



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2017 – 06:20 AM EDT

PDB ID : 1FNV  
Title : STRUCTURE OF STREPTOCOCCAL PYROGENIC EXOTOXIN A  
Authors : Earhart, C.A.; Vath, G.M.; Roggiani, M.; Schlievert, P.M.; Ohlendorf, D.H.  
Deposited on : unknown  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

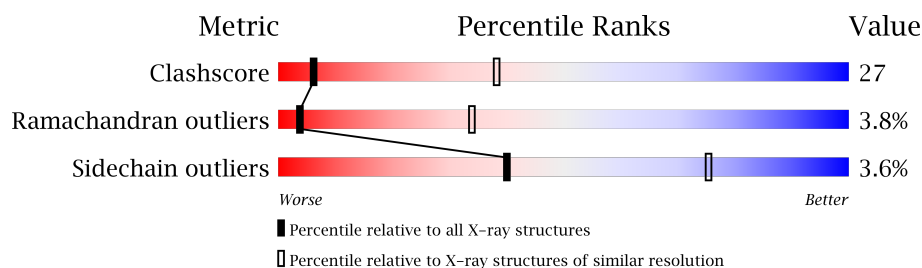
# 1 Overall quality at a glance

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	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

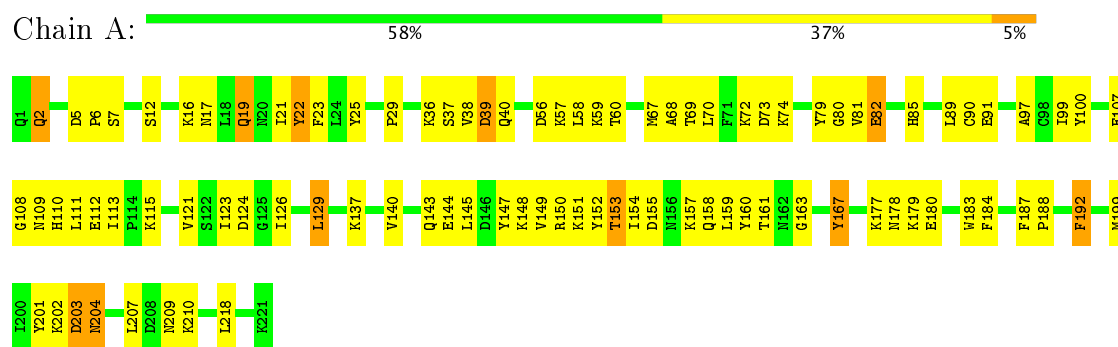
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total 4	Cd 4	0	0
2	A	3	Total 3	Cd 3	0	0
2	D	4	Total 4	Cd 4	0	0
2	C	5	Total 5	Cd 5	0	0

### 3 Residue-property plots

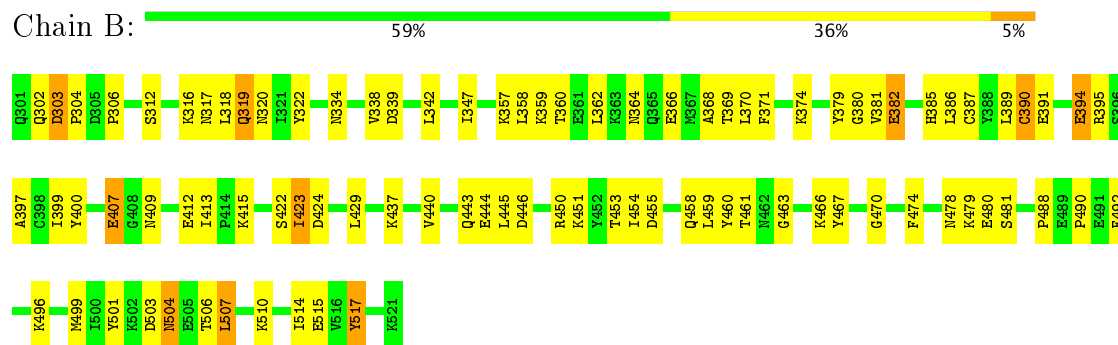
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

