Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 01:59 AM EDT

PDB ID	:	1TT7
Title	:	Crystal structure of Bacillus subtilis protein yhfP
Authors	:	Min, T.; Gorman, J.; Shapiro, L.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2004-06-22
Resolution	:	2.70 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:

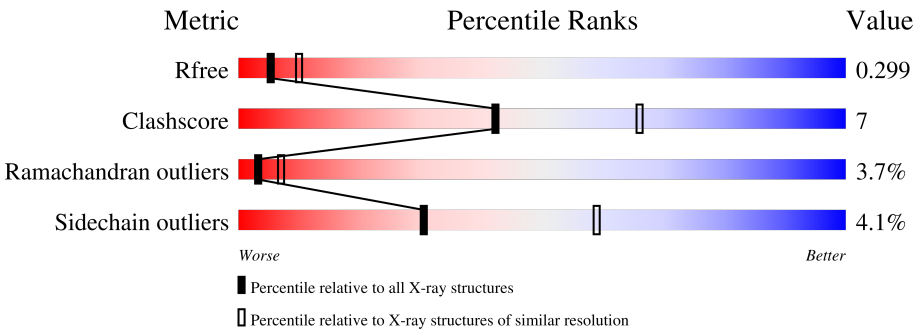
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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%

Mol	Chain	Length	Quality of chain
1	A	330	79% 18% •
1	B	330	77% 21% •
1	C	330	75% 22% •
1	D	330	78% 18% •
1	E	330	78% 19% •
1	F	330	76% 20% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14777 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 YHFP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	329	2436	1533	414	484	1	4	0	0	0
1	B	329	2436	1533	414	484	1	4	0	0	0
1	C	329	2436	1533	414	484	1	4	0	0	0
1	D	329	2436	1533	414	484	1	4	0	0	0
1	E	329	2436	1533	414	484	1	4	0	0	0
1	F	329	2437	1533	414	485	1	4	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	MSE	MET	modified residue	UNP O07615
A	170	MSE	MET	modified residue	UNP O07615
A	278	MSE	MET	modified residue	UNP O07615
A	288	MSE	MET	modified residue	UNP O07615
B	126	MSE	MET	modified residue	UNP O07615
B	170	MSE	MET	modified residue	UNP O07615
B	278	MSE	MET	modified residue	UNP O07615
B	288	MSE	MET	modified residue	UNP O07615
C	126	MSE	MET	modified residue	UNP O07615
C	170	MSE	MET	modified residue	UNP O07615
C	278	MSE	MET	modified residue	UNP O07615
C	288	MSE	MET	modified residue	UNP O07615
D	126	MSE	MET	modified residue	UNP O07615
D	170	MSE	MET	modified residue	UNP O07615
D	278	MSE	MET	modified residue	UNP O07615
D	288	MSE	MET	modified residue	UNP O07615
E	126	MSE	MET	modified residue	UNP O07615

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Chain	Residue	Modelled	Actual	Comment	Reference
E	170	MSE	MET	modified residue	UNP O07615
E	278	MSE	MET	modified residue	UNP O07615
E	288	MSE	MET	modified residue	UNP O07615
F	126	MSE	MET	modified residue	UNP O07615
F	170	MSE	MET	modified residue	UNP O07615
F	278	MSE	MET	modified residue	UNP O07615
F	288	MSE	MET	modified residue	UNP O07615

- Molecule 2 is water.

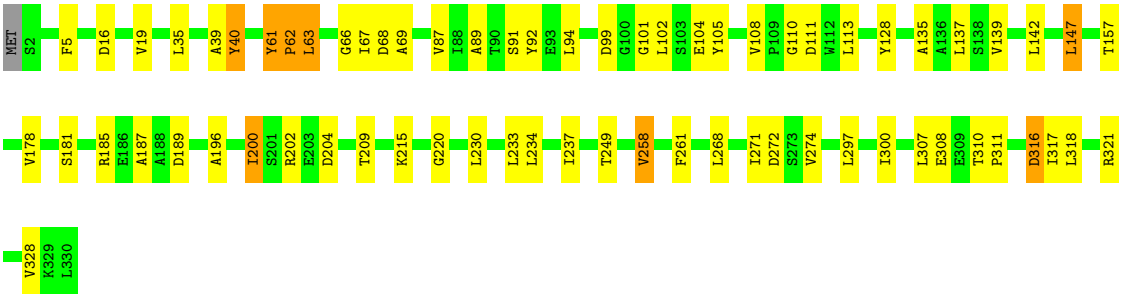
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	25	25	25	0	0
			Total	O		
2	B	26	26	26	0	0
			Total	O		
2	C	29	29	29	0	0
			Total	O		
2	D	19	19	19	0	0
			Total	O		
2	E	30	30	30	0	0
			Total	O		
2	F	31	31	31	0	0

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.

