Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2023 – 02:49 AM EDT

PDB ID	:	3NCW
Title	:	Crystal structure of EHEC O157:H7 intimin
Authors	:	Yi, Y.; Gao, F.; Gao, G.F.; Zou, Q.M.
Deposited on	:	2010-06-06
Resolution	:	2.80 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 (1)) were used in the production of this report:

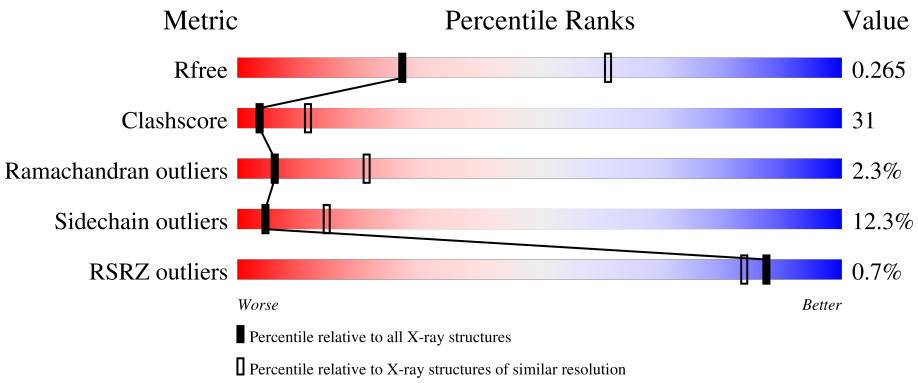
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.80 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))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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% 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.

Mol	Chain	Length	Quality of chain
1	A	189	44% 46% 7% •
1	B	189	% 49% 41% 7% •
1	C	189	% 37% 51% 8% •
1	D	189	% 47% 45% 5% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5795 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 Intimin adherence protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	183	1410	890	231	284	5	0	0	0
1	B	183	1410	890	231	284	5	0	0	0
1	C	183	1410	890	231	284	5	0	0	0
1	D	183	1410	890	231	284	5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	746	MET	-	initiating methionine	UNP C6UYL6
B	746	MET	-	initiating methionine	UNP C6UYL6
C	746	MET	-	initiating methionine	UNP C6UYL6
D	746	MET	-	initiating methionine	UNP C6UYL6

- Molecule 2 is water.

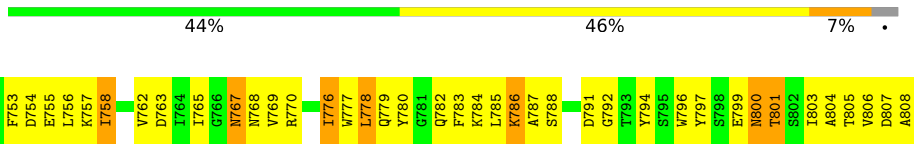
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	59	59	59	0	0
2	B	19	19	19	0	0
2	C	26	26	26	0	0
2	D	51	51	51	0	0

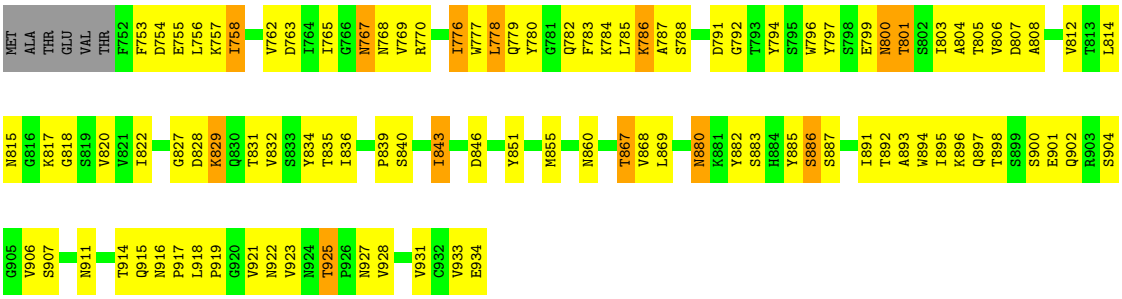
3 Residue-property plots (i)

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 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.

• Molecule 1: Intimin adherence protein

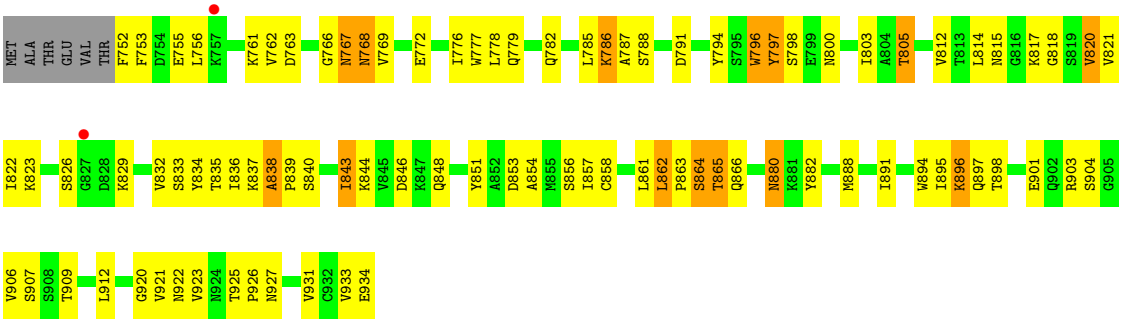
Chain A:





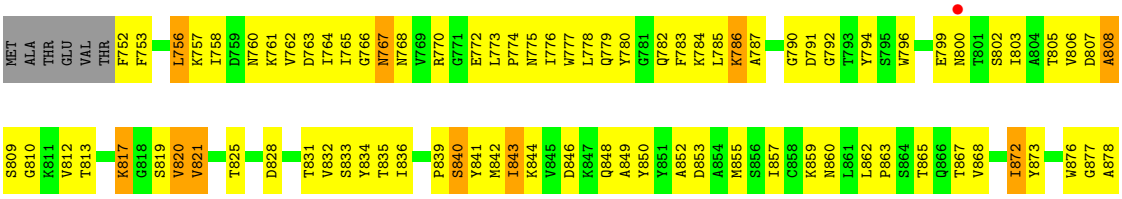
• Molecule 1: Intimin adherence protein

Chain B:



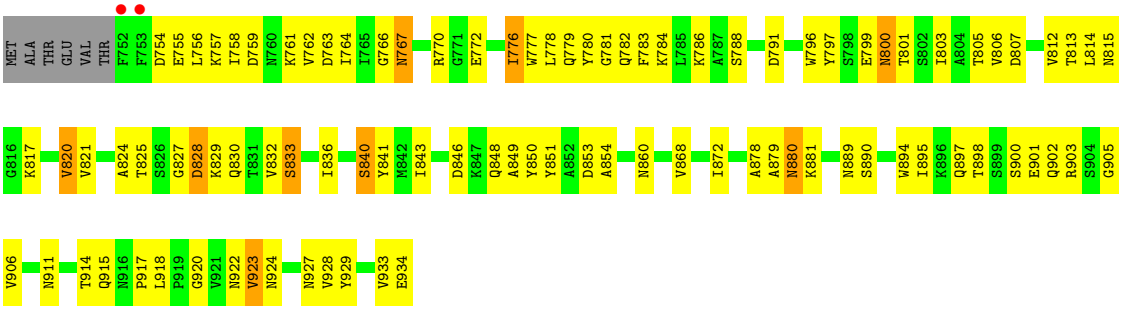
• Molecule 1: Intimin adherence protein

Chain C:



• Molecule 1: Intimin adherence protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	235.16Å 44.81Å 129.12Å 90.00° 97.53° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 27.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.00-2.80) 96.3 (27.94-2.80)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.254 , 0.296 0.257 , 0.265	Depositor DCC
R_{free} test set	1631 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 64.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	5795	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.43	0/1439	0.76	0/1956
1	B	0.39	0/1439	0.76	1/1956 (0.1%)
1	C	0.41	0/1439	0.75	1/1956 (0.1%)
1	D	0.42	0/1439	0.77	0/1956
All	All	0.41	0/5756	0.76	2/7824 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	862	LEU	CB-CG-CD1	-6.13	100.57	111.00
1	C	808	ALA	N-CA-C	5.22	125.08	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1410	0	1379	83	0
1	B	1410	0	1379	74	0
1	C	1410	0	1379	104	0
1	D	1410	0	1379	93	0
2	A	59	0	0	8	0
2	B	19	0	0	1	0
2	C	26	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	51	0	0	8	0
All	All	5795	0	5516	351	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 31.