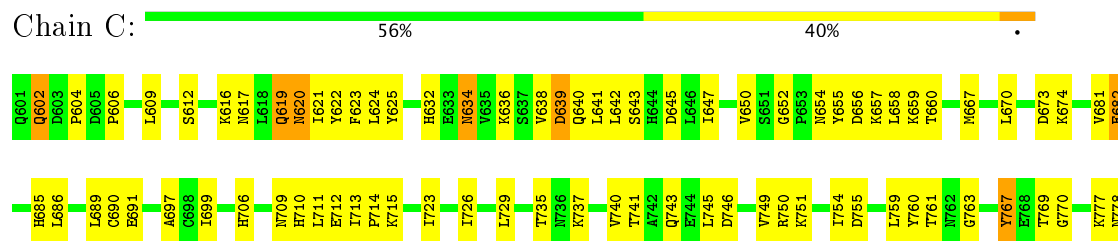
#### • Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

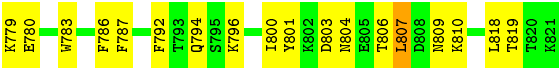


#### • Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

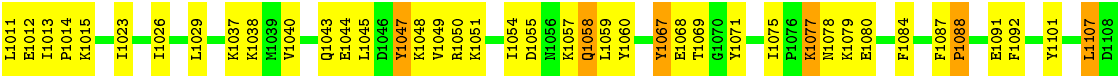


#### • Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)





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



## 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	15.0	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	0.45	0/1865	0.73	0/2522
1	B	0.44	0/1865	0.72	2/2522 (0.1%)
1	C	0.43	0/1865	0.72	0/2522
1	D	0.44	0/1865	0.71	0/2522
All	All	0.44	0/7460	0.72	2/10088 (0.0%)

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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	394	GLU	N-CA-C	-5.17	97.03	111.00
1	B	387	CYS	CA-CB-SG	5.15	123.26	114.00

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 ⓘ

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	104	0
1	B	1823	0	1776	92	0
1	C	1823	0	1776	103	0
1	D	1823	0	1776	104	0
2	A	3	0	0	0	0
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	387	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 27.

