Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2023 – 10:09 AM EST

PDB ID	:	8FC0
Title	:	Crystal structure of a metagenome-derived GH5 endo-beta-1,4-glucanase
Authors	:	Liberato, M.V.; Squina, F.
Deposited on	:	2022-12-01
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

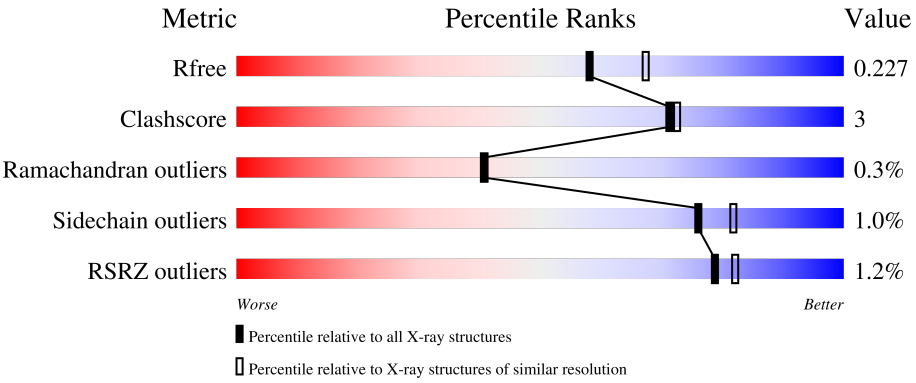
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	381	87% 7% 6%
1	B	381	88% 7% 5%
1	C	381	2% 87% 8% .
1	D	381	. % 88% 7% 5%
1	E	381	85% 9% 6%

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Mol	Chain	Length	Quality of chain
1	F	381	2% 88% 7% 6%
1	G	381	3% 80% 10% 9%
1	H	381	% 83% 11% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	A	501	-	-	X	-
2	BR	D	501	-	-	X	-
2	BR	E	501	-	-	X	-
2	BR	F	501	-	-	X	-
2	BR	H	501	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24419 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 CelE2 (Fragment).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2799	1777	482	534	6			
1	B	362	Total	C	N	O	S	0	1	0
			2831	1798	484	543	6			
1	C	364	Total	C	N	O	S	0	0	0
			2825	1792	488	539	6			
1	D	362	Total	C	N	O	S	0	0	0
			2819	1788	486	539	6			
1	E	360	Total	C	N	O	S	0	0	0
			2794	1776	476	536	6			
1	F	360	Total	C	N	O	S	0	0	0
			2796	1779	480	531	6			
1	G	346	Total	C	N	O	S	0	0	0
			2689	1710	463	510	6			
1	H	359	Total	C	N	O	S	0	0	0
			2783	1768	477	532	6			

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Br	0	0
			2	2		
2	B	2	Total	Br	0	0
			2	2		
2	C	2	Total	Br	0	0
			2	2		
2	D	1	Total	Br	0	0
			1	1		
2	E	1	Total	Br	0	0
			1	1		
2	F	1	Total	Br	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Br 2 2	0	0
2	H	1	Total Br 1 1	0	0

- Molecule 3 is water.

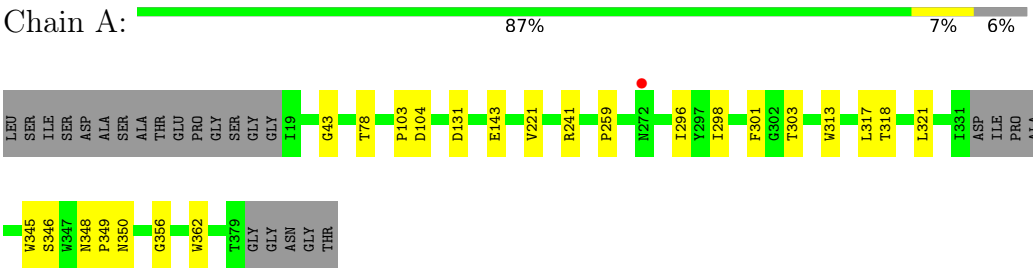
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	304	Total O 304 304	0	0
3	B	292	Total O 292 292	0	0
3	C	275	Total O 275 275	0	0
3	D	273	Total O 273 273	0	0
3	E	199	Total O 199 199	0	0
3	F	258	Total O 258 258	0	0
3	G	211	Total O 211 211	0	0
3	H	259	Total O 259 259	0	0

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.

