG:O	1:C:754:ILE:HD13	1.57	1.01
1:A:137:LYS:HB2	1:A:140:VAL:HG12	1.42	1.00
1:A:178:ASN:H	1:A:178:ASN:ND2	1.46	0.96
1:A:115:LYS:HZ2	1:A:210:LYS:HD3	1.27	0.96
1:A:154:ILE:HD12	1:A:159:LEU:HB3	1.49	0.94
1:A:177:LYS:HG2	1:A:178:ASN:N	1.82	0.93
1:C:750:ARG:O	1:C:754:ILE:CD1	2.16	0.93
1:C:670:LEU:HD23	1:C:670:LEU:O	1.68	0.92
1:D:1015:LYS:HD3	1:D:1110:LYS:HE2	1.52	0.91
1:B:369:THR:HB	3:B:4051:HOH:O	1.69	0.91
1:A:178:ASN:N	1:A:178:ASN:HD22	1.68	0.91
1:D:1012:GLU:HB2	1:D:1013:ILE:HD12	1.51	0.90
1:C:605:ASP:N	1:C:608:GLN:NE2	2.20	0.90
1:B:377:ASP:OD1	1:B:406:HIS:HD2	1.55	0.89
1:C:712:GLU:HG3	3:C:7000:HOH:O	1.70	0.89
1:A:115:LYS:NZ	1:A:210:LYS:HD3	1.87	0.89
1:A:177:LYS:HB2	1:A:177:LYS:NZ	1.85	0.88
1:C:820:THR:O	1:C:821:LYS:OXT	1.90	0.88
1:C:728:SER:O	1:C:729:LEU:HB2	1.74	0.85
1:D:1028:SER:O	1:D:1029:LEU:HB3	1.74	0.84
1:D:977:ASP:OD1	1:D:1006:HIS:HD2	1.62	0.83
1:C:757:LYS:HE3	1:C:757:LYS:HA	1.62	0.82
1:D:1049:VAL:O	1:D:1053:THR:OG1	1.98	0.82
1:D:1120:THR:HG22	1:D:1121:LYS:N	1.93	0.82
1:A:178:ASN:H	1:A:178:ASN:HD22	0.85	0.82
1:C:605:ASP:HB3	1:C:608:GLN:CD	2.04	0.82
1:C:604:PRO:HD3	1:C:783:TRP:CE2	2.16	0.81
1:D:1054:ILE:HD11	1:D:1060:TYR:HD2	1.45	0.81
1:A:5:ASP:HB3	1:A:8:GLN:HG3	1.62	0.81
1:B:493:THR:OG1	1:B:496:LYS:HB2	1.80	0.81
1:C:669:THR:HG21	3:C:4227:HOH:O	1.78	0.80
1:D:1013:ILE:HD12	1:D:1013:ILE:N	1.96	0.80
1:C:737:LYS:HB2	1:C:740:VAL:HG12	1.61	0.80
1:D:1037:LYS:O	1:D:1109:ASN:ND2	2.15	0.80
1:D:1120:THR:CG2	1:D:1121:LYS:H	1.95	0.79
1:C:670:LEU:HD23	1:C:670:LEU:C	2.08	0.79
1:A:177:LYS:NZ	1:A:177:LYS:CB	2.44	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:729:LEU:HD12	1:C:730:SER:H	1.47	0.78
1:D:970:LEU:C	1:D:970:LEU:HD23	2.09	0.78
1:B:451:LYS:HE2	1:B:455:ASP:OD2	1.83	0.77
1:A:151:LYS:HE2	1:A:155:ASP:OD2	1.83	0.77
1:B:454:ILE:HD12	1:B:459:LEU:HB3	1.68	0.76
1:D:1068:GLU:OE1	1:D:1068:GLU:HA	1.84	0.76
1:A:177:LYS:CG	1:A:178:ASN:N	2.49	0.76
1:D:1096:LYS:HE2	3:D:2104:HOH:O	1.85	0.76
1:B:377:ASP:OD1	1:B:406:HIS:CD2	2.38	0.76
1:C:605:ASP:H	1:C:608:GLN:HE21	1.33	0.75
1:B:301:GLN:HE21	1:B:482:PHE:HA	1.50	0.74
1:C:820:THR:O	1:C:821:LYS:C	2.30	0.74
1:D:1096:LYS:HG2	1:D:1097:TYR:N	1.97	0.74
1:B:477:LYS:NZ	3:B:5103:HOH:O	2.19	0.74
1:B:520:THR:O	1:B:521:LYS:HB2	1.86	0.73
1:B:369:THR:HG22	3:B:4178:HOH:O	1.88	0.73
