Full wwPDB X-ray Structure Validation Report ⓘ

Dec 5, 2023 – 01:49 am GMT

PDB ID	:	1UUP
Title	:	Crystal Structure of A Dimeric Form of Streptococcal Pyrogenic Exotoxin A (SpeA1).
Authors	:	Baker, M.D.; Gendlina, I.; Collins, C.M.; Acharya, K.R.
Deposited on	:	2004-01-08
Resolution	:	2.60 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:

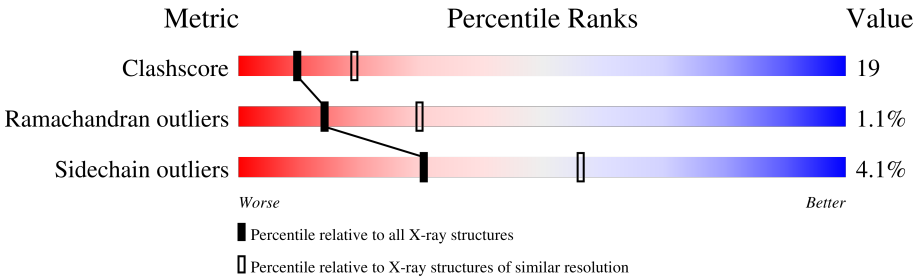
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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	62% 35% .
1	B	221	67% 28% 5%
1	C	221	69% 28% .
1	D	221	65% 33% .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7388 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1812	1158	291	357	6			
1	B	221	Total	C	N	O	S	0	0	0
			1812	1158	291	357	6			
1	C	221	Total	C	N	O	S	0	0	0
			1812	1158	291	357	6			
1	D	221	Total	C	N	O	S	0	0	0
			1812	1158	291	357	6			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	27	Total	O	0	0
			27	27		
3	C	37	Total	O	0	0
			37	37		
3	D	36	Total	O	0	0
			36	36		

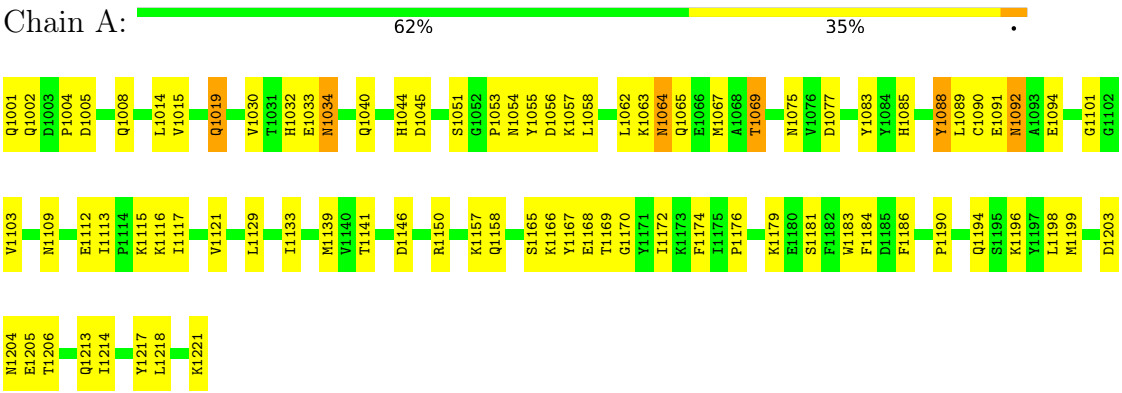
3 Residue-property plots (i)

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.

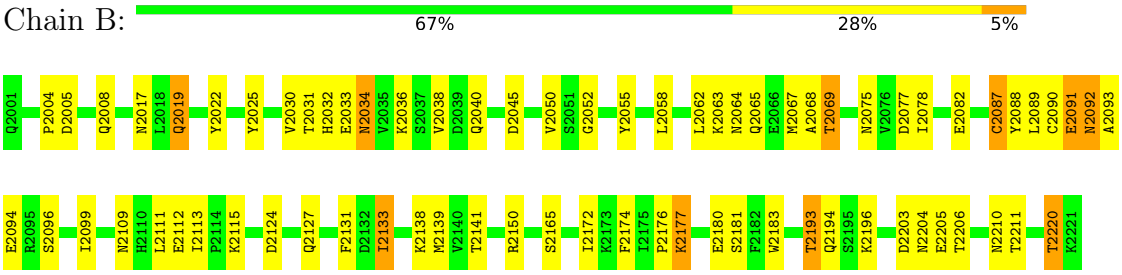
• Molecule 1: EXOTOXIN TYPE A

Chain A:



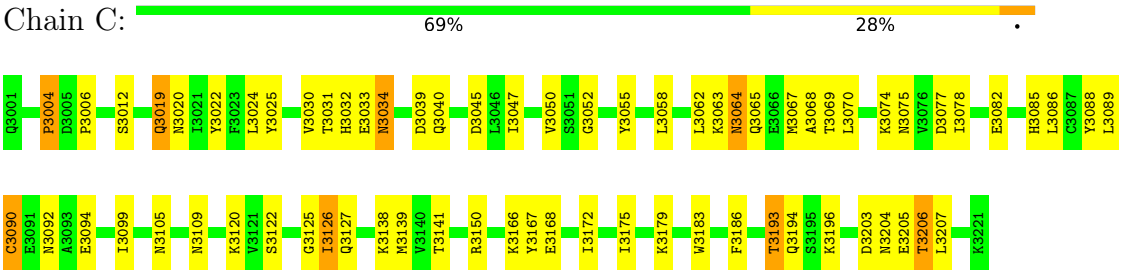
• Molecule 1: EXOTOXIN TYPE A

Chain B:



• Molecule 1: EXOTOXIN TYPE A

Chain C:



• Molecule 1: EXOTOXIN TYPE A

Chain D:


Q4001
P4004
Q4008
L4009
H4010
R4011
L4014
V4015
K4016
N4017
L4018
Q4019
Y4022
E4026
V4030
T4031
N4034
V4035
K4036
D4039
Q4040
L4041
H4044
D4045
L4046
I4047
G4052
Y4055
D4056
E4061
L4062
K4063
N4064
Q4065
E4066
M4067
A4068
T4069
L4070
D4073
K4074
N4075
V4076
D4077
I4078
Y4079
E4082
C4087
Y4088
L4089
C4090
E4091
N4092
A4093
E4094
R4095
I4099
T4104
N4109
K4115
I4133
K4138
M4139
V4140
T4141
E4144
K4148
K4151
Y4152
D4155
N4156
T4161
N4162
G4163
K4166
G4170
K4177
N4178
F4182
W4183
F4187
E4191
F4192
T4193
K4196
N4204
E4205
T4206
N4210
Y4217
K4221

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	53.30Å 127.20Å 148.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	89.0 (20.00-2.60)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7388	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.42	0/1854	0.65	0/2510
1	B	0.38	0/1854	0.66	0/2510
1	C	0.40	0/1854	0.64	0/2510
1	D	0.38	0/1854	0.62	0/2510
All	All	0.40	0/7416	0.64	0/10040

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1812	0	1752	75	0
1	B	1812	0	1752	65	0
1	C	1812	0	1752	63	0
1	D	1812	0	1752	82	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	36	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	0	2	0
3	C	37	0	0	7	0
3	D	36	0	0	0	0
All	All	7388	0	7008	277	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 19.

