



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:51 AM UTC

PDB ID : 1FNV / pdb_00001fnv
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 : 3.60 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

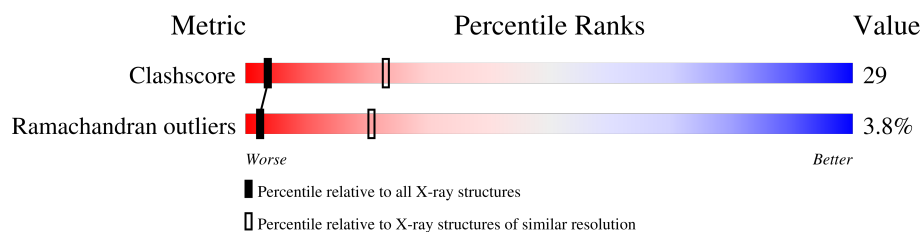
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)

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 2 unique types of molecules in this entry. The entry contains 7308 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	0	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).

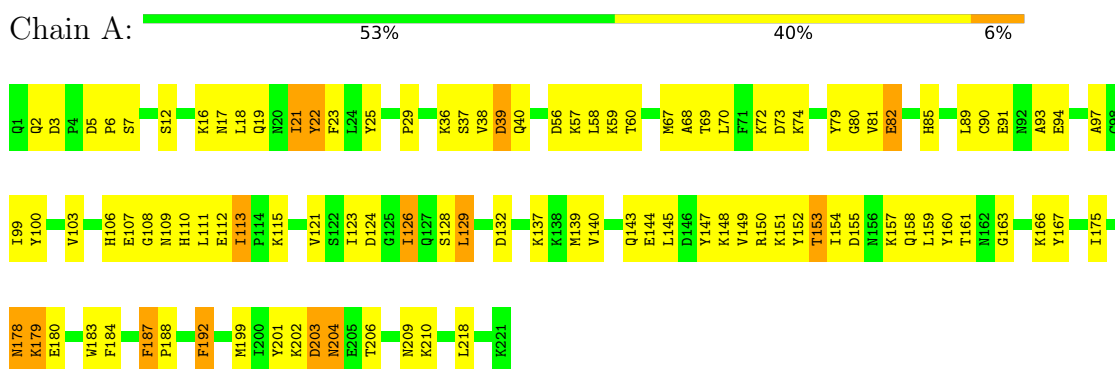
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Cd 3	0	0
2	B	4	Total 4	Cd 4	0	0
2	C	5	Total 5	Cd 5	0	0
2	D	4	Total 4	Cd 4	0	0

3 Residue-property plots [i](#)

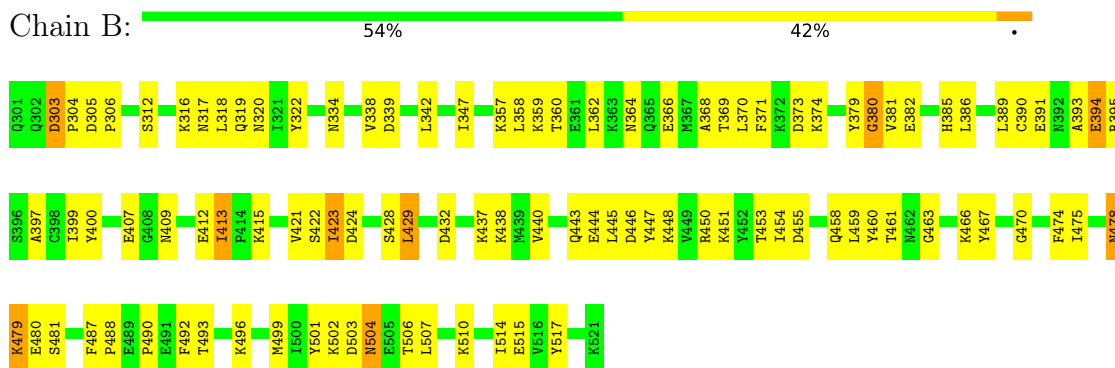
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

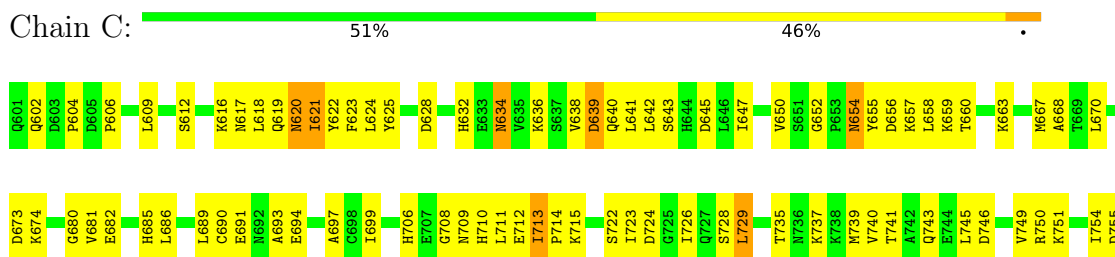
- Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)



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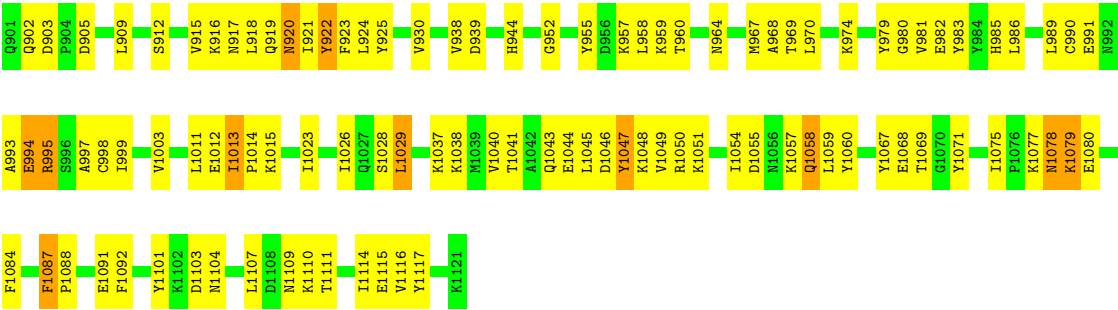


- Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)





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



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 2	Depositor
Cell constants a, b, c, α , β , γ	105.48Å 130.71Å 84.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.60	Depositor
% Data completeness (in resolution range)	75.2 (20.00-3.60)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7308	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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	0.55	0/1865	1.11	20/2522 (0.8%)
1	B	0.49	0/1865	1.14	21/2522 (0.8%)
1	C	0.53	0/1865	1.10	14/2522 (0.6%)
1	D	0.51	0/1865	1.09	20/2522 (0.8%)
All	All	0.52	0/7460	1.11	75/10088 (0.7%)

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

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	487	PHE	CA-C-N	9.29	129.12	120.21
1	B	487	PHE	C-N-CA	9.29	129.12	120.21
1	C	729	LEU	N-CA-C	9.09	119.90	108.45
1	B	394	GLU	N-CA-C	-9.07	97.03	110.46
1	A	94	GLU	N-CA-C	-8.36	98.47	110.59
1	D	1028	SER	N-CA-C	7.89	123.20	113.50
1	B	429	LEU	N-CA-C	7.83	118.57	108.24
1	C	693	ALA	N-CA-C	7.82	121.16	108.41
1	A	187	PHE	CA-C-N	7.80	128.25	120.52
1	A	187	PHE	C-N-CA	7.80	128.25	120.52
1	A	179	LYS	N-CA-C	7.31	119.25	108.14
1	A	129	LEU	N-CA-C	7.29	118.15	107.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	680	GLY	N-CA-C	7.27	122.63	110.56
1	B	303	ASP	CA-C-N	7.21	127.63	119.92
1	B	303	ASP	C-N-CA	7.21	127.63	119.92
1	A	93	ALA	N-CA-C	7.15	120.54	108.02
1	B	393	ALA	N-CA-C	7.15	120.18	108.52
1	B	428	SER	N-CA-C	7.14	119.14	111.36
1	D	994	GLU	N-CA-C	-7.09	98.68	109.95
1	C	694	GLU	N-CA-C	-6.96	99.35	110.14
1	D	905	ASP	CA-C-N	6.91	128.48	119.84
1	D	905	ASP	C-N-CA	6.91	128.48	119.84
1	D	1029	LEU	N-CA-C	6.87	116.93	107.73
1	A	3	ASP	CA-C-N	6.83	126.74	119.85
1	A	3	ASP	C-N-CA	6.83	126.74	119.85
1	A	166	LYS	N-CA-C	-6.69	105.25	113.41
1	A	21	ILE	N-CA-C	-6.56	104.37	110.53
1	D	993	ALA	N-CA-C	6.44	118.89	108.34
1	C	713	ILE	CA-C-N	6.40	127.40	119.98
1	C	713	ILE	C-N-CA	6.40	127.40	119.98
1	D	903	ASP	CA-C-N	6.38	126.36	119.78
1	D	903	ASP	C-N-CA	6.38	126.36	119.78
1	C	778	ASN	N-CA-C	6.35	118.00	111.14
1	B	413	ILE	CA-C-N	6.33	126.70	119.93
1	B	413	ILE	C-N-CA	6.33	126.70	119.93
1	C	775	ILE	CA-C-N	6.22	126.14	119.85
1	C	775	ILE	C-N-CA	6.22	126.14	119.85
1	D	944	HIS	N-CA-C	6.15	119.73	112.72
1	D	1079	LYS	N-CA-C	6.12	117.59	107.73
1	D	1013	ILE	CA-C-N	6.11	127.47	119.84
1	D	1013	ILE	C-N-CA	6.11	127.47	119.84
1	B	475	ILE	CA-C-N	6.10	126.31	119.90
1	B	475	ILE	C-N-CA	6.10	126.31	119.90
1	D	964	ASN	N-CA-C	6.04	116.53	108.38
1	B	479	LYS	N-CA-C	6.03	117.71	108.42
1	D	1003	VAL	N-CA-C	6.00	116.50	107.80
1	A	113	ILE	CA-C-N	5.97	127.31	119.84
1	A	113	ILE	C-N-CA	5.97	127.31	119.84
1	C	628	ASP	CA-C-N	5.96	125.93	120.03
1	C	628	ASP	C-N-CA	5.96	125.93	120.03
1	D	980	GLY	N-CA-C	5.91	122.08	111.03
1	B	432	ASP	N-CA-C	5.88	119.14	109.85
1	D	1111	THR	N-CA-C	5.87	117.95	110.61
1	A	126	ILE	N-CA-C	5.75	116.48	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	478	ASN	N-CA-C	5.58	118.43	111.24
1	C	654	ASN	N-CA-C	5.58	117.13	110.44
1	A	132	ASP	N-CA-C	5.54	118.25	109.50
1	A	128	SER	N-CA-C	5.52	119.74	112.89
1	B	493	THR	N-CA-C	-5.52	101.74	109.69
1	B	438	LYS	N-CA-C	-5.50	105.69	112.90
1	B	421	VAL	N-CA-C	5.50	115.87	108.17
1	D	982	GLU	N-CA-C	5.49	118.65	110.14
1	D	1078	ASN	N-CA-C	5.48	117.06	111.14
1	D	1087	PHE	CA-C-N	5.46	126.82	120.98
1	D	1087	PHE	C-N-CA	5.46	126.82	120.98
1	C	621	ILE	N-CA-C	-5.37	105.89	111.58
1	B	305	ASP	CA-C-N	5.33	126.50	119.84
1	B	305	ASP	C-N-CA	5.33	126.50	119.84
1	C	728	SER	N-CA-C	5.30	117.97	111.82
1	A	178	ASN	N-CA-C	5.26	116.70	110.97
1	A	175	ILE	CA-C-N	5.14	125.07	119.78
1	A	175	ILE	C-N-CA	5.14	125.07	119.78
1	A	82	GLU	N-CA-C	5.12	118.08	109.95
1	A	103	VAL	N-CA-C	5.03	115.16	108.11
1	B	380	GLY	N-CA-C	5.01	120.39	110.83