1:C:601:GLN:NE2	1:C:782:PHE:HB2	2.04	0.72
1:D:911:ARG:NH1	1:D:914:LEU:HD11	2.04	0.72
1:D:1023:ILE:O	1:D:1026:ILE:HD13	1.89	0.72
1:D:1050:ARG:O	1:D:1054:ILE:HG13	1.90	0.72
1:B:301:GLN:NE2	1:B:483:TRP:H	1.88	0.71
1:A:77:ASP:OD1	1:A:106:HIS:HD2	1.73	0.71
1:D:1015:LYS:CD	1:D:1110:LYS:HE2	2.20	0.71
1:A:4:PRO:HD3	1:A:183:TRP:CE2	2.26	0.71
1:A:177:LYS:HG2	1:A:178:ASN:HD22	1.55	0.70
1:A:178:ASN:ND2	1:A:178:ASN:N	2.30	0.70
1:A:1:GLN:HB2	1:A:182:PHE:CA	2.13	0.70
1:A:110:HIS:O	1:A:138:LYS:HE3	1.92	0.70
1:A:129:LEU:C	1:A:129:LEU:HD12	2.17	0.70
1:D:901:GLN:N	1:D:1080:GLU:HG2	2.07	0.69
1:C:630:VAL:HG13	1:C:655:TYR:OH	1.92	0.69
1:D:977:ASP:OD1	1:D:1006:HIS:CD2	2.44	0.69
1:B:344:HIS:CD2	1:B:502:LYS:HZ1	2.11	0.68
1:B:415:LYS:HG2	1:B:509:ASN:ND2	2.08	0.68
1:D:1013:ILE:HD12	1:D:1013:ILE:H	1.57	0.68
1:C:715:LYS:HE3	1:C:810:LYS:CE	2.23	0.68
1:B:391:GLU:OE1	1:D:991:GLU:HG2	1.94	0.67
1:A:154:ILE:HD11	1:A:160:TYR:CD2	2.30	0.67
1:A:129:LEU:C	1:A:129:LEU:CD1	2.68	0.67
1:A:1:GLN:HB3	1:A:183:TRP:CD1	2.30	0.67
1:B:344:HIS:CD2	1:B:502:LYS:NZ	2.63	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:GLN:O	1:B:369:THR:HG23	1.96	0.66
1:A:4:PRO:HD3	1:A:183:TRP:NE1	2.11	0.66
1:B:344:HIS:HD2	1:B:502:LYS:HZ1	1.41	0.66
1:A:89:LEU:HD13	1:A:96:SER:CB	2.26	0.65
1:A:69:THR:HB	3:A:5040:HOH:O	1.97	0.65
3:B:7070:HOH:O	1:C:796:LYS:HE2	1.97	0.65
1:A:1:GLN:HG3	1:A:183:TRP:H	1.63	0.64
1:C:622:TYR:CZ	1:C:626:GLU:HG2	2.31	0.64
1:C:670:LEU:C	1:C:670:LEU:CD2	2.70	0.64
1:A:89:LEU:HD13	1:A:96:SER:HB2	1.78	0.64
1:D:981:VAL:H	1:D:1043:GLN:NE2	1.94	0.64
1:C:605:ASP:CB	1:C:608:GLN:CD	2.71	0.64
1:B:381:VAL:H	1:B:443:GLN:NE2	1.94	0.64
1:C:707:GLU:O	1:C:707:GLU:HG2	1.96	0.64
1:B:453:THR:CG2	3:B:7001:HOH:O	2.46	0.64
1:D:904:PRO:HB3	1:D:1083:TRP:CZ2	2.33	0.63
1:D:906:PRO:O	1:D:908:GLN:N	2.31	0.63
1:B:301:GLN:NE2	1:B:482:PHE:HA	2.13	0.63
1:C:683:TYR:CE2	1:C:795:SER:HB3	2.33	0.63
1:C:754:ILE:HD11	1:C:760:TYR:CD2	2.34	0.63
1:D:1016:LYS:HB3	1:D:1032:ASP:OD2	1.98	0.63
1:A:129:LEU:HD12	1:A:129:LEU:O	1.98	0.63
1:B:370:LEU:HD13	1:B:370:LEU:C	2.23	0.63
1:B:301:GLN:HE22	1:B:483:TRP:H	1.43	0.63
1:C:605:ASP:H	1:C:608:GLN:HE22	1.40	0.63
1:A:177:LYS:HG2	1:A:178:ASN:H	1.61	0.62
1:D:1035:THR:HG23	1:D:1109:ASN:HD22	1.64	0.62
1:D:1045:LEU:O	1:D:1049:VAL:HG23	2.00	0.62