All (277) 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:B:2063:LYS:H	1:B:2067:MET:HE2	1.04	1.09
1:C:3062:LEU:HB3	1:C:3067:MET:HE2	1.33	1.03
1:B:2115:LYS:HE2	1:B:2210:ASN:HA	1.43	1.00
1:A:1063:LYS:H	1:A:1067:MET:HE2	1.31	0.95
1:D:4062:LEU:HB3	1:D:4067:MET:HE2	1.47	0.94
1:B:2092:ASN:HD22	1:B:2092:ASN:H	1.16	0.93
1:B:2088:TYR:HE1	1:B:2090:CYS:HB3	1.31	0.92
1:B:2063:LYS:N	1:B:2067:MET:HE2	1.86	0.90
1:B:2109:ASN:HD21	1:B:2139:MET:H	1.13	0.90
1:A:1062:LEU:HB3	1:A:1067:MET:HE2	1.53	0.89
1:A:1109:ASN:HD21	1:A:1139:MET:H	1.20	0.88
1:D:4193:THR:HG22	1:D:4196:LYS:H	1.38	0.86
3:A:2003:HOH:O	1:D:4094:GLU:HG3	1.75	0.86
1:D:4011:ARG:HB2	1:D:4014:LEU:HD13	1.55	0.85
1:D:4063:LYS:H	1:D:4067:MET:HE2	1.39	0.84
1:D:4063:LYS:H	1:D:4067:MET:CE	1.94	0.80
1:B:2193:THR:HG22	1:B:2196:LYS:H	1.46	0.79
1:A:1103:VAL:H	1:A:1204:ASN:HD21	1.29	0.79
1:C:3019:GLN:H	1:C:3019:GLN:HE21	1.32	0.78
1:A:1034:ASN:ND2	1:A:1075:ASN:HB3	1.98	0.78
1:C:3033:GLU:HG2	3:C:2005:HOH:O	1.84	0.78
1:A:1063:LYS:H	1:A:1067:MET:CE	2.00	0.75
1:B:2089:LEU:HG	1:D:4088:TYR:OH	1.87	0.75
1:D:4017:ASN:HA	1:D:4019:GLN:HE22	1.52	0.74
1:D:4062:LEU:HD22	1:D:4067:MET:HE3	1.68	0.74
1:C:3109:ASN:HD21	1:C:3139:MET:H	1.36	0.73
1:C:3019:GLN:H	1:C:3019:GLN:NE2	1.86	0.73
1:D:4019:GLN:H	1:D:4019:GLN:NE2	1.89	0.71
1:D:4088:TYR:HD1	1:D:4090:CYS:H	1.39	0.70
1:C:3069:THR:HG23	3:C:2006:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4010:HIS:HD2	1:D:4187:PHE:O	1.73	0.70
1:B:2019:GLN:H	1:B:2019:GLN:NE2	1.89	0.70
1:A:1005:ASP:HB3	1:A:1008:GLN:HB2	1.74	0.69
1:A:1116:LYS:HE2	3:A:2024:HOH:O	1.92	0.69
1:A:1067:MET:HE3	1:A:1204:ASN:HB2	1.73	0.69
1:A:1069:THR:HG21	3:A:2012:HOH:O	1.91	0.69
1:A:1019:GLN:H	1:A:1019:GLN:NE2	1.91	0.69
1:B:2065:GLN:O	1:B:2069:THR:HG23	1.92	0.68
1:A:1121:VAL:HB	1:A:1129:LEU:HB3	1.75	0.68
1:D:4133:ILE:HD12	1:D:4148:LYS:HB3	1.76	0.68
1:C:3193:THR:HG21	3:C:2030:HOH:O	1.93	0.67
1:D:4089:LEU:O	1:D:4090:CYS:HB2	1.93	0.67
1:C:3120:LYS:HD3	1:C:3127:GLN:HE22	1.60	0.67
1:D:4040:GLN:HG3	1:D:4045:ASP:O	1.96	0.66
1:C:3090:CYS:HB3	1:C:3092:ASN:OD1	1.96	0.65
1:C:3085:HIS:O	1:C:3086:LEU:HB2	1.95	0.65
1:C:3063:LYS:H	1:C:3067:MET:HE2	1.61	0.65
1:D:4089:LEU:HD12	1:D:4089:LEU:N	2.12	0.65
1:B:2019:GLN:H	1:B:2019:GLN:HE21	1.44	0.64
1:C:3109:ASN:ND2	1:C:3138:LYS:HB2	2.12	0.64
1:B:2092:ASN:HD22	1:B:2092:ASN:N	1.88	0.64
1:A:1063:LYS:N	1:A:1067:MET:HE2	2.10	0.64
1:D:4030:VAL:HG13	1:D:4055:TYR:OH	1.97	0.64
1:C:3089:LEU:HD12	1:C:3089:LEU:N	2.12	0.64
1:B:2040:GLN:HG3	1:B:2045:ASP:O	1.98	0.63
1:A:1088:TYR:HE1	1:A:1090:CYS:HB2	1.64	0.63
1:C:3206:THR:HG21	3:C:2015:HOH:O	1.98	0.63
1:D:4017:ASN:HA	1:D:4019:GLN:NE2	2.14	0.63
1:D:4193:THR:CG2	1:D:4196:LYS:H	2.12	0.63
1:B:2091:GLU:CD	1:B:2091:GLU:H	2.00	0.62
1:A:1062:LEU:HD22	1:A:1067:MET:HE3	1.80	0.62
1:A:1019:GLN:H	1:A:1019:GLN:HE21	1.47	0.62
1:A:1033:GLU:O	1:A:1077:ASP:OD1	2.16	0.62
1:C:3175:ILE:HD12	1:C:3175:ILE:N	2.14	0.62
1:C:3193:THR:HG22	1:C:3196:LYS:H	1.64	0.62
1:B:2082:GLU:HA	1:B:2099:ILE:HG22	1.82	0.62
1:C:3063:LYS:H	1:C:3067:MET:CE	2.12	0.62
1:C:3125:GLY:O	1:C:3126:ILE:HG13	2.00	0.61
1:D:4063:LYS:N	1:D:4067:MET:HE2	2.14	0.61