All (387) 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:NE2	1:B:319:GLN:H	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:NE2	1:D:919:GLN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:VAL:H	1:B:443:GLN:HE21	1.20	0.83
1:D:919:GLN:N	1:D:919:GLN:HE21	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
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: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:NE2	1:A:2:GLN:H	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:437:LYS:HB2	1:B:440:VAL:HG12	1.74	0.69
1:B:379:TYR:CD2	1:B:444:GLU:HG3	2.28	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:112:GLU:C	1:A:113:ILE:HD12	2.14	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:660:THR:O	1:C:660:THR:HG23	1.95	0.64
1:A:167:TYR:N	1:A:167:TYR:CD1	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:CD1	1:D:1067:TYR:N	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:192:PHE:CD1	1:A:192:PHE:C	2.71	0.62
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:C:806:THR:HG22	1:C:807:LEU:N	2.15	0.62
1:A:70:LEU:O	1:A:70:LEU:HD23	2.00	0.61
1:C:619:GLN:H	1:C:619:GLN:NE2	1.98	0.61
1:A:115:LYS:CE	1:A:210:LYS:HD3	2.31	0.61
1:C:658:LEU:HD12	1:C:697:ALA:O	2.00	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:D:1012:GLU:C	1:D:1013:ILE:HD12	2.21	0.60
1:D:1015:LYS:HG2	1:D:1109:ASN:ND2	2.15	0.60
1:B:412:GLU:C	1:B:413:ILE:HD12	2.22	0.59
1:B:370:LEU:O	1:B:370:LEU:HD23	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:N	1:C:602:GLN:NE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:767:TYR:CD1	1:C:767:TYR:N	2.71	0.59
1:B:407:GLU:N	1:B:407:GLU:OE1	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:N	1:B:374:LYS:HD2	2.17	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: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:A:202:LYS:C	1:A:204:ASN:H	2.08	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:1088:PRO:HG3	1:D:1092:PHE:CE2	2.40	0.56
1:D:967:MET:O	1:D:970:LEU:HB3	2.05	0.56
1:A:19:GLN:N	1:A:19:GLN:NE2	2.46	0.56
1:B:492:PHE:CD1	1:B:492:PHE:C	2.77	0.56
1:B:368:ALA:C	1:B:370:LEU:H	2.09	0.56
1:A:123:ILE:O	1:A:126:ILE:HG12	2.06	0.56
1:A:143:GLN:HG3	1:A:201:TYR:CE1	2.40	0.56
1:A:68:ALA:C	1:A:70:LEU:H	2.09	0.56
1:C:616:LYS:HG3	1:C:617:ASN:N	2.20	0.56
1:D:1050:ARG:O	1:D:1051:LYS:C	2.43	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: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:A:150:ARG:O	1:A:151:LYS:C	2.45	0.55
1:D:1037:LYS:HB2	1:D:1040:VAL:HG12	1.88	0.55
1:D:925:TYR:CD2	1:D:1050:ARG:HD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:503:ASP:O	1:B:504:ASN:C	2.46	0.54
1:A:90:CYS:SG	1:C:691:GLU:OE1	2.59	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:B:488:PRO:HG3	1:B:492:PHE:CE2	2.44	0.53
1:C:792:PHE:CD1	1:C:792:PHE:C	2.81	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:C:682:GLU:HA	1:C:699:ILE:HG22	1.90	0.53
1:B:382:GLU:HA	1:B:399:ILE:HG22	1.89	0.53
1:C:670:LEU:O	1:C:670:LEU:HD23	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:N	1:A:19:GLN:HE21	2.05	0.52
1:D:1050:ARG:HB3	1:D:1054:ILE:HD11	1.90	0.52
1:D:968:ALA:C	1:D:970:LEU:H	2.12	0.52
1:B:391:GLU:HG2	1:D:991:GLU:OE1	2.10	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:B:454:ILE:O	1:B:458:GLN:HA	2.09	0.51
1:C:761:THR:C	1:C:763:GLY:H	2.12	0.51
1:D:1078:ASN:O	1:D:1079:LYS:HB3	2.10	0.51
1:D:970:LEU:C	1:D:970:LEU:HD23	2.31	0.51
1:C:723:ILE:O	1:C:726:ILE:HG12	2.11	0.51
1:A:107:GLU:N	1:A:107:GLU:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LYS:HG2	1:A:209:ASN:ND2	2.24	0.51
1:D:1029:LEU:C	1:D:1029:LEU:HD12	2.31	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:C:769:THR:HG1	1:C:819:THR:HG1	1.59	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: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:D:912:SER:HB3	1:D:1087:PHE:CE2	2.47	0.49
1:C:623:PHE:CE2	1:D:995:ARG:NH1	2.81	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:A:161:THR:C	1:A:163:GLY:H	2.16	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:C:619:GLN:HG2	1:C:620:ASN:N	2.29	0.48
1:D:1026:ILE:HG13	1:D:1026:ILE:O	2.14	0.48
1:A:203:ASP:O	1:A:204:ASN:C	2.52	0.48
1:C:619:GLN:O	1:C:621:ILE:N	2.46	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:979:TYR:CE2	1:D:1044:GLU:HG3	2.49	0.48
1:A:113:ILE:HD12	1:A:113:ILE:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:SER:OG	1:A:72:LYS:O	2.31	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:1015:LYS:HE2	1:D:1110:LYS:HD3	1.96	0.47
1:D:970:LEU:O	1:D:970:LEU:HD23	2.14	0.47
1:A:121:VAL:HB	1:A:129:LEU:CD1	2.45	0.47
1:A:100:TYR:CE2	1:A:199:MET:HG2	2.49	0.47
1:D:998:CYS:O	1:D:999:ILE:CG2	2.62	0.47