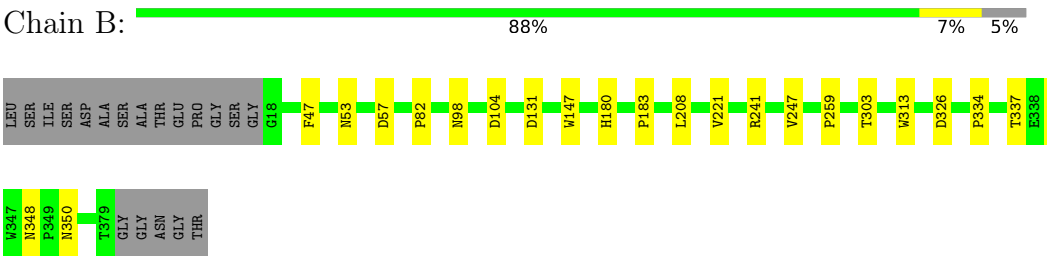
• Molecule 1: CelE2 (Fragment)

Chain A:



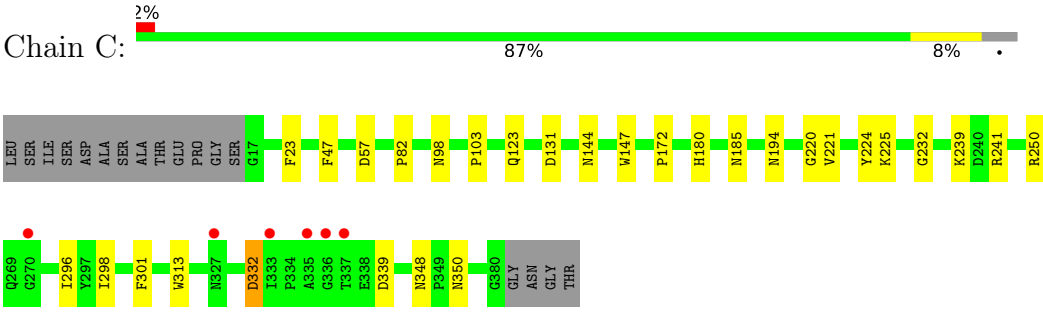
• Molecule 1: CelE2 (Fragment)

Chain B:



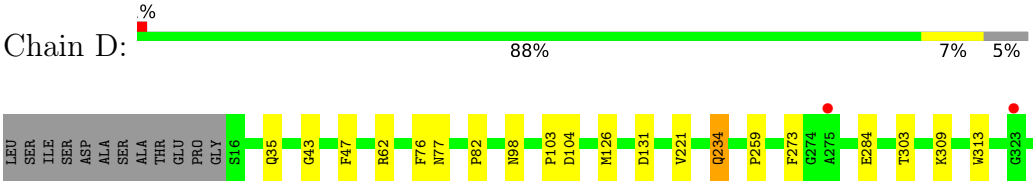
• Molecule 1: CelE2 (Fragment)

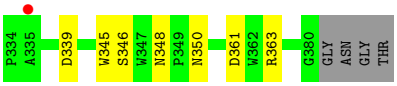
Chain C:



• Molecule 1: CelE2 (Fragment)

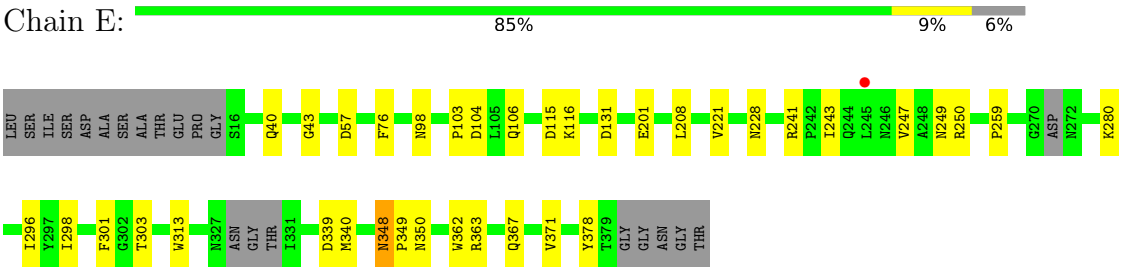
Chain D:





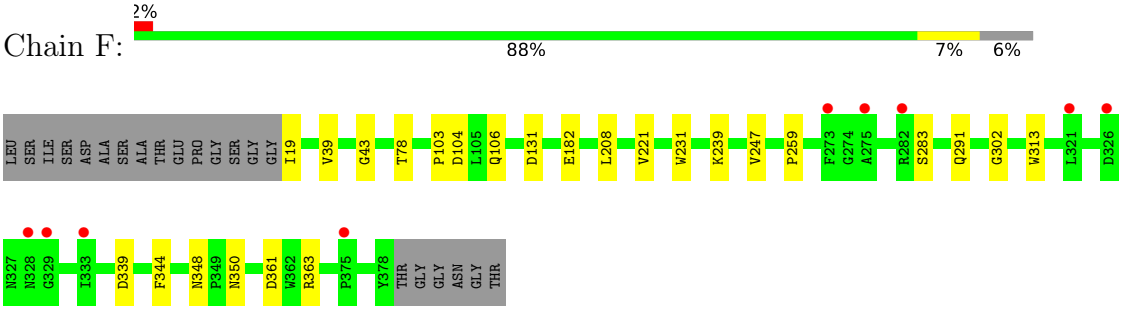
• Molecule 1: CelE2 (Fragment)

Chain E:



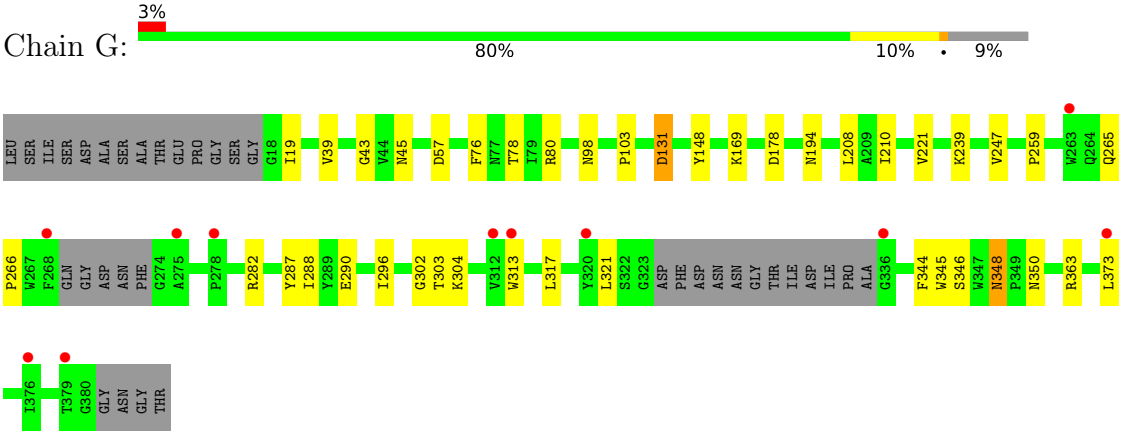
• Molecule 1: CelE2 (Fragment)

Chain F:



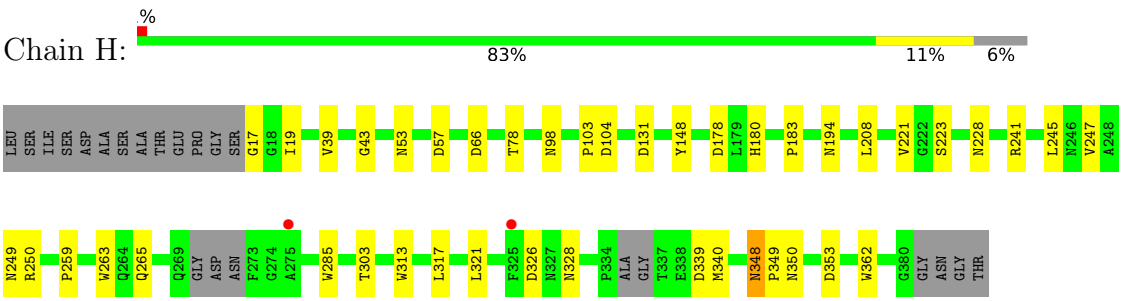
• Molecule 1: CelE2 (Fragment)