1:A:1139:MET:HG3	3:A:2033:HOH:O	1.99	0.61
1:B:2033:GLU:O	1:B:2077:ASP:OD1	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4109:ASN:HD21	1:D:4139:MET:H	1.47	0.61
1:A:1030:VAL:HG11	1:A:1058:LEU:HD22	1.82	0.61
1:D:4141:THR:HA	1:D:4206:THR:HA	1.82	0.61
1:D:4016:LYS:HD2	1:D:4191:GLU:OE1	2.01	0.61
1:A:1062:LEU:HD23	1:A:1101:GLY:HA2	1.83	0.60
1:C:3062:LEU:CB	1:C:3067:MET:HE2	2.21	0.60
1:A:1064:ASN:ND2	1:A:1067:MET:H	1.98	0.60
1:A:1109:ASN:ND2	1:A:1139:MET:H	1.98	0.60
1:A:1170:GLY:HA2	1:A:1217:TYR:O	2.01	0.60
1:C:3089:LEU:O	1:C:3090:CYS:HB2	2.00	0.59
1:D:4004:PRO:HA	1:D:4008:GLN:OE1	2.02	0.59
1:B:2088:TYR:CE1	1:B:2090:CYS:HB3	2.24	0.59
1:A:1205:GLU:OE2	1:A:1205:GLU:HA	2.03	0.58
1:C:3004:PRO:HB3	1:C:3183:TRP:CZ2	2.38	0.58
1:A:1085:HIS:ND1	1:D:4094:GLU:OE1	2.37	0.58
1:B:2005:ASP:N	1:B:2008:GLN:OE1	2.36	0.58
1:A:1030:VAL:HG13	1:A:1055:TYR:OH	2.03	0.57
1:B:2094:GLU:OE2	1:C:3085:HIS:HD2	1.87	0.57
1:C:3030:VAL:HG13	1:C:3055:TYR:OH	2.05	0.57
1:B:2177:LYS:HB3	3:B:3018:HOH:O	2.03	0.57
1:B:2092:ASN:H	1:B:2092:ASN:ND2	1.96	0.56
1:C:3062:LEU:HD12	1:C:3068:ALA:HA	1.87	0.56
1:B:2124:ASP:OD2	1:B:2220:THR:HG23	2.06	0.56
1:D:4089:LEU:O	1:D:4090:CYS:CB	2.53	0.56
1:B:2131:PHE:HE1	1:B:2133:ILE:HD13	1.70	0.56
1:C:3012:SER:HB3	3:C:2037:HOH:O	2.05	0.56
1:A:1067:MET:CE	1:A:1204:ASN:HB2	2.35	0.56
1:B:2062:LEU:HB3	1:B:2067:MET:HG2	1.87	0.56
1:C:3082:GLU:HA	1:C:3099:ILE:HG22	1.88	0.56
1:D:4151:LYS:HE3	1:D:4155:ASP:OD1	2.06	0.56
1:C:3067:MET:HE3	1:C:3204:ASN:HB2	1.89	0.55
1:B:2141:THR:HA	1:B:2206:THR:HA	1.87	0.55
1:C:3034:ASN:ND2	1:C:3075:ASN:HB3	2.22	0.55
1:B:2091:GLU:OE2	1:B:2091:GLU:N	2.28	0.55
1:D:4019:GLN:H	1:D:4019:GLN:HE21	1.52	0.55
1:A:1051:SER:CB	1:A:1056:ASP:HA	2.36	0.55
1:B:2194:GLN:HG3	1:C:3094:GLU:OE1	2.07	0.54
1:A:1001:GLN:HG3	1:A:1002:GLN:H	1.73	0.54
1:D:4062:LEU:CB	1:D:4067:MET:HE2	2.31	0.54
1:D:4089:LEU:N	1:D:4089:LEU:CD1	2.71	0.54
1:D:4166:LYS:O	1:D:4166:LYS:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3019:GLN:O	1:C:3022:TYR:HB3	2.08	0.53
1:C:3141:THR:HA	1:C:3206:THR:HA	1.91	0.53
1:D:4182:PHE:CZ	1:D:4205:GLU:HG2	2.43	0.53
1:D:4087:CYS:O	1:D:4088:TYR:HB3	2.09	0.53
1:D:4065:GLN:O	1:D:4069:THR:HG23	2.09	0.53
1:D:4026:GLU:OE2	1:D:4026:GLU:HA	2.08	0.53
1:B:2141:THR:HG22	1:B:2206:THR:HG22	1.91	0.52
1:D:4115:LYS:HE2	1:D:4210:ASN:HA	1.91	0.52
1:D:4047:ILE:HD13	1:D:4089:LEU:HD23	1.90	0.52
1:D:4052:GLY:HA3	1:D:4055:TYR:CE2	2.43	0.52
1:A:1088:TYR:CE1	1:A:1090:CYS:HB2	2.43	0.52
1:D:4193:THR:HG22	1:D:4196:LYS:N	2.18	0.52
1:C:3062:LEU:HD22	1:C:3067:MET:HE3	1.92	0.52
1:D:4010:HIS:CD2	1:D:4187:PHE:O	2.60	0.52
1:A:1062:LEU:CB	1:A:1067:MET:HE2	2.35	0.51
1:B:2067:MET:HE3	1:B:2204:ASN:HB2	1.93	0.51
1:A:1176:PRO:HG2	1:A:1179:LYS:O	2.10	0.51
1:D:4070:LEU:O	1:D:4074:LYS:HD2	2.10	0.51
1:A:1064:ASN:C	1:A:1064:ASN:HD22	2.12	0.51
1:B:2088:TYR:HE1	1:B:2090:CYS:CB	2.12	0.50
1:B:2177:LYS:N	3:B:3017:HOH:O	2.45	0.50
1:D:4062:LEU:HB3	1:D:4067:MET:CE	2.29	0.50
1:A:1054:ASN:N	1:A:1054:ASN:HD22	2.07	0.50
1:D:4141:THR:HG22	1:D:4206:THR:HG22	1.92	0.50
1:C:3168:GLU:OE2	1:C:3168:GLU:HA	2.12	0.50
1:B:2174:PHE:O	1:B:2181:SER:HB2	2.12	0.50
1:C:3172:ILE:HB	1:C:3186:PHE:CE2	2.47	0.50