All (351) 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:756:LEU:O	1:D:832:VAL:HG21	1.54	1.06
1:B:906:VAL:HG21	1:B:920:GLY:HA2	1.37	1.03
1:B:844:LYS:HE3	1:B:934:GLU:HG3	1.48	0.95
1:D:800:ASN:HB3	1:D:820:VAL:HG21	1.48	0.95
1:B:821:VAL:HG22	1:B:835:THR:HG22	1.51	0.93
1:D:843:ILE:HD12	1:D:872:ILE:HG12	1.53	0.87
1:B:927:ASN:OD1	1:D:890:SER:HB3	1.75	0.86
1:A:778:LEU:HD12	1:A:779:GLN:N	1.94	0.82
1:B:820:VAL:HG12	1:B:836:ILE:HD12	1.62	0.82
1:A:758:ILE:HG21	1:A:834:TYR:HB2	1.62	0.82
1:A:803:ILE:HD12	1:A:818:GLY:HA3	1.62	0.81
1:C:758:ILE:HD13	1:C:787:ALA:HB2	1.62	0.81
1:C:767:ASN:H	1:C:767:ASN:HD22	1.26	0.81
1:C:880:ASN:N	1:C:880:ASN:HD22	1.78	0.80
1:C:784:LYS:HA	1:C:810:GLY:O	1.82	0.80
1:D:898:THR:OG1	1:D:901:GLU:HG3	1.81	0.80
1:B:898:THR:OG1	1:B:901:GLU:HG3	1.82	0.79
1:A:914:THR:HB	2:A:112:HOH:O	1.83	0.79
1:D:757:LYS:HG3	1:D:758:ILE:N	1.96	0.78
1:A:898:THR:OG1	1:A:901:GLU:HG3	1.84	0.77
1:D:758:ILE:HD13	1:D:832:VAL:HB	1.65	0.77
1:D:906:VAL:HG12	1:D:922:ASN:HD22	1.47	0.77
1:B:821:VAL:CG2	1:B:835:THR:HG22	2.15	0.77
1:A:776:ILE:HD13	1:A:776:ILE:H	1.51	0.75
1:B:864:SER:O	1:B:865:THR:HG23	1.87	0.75
1:C:762:VAL:HG11	1:C:783:PHE:HD1	1.52	0.74
1:A:756:LEU:HD12	1:A:788:SER:O	1.88	0.74
1:C:863:PRO:HA	1:C:933:VAL:HG21	1.68	0.72
1:D:817:LYS:HD2	1:D:934:GLU:O	1.90	0.72
1:C:777:TRP:CH2	1:C:839:PRO:HD3	2.24	0.72
1:D:764:ILE:N	1:D:764:ILE:HD12	2.05	0.72
1:B:880:ASN:N	1:B:880:ASN:HD22	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:ASP:OD2	1:A:827:GLY:HA3	1.90	0.71
1:C:927:ASN:HB3	2:C:59:HOH:O	1.90	0.71
1:B:862:LEU:HB3	1:B:863:PRO:HD2	1.73	0.71
1:A:855:MET:HG2	1:A:860:ASN:OD1	1.92	0.70
1:D:763:ASP:HB3	1:D:784:LYS:HB2	1.73	0.70
1:C:900:SER:O	1:C:903:ARG:HB2	1.92	0.69
1:D:800:ASN:CB	1:D:820:VAL:HG21	2.20	0.69
1:A:797:TYR:HE2	1:A:799:GLU:HG3	1.58	0.69
1:B:848:GLN:NE2	1:B:927:ASN:HA	2.07	0.69
1:A:757:LYS:HG3	1:A:758:ILE:N	2.06	0.68
1:A:801:THR:HA	1:A:804:ALA:O	1.93	0.68
1:B:844:LYS:CE	1:B:934:GLU:HG3	2.20	0.68
1:D:767:ASN:H	1:D:767:ASN:ND2	1.92	0.67
1:B:817:LYS:HE3	1:B:934:GLU:OXT	1.93	0.67
1:A:860:ASN:HB3	2:A:19:HOH:O	1.94	0.67
1:A:769:VAL:HA	1:D:915:GLN:OE1	1.94	0.67
1:C:820:VAL:HG12	1:C:836:ILE:HD12	1.76	0.67
1:B:843:ILE:HD12	1:B:931:VAL:HG12	1.76	0.67
1:C:762:VAL:HG11	1:C:783:PHE:CD1	2.30	0.67
1:A:897:GLN:HE21	1:A:907:SER:HB2	1.59	0.66
1:C:767:ASN:HD22	1:C:767:ASN:N	1.88	0.66
1:A:767:ASN:HD22	1:A:768:ASN:N	1.94	0.66
1:C:779:GLN:O	1:C:780:TYR:HB2	1.97	0.65
1:C:756:LEU:HG	1:C:832:VAL:CG2	2.27	0.65
1:C:775:ASN:HD21	1:C:840:SER:HB3	1.61	0.65
1:A:767:ASN:HD22	1:A:767:ASN:C	2.00	0.64
1:C:802:SER:OG	1:C:803:ILE:HD12	1.98	0.64
1:D:755:GLU:HG2	2:D:68:HOH:O	1.95	0.64
1:B:786:LYS:HZ1	1:B:786:LYS:HA	1.63	0.64
1:A:756:LEU:O	1:A:832:VAL:HG21	1.98	0.64
1:B:776:ILE:HG13	1:B:776:ILE:O	1.98	0.64
1:A:778:LEU:HD12	1:A:779:GLN:H	1.61	0.64
1:B:798:SER:HB2	1:B:822:ILE:HD11	1.80	0.64
1:A:904:SER:O	1:A:906:VAL:HG13	1.98	0.63
1:D:897:GLN:NE2	1:D:906:VAL:O	2.31	0.63
1:C:880:ASN:N	1:C:880:ASN:ND2	2.46	0.63
1:C:817:LYS:HB2	1:C:842:MET:HE2	1.80	0.63
1:A:820:VAL:O	1:A:836:ILE:HD13	2.00	0.62
1:C:799:GLU:HG2	1:C:821:VAL:O	2.00	0.62
1:C:758:ILE:CD1	1:C:787:ALA:HB2	2.28	0.62
1:D:879:ALA:HB3	2:D:110:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:906:VAL:HG12	1:D:922:ASN:ND2	2.15	0.61
1:B:843:ILE:HD11	1:B:933:VAL:HG22	1.82	0.61
1:D:762:VAL:HG21	1:D:783:PHE:CD1	2.35	0.61
1:A:836:ILE:N	1:A:836:ILE:HD12	2.15	0.61
1:D:776:ILE:N	1:D:776:ILE:HD13	2.15	0.61
1:B:777:TRP:CZ3	1:B:814:LEU:HD22	2.36	0.60
1:A:782:GLN:HE22	1:A:883:SER:HB2	1.67	0.60
1:B:786:LYS:HA	1:B:786:LYS:NZ	2.15	0.60
1:C:911:ASN:O	1:C:915:GLN:HA	2.02	0.60
1:D:767:ASN:H	1:D:767:ASN:HD22	1.50	0.60
1:A:770:ARG:HG3	1:A:770:ARG:HH11	1.65	0.59
1:C:805:THR:CG2	1:C:806:VAL:N	2.65	0.59
1:B:777:TRP:CH2	1:B:839:PRO:HD3	2.37	0.59
1:C:767:ASN:N	1:C:767:ASN:ND2	2.51	0.59
