Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2024 – 09:34 AM EDT

PDB ID	:	3GYG
Title	:	Crystal structure of yhjK (haloacid dehalogenase-like hydrolase protein) from Bacillus subtilis
Authors	:	Nocek, B.; Stein, A.; Wu, R.; Jedrzejczak, R.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2009-04-03
Resolution	:	2.45 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:

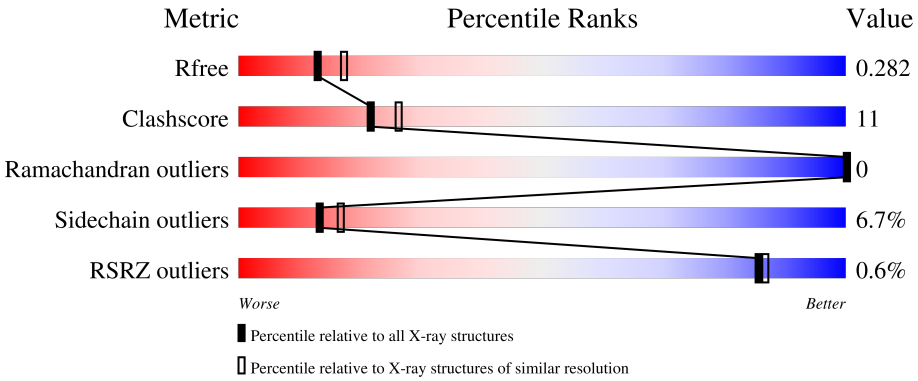
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.45 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}	164625	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (2.46-2.46)

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	289	% 82% 16%
1	B	289	% 63% 16% 20%
1	C	289	75% 18%
1	D	289	60% 23% 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8445 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 NTD biosynthesis operon putative hydrolase ntdB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	Se	0	2	0
			2302	1458	383	453	3	5			
1	B	230	Total	C	N	O	S	Se	0	0	0
			1845	1172	304	362	2	5			
1	C	277	Total	C	N	O	S	Se	0	0	0
			2206	1398	363	439	3	3			
1	D	250	Total	C	N	O	S	Se	0	0	0
			2007	1279	330	390	3	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP O07565
A	-1	ASN	-	expression tag	UNP O07565
A	0	ALA	-	expression tag	UNP O07565
B	-2	SER	-	expression tag	UNP O07565
B	-1	ASN	-	expression tag	UNP O07565
B	0	ALA	-	expression tag	UNP O07565
C	-2	SER	-	expression tag	UNP O07565
C	-1	ASN	-	expression tag	UNP O07565
C	0	ALA	-	expression tag	UNP O07565
D	-2	SER	-	expression tag	UNP O07565
D	-1	ASN	-	expression tag	UNP O07565
D	0	ALA	-	expression tag	UNP O07565

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is water.

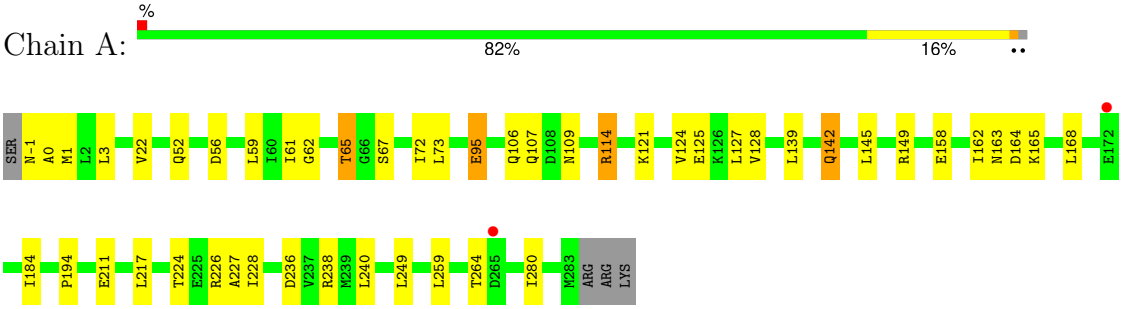
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	24	Total O 24 24	0	0
3	B	15	Total O 15 15	0	0
3	C	25	Total O 25 25	0	0
3	D	17	Total O 17 17	0	0

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.