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	PHE	Sidechain

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	1823	0	1779	107	0
1	B	1823	0	1776	100	0
1	C	1823	0	1776	114	0
1	D	1823	0	1776	114	0
2	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	0	0	0
2	C	5	0	0	0	0
2	D	4	0	0	1	0
All	All	7308	0	7107	417	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (417) 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:D:990:CYS:SG	2:D:1124:CD:CD	1.39	1.29
1:B:454:ILE:HG12	1:B:459:LEU:HB3	1.39	1.05
1:D:919:GLN:H	1:D:919:GLN:HE21	0.97	0.96
1:A:19:GLN:H	1:A:19:GLN:NE2	1.66	0.94
1:C:754:ILE:HG12	1:C:759:LEU:HB3	1.50	0.93
1:B:319:GLN:H	1:B:319:GLN:NE2	1.68	0.91
1:B:319:GLN:H	1:B:319:GLN:HE21	0.95	0.91
1:B:319:GLN:HE21	1:B:319:GLN:N	1.70	0.88
1:D:919:GLN:H	1:D:919:GLN:NE2	1.71	0.88
1:D:958:LEU:HD12	1:D:997:ALA:O	1.74	0.88
1:A:81:VAL:H	1:A:143:GLN:NE2	1.72	0.88
1:D:1054:ILE:HG12	1:D:1059:LEU:HB3	1.54	0.88
1:A:151:LYS:HE2	1:A:155:ASP:OD2	1.73	0.87
1:B:454:ILE:HA	1:B:459:LEU:H	1.39	0.86
1:C:751:LYS:HE2	1:C:755:ASP:OD2	1.76	0.86
1:B:454:ILE:HG23	1:B:460:TYR:H	1.41	0.85
1:B:381:VAL:H	1:B:443:GLN:NE2	1.73	0.85
1:B:415:LYS:HE3	1:B:510:LYS:HA	1.58	0.84
1:D:1015:LYS:HE3	1:D:1110:LYS:HA	1.58	0.84
1:B:381:VAL:H	1:B:443:GLN:HE21	1.20	0.83
1:D:919:GLN:HE21	1:D:919:GLN:N	1.76	0.83
1:A:16:LYS:HG3	1:A:17:ASN:H	1.43	0.83
1:D:1015:LYS:HG2	1:D:1109:ASN:HD22	1.42	0.83
1:B:358:LEU:HD12	1:B:397:ALA:O	1.80	0.82
1:D:916:LYS:HG3	1:D:917:ASN:H	1.46	0.81
1:A:59:LYS:HB2	1:A:89:LEU:CD1	2.10	0.81
1:A:137:LYS:HB2	1:A:140:VAL:HG12	1.61	0.80
1:B:450:ARG:O	1:B:454:ILE:HG13	1.84	0.78
1:C:657:LYS:HB3	1:C:689:LEU:HD21	1.65	0.77
1:D:1050:ARG:O	1:D:1054:ILE:HG13	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:602:GLN:H	1:C:602:GLN:NE2	1.81	0.77
1:D:1054:ILE:HA	1:D:1059:LEU:H	1.49	0.77
1:A:19:GLN:H	1:A:19:GLN:HE21	1.32	0.76
1:D:959:LYS:HB2	1:D:989:LEU:CD1	2.16	0.76
1:A:59:LYS:HB2	1:A:89:LEU:HD11	1.70	0.73
1:C:604:PRO:HB3	1:C:783:TRP:CZ2	2.23	0.73
1:D:981:VAL:H	1:D:1043:GLN:NE2	1.88	0.72
1:A:115:LYS:HE3	1:A:210:LYS:HA	1.72	0.72
1:A:112:GLU:C	1:A:113:ILE:HD12	2.14	0.72
1:A:145:LEU:O	1:A:149:VAL:HG23	1.90	0.71
1:D:957:LYS:HB3	1:D:989:LEU:CD2	2.21	0.70
1:C:625:TYR:CE2	1:C:750:ARG:HD2	2.26	0.70
1:C:715:LYS:HE3	1:C:810:LYS:HA	1.71	0.70
1:A:81:VAL:H	1:A:143:GLN:HE21	1.37	0.70
1:C:770:GLY:O	1:C:786:PHE:HB2	1.91	0.70
1:A:2:GLN:H	1:A:2:GLN:NE2	1.90	0.70
1:B:319:GLN:NE2	1:B:319:GLN:N	2.34	0.70
1:B:359:LYS:HB2	1:B:389:LEU:HD13	1.73	0.69
1:D:981:VAL:H	1:D:1043:GLN:HE21	1.38	0.69
1:B:379:TYR:CD2	1:B:444:GLU:HG3	2.28	0.69
1:B:437:LYS:HB2	1:B:440:VAL:HG12	1.74	0.69
1:C:634:ASN:HB2	1:C:706:HIS:CD2	2.27	0.69
1:A:154:ILE:HG12	1:A:159:LEU:HB3	1.75	0.69
1:D:1115:GLU:HB3	1:D:1117:TYR:HE1	1.58	0.69
1:C:737:LYS:HB2	1:C:740:VAL:HG12	1.75	0.68
1:A:183:TRP:O	1:A:184:PHE:HD2	1.76	0.68
1:B:381:VAL:N	1:B:443:GLN:HE21	1.91	0.68
1:A:115:LYS:HG2	1:A:209:ASN:HD22	1.57	0.68
1:A:192:PHE:CD1	1:A:192:PHE:C	2.71	0.67
1:A:16:LYS:HG3	1:A:17:ASN:N	2.09	0.67
1:A:60:THR:HA	1:A:99:ILE:O	1.94	0.67
1:B:390:CYS:SG	1:D:991:GLU:OE1	2.50	0.67
1:D:912:SER:OG	1:D:1068:GLU:HA	1.94	0.66
1:D:1015:LYS:CE	1:D:1110:LYS:HD3	2.25	0.66