1:A:758:ILE:O	1:A:758:ILE:HG22	2.01	0.59
1:D:758:ILE:HD11	1:D:824:ALA:HB3	1.84	0.59
1:D:782:GLN:HG2	1:D:813:THR:OG1	2.03	0.59
1:D:917:PRO:O	1:D:918:LEU:HD12	2.03	0.58
1:D:820:VAL:HG12	1:D:836:ILE:HD12	1.85	0.58
1:C:786:LYS:HE3	1:C:786:LYS:HA	1.86	0.58
1:C:903:ARG:HH11	1:C:903:ARG:HG3	1.67	0.57
1:C:777:TRP:CZ3	1:C:839:PRO:HD3	2.38	0.57
1:C:849:ALA:HA	2:C:38:HOH:O	2.04	0.57
1:A:777:TRP:CD2	1:A:814:LEU:HD13	2.39	0.57
1:B:767:ASN:ND2	1:B:767:ASN:H	2.01	0.57
1:C:902:GLN:OE1	1:C:902:GLN:C	2.42	0.57
1:C:767:ASN:H	1:C:767:ASN:ND2	2.01	0.57
1:D:786:LYS:HE3	1:D:786:LYS:HA	1.86	0.57
1:B:756:LEU:HD12	1:B:788:SER:O	2.04	0.57
1:D:806:VAL:HG13	1:D:806:VAL:O	2.03	0.57
1:D:851:TYR:O	1:D:854:ALA:HB3	2.04	0.56
1:B:843:ILE:HD12	1:B:931:VAL:CG1	2.35	0.56
1:C:756:LEU:HG	1:C:832:VAL:HG23	1.86	0.56
1:A:822:ILE:HG12	1:A:836:ILE:HD11	1.87	0.56
1:C:904:SER:HB2	2:C:118:HOH:O	2.06	0.56
1:B:891:ILE:HG22	1:B:891:ILE:O	2.06	0.56
1:B:906:VAL:CG2	1:B:920:GLY:HA2	2.23	0.56
1:A:880:ASN:N	1:A:880:ASN:HD22	2.04	0.56
1:D:791:ASP:OD2	1:D:827:GLY:CA	2.54	0.56
1:D:848:GLN:HG2	1:D:929:TYR:CD2	2.41	0.56
1:A:851:TYR:HB3	1:A:923:VAL:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:ALA:HB2	1:A:931:VAL:HG21	1.88	0.55
1:A:767:ASN:C	1:A:767:ASN:ND2	2.60	0.55
1:C:878:ALA:HB1	1:C:880:ASN:HD21	1.72	0.55
1:D:756:LEU:HD23	1:D:832:VAL:HG23	1.88	0.55
1:D:766:GLY:O	1:D:881:LYS:HD2	2.07	0.55
1:B:880:ASN:N	1:B:880:ASN:ND2	2.53	0.55
1:C:773:LEU:HG	1:C:774:PRO:N	2.21	0.55
1:C:782:GLN:HA	1:C:812:VAL:O	2.07	0.55
1:D:767:ASN:ND2	1:D:767:ASN:N	2.54	0.55
1:C:933:VAL:HG12	1:C:933:VAL:O	2.07	0.55
1:D:770:ARG:NH1	1:D:770:ARG:HG3	2.22	0.55
1:D:764:ILE:HD12	1:D:764:ILE:H	1.71	0.54
1:A:753:PHE:CE2	1:A:828:ASP:HB3	2.43	0.54
1:D:757:LYS:HG3	1:D:758:ILE:H	1.72	0.54
1:C:863:PRO:HD3	1:C:933:VAL:HG23	1.88	0.54
1:C:895:ILE:HG22	1:C:896:LYS:O	2.08	0.54
1:D:805:THR:HA	2:D:16:HOH:O	2.07	0.54
1:C:820:VAL:CG1	1:C:836:ILE:HD12	2.37	0.53
1:A:880:ASN:HD22	1:A:880:ASN:H	1.54	0.53
1:B:820:VAL:CG1	1:B:836:ILE:HD12	2.35	0.53
1:A:770:ARG:HG3	1:A:770:ARG:NH1	2.24	0.53
1:A:757:LYS:HE2	1:A:758:ILE:O	2.08	0.53
1:B:796:TRP:N	1:B:796:TRP:CD1	2.77	0.53
1:C:852:ALA:HB3	2:C:44:HOH:O	2.07	0.53
1:D:828:ASP:OD2	1:D:828:ASP:N	2.34	0.53
1:A:784:LYS:HD2	2:A:29:HOH:O	2.08	0.53
1:A:807:ASP:OD2	1:A:807:ASP:C	2.48	0.53
1:A:817:LYS:NZ	2:A:47:HOH:O	2.42	0.53
1:C:776:ILE:HD12	1:C:776:ILE:O	2.09	0.53
1:D:840:SER:HG	1:D:841:TYR:HD2	1.54	0.53
1:B:895:ILE:O	1:B:896:LYS:C	2.47	0.52
1:D:776:ILE:HD13	1:D:776:ILE:H	1.74	0.52
1:D:777:TRP:CD2	1:D:814:LEU:HD13	2.44	0.52
1:A:765:ILE:HG12	1:A:783:PHE:HA	1.90	0.52
1:A:891:ILE:N	1:A:911:ASN:HD21	2.08	0.52
1:D:796:TRP:CD1	1:D:796:TRP:N	2.78	0.52
1:D:849:ALA:HB1	1:D:853:ASP:HB3	1.92	0.52
1:A:792:GLY:HA2	1:A:794:TYR:OH	2.10	0.52
1:C:853:ASP:HB2	2:C:62:HOH:O	2.09	0.52
1:D:851:TYR:HB3	1:D:923:VAL:HB	1.92	0.52
1:C:909:THR:HG23	1:C:921:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:MET:CG	1:A:860:ASN:OD1	2.58	0.51
1:A:762:VAL:CG1	1:A:763:ASP:N	2.73	0.51
1:A:839:PRO:O	1:A:840:SER:C	2.48	0.51
1:D:758:ILE:CD1	1:D:832:VAL:HB	2.38	0.51
1:D:770:ARG:HG3	1:D:770:ARG:HH11	1.74	0.51
1:B:866:GLN:HA	1:B:895:ILE:HD13	1.93	0.51
1:D:914:THR:O	1:D:915:GLN:HB2	2.10	0.51
1:D:783:PHE:CE1	1:D:812:VAL:HB	2.46	0.51
1:B:927:ASN:OD1	1:D:890:SER:CB	2.55	0.51
1:C:863:PRO:CA	1:C:933:VAL:HG21	2.38	0.51
1:B:837:LYS:O	1:B:838:ALA:C	2.49	0.51
1:B:791:ASP:OD1	1:B:826:SER:HB2	2.11	0.50
1:A:817:LYS:HE3	1:A:934:GLU:OXT	2.11	0.50
1:C:778:LEU:HD12	1:C:843:ILE:HG22	1.93	0.50
1:D:879:ALA:CB	2:D:110:HOH:O	2.59	0.50
1:A:906:VAL:HG12	1:A:922:ASN:HA	1.94	0.50
1:D:878:ALA:HB1	1:D:880:ASN:ND2	2.27	0.50
1:B:768:ASN:N	1:B:768:ASN:OD1	2.43	0.50
1:C:791:ASP:N	1:C:828:ASP:OD2	2.45	0.50
1:C:865:THR:O	1:C:868:VAL:HG23	2.12	0.50
1:D:756:LEU:O	1:D:832:VAL:CG2	2.44	0.50
1:C:880:ASN:ND2	1:C:880:ASN:H	2.08	0.49
1:D:803:ILE:HG21	1:D:820:VAL:HB	1.93	0.49