1:D:1051:LYS:HE2	1:D:1055:ASP:OD2	1.99	0.62
1:C:753:THR:CG2	3:C:5010:HOH:O	2.47	0.62
1:D:911:ARG:NH1	1:D:914:LEU:CD1	2.62	0.61
1:A:33:GLU:OE1	1:A:77:ASP:CG	2.43	0.61
1:C:669:THR:HG22	3:C:831:HOH:O	2.01	0.61
1:D:1015:LYS:HE3	1:D:1110:LYS:HD3	1.81	0.60
1:A:5:ASP:HB3	1:A:8:GLN:CG	2.31	0.60
1:D:1012:GLU:HB2	1:D:1013:ILE:CD1	2.30	0.60
1:B:453:THR:HG21	3:B:7001:HOH:O	2.01	0.60
1:C:729:LEU:HD12	1:C:730:SER:N	2.17	0.60
1:D:919:GLN:H	1:D:919:GLN:HE21	1.48	0.59
1:A:164:PRO:HB2	3:A:255:HOH:O	2.01	0.59
1:B:362:LEU:O	1:B:502:LYS:HE3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:740:VAL:C	1:C:806:THR:HG23	2.27	0.59
1:C:622:TYR:OH	1:C:626:GLU:HG2	2.02	0.59
1:C:726:ILE:HG12	1:C:726:ILE:O	2.01	0.59
1:A:126:ILE:HG13	1:A:126:ILE:O	2.03	0.59
1:B:454:ILE:HD11	1:B:460:TYR:CD2	2.37	0.59
1:C:681:VAL:H	1:C:743:GLN:NE2	2.01	0.59
1:B:353:PRO:HD2	3:B:5089:HOH:O	2.02	0.59
1:B:370:LEU:HD22	1:B:370:LEU:O	2.01	0.59
1:D:911:ARG:NH1	1:D:914:LEU:HG	2.18	0.59
1:A:157:LYS:O	1:A:158:GLN:HB2	2.03	0.58
1:C:601:GLN:NE2	1:C:782:PHE:CB	2.66	0.58
1:B:301:GLN:HE21	1:B:482:PHE:CA	2.16	0.58
1:C:750:ARG:O	1:C:754:ILE:HD12	2.00	0.58
1:C:753:THR:HG21	3:C:5010:HOH:O	2.02	0.58
1:A:65:GLN:O	1:A:69:THR:HG22	2.03	0.58
1:C:756:ASN:O	1:C:757:LYS:NZ	2.36	0.58
1:A:81:VAL:H	1:A:143:GLN:NE2	2.02	0.58
1:C:619:GLN:H	1:C:619:GLN:NE2	2.02	0.58
1:A:207:LEU:HD12	1:A:207:LEU:C	2.28	0.57
1:A:137:LYS:HB2	1:A:140:VAL:CG1	2.27	0.57
1:D:916:LYS:C	1:D:916:LYS:HD2	2.29	0.57
1:D:913:SER:OG	1:D:1068:GLU:OE2	2.21	0.57
1:C:712:GLU:CG	3:C:7000:HOH:O	2.42	0.57
1:C:601:GLN:HE22	1:C:782:PHE:HB2	1.69	0.57
1:D:981:VAL:H	1:D:1043:GLN:HE21	1.52	0.57
1:C:605:ASP:O	1:C:608:GLN:HB2	2.05	0.56
1:C:728:SER:O	1:C:729:LEU:CB	2.46	0.56
1:D:970:LEU:C	1:D:970:LEU:CD2	2.77	0.56
1:D:1009:ASN:HD21	1:D:1037:LYS:HB3	1.70	0.56
1:C:665:GLN:O	1:C:669:THR:HG23	2.05	0.56
1:D:919:GLN:H	1:D:919:GLN:NE2	2.03	0.56
1:D:916:LYS:HZ2	1:D:1091:GLU:HG2	1.70	0.56
1:D:983:TYR:CE2	1:D:1095:SER:HB3	2.41	0.56
1:D:989:LEU:HD13	1:D:996:SER:HB2	1.88	0.56
1:D:916:LYS:NZ	1:D:1091:GLU:HG2	2.21	0.56
1:C:715:LYS:HE3	1:C:810:LYS:NZ	2.20	0.56
1:D:1054:ILE:CD1	1:D:1060:TYR:HD2	2.17	0.56
1:C:768:GLU:CB	1:C:821:LYS:HB3	2.35	0.55
1:D:911:ARG:HH12	1:D:914:LEU:CG	2.19	0.55
1:D:911:ARG:HH11	1:D:914:LEU:HD11	1.70	0.55