Chain G:



• Molecule 1: CelE2 (Fragment)

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	97.56Å 97.82Å 100.20Å 66.05° 69.68° 70.02°	Depositor
Resolution (Å)	29.00 – 2.10 49.19 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.7 (29.00-2.10) 94.7 (49.19-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.186 , 0.227 0.186 , 0.227	Depositor DCC
R_{free} test set	8324 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	24419	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: BR

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	0.25	0/2882	0.47	0/3937
1	B	0.25	0/2919	0.47	0/3992
1	C	0.25	0/2910	0.47	0/3978
1	D	0.25	0/2903	0.47	0/3965
1	E	0.24	0/2877	0.46	0/3935
1	F	0.24	0/2881	0.46	0/3940
1	G	0.43	2/2769 (0.1%)	0.71	5/3783 (0.1%)
1	H	0.24	0/2866	0.46	0/3919
All	All	0.27	2/23007 (0.0%)	0.50	5/31449 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	266	PRO	CG-CD	-14.79	1.01	1.50
1	G	266	PRO	CB-CG	-9.13	1.04	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	266	PRO	CB-CG-CD	18.83	179.94	106.50
1	G	266	PRO	CA-CB-CG	-15.77	74.04	104.00
1	G	266	PRO	N-CD-CG	-13.80	82.50	103.20
1	G	266	PRO	CA-N-CD	-12.06	94.61	111.50
1	G	265	GLN	C-N-CD	9.36	148.05	128.40

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	2799	0	2609	16	0
1	B	2831	0	2637	15	0
1	C	2825	0	2619	19	0
1	D	2819	0	2625	17	0
1	E	2794	0	2580	23	0
1	F	2796	0	2590	13	0
1	G	2689	0	2500	23	0
1	H	2783	0	2566	30	0
2	A	2	0	0	2	0
2	B	2	0	0	1	0
2	C	2	0	0	1	0
2	D	1	0	0	2	0
2	E	1	0	0	2	0
2	F	1	0	0	2	0
2	G	2	0	0	1	0
2	H	1	0	0	2	0
3	A	304	0	0	0	0
3	B	292	0	0	0	0
3	C	275	0	0	2	0
3	D	273	0	0	0	0
3	E	199	0	0	3	0
3	F	258	0	0	1	0
3	G	211	0	0	1	0
3	H	259	0	0	2	0
All	All	24419	0	20726	149	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 3.

