Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 07:34 PM EDT

PDB ID	:	1FNU
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 (i) 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 (i)) were used in the production of this report:

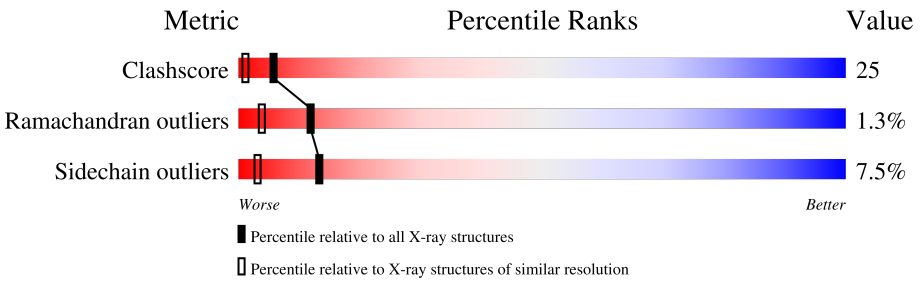
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.94 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	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	221	66% 25% 6% •
1	B	221	73% 20% 5% •
1	C	221	64% 30% 5%
1	D	221	52% 39% 6% •

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	221	1823	1166	293	358	6	5	0	0
1	B	221	1823	1166	293	358	6	0	0	0
1	C	221	1823	1166	293	358	6	0	0	0
1	D	221	1823	1166	293	358	6	0	0	0

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 (three-letter code: CD) (formula: Cd).

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

- Molecule 3 is water.

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

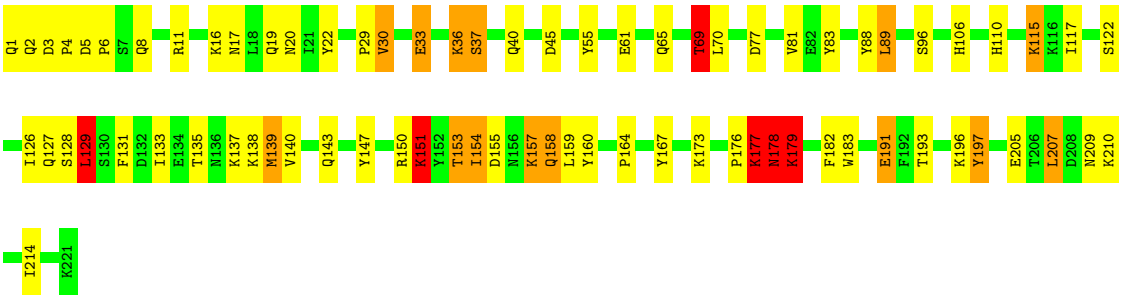
3 Residue-property plots (i)

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.

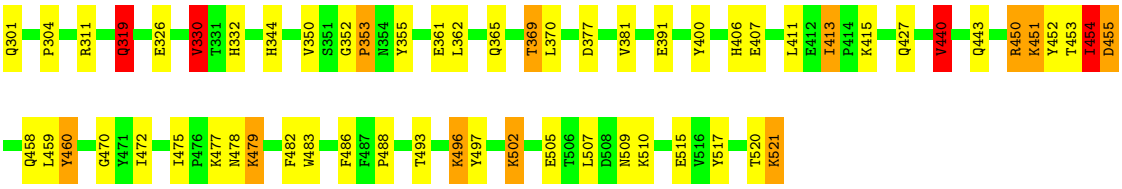
• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

Chain A:



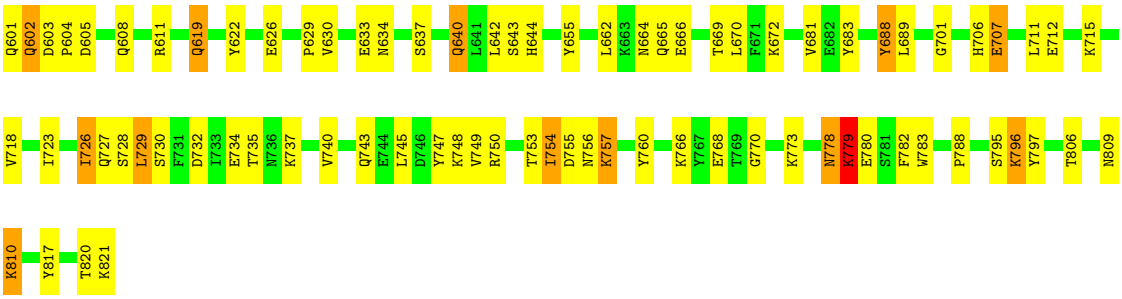
• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