1:B:359:LYS:HB2	1:B:389:LEU:CD1	2.25	0.66
1:C:616:LYS:HG3	1:C:617:ASN:H	1.60	0.65
1:D:1012:GLU:C	1:D:1013:ILE:HD12	2.21	0.65
1:A:19:GLN:O	1:A:22:TYR:HB3	1.97	0.64
1:D:957:LYS:HB3	1:D:989:LEU:HD21	1.78	0.64
1:B:412:GLU:C	1:B:413:ILE:HD12	2.22	0.64
1:C:660:THR:HG23	1:C:660:THR:O	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:TYR:CD1	1:A:167:TYR:N	2.66	0.64
1:C:754:ILE:HA	1:C:759:LEU:H	1.61	0.64
1:A:60:THR:HG23	1:A:60:THR:O	1.98	0.63
1:D:1067:TYR:N	1:D:1067:TYR:CD1	2.65	0.63
1:B:316:LYS:HG3	1:B:317:ASN:N	2.14	0.63
1:D:916:LYS:HE2	1:D:1091:GLU:HG2	1.80	0.63
1:B:470:GLY:HA2	1:B:517:TYR:O	1.99	0.63
1:C:640:GLN:HB2	1:C:645:ASP:O	1.98	0.63
1:C:681:VAL:H	1:C:743:GLN:NE2	1.96	0.63
1:A:154:ILE:HA	1:A:159:LEU:H	1.64	0.62
1:D:959:LYS:HB2	1:D:989:LEU:HD11	1.79	0.62
1:B:415:LYS:HE3	1:B:510:LYS:HD3	1.79	0.62
1:B:316:LYS:HG3	1:B:317:ASN:H	1.64	0.62
1:C:638:VAL:O	1:C:639:ASP:HB2	1.99	0.62
1:A:70:LEU:O	1:A:70:LEU:HD23	2.00	0.61
1:A:202:LYS:C	1:A:204:ASN:H	2.08	0.61
1:C:619:GLN:H	1:C:619:GLN:NE2	1.98	0.61
1:B:492:PHE:CD1	1:B:492:PHE:C	2.77	0.61
1:B:368:ALA:C	1:B:370:LEU:H	2.09	0.61
1:A:115:LYS:CE	1:A:210:LYS:HD3	2.31	0.61
1:A:68:ALA:C	1:A:70:LEU:H	2.09	0.60
1:C:658:LEU:HD12	1:C:697:ALA:O	2.00	0.60
1:D:1050:ARG:O	1:D:1051:LYS:C	2.43	0.60
1:C:625:TYR:CD2	1:C:750:ARG:HD2	2.36	0.60
1:B:490:PRO:HD2	1:C:643:SER:OG	2.02	0.60
1:B:467:TYR:N	1:B:467:TYR:CD1	2.70	0.60
1:C:806:THR:HG22	1:C:807:LEU:N	2.15	0.60
1:A:150:ARG:O	1:A:151:LYS:C	2.45	0.60
1:D:1015:LYS:HG2	1:D:1109:ASN:ND2	2.15	0.60
1:B:370:LEU:HD23	1:B:370:LEU:O	2.02	0.59
1:B:443:GLN:OE1	1:B:501:TYR:HB3	2.02	0.59
1:A:115:LYS:HD3	1:A:210:LYS:NZ	2.17	0.59
1:C:602:GLN:NE2	1:C:602:GLN:N	2.50	0.59
1:B:391:GLU:OE1	1:D:990:CYS:SG	2.56	0.59
1:A:137:LYS:HB2	1:A:140:VAL:CG1	2.32	0.59
1:B:379:TYR:CD2	1:B:444:GLU:HA	2.37	0.59
1:C:767:TYR:CD1	1:C:767:TYR:N	2.71	0.59
1:B:407:GLU:OE1	1:B:407:GLU:N	2.36	0.59
1:C:602:GLN:N	1:C:602:GLN:HE21	2.00	0.59
1:A:38:VAL:O	1:A:39:ASP:HB2	2.03	0.58
1:B:374:LYS:HD2	1:B:374:LYS:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ASP:O	1:B:504:ASN:C	2.46	0.58
1:C:657:LYS:HB3	1:C:689:LEU:CD2	2.33	0.58
1:C:674:LYS:N	1:C:674:LYS:HD2	2.18	0.58
1:B:450:ARG:HB3	1:B:454:ILE:HD11	1.86	0.58
1:B:437:LYS:HB2	1:B:440:VAL:CG1	2.34	0.58
1:D:1011:LEU:HD21	1:D:1038:LYS:HG2	1.84	0.58
1:C:792:PHE:CD1	1:C:792:PHE:C	2.81	0.58
1:A:91:GLU:OE1	1:C:690:CYS:SG	2.58	0.58
1:A:5:ASP:O	1:A:7:SER:N	2.36	0.58
1:C:750:ARG:O	1:C:754:ILE:HG13	2.04	0.57
1:B:319:GLN:O	1:B:322:TYR:N	2.34	0.57
1:A:143:GLN:HG3	1:A:201:TYR:CD1	2.40	0.57
1:D:1051:LYS:HE2	1:D:1055:ASP:OD2	2.04	0.57
1:A:79:TYR:CE2	1:A:144:GLU:HG3	2.40	0.57
1:D:902:GLN:NE2	1:D:902:GLN:H	2.03	0.57
1:A:21:ILE:HG21	1:A:160:TYR:CE2	2.40	0.57
1:C:685:HIS:CD2	1:D:994:GLU:HG2	2.39	0.57
1:D:968:ALA:C	1:D:970:LEU:H	2.12	0.57
1:D:960:THR:HG23	1:D:960:THR:O	2.04	0.56
1:B:461:THR:O	1:B:463:GLY:N	2.35	0.56
1:D:967:MET:O	1:D:970:LEU:HB3	2.05	0.56
1:D:1088:PRO:HG3	1:D:1092:PHE:CE2	2.40	0.56
1:A:19:GLN:NE2	1:A:19:GLN:N	2.46	0.56
1:C:761:THR:C	1:C:763:GLY:H	2.12	0.56
1:A:123:ILE:O	1:A:126:ILE:HG12	2.06	0.56
1:D:970:LEU:C	1:D:970:LEU:HD23	2.31	0.56
1:A:143:GLN:HG3	1:A:201:TYR:CE1	2.40	0.56