1:D:4088:TYR:HD1	1:D:4090:CYS:N	2.07	0.50
1:B:2034:ASN:ND2	1:B:2075:ASN:HB3	2.27	0.50
1:D:4011:ARG:NH2	1:D:4014:LEU:HD11	2.27	0.50
1:A:1065:GLN:O	1:A:1069:THR:HG23	2.12	0.49
1:A:1141:THR:HA	1:A:1206:THR:HA	1.94	0.49
1:D:4221:LYS:OXT	1:D:4221:LYS:HG2	2.12	0.49
1:D:4170:GLY:HA2	1:D:4217:TYR:O	2.13	0.49
1:C:3088:TYR:HD2	1:C:3090:CYS:O	1.96	0.49
1:B:2088:TYR:CD1	1:B:2093:ALA:HB3	2.47	0.49
1:D:4082:GLU:HA	1:D:4099:ILE:HG22	1.94	0.49
1:B:2090:CYS:HB3	1:B:2092:ASN:HD21	1.76	0.49
1:B:2090:CYS:HB3	1:B:2092:ASN:ND2	2.28	0.49
1:D:4044:HIS:HD2	1:D:4061:GLU:HG3	1.77	0.49
1:D:4064:ASN:C	1:D:4064:ASN:HD22	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2004:PRO:HB3	1:B:2183:TRP:CZ2	2.48	0.49
1:C:3064:ASN:C	1:C:3064:ASN:HD22	2.15	0.49
1:A:1165:SER:O	1:A:1221:LYS:HE3	2.13	0.49
1:B:2094:GLU:OE1	1:C:3194:GLN:HG3	2.13	0.49
1:B:2111:LEU:HD21	1:B:2138:LYS:HG2	1.95	0.49
1:C:3020:ASN:O	1:C:3024:LEU:HG	2.12	0.49
1:A:1051:SER:HB3	1:A:1056:ASP:HA	1.95	0.48
1:B:2172:ILE:O	1:B:2172:ILE:HG23	2.13	0.48
1:C:3040:GLN:HG3	1:C:3045:ASP:O	2.13	0.48
1:D:4056:ASP:OD1	1:D:4095:ARG:HB2	2.12	0.48
1:B:2177:LYS:HD3	1:B:2211:THR:OG1	2.12	0.48
1:C:3089:LEU:N	1:C:3089:LEU:CD1	2.75	0.48
1:A:1089:LEU:HB3	1:C:3088:TYR:OH	2.13	0.48
1:C:3052:GLY:HA3	1:C:3055:TYR:CE2	2.47	0.48
1:C:3074:LYS:HD3	1:C:3105:ASN:OD1	2.14	0.48
1:B:2017:ASN:HA	1:B:2019:GLN:NE2	2.29	0.48
1:C:3166:LYS:HD2	1:C:3167:TYR:CZ	2.47	0.48
1:D:4109:ASN:ND2	1:D:4138:LYS:HB2	2.28	0.48
1:C:3064:ASN:ND2	1:C:3067:MET:H	2.11	0.48
1:C:3141:THR:HG23	3:C:2020:HOH:O	2.12	0.48
1:B:2112:GLU:HG3	1:B:2113:ILE:HG13	1.95	0.48
1:A:1034:ASN:HD21	1:A:1075:ASN:HB3	1.71	0.48
1:D:4109:ASN:HD21	1:D:4139:MET:N	2.11	0.48
1:A:1129:LEU:HD22	1:A:1157:LYS:HE3	1.96	0.48
1:A:1146:ASP:O	1:A:1150:ARG:HG3	2.14	0.47
1:B:2093:ALA:HB1	1:B:2096:SER:OG	2.14	0.47
1:A:1103:VAL:H	1:A:1204:ASN:ND2	2.06	0.47
1:B:2082:GLU:CA	1:B:2099:ILE:HG22	2.43	0.47
1:B:2032:HIS:CD2	1:B:2050:VAL:HG21	2.48	0.47
1:C:3065:GLN:HB2	3:C:2006:HOH:O	2.15	0.47
1:A:1213:GLN:C	1:A:1214:ILE:HD13	2.34	0.47
1:B:2052:GLY:HA3	1:B:2055:TYR:CE2	2.48	0.47
1:B:2131:PHE:CE1	1:B:2133:ILE:HD13	2.48	0.47
1:B:2176:PRO:HD3	1:B:2181:SER:HA	1.96	0.47
1:C:3031:THR:HA	1:C:3078:ILE:O	2.15	0.47
1:D:4034:ASN:ND2	1:D:4075:ASN:HB3	2.30	0.47
1:C:3025:TYR:CE2	1:C:3150:ARG:HD2	2.50	0.47
1:C:3019:GLN:HE21	1:C:3019:GLN:N	2.07	0.47
1:B:2036:LYS:HE3	1:B:2075:ASN:OD1	2.16	0.46
1:D:4204:ASN:O	1:D:4206:THR:HG23	2.16	0.46
1:A:1166:LYS:HD2	1:A:1167:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4031:THR:HA	1:D:4078:ILE:O	2.15	0.46
1:D:4076:VAL:HB	1:D:4104:THR:O	2.15	0.46
1:A:1005:ASP:HB3	1:A:1008:GLN:CB	2.42	0.46
1:A:1117:ILE:HB	1:A:1133:ILE:HG22	1.98	0.46
1:D:4004:PRO:HD3	1:D:4183:TRP:CE2	2.51	0.46
1:D:4133:ILE:HD13	1:D:4133:ILE:HA	1.79	0.46
1:A:1053:PRO:O	1:A:1054:ASN:HB2	2.15	0.46
1:A:1194:GLN:HG3	1:D:4094:GLU:OE2	2.16	0.46
1:A:1196:LYS:O	1:A:1199:MET:HG3	2.15	0.46
1:B:2017:ASN:HA	1:B:2019:GLN:HE22	1.81	0.46
1:D:4019:GLN:O	1:D:4022:TYR:HB3	2.16	0.46
1:B:2203:ASP:CG	1:B:2205:GLU:HG2	2.36	0.46
1:A:1053:PRO:O	3:A:2009:HOH:O	2.21	0.45
1:A:1092:ASN:C	1:A:1092:ASN:ND2	2.70	0.45