Chain B:



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

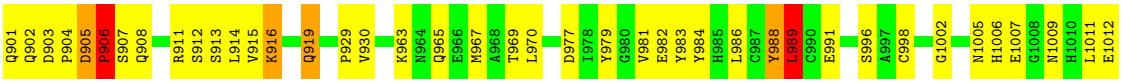
Chain C:

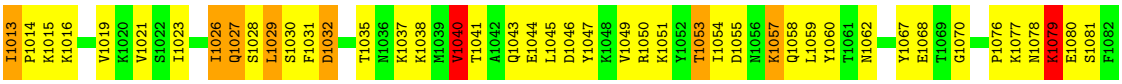


• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

Chain D:

52%
39%
6%


Q901 Q902 D903 P904 D905 P906 S907 Q908 R911 S912 S913 L914 V915 K916 Q919 P929 V930 K963 N964 Q965 E966 M967 A968 T969 L970 D977 I978 Y979 G980 V981 E982 Y983 Y984 H985 L986 C987 Y988 L989 C990 E991 S996 A997 C998 G1002 N1005 H1006 E1007 G1008 N1009 H1010 L1011 E1012


I1013 P1014 K1015 K1016 V1019 K1020 V1021 S1022 I1023 I1026 Q1027 S1028 L1029 S1030 F1031 D1032 T1035 N1036 K1037 K1038 M1039 V1040 T1041 A1042 Q1043 E1044 L1045 D1046 Y1047 K1048 V1049 R1050 K1051 Y1052 T1053 I1054 D1055 N1056 K1057 Q1058 L1059 Y1060 T1061 N1062 Y1067 E1068 T1069 G1070 P1076 K1077 N1078 K1079 E1080 S1081 F1082

W1083 P1088 E1089 P1090 E1091 S1095 K1096 Y1097 L1098 M1099 I1100 Y1101 T1106 L1107 D1108 N1109 K1110 T1111 S1112 Y1117 T1120 K1121

4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	1.25	7/1865 (0.4%)	1.20	8/2522 (0.3%)
1	B	1.28	8/1865 (0.4%)	1.18	12/2522 (0.5%)
1	C	1.24	4/1865 (0.2%)	1.15	7/2522 (0.3%)
1	D	1.13	2/1865 (0.1%)	1.16	8/2522 (0.3%)
All	All	1.23	21/7460 (0.3%)	1.17	35/10088 (0.3%)