1:D:890:SER:OG	1:D:911:ASN:ND2	2.41	0.49
1:D:779:GLN:O	1:D:780:TYR:HB2	2.12	0.49
1:A:782:GLN:HE22	1:A:883:SER:CB	2.25	0.49
1:C:848:GLN:NE2	1:C:927:ASN:HA	2.28	0.49
1:B:894:TRP:HA	1:B:909:THR:HG22	1.95	0.49
1:C:775:ASN:ND2	1:C:840:SER:HB3	2.26	0.49
1:C:785:LEU:HD21	1:C:834:TYR:CE1	2.47	0.49
1:D:894:TRP:CE2	1:D:928:VAL:HG11	2.47	0.49
1:D:933:VAL:HG12	1:D:933:VAL:O	2.12	0.49
1:D:800:ASN:ND2	1:D:803:ILE:HD13	2.28	0.49
1:A:777:TRP:CE3	1:A:814:LEU:HD13	2.48	0.49
1:B:798:SER:HA	1:B:822:ILE:HD13	1.95	0.49
1:D:797:TYR:HE2	1:D:799:GLU:HG3	1.78	0.49
1:C:926:PRO:O	1:C:927:ASN:HB2	2.12	0.49
1:D:853:ASP:HB2	2:D:131:HOH:O	2.13	0.48
1:D:764:ILE:N	1:D:764:ILE:CD1	2.76	0.48
1:C:903:ARG:HG3	1:C:903:ARG:NH1	2.29	0.48
1:C:907:SER:O	1:C:921:VAL:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:796:TRP:N	1:C:796:TRP:CD1	2.81	0.48
1:C:842:MET:HE1	1:C:844:LYS:HE3	1.94	0.48
1:D:840:SER:OG	1:D:841:TYR:HD2	1.97	0.48
1:C:758:ILE:HD13	1:C:787:ALA:CB	2.37	0.48
1:D:850:TYR:O	1:D:851:TYR:C	2.51	0.48
1:A:786:LYS:HA	1:A:786:LYS:NZ	2.29	0.48
1:A:907:SER:O	1:A:921:VAL:HB	2.13	0.48
1:C:807:ASP:O	1:C:809:SER:N	2.47	0.48
1:C:853:ASP:O	1:C:857:ILE:HG13	2.14	0.48
1:D:781:GLY:O	1:D:782:GLN:HG3	2.14	0.48
1:C:865:THR:H	1:C:868:VAL:CG2	2.27	0.48
1:A:787:ALA:HB2	1:A:796:TRP:CH2	2.49	0.47
1:A:928:VAL:HB	2:A:5:HOH:O	2.14	0.47
1:B:752:PHE:N	2:B:141:HOH:O	2.47	0.47
1:B:777:TRP:CZ3	1:B:839:PRO:HD3	2.48	0.47
1:C:832:VAL:HG12	1:C:833:SER:N	2.29	0.47
1:C:880:ASN:HD22	1:C:880:ASN:H	1.57	0.47
1:A:928:VAL:N	2:A:5:HOH:O	2.47	0.47
1:C:778:LEU:O	1:C:779:GLN:C	2.53	0.47
1:A:757:LYS:HG2	2:A:100:HOH:O	2.14	0.47
1:A:779:GLN:O	1:A:780:TYR:HB2	2.15	0.47
1:A:891:ILE:H	1:A:911:ASN:HD21	1.60	0.47
1:C:779:GLN:OE1	1:C:844:LYS:HG2	2.14	0.47
1:C:898:THR:OG1	1:C:901:GLU:HG3	2.14	0.47
1:D:903:ARG:NH1	2:D:125:HOH:O	2.48	0.47
1:C:841:TYR:HA	1:C:934:GLU:OXT	2.13	0.47
1:C:859:LYS:O	1:C:860:ASN:HB2	2.13	0.47
1:C:901:GLU:O	1:C:902:GLN:C	2.53	0.47
1:D:922:ASN:O	1:D:924:ASN:N	2.48	0.47
1:A:885:TYR:O	1:A:887:SER:N	2.48	0.47
1:B:894:TRP:CH2	1:B:923:VAL:HA	2.50	0.47
1:C:756:LEU:HG	1:C:832:VAL:HG21	1.95	0.46
1:B:863:PRO:HA	1:B:933:VAL:HG21	1.96	0.46
1:C:825:THR:OG1	1:C:831:THR:HG23	2.15	0.46
1:D:791:ASP:OD2	1:D:827:GLY:HA3	2.15	0.46
1:A:762:VAL:HG22	1:A:785:LEU:HD23	1.96	0.46
1:A:843:ILE:HG13	1:A:933:VAL:HG22	1.98	0.46
1:A:897:GLN:NE2	1:A:907:SER:HB2	2.30	0.46
1:D:779:GLN:NE2	2:D:126:HOH:O	2.49	0.46
1:B:906:VAL:HG12	1:B:922:ASN:HA	1.98	0.46
1:C:906:VAL:HG12	1:C:922:ASN:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:807:ASP:C	1:D:807:ASP:OD2	2.52	0.46
1:B:891:ILE:HG21	1:B:912:LEU:HD12	1.97	0.46
1:C:914:THR:C	1:C:916:ASN:H	2.19	0.46
1:D:781:GLY:C	1:D:782:GLN:HG3	2.36	0.46
1:D:825:THR:HG23	1:D:830:GLN:O	2.15	0.46
1:B:798:SER:HB2	1:B:822:ILE:CD1	2.45	0.45
1:D:756:LEU:HA	1:D:788:SER:O	2.16	0.45
1:D:868:VAL:O	1:D:872:ILE:HD13	2.16	0.45
1:B:778:LEU:HD23	1:B:779:GLN:O	2.16	0.45
1:B:858:CYS:O	1:B:861:LEU:HB2	2.16	0.45
1:D:843:ILE:HD12	1:D:872:ILE:CG1	2.36	0.45
1:B:803:ILE:HG21	1:B:818:GLY:O	2.16	0.45
1:C:802:SER:HB3	2:C:88:HOH:O	2.17	0.45
1:D:791:ASP:OD2	1:D:827:GLY:N	2.50	0.45
1:A:915:GLN:O	1:A:917:PRO:HD3	2.17	0.45
1:B:777:TRP:CE3	1:B:814:LEU:HD22	2.52	0.45
1:C:859:LYS:O	1:C:860:ASN:CB	2.63	0.45
1:D:805:THR:OG1	1:D:815:ASN:ND2	2.46	0.45
1:B:851:TYR:O	1:B:854:ALA:HB3	2.17	0.45
1:C:765:ILE:HG12	1:C:782:GLN:O	2.17	0.45
1:C:778:LEU:HD12	1:C:843:ILE:CG2	2.47	0.45
1:A:792:GLY:HA2	1:A:794:TYR:CZ	2.52	0.44
1:A:906:VAL:HG12	1:A:922:ASN:HD22	1.82	0.44
1:B:766:GLY:HA3	1:B:882:TYR:OH	2.16	0.44
1:B:797:TYR:C	1:B:797:TYR:CD2	2.90	0.44
1:B:820:VAL:HG22	1:B:821:VAL:H	1.82	0.44
1:C:805:THR:HG23	1:C:806:VAL:N	2.32	0.44
1:D:767:ASN:HD22	1:D:767:ASN:N	2.11	0.44
1:B:921:VAL:O	1:B:922:ASN:C	2.52	0.44
1:B:903:ARG:HG3	1:B:903:ARG:NH1	2.31	0.44
1:C:890:SER:OG	1:C:911:ASN:ND2	2.50	0.44