1:D:1035:THR:CG2	1:D:1109:ASN:HD22	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:SER:HA	1:A:127:GLN:HA	1.88	0.55
1:D:1096:LYS:CE	3:D:2104:HOH:O	2.51	0.55
1:D:911:ARG:NH1	1:D:914:LEU:CG	2.70	0.55
1:A:1:GLN:NE2	1:A:183:TRP:O	2.32	0.54
1:A:4:PRO:HD3	1:A:183:TRP:CD1	2.41	0.54
1:C:810:LYS:HZ3	1:C:810:LYS:HB2	1.72	0.54
1:C:756:ASN:O	1:C:757:LYS:HE3	2.07	0.54
1:D:1013:ILE:N	1:D:1013:ILE:CD1	2.65	0.54
1:C:810:LYS:HZ2	1:C:810:LYS:HA	1.73	0.54
1:A:5:ASP:H	1:A:8:GLN:NE2	2.06	0.54
1:D:967:MET:O	1:D:970:LEU:HB3	2.09	0.53
1:C:735:THR:HG23	1:C:809:ASN:HD22	1.72	0.53
1:A:33:GLU:OE1	1:A:77:ASP:OD1	2.25	0.53
1:D:904:PRO:HD3	1:D:1083:TRP:CE2	2.44	0.53
1:C:715:LYS:HG2	1:C:810:LYS:NZ	2.23	0.53
1:D:1015:LYS:HD2	1:D:1016:LYS:O	2.09	0.53
1:C:603:ASP:OD2	1:C:773:LYS:NZ	2.41	0.53
1:C:734:GLU:O	1:C:748:LYS:HE3	2.08	0.52
1:C:735:THR:CG2	1:C:809:ASN:HD22	2.21	0.52
1:C:810:LYS:NZ	1:C:810:LYS:HB2	2.25	0.52
1:A:36:LYS:O	1:A:37:SER:O	2.28	0.52
1:B:482:PHE:CZ	1:B:505:GLU:HG2	2.44	0.52
1:D:905:ASP:OD1	1:D:906:PRO:N	2.43	0.52
1:D:1002:GLY:HA2	1:D:1041:THR:HG21	1.91	0.52
1:D:1079:LYS:HG2	1:D:1080:GLU:H	1.75	0.52
1:A:137:LYS:HG2	3:A:2147:HOH:O	2.09	0.52
1:C:604:PRO:HD3	1:C:783:TRP:CD2	2.43	0.52
1:D:905:ASP:O	1:D:906:PRO:C	2.51	0.52
1:D:1054:ILE:HD11	1:D:1060:TYR:CD2	2.35	0.52
1:B:301:GLN:NE2	1:B:482:PHE:CA	2.73	0.52
1:C:756:ASN:C	1:C:757:LYS:HZ1	2.18	0.52
1:D:1089:GLU:O	1:D:1090:PRO:C	2.52	0.52
1:D:905:ASP:OD1	1:D:905:ASP:C	2.53	0.51
1:A:115:LYS:HZ2	1:A:210:LYS:HA	1.74	0.51
1:C:601:GLN:N	1:C:780:GLU:CG	2.73	0.51
1:D:1070:GLY:HA2	1:D:1117:TYR:O	2.11	0.51
1:D:1076:PRO:HD3	1:D:1081:SER:HA	1.92	0.51
1:A:196:LYS:HG3	1:A:197:TYR:N	2.26	0.51
1:C:637:SER:OG	1:C:672:LYS:O	2.28	0.51
1:D:1120:THR:O	1:D:1121:LYS:CB	2.59	0.51
1:A:182:PHE:CZ	1:A:205:GLU:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LYS:C	1:A:37:SER:O	2.54	0.50
1:D:929:PRO:HD3	1:D:1047:TYR:CZ	2.46	0.50
1:C:768:GLU:HB3	1:C:821:LYS:HB3	1.93	0.50
1:A:36:LYS:O	1:A:37:SER:C	2.53	0.50
1:C:756:ASN:O	1:C:757:LYS:CE	2.60	0.50
1:C:601:GLN:HE21	1:C:782:PHE:CB	2.25	0.50
1:D:905:ASP:HB3	3:D:4167:HOH:O	2.12	0.50
1:D:1041:THR:HA	1:D:1106:THR:HA	1.92	0.50
1:A:65:GLN:O	1:A:69:THR:CG2	2.60	0.50
1:D:1043:GLN:HG3	1:D:1101:TYR:CD2	2.47	0.50
1:B:470:GLY:HA2	1:B:517:TYR:O	2.12	0.49