All (149) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ASN:HD21	1:H:53:ASN:HD21	1.24	0.86
1:F:208:LEU:HD13	1:F:247:VAL:HB	1.75	0.69
1:H:263:TRP:HD1	1:H:265:GLN:HG2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:259:PRO:HB3	1:G:313:TRP:CE3	2.29	0.68
1:A:318:THR:HA	1:A:321:LEU:HD12	1.75	0.67
1:C:98:ASN:HD21	1:D:98:ASN:HD21	1.47	0.63
1:H:326:ASP:OD2	1:H:328:ASN:ND2	2.31	0.62
1:H:208:LEU:HD13	1:H:247:VAL:HB	1.80	0.62
1:E:103:PRO:HD2	2:E:501:BR:BR	2.56	0.61
1:H:148:TYR:OH	1:H:194:ASN:OD1	2.19	0.61
1:F:106:GLN:NE2	3:F:601:HOH:O	2.34	0.61
1:D:35:GLN:HG2	1:E:115:ASP:OD2	2.01	0.61
1:D:104:ASP:HB2	2:D:501:BR:BR	2.56	0.60
1:G:317:LEU:O	1:G:321:LEU:HD22	2.02	0.59
1:G:19:ILE:HG23	1:G:39:VAL:HG11	1.85	0.59
1:A:339:ASP:OD2	1:A:339:ASP:N	2.35	0.59
1:H:98:ASN:ND2	3:H:606:HOH:O	2.35	0.58
1:B:98:ASN:HD21	1:G:98:ASN:HD21	1.51	0.57
1:G:304:LYS:NZ	3:G:504:HOH:O	2.37	0.57
1:F:348:ASN:HB3	1:F:350:ASN:OD1	2.05	0.56
1:E:98:ASN:HD21	1:H:98:ASN:HD21	1.53	0.56
1:F:239:LYS:HE3	1:F:291:GLN:OE1	2.05	0.56
1:C:194:ASN:ND2	3:C:607:HOH:O	2.38	0.54
1:F:339:ASP:OD1	1:F:339:ASP:N	2.37	0.54
1:H:104:ASP:HB2	2:H:501:BR:BR	2.64	0.53
1:H:317:LEU:O	1:H:321:LEU:HG	2.08	0.53
1:C:239:LYS:NZ	3:C:603:HOH:O	2.37	0.53
1:A:103:PRO:HD2	2:A:501:BR:BR	2.64	0.53
1:B:259:PRO:HG3	1:B:303:THR:HB	1.91	0.52
1:E:104:ASP:HB2	2:E:501:BR:BR	2.65	0.52
1:E:296:ILE:HG21	1:E:340:MET:HE2	1.92	0.52
1:H:259:PRO:HG3	1:H:303:THR:HB	1.89	0.52
1:G:148:TYR:OH	1:G:194:ASN:OD1	2.25	0.52
1:B:348:ASN:HB3	1:B:350:ASN:OD1	2.10	0.51
1:A:348:ASN:HB3	1:A:350:ASN:OD1	2.10	0.51
1:G:43:GLY:HA2	1:G:76:PHE:HB3	1.93	0.51
1:F:361:ASP:O	1:F:363:ARG:HG3	2.11	0.51
1:G:288:ILE:HB	1:G:296:ILE:HD11	1.93	0.51
1:B:339:ASP:OD1	1:B:339:ASP:N	2.43	0.50
1:C:348:ASN:HB3	1:C:350:ASN:OD1	2.11	0.50
1:E:249:ASN:O	1:E:250:ARG:HD3	2.12	0.50
1:H:348:ASN:HB3	1:H:350:ASN:OD1	2.11	0.50
1:D:259:PRO:HG3	1:D:303:THR:HB	1.93	0.50
1:D:339:ASP:OD1	1:D:339:ASP:N	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:259:PRO:HG3	1:G:303:THR:HB	1.93	0.49
1:F:104:ASP:HB2	2:F:501:BR:BR	2.67	0.49
1:D:361:ASP:O	1:D:363:ARG:HG3	2.12	0.49
1:C:224:TYR:CE2	1:C:225:LYS:HD3	2.47	0.49
1:E:43:GLY:HA2	1:E:76:PHE:HB3	1.95	0.49
1:H:19:ILE:HG23	1:H:39:VAL:HG11	1.94	0.49
1:H:223:SER:OG	1:H:228:ASN:OD1	2.27	0.49
1:H:285:TRP:HZ3	1:H:340:MET:HE1	1.78	0.49