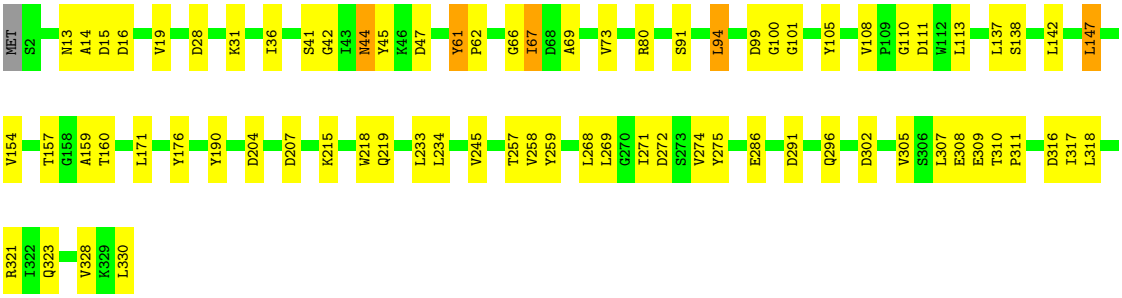
- Molecule 1: YHFP

Chain A:



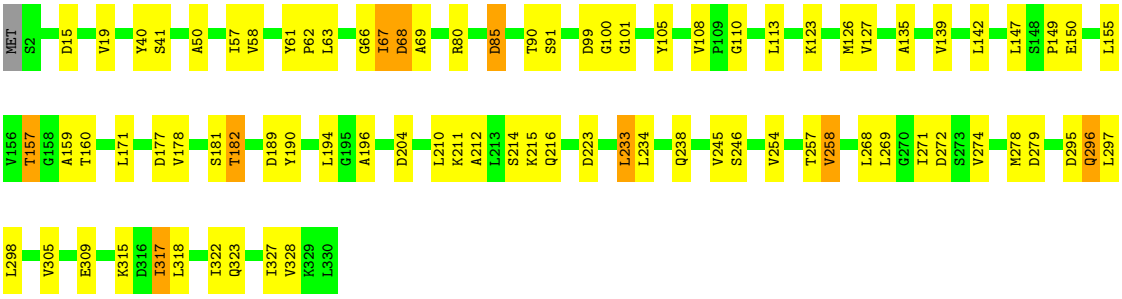
- Molecule 1: YHFP

Chain B:



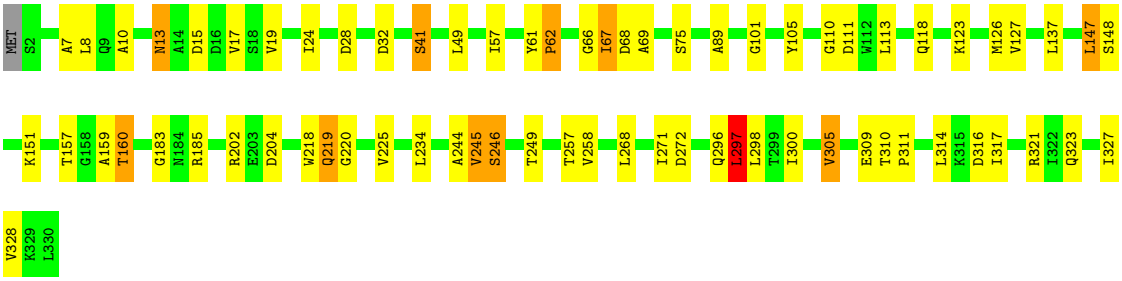
- Molecule 1: YHFP

Chain C:



- Molecule 1: YHFP

Chain D:

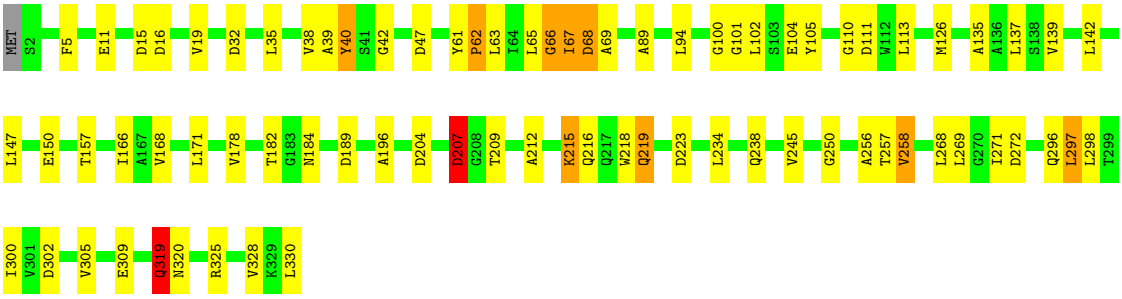


- Molecule 1: YHFP

Chain E:

- Molecule 1: YHFP

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.22Å 133.55Å 166.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.85 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.70) 98.7 (19.85-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.07 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.187 , 0.262 0.282 , 0.299	Depositor DCC
R_{free} test set	3148 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.828	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 28.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	14777	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 2.98% 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	0.29	0/2468	0.69	6/3343 (0.2%)
1	B	0.29	0/2468	0.71	11/3343 (0.3%)
1	C	0.29	0/2468	0.70	9/3343 (0.3%)
1	D	0.29	0/2468	0.69	7/3343 (0.2%)
1	E	0.29	0/2468	0.69	10/3343 (0.3%)
1	F	0.29	0/2469	0.69	10/3343 (0.3%)
All	All	0.29	0/14809	0.69	53/20058 (0.3%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	16	ASP	CB-CG-OD2	6.28	123.95	118.30
1	B	291	ASP	CB-CG-OD2	6.16	123.84	118.30
1	C	15	ASP	CB-CG-OD2	6.10	123.79	118.30
1	C	177	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	316	ASP	CB-CG-OD2	5.99	123.69	118.30
1	F	15	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	189	ASP	CB-CG-OD2	5.91	123.62	118.30
1	C	279	ASP	CB-CG-OD2	5.90	123.61	118.30
1	D	316	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	15	ASP	CB-CG-OD2	5.84	123.56	118.30
1	E	291	ASP	CB-CG-OD2	5.83	123.55	118.30
1	E	295	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	28	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	99	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	207	ASP	CB-CG-OD2	5.77	123.50	118.30
1	D	28	ASP	CB-CG-OD2	5.77	123.49	118.30
1	B	99	ASP	CB-CG-OD2	5.76	123.48	118.30
1	F	16	ASP	CB-CG-OD2	5.74	123.47	118.30
1	F	302	ASP	CB-CG-OD2	5.73	123.46	118.30
1	C	85	ASP	CB-CG-OD2	5.71	123.44	118.30
1	E	207	ASP	CB-CG-OD2	5.68	123.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	223	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	111	ASP	CB-CG-OD2	5.64	123.38	118.30
1	F	207	ASP	CB-CG-OD2	5.62	123.36	118.30
1	F	111	ASP	CB-CG-OD2	5.59	123.34	118.30
1	B	111	ASP	CB-CG-OD2	5.54	123.29	118.30
1	D	15	ASP	CB-CG-OD2	5.50	123.25	118.30
1	D	272	ASP	CB-CG-OD2	5.45	123.21	118.30
1	C	272	ASP	CB-CG-OD2	5.27	123.04	118.30
1	E	99	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	272	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	189	ASP	CB-CG-OD2	5.13	122.92	118.30
1	F	272	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	47	ASP	CB-CG-OD2	5.12	122.90	118.30
1	E	68	ASP	CB-CG-OD2	5.09	122.88	118.30
1	F	204	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	99	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	272	ASP	CB-CG-OD2	5.08	122.88	118.30
1	E	272	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	111	ASP	CB-CG-OD2	5.07	122.86	118.30
1	E	47	ASP	CB-CG-OD2	5.07	122.86	118.30
1	F	47	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	204	ASP	CB-CG-OD2	5.06	122.86	118.30
1	B	204	ASP	CB-CG-OD2	5.06	122.85	118.30
1	F	189	ASP	CB-CG-OD2	5.05	122.85	118.30
1	E	111	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	16	ASP	CB-CG-OD2	5.03	122.83	118.30
1	E	16	ASP	CB-CG-OD2	5.03	122.83	118.30
1	D	32	ASP	CB-CG-OD2	5.03	122.83	118.30
1	E	302	ASP	CB-CG-OD2	5.03	122.82	118.30
1	F	32	ASP	CB-CG-OD2	5.03	122.82	118.30
1	B	302	ASP	CB-CG-OD2	5.02	122.81	118.30
1	D	204	ASP	CB-CG-OD2	5.00	122.80	118.30

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	2436	0	2462	32	0
1	B	2436	0	2462	35	0
1	C	2436	0	2462	37	0
1	D	2436	0	2462	38	0
1	E	2436	0	2462	32	0
1	F	2437	0	2462	33	0
2	A	25	0	0	1	0
2	B	26	0	0	1	0
2	C	29	0	0	0	0
2	D	19	0	0	1	0
2	E	30	0	0	0	0
2	F	31	0	0	0	0
All	All	14777	0	14772	203	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 7.