1:D:895:ILE:HD12	1:D:895:ILE:N	2.33	0.44
1:A:897:GLN:HB3	1:A:907:SER:HB2	2.00	0.44
1:C:933:VAL:HG11	2:C:10:HOH:O	2.18	0.44
1:A:835:THR:C	1:A:836:ILE:HD12	2.38	0.44
1:B:800:ASN:HB3	1:B:820:VAL:HG21	1.99	0.44
1:A:843:ILE:CG1	1:A:933:VAL:HG22	2.48	0.44
1:B:762:VAL:CG1	1:B:763:ASP:N	2.81	0.44
1:B:823:LYS:HG2	1:B:833:SER:OG	2.17	0.44
1:D:778:LEU:O	1:D:779:GLN:C	2.56	0.44
1:B:767:ASN:H	1:B:767:ASN:HD22	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:897:GLN:HB3	1:B:907:SER:HB2	2.01	0.43
1:A:922:ASN:O	1:A:925:THR:OG1	2.36	0.43
1:B:763:ASP:OD2	1:B:763:ASP:C	2.55	0.43
1:C:766:GLY:HA3	1:C:876:TRP:O	2.18	0.43
1:D:878:ALA:HB1	1:D:880:ASN:HD21	1.82	0.43
1:A:800:ASN:HB3	1:A:820:VAL:HG23	2.00	0.43
1:A:851:TYR:CD1	1:A:851:TYR:C	2.90	0.43
1:B:767:ASN:ND2	1:B:767:ASN:N	2.62	0.43
1:B:925:THR:HA	1:B:926:PRO:HD3	1.77	0.43
1:C:762:VAL:CG1	1:C:763:ASP:N	2.82	0.43
1:C:762:VAL:HG12	1:C:763:ASP:N	2.33	0.43
1:C:779:GLN:HB3	1:C:843:ILE:O	2.18	0.43
1:B:851:TYR:HB3	1:B:923:VAL:HG12	2.01	0.43
1:D:848:GLN:HG2	1:D:929:TYR:CE2	2.53	0.43
1:C:903:ARG:NE	2:C:3:HOH:O	2.49	0.43
1:D:800:ASN:HD21	1:D:803:ILE:HD13	1.83	0.43
1:B:901:GLU:HB3	1:B:906:VAL:O	2.18	0.43
1:D:796:TRP:O	1:D:797:TYR:HB2	2.18	0.43
1:D:848:GLN:O	1:D:849:ALA:HB2	2.19	0.43
1:B:903:ARG:HG3	1:B:903:ARG:HH11	1.84	0.43
1:C:764:ILE:HG21	1:C:767:ASN:HD21	1.82	0.43
1:C:782:GLN:HG2	1:C:813:THR:OG1	2.19	0.42
1:C:805:THR:HG23	1:C:806:VAL:H	1.83	0.42
1:C:922:ASN:O	1:C:925:THR:HB	2.18	0.42
1:C:821:VAL:HG23	1:C:835:THR:HG22	2.02	0.42
1:A:805:THR:HB	1:A:815:ASN:HD21	1.84	0.42
1:B:756:LEU:HG	1:B:832:VAL:CG2	2.49	0.42
1:C:819:SER:HA	1:C:836:ILE:O	2.18	0.42
1:C:842:MET:CE	1:C:844:LYS:HE3	2.50	0.42
1:A:894:TRP:CE2	1:A:928:VAL:HG11	2.54	0.42
1:B:782:GLN:HA	1:B:812:VAL:O	2.20	0.42
1:C:783:PHE:N	1:C:783:PHE:CD2	2.88	0.42
1:D:905:GLY:O	1:D:923:VAL:HG13	2.18	0.42
1:A:776:ILE:O	1:A:776:ILE:HG12	2.18	0.42
1:B:785:LEU:HD21	1:B:834:TYR:CE1	2.55	0.42
1:C:872:ILE:HG22	1:C:873:TYR:N	2.33	0.42
1:C:756:LEU:HD12	1:C:757:LYS:N	2.35	0.42
1:A:893:ALA:CB	1:A:931:VAL:HG21	2.49	0.42
1:B:862:LEU:HB3	1:B:863:PRO:CD	2.47	0.42
1:D:758:ILE:HD13	1:D:832:VAL:CB	2.42	0.42
1:B:853:ASP:O	1:B:857:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:760:ASN:ND2	1:C:772:GLU:OE2	2.51	0.42
1:D:766:GLY:HA2	1:D:881:LYS:HD2	2.02	0.42
1:A:805:THR:O	1:A:812:VAL:HG13	2.20	0.41
1:C:850:TYR:HB2	2:C:44:HOH:O	2.18	0.41
1:C:841:TYR:CD1	1:C:841:TYR:C	2.94	0.41
1:B:848:GLN:HE22	1:B:927:ASN:HA	1.84	0.41
1:D:806:VAL:O	1:D:806:VAL:CG1	2.67	0.41
1:C:790:GLY:C	1:C:792:GLY:H	2.24	0.41
1:A:895:ILE:O	1:A:896:LYS:C	2.57	0.41
1:A:803:ILE:HD12	1:A:818:GLY:CA	2.41	0.41
1:A:827:GLY:C	1:A:829:LYS:H	2.24	0.41
1:C:820:VAL:O	1:C:836:ILE:HG13	2.20	0.41
1:D:889:ASN:ND2	2:D:26:HOH:O	2.53	0.41
1:A:788:SER:HB3	2:A:46:HOH:O	2.21	0.41
1:A:892:THR:N	1:A:911:ASN:ND2	2.69	0.41
1:C:913:ILE:HD12	1:C:913:ILE:N	2.35	0.41
1:D:821:VAL:CG1	1:D:833:SER:HB3	2.51	0.41
1:A:880:ASN:C	1:A:882:TYR:H	2.24	0.41
1:C:779:GLN:O	1:C:780:TYR:CB	2.63	0.41
1:D:827:GLY:C	1:D:829:LYS:N	2.74	0.41
1:B:787:ALA:HB3	1:B:794:TYR:CD2	2.56	0.40
1:C:879:ALA:HB3	1:C:913:ILE:HD11	2.02	0.40
1:A:805:THR:CG2	1:A:806:VAL:N	2.84	0.40
1:C:873:TYR:CD1	1:C:877:GLY:C	2.95	0.40
1:A:867:THR:O	1:A:869:LEU:N	2.54	0.40
1:A:916:ASN:ND2	1:A:918:LEU:HD13	2.37	0.40
1:D:764:ILE:CG2	1:D:767:ASN:HD21	2.34	0.40
1:B:843:ILE:HD13	1:B:843:ILE:HA	1.85	0.40
1:C:873:TYR:O	1:C:877:GLY:N	2.41	0.40
1:B:805:THR:HB	1:B:815:ASN:HD21	1.85	0.40
1:C:855:MET:HA	1:C:862:LEU:HD11	2.04	0.40
1:D:848:GLN:HA	1:D:929:TYR:HA	2.02	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	181/189 (96%)	156 (86%)	19 (10%)	6 (3%)	4	13
1	B	181/189 (96%)	156 (86%)	22 (12%)	3 (2%)	9	29
1	C	181/189 (96%)	161 (89%)	16 (9%)	4 (2%)	6	22
1	D	181/189 (96%)	155 (86%)	22 (12%)	4 (2%)	6	22
All	All	724/756 (96%)	628 (87%)	79 (11%)	17 (2%)	6	21