1:C:745:LEU:O	1:C:749:VAL:HG23	2.12	0.49
1:A:4:PRO:HB3	1:A:183:TRP:CZ2	2.47	0.49
1:A:129:LEU:HD23	1:A:157:LYS:HE2	1.94	0.49
1:B:301:GLN:NE2	1:B:482:PHE:HB2	2.28	0.49
1:D:979:TYR:CD1	1:D:1044:GLU:HA	2.47	0.49
1:B:415:LYS:HE2	1:B:510:LYS:HA	1.95	0.49
1:A:135:THR:HG23	1:A:209:ASN:HD22	1.77	0.49
1:A:135:THR:CG2	1:A:209:ASN:HD22	2.26	0.49
1:C:729:LEU:CD1	1:C:730:SER:H	2.21	0.49
1:C:662:LEU:HD23	1:C:701:GLY:HA2	1.95	0.48
1:D:979:TYR:CD1	1:D:1044:GLU:HG3	2.49	0.48
1:B:454:ILE:N	1:B:454:ILE:CD1	2.74	0.48
1:B:326:GLU:OE1	1:B:455:ASP:OD1	2.31	0.48
1:C:601:GLN:N	1:C:780:GLU:CD	2.71	0.48
1:C:619:GLN:H	1:C:619:GLN:HE21	1.61	0.48
1:A:135:THR:HG21	1:A:140:VAL:HG11	1.95	0.48
1:D:1097:TYR:C	1:D:1097:TYR:CD2	2.92	0.48
1:B:415:LYS:CG	1:B:509:ASN:ND2	2.77	0.48
1:D:1120:THR:CG2	1:D:1121:LYS:N	2.61	0.48
1:B:304:PRO:HD3	1:B:483:TRP:CE2	2.49	0.48
1:D:1058:GLN:N	1:D:1058:GLN:CD	2.72	0.48
1:A:137:LYS:O	1:A:209:ASN:ND2	2.47	0.48
1:A:117:ILE:HD11	1:A:209:ASN:HB2	1.96	0.47
1:B:330:VAL:HG22	1:B:355:TYR:OH	2.13	0.47
1:D:1029:LEU:HG	1:D:1030:SER:N	2.27	0.47
1:A:177:LYS:CB	1:A:177:LYS:HZ3	2.26	0.47
1:B:407:GLU:HB2	3:B:7057:HOH:O	2.14	0.47
1:B:332:HIS:CE1	1:B:350:VAL:HB	2.49	0.47
1:A:89:LEU:HD13	1:A:96:SER:HB3	1.96	0.47
1:A:177:LYS:HG2	1:A:178:ASN:ND2	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:715:LYS:HG2	1:C:810:LYS:HZ2	1.79	0.47
1:D:1037:LYS:HB2	1:D:1040:VAL:HG13	1.96	0.47
1:D:1046:ASP:O	1:D:1050:ARG:HG3	2.15	0.47
1:D:1079:LYS:CG	1:D:1080:GLU:H	2.22	0.47
1:D:1108:ASP:OD2	1:D:1111:THR:OG1	2.24	0.47
1:A:193:THR:O	1:A:196:LYS:HG2	2.15	0.47
1:D:1028:SER:O	1:D:1029:LEU:CB	2.48	0.47
1:D:1037:LYS:O	1:D:1109:ASN:CG	2.58	0.47
1:D:1040:VAL:HG22	1:D:1109:ASN:HB3	1.97	0.47
1:D:1079:LYS:NZ	1:D:1079:LYS:HB3	2.30	0.47
1:C:778:ASN:O	1:C:779:LYS:HG3	2.15	0.47
1:A:36:LYS:HD2	1:A:37:SER:O	2.14	0.46
1:D:1013:ILE:H	1:D:1013:ILE:CD1	2.24	0.46
1:D:1057:LYS:HD3	1:D:1057:LYS:HA	1.44	0.46
1:D:1077:LYS:O	3:D:7088:HOH:O	2.20	0.46
1:A:129:LEU:HD11	1:A:131:PHE:HD1	1.80	0.46
1:A:138:LYS:O	1:A:209:ASN:OD1	2.33	0.46
1:D:901:GLN:HE22	1:D:1083:TRP:H	1.63	0.46
1:D:1015:LYS:NZ	1:D:1016:LYS:O	2.48	0.46
1:B:454:ILE:HD12	1:B:454:ILE:N	2.28	0.46
1:C:737:LYS:O	1:C:809:ASN:ND2	2.49	0.46
1:D:1079:LYS:HG2	1:D:1080:GLU:N	2.30	0.46
1:A:176:PRO:O	1:A:177:LYS:C	2.58	0.46