1:C:670:LEU:HD23	1:C:670:LEU:C	2.35	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:D:1023:ILE:O	1:D:1026:ILE:HG12	2.15	0.47
1:A:25:TYR:CE2	1:A:150:ARG:HD2	2.49	0.47
1:A:2:GLN:N	1:A:2:GLN:NE2	2.61	0.47
1:C:624:LEU:HD11	1:C:794:GLN:HG2	1.96	0.47
1:C:796:LYS:C	1:C:796:LYS:HD3	2.34	0.47
1:D:902:GLN:NE2	1:D:902:GLN:N	2.63	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:1045:LEU:O	1:D:1049:VAL:HG23	2.15	0.47
1:D:919:GLN:O	1:D:922:TYR:N	2.47	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:750:ARG:O	1:C:751:LYS:C	2.53	0.47
1:D:1107:LEU:HD12	1:D:1107:LEU:O	2.15	0.47
1:B:303:ASP:HA	1:B:304:PRO:HD2	1.73	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:GLU:CD	1:B:407:GLU:H	2.19	0.46
1:C:713:ILE:HA	1:C:714:PRO:HD3	1.75	0.46
1:C:729:LEU:HD12	1:C:729:LEU:C	2.36	0.46
1:A:183:TRP:C	1:A:184:PHE:CD2	2.89	0.46
1:B:423:ILE:O	1:B:424:ASP:HB2	2.14	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:A:5:ASP:C	1:A:7:SER:H	2.18	0.46
1:D:922:TYR:O	1:D:923:PHE:C	2.54	0.46
1:A:157:LYS:O	1:A:158:GLN:HB2	2.15	0.46
1:A:2:GLN:HE21	1:A:2:GLN:H	1.64	0.46
1:B:371:PHE:N	1:B:371:PHE:CD1	2.83	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:D:994:GLU:O	1:D:995:ARG:CB	2.64	0.45
1:A:56:ASP:OD2	1:A:56:ASP:N	2.49	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:CD1	1:B:517:TYR:N	2.84	0.45
1:C:604:PRO:HB3	1:C:783:TRP:CH2	2.50	0.45
1:B:488:PRO:CG	1:B:492:PHE:CE2	3.00	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: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:A:167:TYR:HD1	1:A:167:TYR:N	2.12	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:1092:PHE:C	1:D:1092:PHE:CD1	2.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:HD12	1:A:129:LEU:C	2.38	0.44
1:D:1114:ILE:HG22	1:D:1115:GLU:N	2.32	0.44
1:B:391:GLU:OE2	1:D:990:CYS:SG	2.76	0.44
1:C:670:LEU:O	1:C:674:LYS:HD3	2.18	0.43
1:D:1077:LYS:HD3	1:D:1077:LYS:C	2.39	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:A:147:TYR:O	1:A:148:LYS:C	2.57	0.43
1:A:183:TRP:O	1:A:184:PHE:CD2	2.63	0.43
1:D:909:LEU:HD13	1:D:1069:THR:HB	2.00	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: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:N	1:B:382:GLU:OE1	2.42	0.43
1:C:743:GLN:HG3	1:C:801:TYR:CE1	2.54	0.43
1:C:803:ASP:O	1:C:804:ASN:C	2.56	0.43
1:D:1117:TYR:CD1	1:D:1117:TYR:N	2.85	0.43
1:B:445:LEU:O	1:B:446:ASP:C	2.57	0.43
1:B:496:LYS:O	1:B:496:LYS:HD3	2.18	0.43
1:C:726:ILE:HG13	1:C:726:ILE:O	2.19	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:1067:TYR:H	1:D:1067:TYR:HD1	1.66	0.42
1:D:983:TYR:HE2	1:D:986:LEU:O	2.02	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:741:THR:C	1:C:743:GLN:N	2.71	0.42
1:B:450:ARG:O	1:B:451:LYS:C	2.58	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:B:429:LEU:HD12	1:B:429:LEU:C	2.40	0.42
1:D:957:LYS:CB	1:D:989:LEU:CD2	2.96	0.42
1:C:735:THR:OG1	1:C:740:VAL:HG11	2.20	0.42
1:D:1013:ILE:HG23	1:D:1014:PRO:HD2	2.02	0.42
1:D:1069:THR:HG1	1:D:1119:THR:HG1	1.62	0.42
1:C:659:LYS:HB2	1:C:689:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:LEU:O	1:B:319:GLN:C	2.58	0.42
1:B:454:ILE:HD13	1:B:460:TYR:CD1	2.55	0.42
1:C:654:ASN:O	1:C:655:TYR:HB3	2.19	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:C:712:GLU:C	1:C:713:ILE:HD12	2.39	0.42
1:C:761:THR:C	1:C:763:GLY:N	2.73	0.42
1:A:108:GLY:C	1:A:110:HIS:H	2.24	0.41
1:A:153:THR:O	1:A:158:GLN:N	2.53	0.41
1:D:924:LEU:HA	1:D:924:LEU:HD23	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:183:TRP:C	1:A:184:PHE:HD2	2.21	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:B:461:THR:C	1:B:463:GLY:N	2.74	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:B:496:LYS:C	1:B:496:LYS:HD3	2.41	0.41
1:C:689:LEU:HD12	1:C:689:LEU:HA	1.87	0.41
1:A:70:LEU:C	1:A:70:LEU:HD23	2.41	0.41
1:A:161:THR:C	1:A:163:GLY:N	2.73	0.41
1:A:202:LYS:C	1:A:204:ASN:N	2.72	0.41
1:C:636:LYS:HD2	1:C:673:ASP:O	2.21	0.41
1:D:1013:ILE:HD12	1:D:1013:ILE:N	2.36	0.41
1:B:400:TYR:CE2	1:B:499:MET:HG2	2.56	0.41
1:C:713:ILE:N	1:C:713:ILE:HD12	2.35	0.41
1:C:715:LYS:HE3	1:C:810:LYS:HD3	2.03	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:HE21	1:D:902:GLN:N	2.19	0.40
1:D:919:GLN:C	1:D:921:ILE:H	2.25	0.40
1:A:68:ALA:C	1:A:70:LEU:N	2.74	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:800:ILE:HG13	1:C:801:TYR:CD2	2.57	0.40
1:D:1047:TYR:O	1:D:1048:LYS:C	2.60	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%)	3	29
1	B	219/221 (99%)	179 (82%)	30 (14%)	10 (5%)	3	29
1	C	219/221 (99%)	180 (82%)	33 (15%)	6 (3%)	6	42
1	D	219/221 (99%)	178 (81%)	34 (16%)	7 (3%)	5	38
All	All	876/884 (99%)	721 (82%)	122 (14%)	33 (4%)	4	34