1:C:616:LYS:HG3	1:C:617:ASN:N	2.20	0.56
1:B:391:GLU:OE1	1:D:991:GLU:HG2	2.05	0.56
1:D:1015:LYS:HE3	1:D:1110:LYS:HD3	1.86	0.56
1:C:710:HIS:CD2	1:C:711:LEU:H	2.24	0.55
1:D:1029:LEU:C	1:D:1029:LEU:HD12	2.31	0.55
1:D:1037:LYS:HB2	1:D:1040:VAL:CG1	2.37	0.55
1:D:1054:ILE:HG23	1:D:1060:TYR:H	1.71	0.55
1:D:1037:LYS:HB2	1:D:1040:VAL:HG12	1.88	0.55
1:C:663:LYS:HB3	1:C:667:MET:HE3	1.89	0.55
1:D:925:TYR:CD2	1:D:1050:ARG:HD2	2.42	0.55
1:A:57:LYS:HB3	1:A:89:LEU:CD2	2.37	0.55
1:B:379:TYR:CE2	1:B:444:GLU:HG3	2.42	0.54
1:D:916:LYS:HG3	1:D:917:ASN:N	2.19	0.54
1:C:737:LYS:HB2	1:C:740:VAL:CG1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:925:TYR:CE2	1:D:1050:ARG:HD2	2.43	0.54
1:A:40:GLN:NE2	1:A:72:LYS:HE2	2.23	0.54
1:B:440:VAL:O	1:B:506:THR:HG23	2.07	0.54
1:B:443:GLN:HG3	1:B:501:TYR:CE1	2.43	0.54
1:B:451:LYS:HE2	1:B:455:ASP:OD2	2.08	0.54
1:C:796:LYS:O	1:C:796:LYS:HD3	2.08	0.54
1:C:710:HIS:HD2	1:C:711:LEU:H	1.54	0.54
1:A:58:LEU:HD12	1:A:97:ALA:O	2.08	0.53
1:A:167:TYR:CD2	1:A:218:LEU:HD13	2.44	0.53
1:B:443:GLN:HG3	1:B:501:TYR:CD1	2.42	0.53
1:A:161:THR:C	1:A:163:GLY:H	2.16	0.53
1:B:488:PRO:HG3	1:B:492:PHE:CE2	2.44	0.53
1:B:415:LYS:CE	1:B:510:LYS:HD3	2.39	0.53
1:B:319:GLN:O	1:B:322:TYR:HB3	2.08	0.53
1:A:74:LYS:HD2	1:A:74:LYS:N	2.23	0.53
1:A:203:ASP:O	1:A:204:ASN:C	2.52	0.53
1:C:682:GLU:HA	1:C:699:ILE:HG22	1.90	0.53
1:A:139:MET:HE3	1:A:206:THR:HG22	1.90	0.53
1:B:382:GLU:HA	1:B:399:ILE:HG22	1.89	0.53
1:C:670:LEU:HD23	1:C:670:LEU:O	2.08	0.53
1:A:67:MET:O	1:A:70:LEU:HB3	2.09	0.53
1:A:81:VAL:N	1:A:143:GLN:HE21	2.04	0.52
1:C:745:LEU:O	1:C:749:VAL:HG23	2.09	0.52
1:D:998:CYS:O	1:D:999:ILE:HG23	2.08	0.52
1:A:19:GLN:HE21	1:A:19:GLN:N	2.05	0.52
1:D:1050:ARG:HB3	1:D:1054:ILE:HD11	1.90	0.52
1:B:391:GLU:HG2	1:D:991:GLU:OE1	2.10	0.52
1:C:670:LEU:HD23	1:C:670:LEU:C	2.35	0.52
1:A:23:PHE:CE2	1:B:395:ARG:NH1	2.78	0.52
1:B:342:LEU:HD22	1:C:792:PHE:HA	1.92	0.52
1:C:715:LYS:HG2	1:C:809:ASN:HD22	1.74	0.52
1:C:796:LYS:HD3	1:C:796:LYS:C	2.34	0.52
1:B:454:ILE:O	1:B:458:GLN:HA	2.09	0.51
1:D:1078:ASN:O	1:D:1079:LYS:HB3	2.10	0.51
1:C:750:ARG:O	1:C:751:LYS:C	2.53	0.51
1:C:723:ILE:O	1:C:726:ILE:HG12	2.11	0.51
1:A:107:GLU:OE1	1:A:107:GLU:N	2.43	0.51
1:B:407:GLU:CD	1:B:407:GLU:H	2.19	0.51
1:C:729:LEU:HD12	1:C:729:LEU:C	2.36	0.51
1:A:115:LYS:HG2	1:A:209:ASN:ND2	2.24	0.51
1:A:183:TRP:C	1:A:184:PHE:CD2	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ASP:C	1:A:7:SER:H	2.18	0.51
1:A:110:HIS:HD2	1:A:111:LEU:H	1.59	0.51
1:A:115:LYS:HE2	1:A:210:LYS:HD3	1.93	0.51
1:C:658:LEU:HD12	1:C:659:LYS:H	1.75	0.51
1:D:922:TYR:O	1:D:923:PHE:C	2.54	0.51
1:A:150:ARG:O	1:A:154:ILE:HG13	2.11	0.51
1:B:454:ILE:HD13	1:B:460:TYR:HD1	1.76	0.51
1:C:609:LEU:HD13	1:C:769:THR:HB	1.93	0.51
1:C:619:GLN:H	1:C:619:GLN:HE21	1.58	0.50
1:D:960:THR:HA	1:D:999:ILE:O	2.11	0.50
1:A:110:HIS:CD2	1:A:111:LEU:N	2.80	0.50
1:C:657:LYS:CB	1:C:689:LEU:HD21	2.39	0.50
1:B:385:HIS:CD2	1:B:386:LEU:HG	2.46	0.50
1:C:710:HIS:CD2	1:C:711:LEU:N	2.80	0.50
1:D:1057:LYS:O	1:D:1058:GLN:HB2	2.12	0.50
1:A:121:VAL:HB	1:A:129:LEU:HD12	1.94	0.50
1:C:639:ASP:O	1:C:647:ILE:HB	2.12	0.49
1:C:739:MET:HE3	1:C:806:THR:HG22	1.94	0.49
1:C:713:ILE:HG23	1:C:714:PRO:HD2	1.93	0.49