1:C:770:GLY:HA2	1:C:817:TYR:O	2.15	0.46
1:D:1027:GLN:NE2	1:D:1030:SER:OG	2.47	0.46
1:A:129:LEU:CD1	1:A:131:PHE:HD1	2.29	0.46
1:C:706:HIS:ND1	1:C:706:HIS:C	2.74	0.46
1:A:209:ASN:OD1	1:A:209:ASN:N	2.47	0.45
1:B:301:GLN:NE2	1:B:483:TRP:N	2.62	0.45
1:C:711:LEU:HD11	1:C:809:ASN:HD21	1.81	0.45
1:D:901:GLN:NE2	1:D:1083:TRP:H	2.12	0.45
1:C:737:LYS:HB2	1:C:740:VAL:CG1	2.40	0.45
1:D:1051:LYS:CE	1:D:1055:ASP:OD2	2.64	0.45
1:A:207:LEU:HD12	1:A:207:LEU:O	2.17	0.45
1:B:352:GLY:HA3	1:B:355:TYR:CE1	2.52	0.45
1:D:1096:LYS:O	1:D:1099:MET:HG3	2.17	0.45
1:A:146:ASP:O	1:A:147:TYR:C	2.59	0.45
1:B:301:GLN:HE21	1:B:482:PHE:CB	2.29	0.44
1:C:601:GLN:HE22	1:C:783:TRP:H	1.65	0.44
1:D:901:GLN:O	1:D:902:GLN:C	2.59	0.44
1:A:81:VAL:H	1:A:143:GLN:HE21	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:979:TYR:CG	1:D:1044:GLU:HG3	2.51	0.44
1:A:16:LYS:O	1:A:17:ASN:HB2	2.16	0.44
1:B:472:ILE:HB	1:B:486:PHE:CE1	2.53	0.44
1:D:1013:ILE:HA	1:D:1014:PRO:HD3	1.80	0.44
1:D:1043:GLN:HG3	1:D:1101:TYR:CG	2.53	0.44
1:B:475:ILE:HD11	1:B:515:GLU:OE1	2.18	0.44
1:A:133:ILE:HD11	1:A:214:ILE:CD1	2.48	0.44
1:A:129:LEU:HD11	1:A:131:PHE:CD1	2.52	0.44
1:C:757:LYS:HA	1:C:757:LYS:CE	2.38	0.44
1:B:381:VAL:H	1:B:443:GLN:HE21	1.62	0.44
1:D:1077:LYS:HB2	1:D:1111:THR:HB	1.99	0.44
1:C:715:LYS:HE3	1:C:810:LYS:HE3	1.98	0.44
1:D:1021:VAL:HG21	1:D:1031:PHE:CE1	2.52	0.44
1:D:1079:LYS:HE2	1:D:1080:GLU:HB2	1.99	0.43
1:B:369:THR:HG21	3:B:5032:HOH:O	2.17	0.43
1:B:440:VAL:CG2	1:B:509:ASN:HB3	2.49	0.43
1:C:718:VAL:HA	1:C:732:ASP:OD1	2.19	0.43
1:D:1079:LYS:HB3	1:D:1079:LYS:HZ3	1.83	0.43
1:D:915:VAL:HA	1:D:1090:PRO:HA	2.01	0.43
1:D:911:ARG:HH11	1:D:914:LEU:CD1	2.29	0.43
1:B:475:ILE:HD11	1:B:515:GLU:CD	2.44	0.43
1:C:626:GLU:OE1	1:C:755:ASP:OD1	2.37	0.43
1:D:1021:VAL:HG21	1:D:1031:PHE:HE1	1.84	0.43
1:A:135:THR:HG23	1:A:209:ASN:ND2	2.34	0.43
1:B:319:GLN:HE21	1:B:319:GLN:HB2	0.96	0.43
1:C:634:ASN:HB2	1:C:706:HIS:CD2	2.54	0.43
1:D:1121:LYS:NZ	3:D:5167:HOH:O	2.52	0.43
1:C:602:GLN:HE21	1:C:602:GLN:HB3	1.61	0.43
1:D:936:LYS:HB3	1:D:936:LYS:HZ2	1.84	0.43
1:A:30:VAL:HG22	1:A:55:TYR:OH	2.18	0.43
1:A:127:GLN:O	1:A:127:GLN:HG2	2.17	0.43
1:A:210:LYS:HB2	1:A:210:LYS:HE2	1.81	0.43
1:C:642:LEU:HD12	1:C:644:HIS:HE1	1.83	0.43
1:D:1011:LEU:HD21	1:D:1038:LYS:HG2	2.01	0.43