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	800	ASN
1	A	886	SER
1	B	829	LYS
1	C	808	ALA
1	A	755	GLU
1	D	920	GLY
1	D	923	VAL
1	C	920	GLY
1	D	772	GLU
1	D	800	ASN
1	B	896	LYS
1	A	808	ALA
1	C	768	ASN
1	A	868	VAL
1	A	919	PRO
1	B	838	ALA
1	C	916	ASN

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	158/163 (97%)	140 (89%)	18 (11%)	5 18
1	B	158/163 (97%)	137 (87%)	21 (13%)	4 12
1	C	158/163 (97%)	135 (85%)	23 (15%)	3 9
1	D	158/163 (97%)	142 (90%)	16 (10%)	7 22
All	All	632/652 (97%)	554 (88%)	78 (12%)	4 15

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	754	ASP
1	A	758	ILE
1	A	767	ASN
1	A	776	ILE
1	A	778	LEU
1	A	786	LYS
1	A	801	THR
1	A	829	LYS
1	A	831	THR
1	A	843	ILE
1	A	846	ASP
1	A	867	THR
1	A	880	ASN
1	A	886	SER
1	A	900	SER
1	A	902	GLN
1	A	925	THR
1	A	927	ASN
1	B	753	PHE
1	B	755	GLU
1	B	761	LYS
1	B	767	ASN
1	B	768	ASN
1	B	769	VAL
1	B	772	GLU
1	B	786	LYS
1	B	796	TRP
1	B	797	TYR
1	B	805	THR
1	B	820	VAL
1	B	840	SER
1	B	843	ILE
1	B	846	ASP