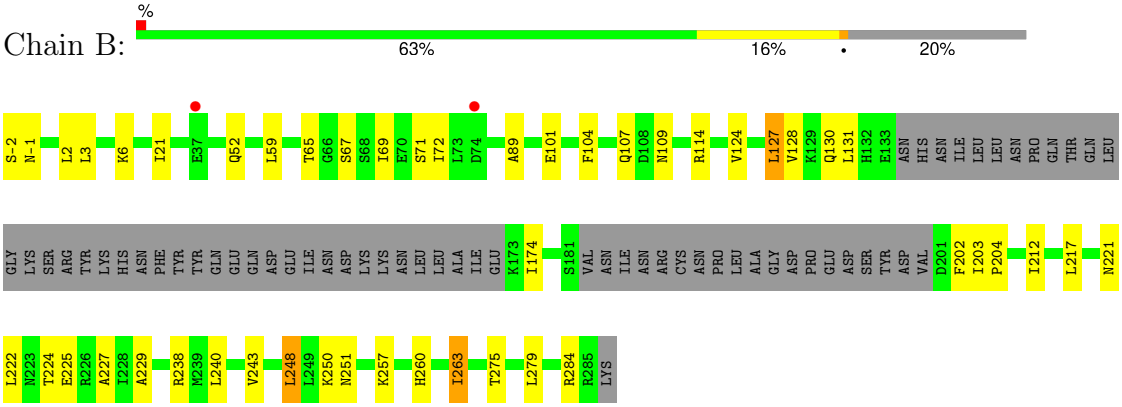
• Molecule 1: NTD biosynthesis operon putative hydrolase ntdB

Chain A:



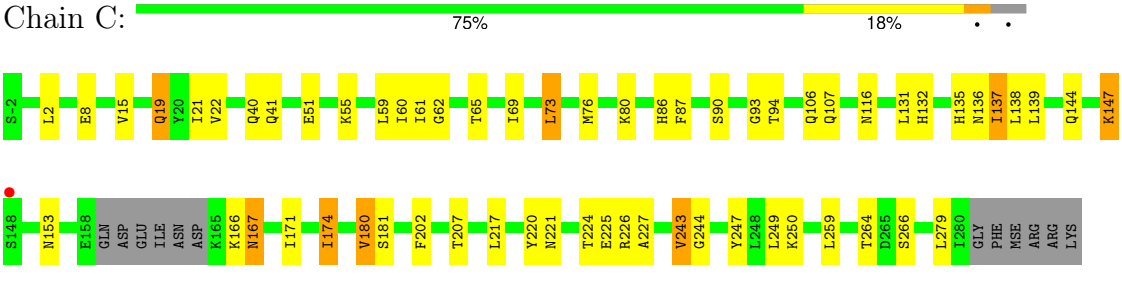
• Molecule 1: NTD biosynthesis operon putative hydrolase ntdB

Chain B:



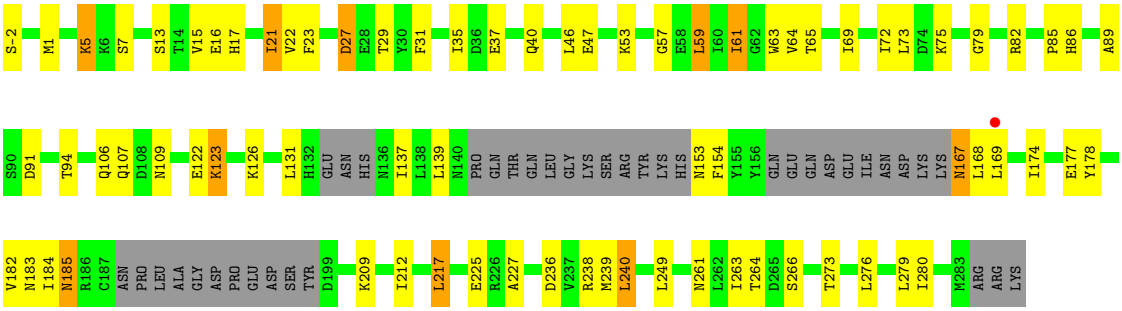
• Molecule 1: NTD biosynthesis operon putative hydrolase ntdB

Chain C:



• Molecule 1: NTD biosynthesis operon putative hydrolase ntdB

Chain D:


S-2 M1 K5 K6 S7 S13 T14 V15 E16 H17 I21 V22 F23 D27 E28 T29 Y30 F31 I35 D36 E37 Q40 L46 E47 K53 G57 E58 L59 I60 I61 G62 W63 V64 T65 I69 I72 L73 D74 K75 G79 R82 P85 H86 A89
S90 D91 T94 Q106 Q107 D108 N109 E122 K123 K126 L131 H132 GLU ASN HIS N136 I137 L138 L139 N140 PRO GLN THR GLN LEU GLY LYS SER ARG TYR LYS HIS N153 F154 Y155 Y156 GLN GLU GLN ASP GLU ILE ASN ASP LYS LYS N167 L168 L169 I174 E177 Y178
V182 N183 I184 N185 R186 C187 ASN PRO LEU ALA GLY ASP PRO GLU ASP SER TYR D199 K209 I212 L217 E225 R226 A227 D236 V237 R238 M239 L240 L249 N261 L262 I263 T264 D265 S266 T273 L276 L279 I280 M283 ARG ARG LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.08Å 111.73Å 135.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.45 40.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	93.4 (40.00-2.45) 93.4 (40.00-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.00 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, R_{free}	0.210 , 0.277 0.224 , 0.282	Depositor DCC
R_{free} test set	1919 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8445	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.51	0/2350	0.57	0/3164
1	B	0.53	0/1875	0.59	0/2515
1	C	0.52	0/2247	0.61	0/3033
1	D	0.54	0/2037	0.63	0/2733
All	All	0.52	0/8509	0.60	0/11445

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	2302	0	2210	36	0
1	B	1845	0	1775	43	0
1	C	2206	0	2086	53	0
1	D	2007	0	1945	55	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	24	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	0	0	0
3	C	25	0	0	0	0
3	D	17	0	0	1	0
All	All	8445	0	8016	174	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 11.