1:B:338:VAL:O	1:B:339:ASP:HB2	2.12	0.49
1:D:915:VAL:HG11	1:D:918:LEU:HD13	1.93	0.49
1:C:623:PHE:CE2	1:D:995:ARG:NH1	2.81	0.49
1:D:912:SER:HB3	1:D:1087:PHE:CE2	2.47	0.49
1:A:57:LYS:HB3	1:A:89:LEU:HD23	1.94	0.49
1:C:681:VAL:H	1:C:743:GLN:HE21	1.60	0.49
1:D:1092:PHE:CD1	1:D:1092:PHE:C	2.90	0.49
1:A:129:LEU:HD12	1:A:129:LEU:C	2.38	0.49
1:D:1078:ASN:OD1	1:D:1079:LYS:N	2.46	0.49
1:D:994:GLU:O	1:D:995:ARG:HB2	2.13	0.48
1:B:362:LEU:HD12	1:B:368:ALA:HA	1.95	0.48
1:B:422:SER:O	1:B:423:ILE:HG13	2.13	0.48
1:C:632:HIS:CD2	1:C:650:VAL:HG21	2.48	0.48
1:C:778:ASN:O	1:C:779:LYS:HB3	2.14	0.48
1:B:478:ASN:OD1	1:B:479:LYS:N	2.46	0.48
1:D:1026:ILE:O	1:D:1026:ILE:HG13	2.14	0.48
1:A:147:TYR:O	1:A:148:LYS:C	2.57	0.48
1:C:619:GLN:O	1:C:621:ILE:N	2.46	0.48
1:C:619:GLN:HG2	1:C:620:ASN:N	2.29	0.48
1:D:1015:LYS:HD3	1:D:1110:LYS:NZ	2.29	0.48
1:D:916:LYS:CG	1:D:917:ASN:H	2.22	0.48
1:D:1077:LYS:HD3	1:D:1077:LYS:C	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:TRP:C	1:A:184:PHE:HD2	2.21	0.48
1:C:803:ASP:O	1:C:804:ASN:C	2.56	0.48
1:D:979:TYR:CE2	1:D:1044:GLU:HG3	2.49	0.48
1:A:37:SER:OG	1:A:72:LYS:O	2.31	0.48
1:A:113:ILE:HD12	1:A:113:ILE:N	2.28	0.48
1:B:445:LEU:O	1:B:446:ASP:C	2.57	0.48
1:B:474:PHE:O	1:B:481:SER:HB2	2.14	0.47
1:C:612:SER:HB3	1:C:787:PHE:CE2	2.49	0.47
1:D:970:LEU:HD23	1:D:970:LEU:O	2.14	0.47
1:D:1015:LYS:HE2	1:D:1110:LYS:HD3	1.96	0.47
1:A:100:TYR:CE2	1:A:199:MET:HG2	2.49	0.47
1:A:121:VAL:HB	1:A:129:LEU:CD1	2.45	0.47
1:D:998:CYS:O	1:D:999:ILE:CG2	2.62	0.47
1:D:1071:TYR:HB2	1:D:1084:PHE:O	2.15	0.47
1:A:81:VAL:N	1:A:143:GLN:NE2	2.51	0.47
1:A:91:GLU:OE1	1:C:691:GLU:HG2	2.14	0.47
1:B:450:ARG:O	1:B:451:LYS:C	2.58	0.47
1:C:741:THR:C	1:C:743:GLN:N	2.71	0.47
1:C:761:THR:C	1:C:763:GLY:N	2.73	0.47
1:D:1023:ILE:O	1:D:1026:ILE:HG12	2.15	0.47
1:A:2:GLN:NE2	1:A:2:GLN:N	2.61	0.47
1:A:25:TYR:CE2	1:A:150:ARG:HD2	2.49	0.47
1:C:624:LEU:HD11	1:C:794:GLN:HG2	1.96	0.47
1:D:902:GLN:NE2	1:D:902:GLN:N	2.63	0.47
1:B:429:LEU:C	1:B:429:LEU:HD12	2.40	0.47
1:C:619:GLN:O	1:C:622:TYR:HB3	2.15	0.47
1:C:746:ASP:OD1	1:C:801:TYR:OH	2.22	0.47
1:D:930:VAL:HG13	1:D:955:TYR:OH	2.14	0.47
1:B:364:ASN:OD1	1:B:366:GLU:HB2	2.14	0.47
1:C:754:ILE:HD13	1:C:760:TYR:HD1	1.79	0.47
1:D:919:GLN:O	1:D:922:TYR:N	2.47	0.47
1:D:1045:LEU:O	1:D:1049:VAL:HG23	2.15	0.47
1:A:2:GLN:N	1:A:2:GLN:HE21	2.12	0.47
1:B:368:ALA:O	1:B:370:LEU:N	2.47	0.47
1:C:652:GLY:HA3	1:C:655:TYR:CZ	2.50	0.47
1:C:712:GLU:C	1:C:713:ILE:HD12	2.39	0.47
1:D:1107:LEU:O	1:D:1107:LEU:HD12	2.15	0.47
1:B:303:ASP:HA	1:B:304:PRO:HD2	1.73	0.46
1:B:318:LEU:O	1:B:319:GLN:C	2.58	0.46
1:C:685:HIS:O	1:C:686:LEU:HB2	2.15	0.46
1:A:25:TYR:CD2	1:A:150:ARG:HD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:657:LYS:CB	1:C:689:LEU:CD2	2.94	0.46
1:D:1043:GLN:HG3	1:D:1101:TYR:CD1	2.50	0.46
1:A:68:ALA:O	1:A:70:LEU:N	2.45	0.46
1:D:919:GLN:NE2	1:D:919:GLN:N	2.46	0.46
1:D:919:GLN:O	1:D:921:ILE:N	2.48	0.46
1:D:985:HIS:O	1:D:986:LEU:HB2	2.14	0.46
1:A:12:SER:HB3	1:A:187:PHE:CE2	2.50	0.46
1:A:80:GLY:HA2	1:A:143:GLN:NE2	2.31	0.46
1:C:713:ILE:HA	1:C:714:PRO:HD3	1.75	0.46
1:B:423:ILE:O	1:B:424:ASP:HB2	2.14	0.46
1:B:461:THR:C	1:B:463:GLY:N	2.74	0.46