1:D:1080:GLU:C	1:D:1081:SER:O	2.57	0.43
1:D:911:ARG:HH12	1:D:914:LEU:HG	1.84	0.42
1:A:40:GLN:NE2	3:A:7090:HOH:O	2.48	0.42
1:C:601:GLN:N	1:C:780:GLU:HG2	2.34	0.42
1:D:1059:LEU:O	1:D:1059:LEU:HD12	2.20	0.42
1:A:36:LYS:HB3	1:A:36:LYS:HE3	1.55	0.42
1:A:139:MET:CE	3:A:7036:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:665:GLN:NE2	3:C:6033:HOH:O	2.40	0.42
1:C:810:LYS:NZ	1:C:810:LYS:CB	2.83	0.42
1:A:19:GLN:O	1:A:22:TYR:HB3	2.19	0.42
1:D:1019:VAL:HG12	1:D:1021:VAL:HG23	2.01	0.42
1:A:177:LYS:CG	1:A:178:ASN:HD22	2.27	0.42
1:B:369:THR:CG2	3:B:4051:HOH:O	2.68	0.42
1:B:454:ILE:HG13	1:B:460:TYR:HB2	2.01	0.42
1:A:1:GLN:HG3	1:A:182:PHE:HB2	2.02	0.41
1:A:3:ASP:OD2	1:A:173:LYS:NZ	2.44	0.41
1:D:1067:TYR:CD2	1:D:1067:TYR:N	2.87	0.41
1:A:29:PRO:HD3	1:A:147:TYR:CZ	2.55	0.41
1:B:413:ILE:HD12	1:B:413:ILE:HA	1.77	0.41
1:A:19:GLN:HG2	1:A:20:ASN:N	2.35	0.41
1:C:603:ASP:HB3	1:C:604:PRO:HD2	2.02	0.41
1:D:1015:LYS:HD2	1:D:1016:LYS:N	2.35	0.41
1:A:115:LYS:NZ	1:A:210:LYS:CD	2.73	0.41
1:B:319:GLN:H	1:B:319:GLN:HG3	1.35	0.41
1:D:979:TYR:CE1	1:D:1044:GLU:HG3	2.56	0.41
1:B:415:LYS:CG	1:B:509:ASN:HD22	2.34	0.41
1:B:479:LYS:HE2	1:B:479:LYS:HB3	1.92	0.41
1:C:605:ASP:CB	1:C:608:GLN:NE2	2.83	0.41
1:D:904:PRO:HB3	1:D:1083:TRP:CH2	2.55	0.41
1:D:982:GLU:HA	1:D:998:CYS:O	2.21	0.41
1:D:986:LEU:O	1:D:988:TYR:CD1	2.73	0.41
1:D:1007:GLU:CD	1:D:1007:GLU:H	2.28	0.41
1:A:178:ASN:HB2	1:A:179:LYS:H	1.60	0.41
1:D:965:GLN:O	1:D:969:THR:HG23	2.21	0.41
1:D:1011:LEU:HD11	1:D:1109:ASN:HD21	1.85	0.41
1:D:1057:LYS:HD2	1:D:1057:LYS:O	2.21	0.41
1:C:754:ILE:HD11	1:C:760:TYR:HD2	1.85	0.40
1:D:1110:LYS:HE3	1:D:1110:LYS:HA	2.01	0.40
1:A:126:ILE:O	1:A:126:ILE:CG1	2.66	0.40
1:C:643:SER:O	1:C:665:GLN:HA	2.22	0.40
1:C:629:PRO:HD3	1:C:747:TYR:CZ	2.56	0.40
1:D:1077:LYS:HD2	1:D:1111:THR:HB	2.03	0.40
1:C:664:ASN:OD1	1:C:666:GLU:HB2	2.22	0.40
1:D:906:PRO:C	1:D:908:GLN:N	2.79	0.40
1:D:989:LEU:HD13	1:D:996:SER:CB	2.50	0.40
1:D:1068:GLU:OE1	1:D:1068:GLU:CA	2.60	0.40

All (2) 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)
3:A:2128:HOH:O	3:A:3010:HOH:O[1_655]	1.69	0.51
1:B:455:ASP:O	3:C:5073:HOH:O[3_545]	2.18	0.02

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	219/221 (99%)	206 (94%)	9 (4%)	4 (2%)	6	1
1	B	219/221 (99%)	208 (95%)	11 (5%)	0	100	100