1:E:259:PRO:HB3	1:E:313:TRP:CE3	2.48	0.48
1:E:280:LYS:NZ	3:E:612:HOH:O	2.47	0.48
1:H:339:ASP:OD1	1:H:339:ASP:N	2.33	0.48
1:B:47:PHE:HA	1:B:82:PRO:HD2	1.96	0.48
1:B:208:LEU:HD13	1:B:247:VAL:HB	1.96	0.48
1:D:62:ARG:HD3	1:D:363:ARG:HG2	1.96	0.48
1:D:103:PRO:HD2	2:D:501:BR:BR	2.69	0.48
1:D:77:ASN:HA	1:D:126:MET:HG2	1.96	0.47
1:B:259:PRO:HB3	1:B:313:TRP:CE3	2.49	0.47
1:H:43:GLY:HA3	1:H:78:THR:O	2.14	0.47
1:G:45:ASN:OD1	1:G:80:ARG:HD3	2.15	0.47
1:G:317:LEU:HG	1:G:321:LEU:HD21	1.96	0.47
1:C:103:PRO:HD2	2:C:501:BR:BR	2.70	0.47
1:B:180:HIS:HD2	1:B:183:PRO:HB3	1.80	0.47
1:G:282:ARG:NE	1:G:290:GLU:OE1	2.48	0.47
1:E:201:GLU:HG3	1:E:243:ILE:HG23	1.96	0.46
1:F:182:GLU:HB3	1:F:231:TRP:HB3	1.97	0.46
1:H:57:ASP:HB2	1:H:348:ASN:ND2	2.31	0.46
1:E:57:ASP:HB2	1:E:348:ASN:ND2	2.30	0.46
1:G:239:LYS:HG2	1:G:287:TYR:CE2	2.51	0.46
1:H:263:TRP:CD1	1:H:265:GLN:HG2	2.47	0.46
1:E:208:LEU:HD13	1:E:247:VAL:HB	1.98	0.46
1:A:296:ILE:HB	1:A:340:MET:HG2	1.97	0.46
1:B:326:ASP:OD1	1:B:326:ASP:N	2.49	0.46
1:H:259:PRO:HB3	1:H:313:TRP:CE3	2.51	0.46
1:A:104:ASP:HB2	2:A:501:BR:BR	2.71	0.46
1:G:57:ASP:HB2	1:G:348:ASN:ND2	2.32	0.45
1:B:57:ASP:HB2	1:B:348:ASN:ND2	2.31	0.45
1:E:298:ILE:HD11	1:E:301:PHE:HB3	1.97	0.45
1:C:224:TYR:CZ	1:C:225:LYS:HD3	2.51	0.45
1:D:345:TRP:HA	1:D:346:SER:HA	1.77	0.45
1:G:208:LEU:HD13	1:G:247:VAL:HB	1.99	0.45
1:C:47:PHE:HA	1:C:82:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:353:ASP:OD2	1:H:353:ASP:N	2.50	0.45
1:H:321:LEU:O	1:H:339:ASP:HB2	2.17	0.44
1:C:57:ASP:HB2	1:C:348:ASN:ND2	2.32	0.44
1:G:348:ASN:HB3	1:G:350:ASN:OD1	2.17	0.44
1:G:103:PRO:HD2	2:G:402:BR:BR	2.72	0.44
1:G:344:PHE:CD2	1:G:373:LEU:HD11	2.52	0.44
1:C:339:ASP:OD1	1:C:339:ASP:N	2.34	0.44
1:D:273:PHE:CE2	1:D:309:LYS:HG2	2.53	0.44
1:C:259:PRO:HB3	1:C:313:TRP:CE3	2.52	0.44
1:H:208:LEU:HD11	1:H:245:LEU:HD23	1.99	0.44
1:H:249:ASN:O	1:H:250:ARG:HD3	2.17	0.44
1:C:298:ILE:HD11	1:C:301:PHE:HB3	1.98	0.44
1:D:43:GLY:HA2	1:D:76:PHE:HB3	2.00	0.44
1:A:43:GLY:HA3	1:A:78:THR:O	2.18	0.43
1:A:143:GLU:CD	1:A:143:GLU:H	2.21	0.43
1:A:321:LEU:O	1:A:339:ASP:HB2	2.18	0.43
1:H:349:PRO:HD2	1:H:362:TRP:CZ2	2.53	0.43
1:F:259:PRO:HB3	1:F:313:TRP:CE3	2.54	0.43
1:C:220:GLY:O	1:C:232:GLY:HA2	2.18	0.43
1:C:147:TRP:HA	1:C:180:HIS:CE1	2.53	0.43
1:G:169:LYS:NZ	1:G:210:ILE:O	2.51	0.43
1:H:103:PRO:HD2	2:H:501:BR:BR	2.73	0.43