All (203) 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:F:68:ASP:HB3	1:F:126:MSE:HE1	1.57	0.86
1:D:66:GLY:HA3	1:D:101:GLY:H	1.43	0.83
1:E:68:ASP:HB3	1:E:126:MSE:HE1	1.63	0.81
1:D:245:VAL:O	1:D:246:SER:HB3	1.83	0.79
1:C:257:THR:O	1:C:258:VAL:HB	1.85	0.75
1:A:66:GLY:HA3	1:A:101:GLY:H	1.52	0.75
1:F:39:ALA:HA	1:F:330:LEU:HB2	1.71	0.72
1:D:160:THR:HG23	1:D:323:GLN:HG3	1.72	0.72
1:B:257:THR:O	1:B:259:TYR:N	2.22	0.72
1:C:57:ILE:HD12	1:C:58:VAL:H	1.55	0.72
1:F:39:ALA:O	1:F:40:TYR:HB2	1.90	0.70
1:C:66:GLY:HA3	1:C:100:GLY:HA3	1.73	0.70
1:D:218:TRP:O	1:D:219:GLN:HB3	1.93	0.67
1:A:261:PHE:HB3	1:D:245:VAL:HG21	1.77	0.67
1:D:13:ASN:HD22	1:D:13:ASN:H	1.40	0.66
1:F:67:ILE:O	1:F:68:ASP:HB2	1.97	0.65
1:C:159:ALA:O	1:C:160:THR:HB	1.96	0.65
1:C:160:THR:HG23	1:C:323:GLN:HG3	1.78	0.64
1:E:66:GLY:HA3	1:E:101:GLY:H	1.63	0.64
1:D:310:THR:N	1:D:311:PRO:HD2	2.13	0.63
1:C:68:ASP:HA	1:C:90:THR:HG22	1.82	0.62
1:C:305:VAL:HG13	1:C:309:GLU:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:SER:HB3	1:B:328:VAL:H	1.65	0.61
1:B:41:SER:CB	1:B:328:VAL:H	2.13	0.60
1:B:160:THR:HG23	1:B:323:GLN:HG3	1.84	0.60
1:F:66:GLY:HA3	1:F:100:GLY:HA3	1.84	0.60
1:B:66:GLY:HA3	1:B:100:GLY:HA3	1.85	0.59
1:F:61:TYR:N	1:F:62:PRO:HD2	2.18	0.59
1:D:69:ALA:HB2	1:D:101:GLY:HA3	1.83	0.58
1:C:67:ILE:O	1:C:68:ASP:HB2	2.03	0.58
1:B:91:SER:HB2	1:B:274:VAL:HA	1.85	0.58
1:C:50:ALA:HA	1:C:57:ILE:HD13	1.86	0.57
1:D:159:ALA:O	1:D:160:THR:HB	2.04	0.57
1:A:317:ILE:O	1:A:318:LEU:HB2	2.05	0.56
1:C:149:PRO:O	1:D:118:GLN:HB2	2.05	0.56
1:D:10:ALA:O	2:D:335:HOH:O	2.18	0.55
1:D:148:SER:HB2	1:D:151:LYS:HD3	1.88	0.55
1:C:246:SER:HB3	1:C:271:ILE:HB	1.89	0.55
1:A:69:ALA:HB3	1:A:89:ALA:HB3	1.89	0.55
1:D:41:SER:HA	1:D:328:VAL:H	1.72	0.55
1:B:61:TYR:N	1:B:62:PRO:HD2	2.22	0.54
1:D:159:ALA:O	1:D:160:THR:CB	2.54	0.54
1:F:182:THR:HG22	1:F:184:ASN:H	1.72	0.54
1:D:41:SER:HB3	1:D:126:MSE:HB3	1.89	0.54
1:C:317:ILE:O	1:C:318:LEU:HB3	2.08	0.53
1:B:307:LEU:HD12	1:B:330:LEU:HD22	1.90	0.53
1:F:67:ILE:O	1:F:68:ASP:CB	2.57	0.53
1:B:310:THR:N	1:B:311:PRO:CD	2.72	0.53
1:C:40:TYR:HB3	1:C:126:MSE:HG3	1.91	0.53
1:E:142:LEU:HD23	1:E:269:LEU:HD12	1.91	0.52
1:C:178:VAL:HB	1:C:196:ALA:HA	1.91	0.52
1:C:212:ALA:HA	1:C:257:THR:HG21	1.91	0.52
1:F:296:GLN:O	1:F:298:LEU:N	2.43	0.52
1:C:305:VAL:O	1:C:328:VAL:HA	2.10	0.52
1:A:39:ALA:O	1:A:40:TYR:HB2	2.10	0.51
1:A:61:TYR:O	1:A:63:LEU:HB2	2.10	0.51
1:E:159:ALA:O	1:E:160:THR:HB	2.09	0.51
1:A:110:GLY:HA2	1:A:113:LEU:HD12	1.93	0.51
1:D:305:VAL:HG22	1:D:309:GLU:HB2	1.93	0.51
1:B:41:SER:HA	1:B:328:VAL:HB	1.91	0.51
1:B:44:ASN:HD22	1:B:45:TYR:H	1.58	0.51
1:C:69:ALA:HB2	1:C:101:GLY:HA3	1.91	0.51
1:A:137:LEU:HD23	1:A:271:ILE:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ALA:HB3	1:D:89:ALA:HB3	1.93	0.50
1:E:211:LYS:O	1:E:212:ALA:HB3	2.11	0.50
1:F:69:ALA:HB2	1:F:101:GLY:HA3	1.92	0.50
1:F:166:ILE:HG12	1:F:300:ILE:HD13	1.93	0.50
1:A:69:ALA:HB2	1:A:101:GLY:HA3	1.94	0.50
1:D:66:GLY:C	1:D:68:ASP:H	2.15	0.50
1:E:61:TYR:N	1:E:62:PRO:HD3	2.25	0.50
1:E:157:THR:HA	1:E:181:SER:HB3	1.94	0.50