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Mol	Chain	Res	Type
1	B	856	SER
1	B	864	SER
1	B	865	THR
1	B	880	ASN
1	B	888	MET
1	B	904	SER
1	C	752	PHE
1	C	753	PHE
1	C	756	LEU
1	C	761	LYS
1	C	767	ASN
1	C	770	ARG
1	C	786	LYS
1	C	794	TYR
1	C	800	ASN
1	C	817	LYS
1	C	820	VAL
1	C	821	VAL
1	C	840	SER
1	C	843	ILE
1	C	846	ASP
1	C	867	THR
1	C	872	ILE
1	C	880	ASN
1	C	883	SER
1	C	902	GLN
1	C	915	GLN
1	C	922	ASN
1	C	925	THR
1	D	754	ASP
1	D	759	ASP
1	D	761	LYS
1	D	767	ASN
1	D	776	ILE
1	D	801	THR
1	D	820	VAL
1	D	828	ASP
1	D	833	SER
1	D	840	SER
1	D	846	ASP
1	D	860	ASN
1	D	880	ASN

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Mol	Chain	Res	Type
1	D	900	SER
1	D	902	GLN
1	D	927	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	767	ASN
1	A	779	GLN
1	A	782	GLN
1	A	815	ASN
1	A	880	ASN
1	A	897	GLN
1	A	911	ASN
1	A	916	ASN
1	A	922	ASN
1	A	927	ASN
1	B	767	ASN
1	B	782	GLN
1	B	815	ASN
1	B	880	ASN
1	B	897	GLN
1	B	915	GLN
1	C	760	ASN
1	C	767	ASN
1	C	775	ASN
1	C	848	GLN
1	C	880	ASN
1	C	915	GLN
1	D	767	ASN
1	D	779	GLN
1	D	815	ASN
1	D	880	ASN
1	D	889	ASN
1	D	897	GLN
1	D	922	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)

There are no ligands in this entry.

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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	183/189 (96%)	-0.69	0	100	100	2, 18, 40, 61	0
1	B	183/189 (96%)	-0.43	2 (1%)	80	75	4, 35, 68, 80	0
1	C	183/189 (96%)	-0.37	1 (0%)	91	88	5, 37, 68, 87	0
1	D	183/189 (96%)	-0.63	2 (1%)	80	75	1, 19, 41, 75	0
All	All	732/756 (96%)	-0.53	5 (0%)	87	84	1, 26, 62, 87	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	800	ASN	2.9
1	B	757	LYS	2.4
1	D	752	PHE	2.2
1	B	827	GLY	2.2
1	D	753	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.