1:C:3030:VAL:HG11	1:C:3058:LEU:HD22	1.98	0.45
1:D:4036:LYS:NZ	1:D:4073:ASP:O	2.38	0.45
1:A:1094:GLU:OE1	1:D:4193:THR:HA	2.17	0.45
1:B:2176:PRO:CD	1:B:2181:SER:HA	2.47	0.45
1:C:3039:ASP:HB3	1:C:3047:ILE:HB	1.99	0.45
1:D:4088:TYR:C	1:D:4089:LEU:HD12	2.37	0.45
1:A:1067:MET:HE3	1:A:1204:ASN:CB	2.45	0.45
1:C:3064:ASN:HD22	1:C:3067:MET:H	1.63	0.45
1:C:3082:GLU:CA	1:C:3099:ILE:HG22	2.47	0.45
1:D:4152:TYR:CE1	1:D:4156:ASN:ND2	2.85	0.45
1:C:3203:ASP:OD2	1:C:3205:GLU:HB2	2.17	0.44
1:A:1112:GLU:HG3	1:A:1113:ILE:HG13	1.98	0.44
1:C:3033:GLU:HA	1:C:3077:ASP:OD1	2.18	0.44
1:A:1054:ASN:N	1:A:1054:ASN:ND2	2.65	0.44
1:B:2030:VAL:HG11	1:B:2058:LEU:HD22	1.98	0.44
1:C:3032:HIS:CD2	1:C:3050:VAL:HB	2.52	0.44
1:A:1170:GLY:HA3	1:A:1218:LEU:HD23	2.00	0.44
1:A:1069:THR:HG22	3:A:2006:HOH:O	2.17	0.44
1:A:1206:THR:HG21	3:A:2022:HOH:O	2.18	0.44
1:D:4067:MET:CE	1:D:4204:ASN:HB2	2.47	0.44
1:D:4161:THR:O	1:D:4163:GLY:N	2.50	0.44
1:B:2019:GLN:O	1:B:2022:TYR:HB3	2.18	0.43
1:D:4079:TYR:CD2	1:D:4144:GLU:HG3	2.53	0.43
1:A:1203:ASP:OD1	1:A:1205:GLU:N	2.45	0.43
1:D:4193:THR:HG22	1:D:4196:LYS:HG2	2.00	0.43
1:B:2087:CYS:SG	1:B:2088:TYR:N	2.90	0.43
1:D:4193:THR:CG2	1:D:4196:LYS:HG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4067:MET:HE3	1:D:4204:ASN:HB2	2.00	0.43
1:A:1089:LEU:O	1:A:1090:CYS:SG	2.77	0.43
1:A:1172:ILE:HB	1:A:1186:PHE:CE2	2.53	0.43
1:B:2067:MET:CE	1:B:2204:ASN:HB2	2.48	0.43
1:A:1169:THR:HA	3:A:2026:HOH:O	2.19	0.42
1:C:3032:HIS:NE2	1:C:3050:VAL:HB	2.34	0.42
1:D:4030:VAL:HG23	1:D:4082:GLU:OE2	2.19	0.42
1:A:1168:GLU:OE2	1:A:1168:GLU:HA	2.18	0.42
1:A:1015:VAL:HA	1:A:1190:PRO:HA	2.01	0.42
1:A:1157:LYS:O	1:A:1158:GLN:HB2	2.20	0.42
1:A:1040:GLN:HG3	1:A:1045:ASP:O	2.19	0.42
1:B:2180:GLU:OE2	1:B:2180:GLU:HA	2.20	0.42
1:D:4011:ARG:HH21	1:D:4014:LEU:HD11	1.83	0.42
1:A:1032:HIS:HE1	1:A:1055:TYR:OH	2.02	0.42
1:C:3067:MET:CE	1:C:3204:ASN:HB2	2.49	0.42
1:C:3085:HIS:CE1	1:C:3086:LEU:HD13	2.55	0.42
1:D:4011:ARG:NE	1:D:4014:LEU:HD11	2.35	0.42
1:D:4019:GLN:HE21	1:D:4019:GLN:N	2.16	0.42
1:D:4089:LEU:H	1:D:4093:ALA:CB	2.33	0.42
1:A:1174:PHE:CE2	1:A:1214:ILE:HD12	2.55	0.42
1:B:2025:TYR:CE2	1:B:2150:ARG:HD2	2.55	0.42
1:B:2062:LEU:HD12	1:B:2068:ALA:HA	2.01	0.42
1:D:4079:TYR:CG	1:D:4144:GLU:HG3	2.55	0.42
1:D:4082:GLU:CA	1:D:4099:ILE:HG22	2.49	0.42
1:A:1083:TYR:CD2	1:A:1198:LEU:HD12	2.55	0.42
1:D:4177:LYS:HG3	1:D:4178:ASN:ND2	2.34	0.42
1:C:3109:ASN:HA	1:C:3138:LYS:HD2	2.01	0.41
1:A:1213:GLN:O	1:A:1214:ILE:HD13	2.20	0.41
1:A:1172:ILE:HG22	1:A:1184:PHE:HB2	2.02	0.41
1:B:2004:PRO:HD3	1:B:2183:TRP:CD1	2.56	0.41
1:B:2193:THR:HG22	1:B:2196:LYS:HG2	2.02	0.41
1:D:4041:LEU:HB3	1:D:4045:ASP:OD2	2.21	0.41
1:B:2034:ASN:HD21	1:B:2075:ASN:HB3	1.85	0.41
1:C:3126:ILE:O	1:C:3127:GLN:C	2.57	0.41
1:D:4039:ASP:CG	1:D:4040:GLN:H	2.23	0.41
1:A:1176:PRO:HD2	1:A:1181:SER:HA	2.03	0.40
1:B:2088:TYR:CD1	1:B:2088:TYR:C	2.94	0.40
1:D:4079:TYR:CD1	1:D:4144:GLU:HG3	2.56	0.40
1:A:1004:PRO:HB3	1:A:1183:TRP:CZ2	2.56	0.40
1:B:2031:THR:HA	1:B:2078:ILE:O	2.22	0.40
1:C:3070:LEU:O	1:C:3074:LYS:NZ	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1203:ASP:OD1	1:A:1203:ASP:C	2.60	0.40