All (174) 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:A:114[A]:ARG:HG3	1:A:114[A]:ARG:NH1	1.56	1.09
1:D:65:THR:HG21	1:D:72:ILE:HD11	1.31	1.06
1:A:114[A]:ARG:HH11	1:A:114[A]:ARG:CG	1.69	1.05
1:D:22:VAL:HB	1:D:61:ILE:HD12	1.48	0.96
1:A:114[A]:ARG:HG3	1:A:114[A]:ARG:HH11	0.78	0.92
1:D:21:ILE:HD12	1:D:23:PHE:CZ	2.06	0.91
1:B:107:GLN:HE22	1:C:106:GLN:HA	1.38	0.88
1:D:21:ILE:HD12	1:D:23:PHE:CE2	2.10	0.86
1:B:65:THR:HG21	1:B:72:ILE:HD11	1.59	0.82
1:D:185:ASN:HD22	1:D:185:ASN:N	1.81	0.78
1:D:65:THR:CG2	1:D:72:ILE:HD11	2.14	0.76
1:B:131:LEU:CD1	1:B:174:ILE:HD13	2.18	0.74
1:A:1:MSE:HE3	1:A:73:LEU:HD12	1.71	0.71
1:C:137:ILE:HD12	1:C:167:ASN:ND2	2.05	0.70
1:B:65:THR:CG2	1:B:72:ILE:HD11	2.21	0.70
1:D:47:GLU:OE2	1:D:82:ARG:NH2	2.26	0.69
1:A:168:LEU:HD13	1:A:184:ILE:HG21	1.75	0.68
1:B:107:GLN:HE21	1:B:109:ASN:HD22	1.42	0.67
1:A:3:LEU:HD22	1:D:94:THR:HB	1.77	0.67
1:D:21:ILE:CD1	1:D:23:PHE:CZ	2.79	0.66
1:B:250:LYS:HA	1:B:263:ILE:HD11	1.76	0.66
1:C:249:LEU:HA	1:C:264:THR:HG22	1.79	0.65
1:C:227:ALA:CB	1:C:243:VAL:HG22	2.27	0.64
1:A:121:LYS:O	1:A:125:GLU:HG2	1.97	0.64
1:D:21:ILE:CD1	1:D:23:PHE:CE2	2.80	0.64
1:B:127:LEU:C	1:B:127:LEU:HD12	2.17	0.64
1:A:107:GLN:HE21	1:A:109:ASN:HD22	1.47	0.63
1:D:264:THR:HG22	1:D:266:SER:H	1.62	0.63
1:D:29:THR:HG23	1:D:249:LEU:HD11	1.81	0.62
1:A:128:VAL:HG22	1:A:139:LEU:HD22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:LYS:HB3	1:D:59:LEU:HD23	1.85	0.59
1:D:22:VAL:CB	1:D:61:ILE:HD12	2.28	0.59
1:C:217:LEU:HD21	1:C:227:ALA:HB2	1.85	0.58
1:B:131:LEU:HD11	1:B:174:ILE:HG21	1.85	0.58
1:B:131:LEU:HD11	1:B:174:ILE:HD13	1.84	0.58
1:B:240:LEU:CD1	1:B:248:LEU:HD13	2.34	0.58
1:D:29:THR:HG23	1:D:249:LEU:CD1	2.35	0.57
1:A:1:MSE:HE3	1:A:73:LEU:CD1	2.35	0.57
1:D:16:GLU:HG2	1:D:17:HIS:CE1	2.39	0.57
1:C:19:GLN:O	1:C:226:ARG:HD2	2.06	0.56
1:B:6:LYS:HZ2	1:C:116:ASN:HD22	1.53	0.56
1:B:127:LEU:HD12	1:B:128:VAL:N	2.21	0.55
1:D:139:LEU:HB3	1:D:154:PHE:HB3	1.88	0.55
1:D:13:SER:O	1:D:86:HIS:HE1	1.89	0.55
1:A:-1:ASN:HD21	1:A:1:MSE:HB3	1.70	0.55
1:C:131:LEU:HD23	1:C:174:ILE:HD11	1.89	0.55
1:B:6:LYS:NZ	1:C:116:ASN:HD22	2.04	0.54
1:B:21:ILE:HD12	1:B:217:LEU:HD23	1.88	0.54
1:B:21:ILE:HD11	1:B:222:LEU:HD12	1.90	0.54
1:A:127:LEU:C	1:A:127:LEU:HD23	2.28	0.54
1:D:131:LEU:HG	1:D:174:ILE:HD12	1.89	0.54
1:C:65:THR:O	1:C:90:SER:HA	2.07	0.53
1:C:264:THR:HG23	1:C:266:SER:O	2.08	0.53
1:A:52:GLN:NE2	1:A:56:ASP:OD1	2.41	0.53
1:C:227:ALA:HB1	1:C:243:VAL:CG2	2.39	0.53
1:C:224:THR:HG22	1:C:244:GLY:N	2.23	0.53
1:B:275:THR:HG22	1:B:279:LEU:HD12	1.91	0.53
1:C:167:ASN:HD22	1:C:167:ASN:C	2.13	0.53
1:A:0:ALA:HB2	1:D:91:ASP:HB3	1.90	0.52
1:B:248:LEU:HD22	1:B:260:HIS:HB3	1.91	0.52
1:C:249:LEU:HA	1:C:264:THR:CG2	2.39	0.52
1:C:250:LYS:H	1:C:264:THR:HG22	1.73	0.52
1:A:107:GLN:HE22	1:D:106:GLN:HA	1.73	0.52
1:C:144:GLN:O	1:C:147:LYS:HB3	2.09	0.52
1:D:153:ASN:HB3	1:D:154:PHE:HD1	1.76	0.51
1:B:59:LEU:O	1:B:59:LEU:HD12	2.10	0.51
1:C:59:LEU:HD12	1:C:59:LEU:C	2.31	0.51
1:B:59:LEU:HD12	1:B:59:LEU:C	2.31	0.51
1:B:131:LEU:HD12	1:B:174:ILE:HD13	1.93	0.51
1:C:61:ILE:H	1:C:86:HIS:HD2	1.59	0.51
1:D:236:ASP:O	1:D:240:LEU:HD22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-1:ASN:ND2	1:A:1:MSE:HE2	2.26	0.50
1:D:27:ASP:OD2	1:D:27:ASP:N	2.41	0.50
1:A:95:GLU:HG3	1:D:-2:SER:O	2.11	0.50
1:A:106:GLN:HA	1:D:107:GLN:HE22	1.77	0.50
1:C:132:HIS:O	1:C:136:ASN:HA	2.12	0.50
1:C:264:THR:CG2	1:C:266:SER:O	2.60	0.50
1:D:123:LYS:NZ	1:D:178:TYR:O	2.37	0.50
1:C:2:LEU:C	1:C:2:LEU:HD23	2.32	0.49
1:C:132:HIS:HD2	1:C:138:LEU:HD13	1.78	0.49
1:D:137:ILE:HD11	1:D:167:ASN:HB2	1.94	0.49
1:D:263:ILE:HG22	1:D:264:THR:O	2.13	0.48
1:D:35:ILE:HD12	1:D:79:GLY:HA2	1.95	0.48
1:A:163:ASN:O	1:A:164:ASP:C	2.52	0.47
1:B:21:ILE:CD1	1:B:222:LEU:HD12	2.44	0.47
1:B:257:LYS:HE2	1:B:263:ILE:HD13	1.95	0.47
1:D:31:PHE:CE2	1:D:75:LYS:HD3	2.49	0.47
1:D:185:ASN:N	1:D:185:ASN:ND2	2.51	0.47
1:C:153:ASN:ND2	1:C:202:PHE:H	2.13	0.47
1:C:40:GLN:NE2	1:C:80:LYS:HD2	2.28	0.47
1:A:61:ILE:HD12	1:A:62:GLY:N	2.30	0.47
1:B:250:LYS:HA	1:B:263:ILE:CD1	2.43	0.47
1:B:131:LEU:HD12	1:B:174:ILE:CD1	2.44	0.47