1:A:259:PRO:HG3	1:A:303:THR:HB	2.00	0.43
1:E:116:LYS:HA	1:E:116:LYS:HD3	1.82	0.43
1:H:17:GLY:N	3:H:623:HOH:O	2.52	0.43
1:A:345:TRP:HA	1:A:346:SER:HA	1.72	0.43
1:C:332:ASP:N	1:C:332:ASP:OD1	2.51	0.43
1:D:259:PRO:HB3	1:D:313:TRP:CE3	2.54	0.43
1:B:334:PRO:HG2	1:B:337:THR:HG21	2.00	0.42
1:E:363:ARG:HD2	1:H:66:ASP:OD1	2.18	0.42
1:E:367:GLN:O	1:E:371:VAL:HG23	2.19	0.42
1:G:43:GLY:HA3	1:G:78:THR:O	2.19	0.42
1:H:180:HIS:HD2	1:H:183:PRO:HB3	1.83	0.42
1:D:348:ASN:HB3	1:D:350:ASN:OD1	2.19	0.42
1:H:208:LEU:CD1	1:H:245:LEU:HD23	2.50	0.42
1:H:131:ASP:HA	1:H:178:ASP:HB3	2.01	0.42
1:C:144:ASN:O	1:C:185:ASN:ND2	2.39	0.42
1:E:40:GLN:HB3	1:E:378:TYR:CD1	2.55	0.42
1:A:317:LEU:HG	1:A:321:LEU:HD11	2.01	0.41
1:B:104:ASP:HB2	2:B:501:BR:BR	2.75	0.41
1:G:345:TRP:HA	1:G:346:SER:HA	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:ILE:HD13	1:C:296:ILE:HA	1.97	0.41
1:E:339:ASP:OD1	1:E:339:ASP:N	2.49	0.41
1:C:23:PHE:CE1	1:C:172:PRO:HA	2.56	0.41
1:D:234:GLN:NE2	1:D:284:GLU:OE1	2.53	0.41
1:F:103:PRO:HD2	2:F:501:BR:BR	2.75	0.41
1:C:98:ASN:ND2	1:D:98:ASN:HD21	2.16	0.41
1:F:19:ILE:HG23	1:F:39:VAL:HG11	2.02	0.41
1:F:302:GLY:HA2	1:F:344:PHE:CZ	2.56	0.41
1:D:47:PHE:HA	1:D:82:PRO:HD2	2.02	0.41
1:E:296:ILE:HD13	1:E:296:ILE:HA	1.85	0.41
1:E:363:ARG:NH2	3:E:611:HOH:O	2.46	0.41
1:F:43:GLY:HA3	1:F:78:THR:O	2.21	0.41
1:B:147:TRP:HA	1:B:180:HIS:CE1	2.57	0.40
1:E:348:ASN:HB3	1:E:350:ASN:OD1	2.21	0.40
1:G:302:GLY:HA2	1:G:344:PHE:CZ	2.56	0.40
1:A:348:ASN:O	1:A:356:GLY:HA3	2.21	0.40
1:A:349:PRO:HD2	1:A:362:TRP:CZ2	2.55	0.40
1:A:259:PRO:HB3	1:A:313:TRP:CE3	2.57	0.40
1:G:131:ASP:HA	1:G:178:ASP:HB3	2.02	0.40
1:A:298:ILE:HD11	1:A:301:PHE:HB3	2.03	0.40
1:B:345:TRP:HA	1:B:346:SER:HA	1.70	0.40
1:E:106:GLN:NE2	3:E:625:HOH:O	2.55	0.40
1:E:349:PRO:HD2	1:E:362:TRP:CZ2	2.57	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	353/381 (93%)	338 (96%)	14 (4%)	1 (0%)	41	41
1	B	361/381 (95%)	348 (96%)	12 (3%)	1 (0%)	41	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	362/381 (95%)	348 (96%)	13 (4%)	1 (0%)	41	41
1	D	358/381 (94%)	345 (96%)	12 (3%)	1 (0%)	41	41
1	E	354/381 (93%)	343 (97%)	10 (3%)	1 (0%)	41	41
1	F	358/381 (94%)	343 (96%)	14 (4%)	1 (0%)	41	41
1	G	340/381 (89%)	329 (97%)	10 (3%)	1 (0%)	41	41
1	H	353/381 (93%)	340 (96%)	12 (3%)	1 (0%)	41	41
All	All	2839/3048 (93%)	2734 (96%)	97 (3%)	8 (0%)	41	41