There are no symmetry-related clashes.

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%)	200 (91%)	18 (8%)	1 (0%)	29	52
1	B	219/221 (99%)	200 (91%)	16 (7%)	3 (1%)	11	22
1	C	219/221 (99%)	203 (93%)	11 (5%)	5 (2%)	6	11
1	D	219/221 (99%)	204 (93%)	14 (6%)	1 (0%)	29	52
All	All	876/884 (99%)	807 (92%)	59 (7%)	10 (1%)	14	30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1091	GLU
1	C	3090	CYS
1	D	4090	CYS
1	B	2087	CYS
1	B	2091	GLU
1	C	3179	LYS
1	B	2177	LYS
1	C	3006	PRO
1	C	3004	PRO
1	C	3126	ILE

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	206/208 (99%)	196 (95%)	10 (5%)	25 48
1	B	206/208 (99%)	195 (95%)	11 (5%)	22 45
1	C	206/208 (99%)	199 (97%)	7 (3%)	37 63
1	D	206/208 (99%)	200 (97%)	6 (3%)	42 68
All	All	824/832 (99%)	790 (96%)	34 (4%)	30 56

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1014	LEU
1	A	1019	GLN
1	A	1034	ASN
1	A	1044	HIS
1	A	1057	LYS
1	A	1064	ASN
1	A	1069	THR
1	A	1088	TYR
1	A	1092	ASN
1	A	1115	LYS
1	B	2019	GLN
1	B	2034	ASN
1	B	2038	VAL
1	B	2064	ASN
1	B	2069	THR
1	B	2092	ASN
1	B	2127	GLN
1	B	2133	ILE
1	B	2165	SER
1	B	2193	THR
1	B	2220	THR
1	C	3019	GLN
1	C	3034	ASN
1	C	3064	ASN