1:B:317:ILE:O	1:B:318:LEU:HB2	2.12	0.49
1:E:160:THR:HG23	1:E:323:GLN:HG3	1.93	0.49
1:E:69:ALA:HB2	1:E:101:GLY:HA3	1.93	0.49
1:E:69:ALA:HB3	1:E:89:ALA:HB3	1.93	0.49
1:F:69:ALA:HB3	1:F:89:ALA:HB3	1.94	0.49
1:A:178:VAL:HB	1:A:196:ALA:HA	1.95	0.49
1:E:66:GLY:C	1:E:68:ASP:H	2.16	0.49
1:B:159:ALA:O	1:B:160:THR:HB	2.13	0.49
1:B:308:GLU:O	1:B:309:GLU:HB3	2.13	0.49
1:D:183:GLY:HA2	1:D:202:ARG:HD2	1.95	0.49
1:B:275:TYR:HB3	1:C:80:ARG:HD2	1.95	0.48
1:A:91:SER:HB3	1:A:274:VAL:HA	1.94	0.48
1:F:216:GLN:HB3	1:F:238:GLN:HG2	1.95	0.48
1:C:157:THR:HA	1:C:181:SER:HB3	1.94	0.48
1:B:305:VAL:O	1:B:328:VAL:HA	2.14	0.48
1:D:147:LEU:HD21	1:D:220:GLY:HA3	1.95	0.48
1:B:154:VAL:HB	1:B:171:LEU:HD21	1.96	0.47
1:C:317:ILE:HG23	1:C:322:ILE:HD12	1.95	0.47
1:D:49:LEU:HB2	1:D:57:ILE:HD12	1.96	0.47
1:E:185:ARG:H	1:E:185:ARG:HH11	1.61	0.47
1:A:66:GLY:C	1:A:68:ASP:H	2.18	0.47
1:E:211:LYS:O	1:E:212:ALA:CB	2.62	0.47
1:D:137:LEU:HD23	1:D:271:ILE:HG23	1.95	0.47
1:E:137:LEU:HD23	1:E:271:ILE:HG23	1.96	0.47
1:A:200:ILE:HG23	1:A:204:ASP:HB2	1.96	0.47
1:F:319:GLN:HB3	1:F:320:ASN:H	1.56	0.47
1:E:91:SER:HB3	1:E:274:VAL:HA	1.96	0.47
1:F:5:PHE:HB2	1:F:104:GLU:HB2	1.97	0.47
1:A:87:VAL:HG21	1:A:113:LEU:HB3	1.96	0.46
1:B:218:TRP:O	1:B:219:GLN:HB3	2.15	0.46
1:C:50:ALA:HA	1:C:57:ILE:CD1	2.45	0.46
1:A:202:ARG:HG2	2:A:348:HOH:O	2.15	0.46
1:F:215:LYS:H	1:F:215:LYS:HD3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:VAL:HG22	1:E:309:GLU:HB3	1.98	0.46
1:F:234:LEU:HD21	1:F:268:LEU:HD13	1.97	0.46
1:C:135:ALA:O	1:C:139:VAL:HG23	2.16	0.46
1:F:168:VAL:HG13	1:F:178:VAL:HG11	1.98	0.46
1:D:202:ARG:HH22	1:D:225:VAL:HG21	1.81	0.46
1:A:157:THR:HA	1:A:181:SER:HB3	1.97	0.46
1:E:138:SER:O	1:E:142:LEU:HG	2.15	0.45
1:D:41:SER:HB2	1:D:327:ILE:HG23	1.98	0.45
1:D:123:LYS:O	1:D:127:VAL:HG23	2.17	0.45
1:F:39:ALA:O	1:F:40:TYR:CB	2.62	0.45
1:D:66:GLY:HA3	1:D:101:GLY:N	2.20	0.45
1:E:110:GLY:HA2	1:E:113:LEU:HD12	1.98	0.45
1:C:110:GLY:HA2	1:C:113:LEU:HD12	1.99	0.45
1:B:234:LEU:HD21	1:B:268:LEU:HD13	1.98	0.45
1:E:159:ALA:O	1:E:160:THR:CB	2.65	0.45
1:F:137:LEU:HD23	1:F:271:ILE:HG23	1.97	0.45
1:A:5:PHE:HB2	1:A:104:GLU:HB2	1.99	0.45
1:D:41:SER:CB	1:D:126:MSE:HB3	2.46	0.45
1:D:225:VAL:HG13	1:D:249:THR:O	2.17	0.45
1:A:147:LEU:HD21	1:A:220:GLY:HA3	1.99	0.44
1:B:157:THR:HG21	2:B:339:HOH:O	2.16	0.44
1:E:310:THR:N	1:E:311:PRO:CD	2.80	0.44
1:F:305:VAL:HG13	1:F:309:GLU:HB2	1.99	0.44
1:A:61:TYR:O	1:A:62:PRO:C	2.55	0.44
1:C:155:LEU:HD11	1:C:157:THR:HG23	1.98	0.44
1:B:308:GLU:O	1:B:309:GLU:CB	2.65	0.44
1:B:138:SER:O	1:B:142:LEU:HG	2.17	0.44
1:C:155:LEU:HD12	1:C:233:LEU:HD21	2.00	0.44
1:B:36:ILE:HG13	1:B:73:VAL:HA	2.00	0.44
1:B:142:LEU:HD23	1:B:269:LEU:HD12	1.99	0.44
1:C:91:SER:HB3	1:C:274:VAL:HA	2.00	0.44
1:D:234:LEU:HD21	1:D:268:LEU:HD13	1.99	0.44
1:E:185:ARG:O	1:E:186:GLU:HB2	2.18	0.44
1:B:215:LYS:H	1:B:215:LYS:HD2	1.82	0.44
1:A:234:LEU:HD21	1:A:268:LEU:HD13	2.00	0.44
1:C:211:LYS:HB3	1:C:214:SER:HB3	2.00	0.44
1:F:178:VAL:HB	1:F:196:ALA:HA	1.99	0.44
1:A:316:ASP:HA	1:A:321:ARG:HD2	2.00	0.43