1	C	219/221 (99%)	211 (96%)	6 (3%)	2 (1%)	14	6
1	D	219/221 (99%)	195 (89%)	19 (9%)	5 (2%)	5	0
All	All	876/884 (99%)	820 (94%)	45 (5%)	11 (1%)	9	3

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	727	GLN
1	D	907	SER
1	D	1112	SER
1	A	178	ASN
1	C	729	LEU
1	D	1029	LEU
1	A	179	LYS
1	D	1078	ASN
1	D	906	PRO
1	A	37	SER
1	A	177	LYS

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	208/208 (100%)	189 (91%)	19 (9%)	9	1
1	B	208/208 (100%)	192 (92%)	16 (8%)	12	3
1	C	208/208 (100%)	198 (95%)	10 (5%)	23	10
1	D	208/208 (100%)	186 (89%)	22 (11%)	6	1
All	All	832/832 (100%)	765 (92%)	67 (8%)	11	2

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	6	PRO
1	A	30	VAL
1	A	36	LYS
1	A	69	THR
1	A	70	LEU
1	A	115	LYS
1	A	118	VAL
1	A	128	SER
1	A	129	LEU
1	A	151	LYS
1	A	153	THR
1	A	154	ILE
1	A	158	GLN
1	A	177	LYS
1	A	178	ASN
1	A	179	LYS
1	A	191	GLU
1	A	207	LEU
1	B	319	GLN
1	B	330	VAL
1	B	353	PRO
1	B	369	THR
1	B	370	LEU
1	B	413	ILE
1	B	440	VAL
1	B	454	ILE
1	B	458	GLN

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Mol	Chain	Res	Type
1	B	475	ILE
1	B	478	ASN
1	B	480	GLU
1	B	488	PRO
1	B	496	LYS
1	B	507	LEU
1	B	521	LYS
1	C	602	GLN
1	C	619	GLN
1	C	640	GLN
1	C	670	LEU
1	C	726	ILE
1	C	757	LYS
1	C	778	ASN
1	C	779	LYS
1	C	788	PRO
1	C	810	LYS
1	D	902	GLN
1	D	905	ASP
1	D	906	PRO
1	D	912	SER
1	D	916	LYS
1	D	919	GLN
1	D	930	VAL
1	D	972	LYS
1	D	989	LEU
1	D	1005	ASN
1	D	1007	GLU
1	D	1013	ILE
1	D	1026	ILE
1	D	1027	GLN
1	D	1032	ASP
1	D	1040	VAL
1	D	1053	THR
1	D	1057	LYS
1	D	1079	LYS
1	D	1088	PRO
1	D	1090	PRO
1	D	1107	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	8	GLN
1	A	40	GLN
1	A	105	ASN
1	A	106	HIS
1	A	127	GLN
1	A	143	GLN
1	A	178	ASN
1	A	194	GLN
1	B	301	GLN
1	B	302	GLN
1	B	319	GLN
1	B	340	GLN
1	B	344	HIS
1	B	349	ASN
1	B	406	HIS
1	B	410	HIS
1	B	443	GLN
1	B	458	GLN
1	B	494	GLN
1	C	601	GLN
1	C	602	GLN
1	C	608	GLN
1	C	619	GLN
1	C	705	ASN
1	C	736	ASN
1	C	743	GLN
1	C	794	GLN
1	C	809	ASN
1	C	813	GLN
1	D	901	GLN
1	D	919	GLN
1	D	934	ASN
1	D	965	GLN
1	D	1006	HIS
1	D	1043	GLN
1	D	1058	GLN
1	D	1062	ASN
1	D	1094	GLN
1	D	1109	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 15 ligands modelled in this entry, 15 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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.