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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	319	GLN	CB-CG	7.17	1.72	1.52
1	B	452	TYR	CD1-CE1	6.96	1.49	1.39
1	C	688	TYR	CD2-CE2	6.79	1.49	1.39
1	B	502	LYS	CD-CE	6.73	1.68	1.51
1	C	688	TYR	CD1-CE1	6.38	1.49	1.39
1	A	191	GLU	CD-OE1	5.99	1.32	1.25
1	A	153	THR	CA-CB	5.96	1.68	1.53
1	A	83	TYR	CD2-CE2	5.68	1.47	1.39
1	B	502	LYS	CE-NZ	5.54	1.62	1.49
1	D	984	TYR	CD1-CE1	5.46	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	319	GLN	CG-CD	-5.45	1.38	1.51
1	A	157	LYS	CD-CE	5.28	1.64	1.51
1	A	69	THR	CA-CB	5.26	1.67	1.53
1	D	963	LYS	CE-NZ	5.19	1.62	1.49
1	C	633	GLU	CB-CG	5.17	1.61	1.52
1	B	460	TYR	CD2-CE2	5.15	1.47	1.39
1	A	33	GLU	CB-CG	5.11	1.61	1.52
1	B	400	TYR	CE2-CZ	5.11	1.45	1.38
1	B	361	GLU	CD-OE1	5.11	1.31	1.25
1	C	707	GLU	CG-CD	5.08	1.59	1.51
1	A	88	TYR	CD1-CE1	5.06	1.47	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	440	VAL	CB-CA-C	-8.53	95.19	111.40
1	B	451	LYS	CD-CE-NZ	-8.02	93.26	111.70
1	B	311	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	11	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	11	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	754	ILE	CG1-CB-CG2	-6.34	97.45	111.40
1	A	139	MET	CG-SD-CE	6.27	110.23	100.20
1	C	796	LYS	CD-CE-NZ	-6.23	97.37	111.70
1	D	1040	VAL	CB-CA-C	-6.02	99.97	111.40
1	A	89	LEU	CA-CB-CG	5.96	129.01	115.30
1	D	989	LEU	CA-CB-CG	5.96	129.01	115.30
1	C	779	LYS	N-CA-C	5.92	126.98	111.00
1	C	766	LYS	CB-CA-C	-5.88	98.64	110.40
1	B	311	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	D	1107	LEU	CA-CB-CG	5.84	128.74	115.30
1	C	689	LEU	CA-CB-CG	5.83	128.72	115.30
1	A	129	LEU	CA-CB-CG	5.80	128.65	115.30
1	B	411	LEU	CA-CB-CG	5.66	128.33	115.30
1	D	1110	LYS	CD-CE-NZ	5.66	124.71	111.70
1	D	1079	LYS	N-CA-C	5.63	126.19	111.00
1	B	330	VAL	CG1-CB-CG2	5.59	119.84	110.90
1	D	903	ASP	N-CA-C	5.56	126.01	111.00
1	B	450	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	B	479	LYS	N-CA-C	5.16	124.94	111.00
1	A	151	LYS	CB-CG-CD	5.16	125.00	111.60
1	B	440	VAL	CG1-CB-CG2	5.15	119.14	110.90
1	A	45	ASP	CB-CG-OD1	5.14	122.93	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1062	ASN	N-CA-C	-5.14	97.12	111.00
1	C	611	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	61	GLU	OE1-CD-OE2	5.12	129.45	123.30
1	B	454	ILE	CG1-CB-CG2	-5.11	100.15	111.40
1	D	988	TYR	CB-CA-C	-5.10	100.20	110.40
1	B	521	LYS	N-CA-C	5.06	124.66	111.00
1	B	455	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	C	640	GLN	CA-CB-CG	5.02	124.45	113.40

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 (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	1778	94	0
1	B	1823	0	1775	58	1
1	C	1823	0	1775	93	0
1	D	1823	0	1775	121	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	365	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 25.

All (365) 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
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: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:A:115:LYS:NZ	1:A:210:LYS:HD3	1.87	0.89
1:C:712:GLU:HG3	3:C:7000:HOH:O	1.70	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:A:115:LYS:HZ2	1:A:210:LYS:HD3	1.36	0.85
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:177:LYS:NZ	1:A:177:LYS:CB	2.44	0.79
1:C:729:LEU:HD12	1:C:730:SER:H	1.47	0.78
1:C:605:ASP:HB3	1:C:608:GLN:CD	2.04	0.77
1:B:451:LYS:HE2	1:B:455:ASP:OD2	1.83	0.77
1:D:1096:LYS:HG2	1:D:1097:TYR:N	1.97	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:670:LEU:HD23	1:C:670:LEU:C	2.08	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:D:970:LEU:C	1:D:970:LEU:HD23	2.09	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:C:820:THR:O	1:C:821:LYS:C	2.30	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:A:89:LEU:HD13	1:A:96:SER:CB	2.26	0.65
1:A:129:LEU:C	1:A:129:LEU:HD12	2.17	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: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: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: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:A:129:LEU:C	1:A:129:LEU:CD1	2.68	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: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:C:605:ASP:CB	1:C:608:GLN:CD	2.71	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:670:LEU:C	1:C:670:LEU:CD2	2.70	0.59
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
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:B:370:LEU:HD13	1:B:370:LEU:C	2.23	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: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:137:LYS:HB2	1:A:140:VAL:CG1	2.27	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:A:33:GLU:OE1	1:A:77:ASP:CG	2.43	0.57
1:C:756:ASN:O	1:C:757:LYS:NZ	2.36	0.56
1:B:344:HIS:HD2	1:B:502:LYS:HZ1	1.51	0.56
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: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: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:A:115:LYS:HZ2	1:A:210:LYS:HA	1.69	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:344:HIS:CD2	1:B:502:LYS:HZ1	2.23	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:C:740:VAL:C	1:C:806:THR:HG23	2.27	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:A:207:LEU:HD12	1:A:207:LEU:C	2.28	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:D:916:LYS:C	1:D:916:LYS:HD2	2.29	0.52
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:970:LEU:C	1:D:970:LEU:CD2	2.77	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:637:SER:OG	1:C:672:LYS:O	2.28	0.51
1:B:344:HIS:CD2	1:B:502:LYS:HZ3	2.27	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
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: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: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: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: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:D:905:ASP:O	1:D:906:PRO:C	2.51	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