1:D:61:TYR:N	1:D:62:PRO:HD3	2.33	0.43
1:E:317:ILE:HG13	1:E:318:LEU:H	1.83	0.43
1:A:94:LEU:HD21	1:A:108:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:TYR:N	1:E:62:PRO:CD	2.81	0.43
1:A:258:VAL:HA	1:A:261:PHE:HD2	1.84	0.43
1:D:8:LEU:HD21	1:D:314:LEU:HD11	2.01	0.43
1:E:74:VAL:HG23	1:E:75:SER:H	1.82	0.43
1:B:69:ALA:HB2	1:B:101:GLY:HA3	1.99	0.43
1:E:166:ILE:HG12	1:E:300:ILE:HD13	1.99	0.43
1:D:110:GLY:HA2	1:D:113:LEU:HD12	2.00	0.43
1:B:137:LEU:HD23	1:B:271:ILE:HG23	1.99	0.43
1:F:66:GLY:HA3	1:F:101:GLY:H	1.84	0.43
1:A:66:GLY:HA2	1:A:102:LEU:HG	2.01	0.43
1:B:94:LEU:HD21	1:B:108:VAL:HB	2.01	0.43
1:C:216:GLN:HB3	1:C:238:GLN:HG2	2.01	0.43
1:E:260:PRO:O	1:E:264:ARG:HB2	2.18	0.43
1:F:135:ALA:O	1:F:139:VAL:HG23	2.18	0.43
1:A:40:TYR:HA	1:A:328:VAL:O	2.18	0.43
1:D:225:VAL:HG22	1:D:249:THR:HB	2.01	0.43
1:B:142:LEU:HB3	1:B:147:LEU:HG	2.00	0.42
1:F:305:VAL:O	1:F:328:VAL:HA	2.19	0.42
1:A:135:ALA:O	1:A:139:VAL:HG23	2.19	0.42
1:D:297:LEU:O	1:D:300:ILE:HG22	2.19	0.42
1:B:160:THR:HA	1:B:190:TYR:HE2	1.85	0.42
1:D:296:GLN:O	1:D:298:LEU:N	2.49	0.42
1:E:226:GLY:HA2	1:E:230:LEU:HD12	2.00	0.42
1:F:110:GLY:HA2	1:F:113:LEU:HD12	2.01	0.42
1:B:110:GLY:HA2	1:B:113:LEU:HD12	2.02	0.42
1:C:123:LYS:O	1:C:127:VAL:HG23	2.20	0.42
1:E:78:ASP:HA	1:E:79:PRO:HD3	1.85	0.42
1:A:233:LEU:O	1:A:237:ILE:HG12	2.20	0.42
1:C:234:LEU:HD21	1:C:268:LEU:HD13	2.01	0.42
1:F:157:THR:HB	1:F:223:ASP:HA	2.02	0.42
1:E:94:LEU:HD21	1:E:108:VAL:HB	2.02	0.41
1:C:41:SER:HB2	1:C:327:ILE:HG23	2.01	0.41
1:D:7:ALA:HB3	1:D:24:ILE:HD13	2.02	0.41
1:F:218:TRP:O	1:F:219:GLN:HB3	2.18	0.41
1:B:66:GLY:HA3	1:B:101:GLY:H	1.86	0.41
1:C:159:ALA:HB3	1:C:182:THR:HG23	2.02	0.41
1:C:190:TYR:O	1:C:194:LEU:HG	2.20	0.41
1:F:42:GLY:HA3	1:F:325:ARG:NH1	2.35	0.41
1:D:245:VAL:O	1:D:246:SER:CB	2.60	0.41
1:F:142:LEU:HD23	1:F:269:LEU:HD12	2.01	0.41
1:A:128:TYR:CZ	1:A:297:LEU:HD21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:TYR:N	1:C:62:PRO:CD	2.84	0.41
1:B:61:TYR:N	1:B:62:PRO:CD	2.82	0.41
1:B:171:LEU:HG	1:B:176:TYR:HB2	2.03	0.41
1:D:244:ALA:HB1	1:D:271:ILE:HD13	2.02	0.41
1:C:142:LEU:HD23	1:C:269:LEU:HD12	2.03	0.41
1:E:155:LEU:HD21	1:E:200:ILE:HD11	2.02	0.41
1:A:215:LYS:H	1:A:215:LYS:HD2	1.86	0.41
1:F:65:LEU:O	1:F:102:LEU:HB2	2.20	0.41
1:A:310:THR:N	1:A:311:PRO:CD	2.84	0.40
1:E:197:SER:O	1:E:198:GLU:HB2	2.21	0.40
1:E:245:VAL:HB	1:E:246:SER:H	1.71	0.40
1:C:296:GLN:O	1:C:298:LEU:N	2.54	0.40
1:F:219:GLN:HB3	1:F:219:GLN:HE21	1.64	0.40
1:A:142:LEU:HB3	1:A:147:LEU:HG	2.03	0.40
1:A:185:ARG:C	1:A:187:ALA:H	2.24	0.40
1:C:254:VAL:HB	1:F:256:ALA:HB3	2.03	0.40
1:B:316:ASP:HA	1:B:321:ARG:HH11	1.86	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	327/330 (99%)	295 (90%)	22 (7%)	10 (3%)	4 9
1	B	327/330 (99%)	282 (86%)	36 (11%)	9 (3%)	5 11
1	C	327/330 (99%)	280 (86%)	36 (11%)	11 (3%)	3 8
1	D	327/330 (99%)	287 (88%)	26 (8%)	14 (4%)	2 5
1	E	327/330 (99%)	285 (87%)	31 (10%)	11 (3%)	3 8
1	F	327/330 (99%)	285 (87%)	25 (8%)	17 (5%)	2 3
All	All	1962/1980 (99%)	1714 (87%)	176 (9%)	72 (4%)	3 7