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	VAL
1	C	221	VAL
1	D	221	VAL
1	E	221	VAL
1	G	221	VAL
1	B	221	VAL
1	F	221	VAL
1	H	221	VAL

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	284/303 (94%)	282 (99%)	2 (1%)	84	88
1	B	288/303 (95%)	286 (99%)	2 (1%)	84	88
1	C	283/303 (93%)	278 (98%)	5 (2%)	59	65
1	D	285/303 (94%)	283 (99%)	2 (1%)	84	88
1	E	281/303 (93%)	276 (98%)	5 (2%)	59	65
1	F	279/303 (92%)	277 (99%)	2 (1%)	84	88
1	G	269/303 (89%)	266 (99%)	3 (1%)	73	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	279/303 (92%)	277 (99%)	2 (1%)	84 88
All	All	2248/2424 (93%)	2225 (99%)	23 (1%)	76 82

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	ASP
1	A	241	ARG
1	B	131	ASP
1	B	241	ARG
1	C	123	GLN
1	C	131	ASP
1	C	241	ARG
1	C	250	ARG
1	C	332	ASP
1	D	131	ASP
1	D	234	GLN
1	E	131	ASP
1	E	228	ASN
1	E	241	ARG
1	E	303	THR
1	E	348	ASN
1	F	131	ASP
1	F	283	SER
1	G	131	ASP
1	G	348	ASN
1	G	363	ARG
1	H	241	ARG
1	H	348	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	B	151	GLN
1	B	213	ASN
1	D	123	GLN
1	E	106	GLN
1	F	106	GLN
1	H	53	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 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	357/381 (93%)	-0.32	1 (0%) 94 94	19, 27, 39, 72	0
1	B	362/381 (95%)	-0.37	0 100 100	17, 26, 43, 55	0
1	C	364/381 (95%)	-0.21	7 (1%) 66 71	18, 26, 46, 73	0
1	D	362/381 (95%)	-0.17	4 (1%) 80 84	16, 29, 49, 80	0
1	E	360/381 (94%)	-0.06	1 (0%) 94 94	21, 42, 63, 82	0
1	F	360/381 (94%)	-0.09	9 (2%) 57 62	20, 33, 56, 84	0
1	G	346/381 (90%)	0.04	11 (3%) 47 54	19, 36, 56, 79	0
1	H	359/381 (94%)	-0.11	2 (0%) 89 91	19, 33, 55, 80	0
All	All	2870/3048 (94%)	-0.16	35 (1%) 79 82	16, 31, 56, 84	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	335	ALA	4.3
1	F	328	ASN	4.0
1	G	275	ALA	3.8
1	C	333	ILE	3.7
1	F	333	ILE	3.4
1	G	320	TYR	3.3
1	F	326	ASP	3.3
1	G	313	TRP	3.2
1	G	336	GLY	3.2
1	F	329	GLY	3.1
1	G	379	THR	3.1
1	F	275	ALA	3.0
1	G	373	LEU	2.9
1	H	275	ALA	2.8
1	G	312	VAL	2.6
1	G	376	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	337	THR	2.5
1	D	323	GLY	2.5
1	D	335	ALA	2.5
1	D	275	ALA	2.5
1	G	278	PRO	2.4
1	C	336	GLY	2.3
1	G	263	TRP	2.3
1	D	330	THR	2.3
1	A	272	ASN	2.3
1	C	327	ASN	2.2
1	F	273	PHE	2.2
1	H	325	PHE	2.2
1	F	321	LEU	2.2
1	E	245	LEU	2.2
1	F	375	PRO	2.1
1	C	270	GLY	2.1
1	F	282	ARG	2.0
1	C	268	PHE	2.0
1	G	268	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)

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	BR	F	501	1/1	0.98	0.05	46,46,46,46	0
2	BR	C	501	1/1	0.99	0.07	27,27,27,27	0
2	BR	B	501	1/1	1.00	0.07	29,29,29,29	0
2	BR	B	502	1/1	1.00	0.05	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BR	A	501	1/1	1.00	0.08	31,31,31,31	0
2	BR	C	502	1/1	1.00	0.06	35,35,35,35	0
2	BR	D	501	1/1	1.00	0.07	32,32,32,32	0
2	BR	E	501	1/1	1.00	0.06	37,37,37,37	0
2	BR	A	502	1/1	1.00	0.05	34,34,34,34	0
2	BR	G	401	1/1	1.00	0.04	39,39,39,39	0
2	BR	G	402	1/1	1.00	0.07	30,30,30,30	0
2	BR	H	501	1/1	1.00	0.07	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.