1:C:247:TYR:HE2	1:C:279:LEU:HD11	1.80	0.47
1:D:109:ASN:ND2	3:D:424:HOH:O	2.46	0.47
1:D:35:ILE:HG21	1:D:40:GLN:NE2	2.29	0.47
1:C:131:LEU:CD2	1:C:174:ILE:HD11	2.46	0.46
1:D:89:ALA:HB1	1:D:212:ILE:HD13	1.97	0.46
1:B:3:LEU:CD1	1:C:94:THR:HB	2.46	0.46
1:C:137:ILE:HD12	1:C:167:ASN:HD22	1.80	0.46
1:B:275:THR:HG22	1:B:279:LEU:CD1	2.45	0.46
1:D:122:GLU:HG2	1:D:126:LYS:HE2	1.98	0.46
1:A:-1:ASN:ND2	1:A:1:MSE:HB3	2.31	0.45
1:A:59:LEU:HD23	1:A:280:ILE:HD13	1.98	0.45
1:B:229:ALA:CB	1:B:243:VAL:HG21	2.45	0.45
1:B:227:ALA:HB1	1:B:243:VAL:HG12	1.98	0.45
1:A:22:VAL:HB	1:A:61:ILE:HD13	1.99	0.45
1:C:131:LEU:HG	1:C:174:ILE:HD12	1.99	0.45
1:C:227:ALA:HB3	1:C:243:VAL:HG22	1.97	0.45
1:C:61:ILE:HG22	1:C:86:HIS:HD2	1.82	0.45
1:C:73:LEU:O	1:C:76:MSE:HB2	2.17	0.45
1:D:29:THR:HA	1:D:249:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:THR:HG21	1:B:72:ILE:CD1	2.40	0.45
1:D:15:VAL:HG13	1:D:57:GLY:HA2	1.97	0.45
1:D:183:ASN:CG	1:D:185:ASN:HD21	2.20	0.45
1:B:203:ILE:HG22	1:B:204:PRO:HD2	1.98	0.44
1:A:217:LEU:HD21	1:A:227:ALA:HB2	1.99	0.44
1:C:61:ILE:H	1:C:86:HIS:CD2	2.34	0.44
1:A:168:LEU:HD13	1:A:184:ILE:CG2	2.47	0.44
1:C:21:ILE:HD11	1:C:220:TYR:CD2	2.53	0.44
1:A:236:ASP:O	1:A:240:LEU:HG	2.17	0.44
1:B:131:LEU:CD1	1:B:174:ILE:CD1	2.92	0.44
1:C:21:ILE:HD13	1:C:60:ILE:HD11	1.99	0.44
1:A:65:THR:HG21	1:A:72:ILE:HD11	1.98	0.44
1:B:107:GLN:HE21	1:B:109:ASN:ND2	2.11	0.44
1:B:225:GLU:OE1	1:B:225:GLU:N	2.48	0.44
1:C:247:TYR:CE2	1:C:279:LEU:HD11	2.53	0.43
1:C:227:ALA:HB1	1:C:243:VAL:HG22	1.96	0.43
1:D:168:LEU:CD2	1:D:184:ILE:HD13	2.48	0.43
1:C:250:LYS:N	1:C:264:THR:HG22	2.33	0.43
1:A:124:VAL:HG11	1:D:7:SER:HB2	2.00	0.43
1:B:127:LEU:HD11	1:B:202:PHE:CE1	2.54	0.43
1:B:229:ALA:HB3	1:B:243:VAL:HG21	2.00	0.43
1:B:-2:SER:HB2	1:B:2:LEU:HD23	2.01	0.43
1:D:16:GLU:HG2	1:D:17:HIS:NE2	2.34	0.43
1:C:167:ASN:ND2	1:C:167:ASN:C	2.72	0.43
1:C:137:ILE:HD11	1:C:171:ILE:HD11	2.01	0.43
1:C:139:LEU:HD11	1:C:171:ILE:CD1	2.49	0.43
1:A:65:THR:CG2	1:A:72:ILE:HD11	2.49	0.42
1:B:114:ARG:HE	1:B:114:ARG:HB3	1.67	0.42
1:A:107:GLN:H	1:D:107:GLN:NE2	2.18	0.42
1:A:158:GLU:HB2	1:A:164:ASP:OD2	2.20	0.42
1:B:104:PHE:HB3	1:C:116:ASN:HD21	1.84	0.42
1:D:182:VAL:HG22	1:D:184:ILE:HG13	2.00	0.42
1:D:64:VAL:HG11	1:D:209:LYS:HG2	2.01	0.42
1:A:249:LEU:HA	1:A:264:THR:OG1	2.19	0.42
1:D:63:TRP:CD2	1:D:85:PRO:HG3	2.55	0.42
1:B:89:ALA:HB1	1:B:212:ILE:HD13	2.02	0.42
1:C:59:LEU:HD12	1:C:59:LEU:O	2.20	0.42
1:D:46:LEU:HD13	1:D:273:THR:OG1	2.20	0.42
1:D:276:LEU:HD22	1:D:280:ILE:HD12	2.02	0.41
1:D:184:ILE:C	1:D:185:ASN:HD22	2.22	0.41
1:A:145:LEU:HD13	1:A:194:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLN:CB	1:C:107:GLN:HG2	2.50	0.41
1:C:93:GLY:HA3	1:C:207:THR:HB	2.02	0.41
1:D:167:ASN:OD1	1:D:167:ASN:N	2.53	0.41
1:B:127:LEU:C	1:B:127:LEU:CD1	2.87	0.41
1:C:147:LYS:O	1:C:147:LYS:HG3	2.14	0.41
1:D:5:LYS:HG2	1:D:73:LEU:HD22	2.03	0.41
1:D:53:LYS:CB	1:D:59:LEU:HD23	2.50	0.41
1:A:165:LYS:NZ	3:A:467:HOH:O	2.53	0.41
1:C:135:HIS:CD2	1:C:174:ILE:HD11	2.55	0.41
1:C:180:VAL:HG13	1:C:181:SER:N	2.36	0.41
1:D:217:LEU:HD11	1:D:227:ALA:HB2	2.02	0.41
1:C:51:GLU:OE2	1:C:55:LYS:HG3	2.21	0.41
1:A:22:VAL:HA	1:A:228:ILE:O	2.22	0.40
1:C:62:GLY:HA3	1:C:87:PHE:CZ	2.56	0.40
1:C:153:ASN:HD22	1:C:202:PHE:H	1.69	0.40
1:D:1:MSE:HE3	1:D:73:LEU:HD12	2.03	0.40
1:A:142:GLN:HE22	1:A:149:ARG:HE	1.69	0.40
1:B:124:VAL:O	1:B:128:VAL:HG23	2.21	0.40
1:B:251:ASN:H	1:B:251:ASN:ND2	2.20	0.40
1:C:139:LEU:HD11	1:C:171:ILE:HD11	2.04	0.40
1:D:264:THR:HG22	1:D:266:SER:N	2.32	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	285/289 (99%)	276 (97%)	9 (3%)	0	100	100
1	B	224/289 (78%)	216 (96%)	8 (4%)	0	100	100
1	C	273/289 (94%)	260 (95%)	13 (5%)	0	100	100
1	D	240/289 (83%)	229 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1022/1156 (88%)	981 (96%)	41 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	253/257 (98%)	241 (95%)	12 (5%)	22 32
1	B	201/257 (78%)	187 (93%)	14 (7%)	12 15
1	C	240/257 (93%)	223 (93%)	17 (7%)	12 15
1	D	220/257 (86%)	201 (91%)	19 (9%)	8 9
All	All	914/1028 (89%)	852 (93%)	62 (7%)	13 16