1:C:770:GLY:HA3	1:C:818:LEU:CD2	2.46	0.46
1:A:36:LYS:HD2	1:A:73:ASP:O	2.14	0.46
1:B:496:LYS:C	1:B:496:LYS:HD3	2.41	0.46
1:A:2:GLN:H	1:A:2:GLN:HE21	1.64	0.46
1:A:70:LEU:HD23	1:A:70:LEU:C	2.41	0.46
1:A:157:LYS:O	1:A:158:GLN:HB2	2.15	0.46
1:B:371:PHE:CD1	1:B:371:PHE:N	2.83	0.46
1:A:90:CYS:SG	1:C:691:GLU:OE1	2.59	0.46
1:B:413:ILE:HD12	1:B:413:ILE:N	2.31	0.46
1:D:974:LYS:HD2	1:D:974:LYS:N	2.30	0.46
1:C:715:LYS:HG2	1:C:809:ASN:ND2	2.30	0.46
1:A:108:GLY:C	1:A:110:HIS:H	2.24	0.45
1:B:368:ALA:C	1:B:370:LEU:N	2.75	0.45
1:D:994:GLU:O	1:D:995:ARG:CB	2.64	0.45
1:C:770:GLY:HA3	1:C:818:LEU:HD23	1.98	0.45
1:B:514:ILE:HG22	1:B:515:GLU:N	2.31	0.45
1:B:517:TYR:N	1:B:517:TYR:CD1	2.84	0.45
1:C:604:PRO:HB3	1:C:783:TRP:CH2	2.50	0.45
1:D:919:GLN:C	1:D:921:ILE:H	2.25	0.45
1:B:488:PRO:CG	1:B:492:PHE:CE2	3.00	0.45
1:A:161:THR:C	1:A:163:GLY:N	2.73	0.45
1:D:1088:PRO:CG	1:D:1092:PHE:CE2	3.00	0.45
1:A:19:GLN:O	1:A:22:TYR:N	2.50	0.45
1:A:115:LYS:HE3	1:A:210:LYS:HD3	1.99	0.45
1:C:619:GLN:O	1:C:622:TYR:N	2.49	0.45
1:C:681:VAL:HG23	1:C:743:GLN:HE21	1.81	0.45
1:D:1047:TYR:O	1:D:1048:LYS:C	2.60	0.45
1:A:178:ASN:OD1	1:A:179:LYS:N	2.50	0.45
1:A:202:LYS:O	1:A:204:ASN:N	2.50	0.45
1:B:390:CYS:SG	1:D:991:GLU:CD	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASP:OD2	1:A:56:ASP:N	2.49	0.45
1:A:167:TYR:N	1:A:167:TYR:HD1	2.12	0.45
1:B:373:ASP:C	1:B:374:LYS:HD2	2.42	0.45
1:B:370:LEU:O	1:B:374:LYS:HD3	2.16	0.44
1:B:390:CYS:SG	1:D:991:GLU:OE2	2.75	0.44
1:C:641:LEU:HG	1:C:642:LEU:HG	1.99	0.44
1:D:917:ASN:HB3	1:D:920:ASN:ND2	2.32	0.44
1:B:360:THR:HG23	1:B:360:THR:O	2.17	0.44
1:B:466:LYS:HB3	1:B:467:TYR:CE1	2.52	0.44
1:C:806:THR:CG2	1:C:807:LEU:N	2.80	0.44
1:D:957:LYS:HB3	1:D:989:LEU:HD23	1.98	0.44
1:C:632:HIS:CE1	1:C:650:VAL:HB	2.53	0.44
1:D:1011:LEU:HD21	1:D:1038:LYS:CG	2.47	0.44
1:C:619:GLN:C	1:C:621:ILE:N	2.75	0.44
1:C:723:ILE:O	1:C:724:ASP:C	2.61	0.44
1:B:391:GLU:OE2	1:D:990:CYS:SG	2.76	0.44
1:B:502:LYS:C	1:B:504:ASN:H	2.26	0.44
1:D:1114:ILE:HG22	1:D:1115:GLU:N	2.32	0.44
1:C:670:LEU:O	1:C:674:LYS:HD3	2.18	0.43
1:A:82:GLU:OE1	1:A:82:GLU:N	2.43	0.43
1:B:347:ILE:HG12	1:B:389:LEU:HD11	2.00	0.43
1:B:506:THR:HG22	1:B:507:LEU:N	2.33	0.43
1:C:667:MET:O	1:C:670:LEU:HB3	2.18	0.43
1:D:1067:TYR:N	1:D:1067:TYR:HD1	2.14	0.43
1:D:1116:VAL:C	1:D:1117:TYR:HD1	2.27	0.43
1:A:183:TRP:O	1:A:184:PHE:CD2	2.63	0.43
1:B:317:ASN:C	1:B:319:GLN:NE2	2.77	0.43
1:D:909:LEU:HD13	1:D:1069:THR:HB	2.00	0.43
1:A:18:LEU:O	1:A:19:GLN:C	2.59	0.43
1:B:357:LYS:HB3	1:B:389:LEU:CD2	2.48	0.43
1:C:750:ARG:HB3	1:C:754:ILE:HD11	2.00	0.43
1:D:998:CYS:C	1:D:999:ILE:HG23	2.43	0.43
1:B:459:LEU:HD23	1:B:460:TYR:CE1	2.53	0.43
1:A:188:PRO:HB2	1:A:192:PHE:CD2	2.54	0.43
1:B:382:GLU:OE1	1:B:382:GLU:N	2.42	0.43
1:C:743:GLN:HG3	1:C:801:TYR:CE1	2.54	0.43
1:C:777:LYS:HD3	1:C:777:LYS:C	2.44	0.43
1:D:1117:TYR:N	1:D:1117:TYR:CD1	2.85	0.43
1:B:496:LYS:HD3	1:B:496:LYS:O	2.18	0.43
1:D:1103:ASP:O	1:D:1104:ASN:C	2.61	0.43
1:A:202:LYS:C	1:A:204:ASN:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:726:ILE:HG13	1:C:726:ILE:O	2.19	0.43
1:C:741:THR:C	1:C:743:GLN:H	2.27	0.43
1:D:1041:THR:C	1:D:1043:GLN:N	2.73	0.43
1:A:29:PRO:HD3	1:A:147:TYR:CZ	2.54	0.43