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	TYR
1	A	62	PRO
1	A	67	ILE
1	A	258	VAL
1	B	258	VAL
1	C	258	VAL
1	D	67	ILE
1	D	245	VAL
1	E	67	ILE
1	E	212	ALA
1	E	258	VAL
1	F	40	TYR
1	F	67	ILE
1	F	68	ASP
1	F	297	LEU
1	F	319	GLN
1	A	209	THR
1	A	249	THR
1	B	67	ILE
1	B	245	VAL
1	C	210	LEU
1	C	215	LYS
1	C	245	VAL
1	D	160	THR
1	D	246	SER
1	D	258	VAL
1	E	210	LEU
1	F	94	LEU
1	F	258	VAL
1	A	105	TYR
1	B	42	GLY
1	B	94	LEU
1	C	67	ILE
1	C	68	ASP
1	D	75	SER
1	E	14	ALA
1	E	245	VAL
1	F	207	ASP
1	A	92	TYR
1	B	14	ALA
1	B	105	TYR
1	C	105	TYR

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Mol	Chain	Res	Type
1	C	150	GLU
1	C	296	GLN
1	C	297	LEU
1	D	17	VAL
1	D	19	VAL
1	D	41	SER
1	E	105	TYR
1	F	105	TYR
1	F	245	VAL
1	F	250	GLY
1	A	19	VAL
1	A	40	TYR
1	B	13	ASN
1	B	19	VAL
1	C	19	VAL
1	D	105	TYR
1	D	257	THR
1	D	297	LEU
1	E	19	VAL
1	E	160	THR
1	E	309	GLU
1	F	19	VAL
1	F	212	ALA
1	D	62	PRO
1	F	38	VAL
1	F	62	PRO
1	F	209	THR
1	E	61	TYR
1	F	66	GLY
1	D	317	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	261/258 (101%)	253 (97%)	8 (3%)	40 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	261/258 (101%)	252 (97%)	9 (3%)	37	66
1	C	261/258 (101%)	249 (95%)	12 (5%)	27	54
1	D	261/258 (101%)	252 (97%)	9 (3%)	37	66
1	E	261/258 (101%)	248 (95%)	13 (5%)	24	51
1	F	261/258 (101%)	248 (95%)	13 (5%)	24	51
All	All	1566/1548 (101%)	1502 (96%)	64 (4%)	30	59