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	THR
1	A	67	SER
1	A	95	GLU
1	A	114[A]	ARG
1	A	114[B]	ARG
1	A	142	GLN
1	A	162	ILE
1	A	211	GLU
1	A	224	THR
1	A	226	ARG
1	A	238	ARG
1	A	259	LEU
1	B	-1	ASN
1	B	52	GLN
1	B	67	SER
1	B	69	ILE
1	B	71	SER

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Mol	Chain	Res	Type
1	B	101	GLU
1	B	127	LEU
1	B	130	GLN
1	B	221	ASN
1	B	224	THR
1	B	238	ARG
1	B	248	LEU
1	B	263	ILE
1	B	284	ARG
1	C	8	GLU
1	C	15	VAL
1	C	19	GLN
1	C	22	VAL
1	C	41	GLN
1	C	69	ILE
1	C	73	LEU
1	C	137	ILE
1	C	147	LYS
1	C	166	LYS
1	C	167	ASN
1	C	174	ILE
1	C	180	VAL
1	C	221	ASN
1	C	225	GLU
1	C	243	VAL
1	C	259	LEU
1	D	5	LYS
1	D	21	ILE
1	D	27	ASP
1	D	37	GLU
1	D	59	LEU
1	D	61	ILE
1	D	69	ILE
1	D	123	LYS
1	D	167	ASN
1	D	169	LEU
1	D	177	GLU
1	D	185	ASN
1	D	217	LEU
1	D	225	GLU
1	D	238	ARG
1	D	239	MSE