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	201 (97%)	7 (3%)	42	77
1	B	208/208 (100%)	200 (96%)	8 (4%)	38	74
1	C	208/208 (100%)	202 (97%)	6 (3%)	48	80
1	D	208/208 (100%)	199 (96%)	9 (4%)	33	71
All	All	832/832 (100%)	802 (96%)	30 (4%)	40	75

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	19	GLN
1	A	82	GLU
1	A	129	LEU
1	A	167	TYR
1	A	177	LYS
1	A	207	LEU
1	B	302	GLN
1	B	303	ASP
1	B	319	GLN

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Mol	Chain	Res	Type
1	B	382	GLU
1	B	390	CYS
1	B	407	GLU
1	B	507	LEU
1	B	517	TYR
1	C	602	GLN
1	C	619	GLN
1	C	682	GLU
1	C	767	TYR
1	C	777	LYS
1	C	807	LEU
1	D	902	GLN
1	D	919	GLN
1	D	982	GLU
1	D	1067	TYR
1	D	1077	LYS
1	D	1088	PRO
1	D	1107	LEU
1	D	1117	TYR
1	D	1121	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	2	GLN
1	A	8	GLN
1	A	19	GLN
1	A	40	GLN
1	A	85	HIS
1	A	110	HIS
1	A	143	GLN
1	A	156	ASN
1	A	162	ASN
1	A	194	GLN
1	B	301	GLN
1	B	302	GLN
1	B	308	GLN
1	B	317	ASN
1	B	319	GLN
1	B	385	HIS
1	B	410	HIS

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Mol	Chain	Res	Type
1	B	443	GLN
1	B	456	ASN
1	B	494	GLN
1	C	601	GLN
1	C	602	GLN
1	C	608	GLN
1	C	619	GLN
1	C	620	ASN
1	C	640	GLN
1	C	685	HIS
1	C	710	HIS
1	C	743	GLN
1	C	756	ASN
1	C	762	ASN
1	C	794	GLN
1	D	901	GLN
1	D	902	GLN
1	D	908	GLN
1	D	919	GLN
1	D	920	ASN
1	D	940	GLN
1	D	985	HIS
1	D	1010	HIS
1	D	1043	GLN
1	D	1094	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.