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	63	LEU
1	A	147	LEU
1	A	200	ILE
1	A	230	LEU
1	A	300	ILE
1	A	307	LEU
1	A	308	GLU
1	B	31	LYS
1	B	44	ASN
1	B	61	TYR
1	B	67	ILE
1	B	80	ARG
1	B	147	LEU
1	B	233	LEU
1	B	286	GLU
1	B	296	GLN
1	C	63	LEU
1	C	85	ASP
1	C	108	VAL
1	C	147	LEU
1	C	157	THR
1	C	171	LEU
1	C	182	THR
1	C	233	LEU
1	C	278	MSE
1	C	295	ASP
1	C	315	LYS
1	C	317	ILE
1	D	13	ASN

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Mol	Chain	Res	Type
1	D	67	ILE
1	D	147	LEU
1	D	157	THR
1	D	185	ARG
1	D	219	GLN
1	D	297	LEU
1	D	305	VAL
1	D	321	ARG
1	E	8	LEU
1	E	22	LYS
1	E	28	ASP
1	E	35	LEU
1	E	59	ARG
1	E	74	VAL
1	E	147	LEU
1	E	150	GLU
1	E	155	LEU
1	E	185	ARG
1	E	230	LEU
1	E	258	VAL
1	E	319	GLN
1	F	11	GLU
1	F	35	LEU
1	F	63	LEU
1	F	147	LEU
1	F	150	GLU
1	F	171	LEU
1	F	207	ASP
1	F	215	LYS
1	F	219	GLN
1	F	257	THR
1	F	258	VAL
1	F	297	LEU
1	F	319	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	B	119	ASN
1	B	296	GLN
1	C	9	GLN

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Mol	Chain	Res	Type
1	C	229	GLN
1	D	13	ASN
1	D	216	GLN
1	D	219	GLN
1	D	238	GLN
1	E	9	GLN
1	E	238	GLN
1	F	217	GLN
1	F	219	GLN

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.