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Mol	Chain	Res	Type
1	C	3122	SER
1	C	3193	THR
1	C	3206	THR
1	C	3207	LEU
1	D	4019	GLN
1	D	4064	ASN
1	D	4089	LEU
1	D	4092	ASN
1	D	4166	LYS
1	D	4193	THR

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	1001	GLN
1	A	1019	GLN
1	A	1032	HIS
1	A	1034	ASN
1	A	1044	HIS
1	A	1054	ASN
1	A	1064	ASN
1	A	1065	GLN
1	A	1092	ASN
1	A	1109	ASN
1	A	1127	GLN
1	A	1156	ASN
1	A	1204	ASN
1	B	2001	GLN
1	B	2019	GLN
1	B	2034	ASN
1	B	2064	ASN
1	B	2065	GLN
1	B	2092	ASN
1	B	2109	ASN
1	B	2110	HIS
1	C	3008	GLN
1	C	3019	GLN
1	C	3032	HIS
1	C	3034	ASN
1	C	3049	ASN
1	C	3064	ASN
1	C	3065	GLN

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Mol	Chain	Res	Type
1	C	3106	HIS
1	C	3109	ASN
1	C	3156	ASN
1	D	4010	HIS
1	D	4019	GLN
1	D	4034	ASN
1	D	4040	GLN
1	D	4064	ASN
1	D	4065	GLN
1	D	4109	ASN
1	D	4156	ASN
1	D	4178	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.