Continued on next page...

Continued from previous page...

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:916:LYS:HZ2	1:D:1091:GLU:HG2	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:1089:GLU:O	1:D:1090:PRO:C	2.52	0.47
1:A:193:THR:O	1:A:196:LYS:HG2	2.15	0.47
1:D:905:ASP:OD1	1:D:905:ASP:C	2.53	0.47
1:D:1028:SER:O	1:D:1029:LEU:CB	2.48	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: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:16:LYS:O	1:A:17:ASN:HB2	2.16	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:36:LYS:C	1:A:37:SER:O	2.54	0.46
1:A:129:LEU:CD1	1:A:131:PHE:HD1	2.29	0.46
1:A:209:ASN:OD1	1:A:209:ASN:N	2.47	0.46
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:A:36:LYS:O	1:A:37:SER:C	2.53	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: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:1108:ASP:OD2	1:D:1111:THR:OG1	2.24	0.44
1:A:81:VAL:H	1:A:143:GLN:HE21	1.65	0.44

Continued on next page...

Continued from previous page...

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:115:LYS:HZ1	1:A:210:LYS:HD3	1.77	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:C:601:GLN:N	1:C:780:GLU:CD	2.71	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:1097:TYR:CD2	1:D:1097:TYR:C	2.92	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: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:D:1058:GLN:N	1:D:1058:GLN:CD	2.72	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: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:911:ARG:HH12	1:D:914:LEU:HG	1.84	0.42
1:D:970:LEU:HD23	1:D:970:LEU:O	2.19	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

Continued on next page...

Continued from previous page...

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:1037:LYS:O	1:D:1109:ASN:CG	2.58	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:A:176:PRO:O	1:A:177:LYS:C	2.58	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:C:706:HIS:ND1	1:C:706:HIS:C	2.74	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:C:756:ASN:C	1:C:757:LYS:HZ1	2.24	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: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%)	8 2
1	B	219/221 (99%)	208 (95%)	11 (5%)	0	100 100
1	C	219/221 (99%)	211 (96%)	6 (3%)	2 (1%)	17 7
1	D	219/221 (99%)	195 (89%)	19 (9%)	5 (2%)	6 1
All	All	876/884 (99%)	820 (94%)	45 (5%)	11 (1%)	12 4

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%)	190 (91%)	18 (9%)	10 2
1	B	208/208 (100%)	195 (94%)	13 (6%)	18 5
1	C	208/208 (100%)	199 (96%)	9 (4%)	29 14
1	D	208/208 (100%)	186 (89%)	22 (11%)	6 1
All	All	832/832 (100%)	770 (92%)	62 (8%)	13 3

All (62) 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	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	413	ILE
1	B	427	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	440	VAL
1	B	454	ILE
1	B	458	GLN
1	B	478	ASN
1	B	488	PRO
1	B	496	LYS
1	B	507	LEU
1	C	602	GLN
1	C	619	GLN
1	C	640	GLN
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	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
1	D	1110	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	8	GLN
1	A	40	GLN
1	A	106	HIS
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	375	ASN
1	B	406	HIS
1	B	410	HIS
1	B	443	GLN
1	B	458	GLN
1	C	601	GLN
1	C	602	GLN
1	C	608	GLN
1	C	619	GLN
1	C	743	GLN
1	C	794	GLN
1	C	809	ASN
1	D	901	GLN
1	D	908	GLN
1	D	919	GLN
1	D	934	ASN
1	D	965	GLN
1	D	1006	HIS
1	D	1043	GLN
1	D	1056	ASN
1	D	1058	GLN
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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.