1:B:374:LYS:N	1:B:374:LYS:CD	2.82	0.42
1:D:983:TYR:HE2	1:D:986:LEU:O	2.02	0.42
1:D:1067:TYR:HD1	1:D:1067:TYR:H	1.66	0.42
1:A:12:SER:HB3	1:A:187:PHE:CD2	2.55	0.42
1:B:454:ILE:HG12	1:B:459:LEU:CB	2.28	0.42
1:C:668:ALA:C	1:C:670:LEU:H	2.27	0.42
1:A:70:LEU:O	1:A:74:LYS:HD3	2.19	0.42
1:C:625:TYR:CZ	1:C:750:ARG:NH1	2.87	0.42
1:D:952:GLY:HA3	1:D:955:TYR:CE2	2.55	0.42
1:D:957:LYS:CB	1:D:989:LEU:CD2	2.96	0.42
1:D:1045:LEU:O	1:D:1046:ASP:C	2.59	0.42
1:C:708:GLY:C	1:C:710:HIS:H	2.27	0.42
1:C:735:THR:OG1	1:C:740:VAL:HG11	2.20	0.42
1:A:68:ALA:C	1:A:70:LEU:N	2.74	0.42
1:C:619:GLN:C	1:C:621:ILE:H	2.28	0.42
1:D:1013:ILE:HG23	1:D:1014:PRO:HD2	2.02	0.42
1:B:391:GLU:CD	1:D:990:CYS:SG	3.03	0.42
1:C:618:LEU:O	1:C:619:GLN:C	2.61	0.42
1:C:659:LYS:HB2	1:C:689:LEU:CD1	2.50	0.42
1:C:722:SER:C	1:C:723:ILE:HG13	2.45	0.42
1:B:454:ILE:HD13	1:B:460:TYR:CD1	2.55	0.42
1:C:751:LYS:CE	1:C:755:ASP:OD2	2.57	0.42
1:D:938:VAL:O	1:D:939:ASP:HB2	2.20	0.42
1:A:85:HIS:CD2	1:B:394:GLU:HG2	2.55	0.42
1:B:447:TYR:O	1:B:448:LYS:C	2.63	0.42
1:A:153:THR:O	1:A:158:GLN:N	2.53	0.41
1:D:919:GLN:C	1:D:921:ILE:N	2.76	0.41
1:D:924:LEU:HD23	1:D:924:LEU:HA	1.88	0.41
1:C:656:ASP:O	1:C:657:LYS:HG2	2.20	0.41
1:A:16:LYS:CG	1:A:17:ASN:N	2.81	0.41
1:A:29:PRO:HD3	1:A:147:TYR:OH	2.20	0.41
1:B:380:GLY:HA2	1:B:443:GLN:NE2	2.36	0.41
1:C:770:GLY:CA	1:C:818:LEU:HD23	2.50	0.41
1:D:1117:TYR:HD1	1:D:1117:TYR:N	2.18	0.41
1:A:123:ILE:O	1:A:124:ASP:HB2	2.20	0.41
1:C:689:LEU:HD12	1:C:689:LEU:HA	1.87	0.41
1:D:968:ALA:C	1:D:970:LEU:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:654:ASN:O	1:C:655:TYR:HB3	2.19	0.41
1:A:106:HIS:ND1	1:A:106:HIS:C	2.79	0.41
1:D:1071:TYR:CD1	1:D:1071:TYR:C	2.98	0.41
1:B:400:TYR:CE2	1:B:499:MET:HG2	2.56	0.41
1:C:636:LYS:HD2	1:C:673:ASP:O	2.21	0.41
1:C:713:ILE:HD12	1:C:713:ILE:N	2.35	0.41
1:C:715:LYS:HE3	1:C:810:LYS:HD3	2.03	0.41
1:D:1013:ILE:HD12	1:D:1013:ILE:N	2.36	0.41
1:D:952:GLY:HA3	1:D:955:TYR:CZ	2.56	0.41
1:A:16:LYS:CG	1:A:17:ASN:H	2.23	0.40
1:C:761:THR:O	1:C:763:GLY:N	2.44	0.40
1:D:902:GLN:N	1:D:902:GLN:HE21	2.19	0.40
1:A:91:GLU:HG2	1:C:691:GLU:OE1	2.20	0.40
1:D:1075:ILE:O	1:D:1075:ILE:HG22	2.21	0.40
1:C:729:LEU:C	1:C:729:LEU:CD1	2.94	0.40
1:C:800:ILE:HG13	1:C:801:TYR:CD2	2.57	0.40
1:B:422:SER:C	1:B:423:ILE:HG13	2.46	0.40
1:D:1015:LYS:HD3	1:D:1110:LYS:HZ3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	219/221 (99%)	184 (84%)	25 (11%)	10 (5%)	2	17
1	B	219/221 (99%)	179 (82%)	30 (14%)	10 (5%)	2	17
1	C	219/221 (99%)	180 (82%)	33 (15%)	6 (3%)	4	27
1	D	219/221 (99%)	178 (81%)	34 (16%)	7 (3%)	3	24
All	All	876/884 (99%)	721 (82%)	122 (14%)	33 (4%)	2	21

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	GLU
1	B	480	GLU
1	C	780	GLU
1	D	1080	GLU
1	A	6	PRO
1	A	109	ASN
1	A	152	TYR
1	A	203	ASP
1	B	334	ASN
1	B	369	THR
1	A	153	THR
1	B	312	SER
1	B	409	ASN
1	B	423	ILE
1	D	920	ASN
1	D	969	THR
1	A	22	TYR
1	A	69	THR
1	B	320	ASN
1	B	453	THR
1	B	504	ASN
1	C	606	PRO
1	C	620	ASN
1	D	922	TYR
1	D	995	ARG
1	A	39	ASP
1	A	204	ASN
1	B	306	PRO
1	C	639	ASP
1	C	709	ASN
1	D	1047	TYR
1	D	1058	GLN
1	C	634	ASN

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 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.