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Mol	Chain	Res	Type
1	D	240	LEU
1	D	261	ASN
1	D	279	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	19	GLN
1	A	107	GLN
1	A	109	ASN
1	A	130	GLN
1	A	142	GLN
1	A	235	ASN
1	A	251	ASN
1	A	254	GLN
1	B	40	GLN
1	B	107	GLN
1	B	109	ASN
1	B	112	ASN
1	B	210	ASN
1	B	235	ASN
1	B	251	ASN
1	C	40	GLN
1	C	86	HIS
1	C	116	ASN
1	C	132	HIS
1	C	135	HIS
1	C	144	GLN
1	C	153	ASN
1	C	167	ASN
1	D	17	HIS
1	D	40	GLN
1	D	107	GLN
1	D	109	ASN
1	D	130	GLN
1	D	132	HIS
1	D	185	ASN
1	D	254	GLN
1	D	261	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 oligosaccharides 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

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

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, 95^{th} 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	280/289 (96%)	-0.12	2 (0%)	84	85	7, 24, 35, 38	2 (0%)
1	B	225/289 (77%)	-0.23	2 (0%)	81	81	5, 22, 34, 43	0
1	C	273/289 (94%)	-0.02	1 (0%)	89	89	15, 26, 37, 40	0
1	D	245/289 (84%)	-0.10	1 (0%)	89	89	11, 23, 32, 36	0
All	All	1023/1156 (88%)	-0.11	6 (0%)	85	87	5, 24, 35, 43	2 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	GLU	2.9
1	A	265	ASP	2.6
1	C	148	SER	2.5
1	B	74	ASP	2.5
1	D	169	LEU	2.2
1	B	37	GLU	2.2

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	D	301	1/1	0.74	0.15	49,49,49,49	0
2	MG	C	301	1/1	0.82	0.16	49,49,49,49	0
2	MG	A	301	1/1	0.88	0.13	45,45,45,45	0
2	MG	B	301	1/1	0.91	0.09	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.