Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:46 AM GMT

PDB ID	:	2BHV
Title	:	STRUCTURE OF COMB10 OF THE COM TYPE IV SECRETION SYSTEM OF HELICOBACTER PYLORI
Authors	:	Terradot, L.; Oomen, C.; Bayliss, R.; Leonard, G.; Waksman, G.
Deposited on	:	2005-01-18
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

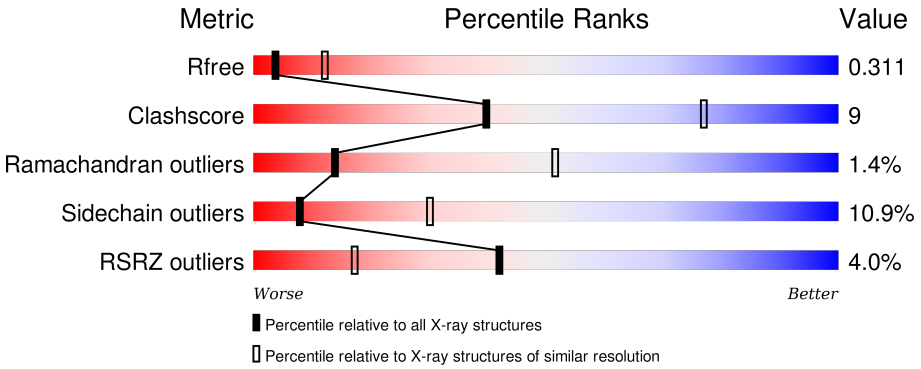
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	246	56% 17% 22%
1	B	246	4% 59% 15% 22%
1	C	246	2% 60% 14% 24%
1	D	246	4% 54% 19% 23%
1	E	246	4% 55% 19% 23%

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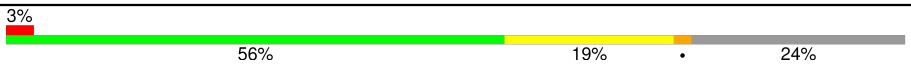
Mol	Chain	Length	Quality of chain
1	F	246	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8759 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 COMB10.

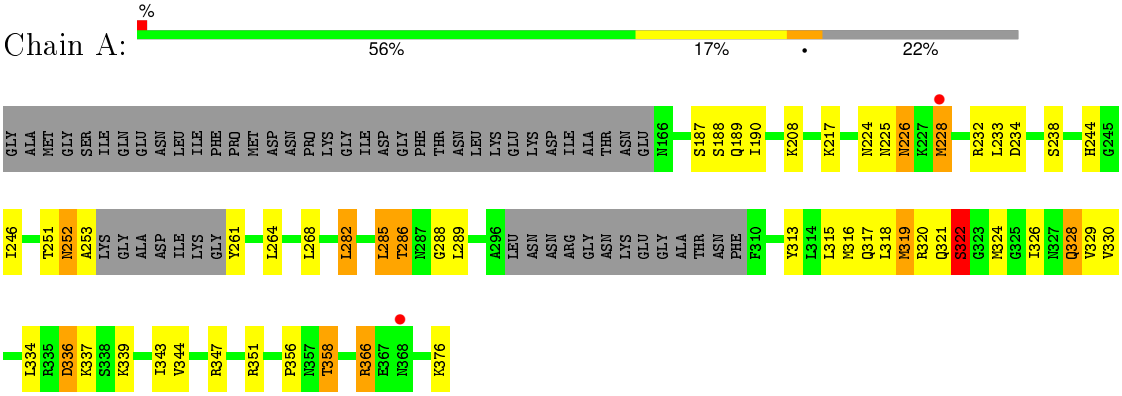
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1468	945	253	263	7			
1	B	192	Total	C	N	O	S	0	0	0
			1466	944	254	261	7			
1	C	188	Total	C	N	O	S	0	0	0
			1457	941	250	259	7			
1	D	189	Total	C	N	O	S	0	0	0
			1464	944	251	262	7			
1	E	190	Total	C	N	O	S	0	0	0
			1447	931	251	258	7			
1	F	188	Total	C	N	O	S	0	0	0
			1457	939	250	261	7			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

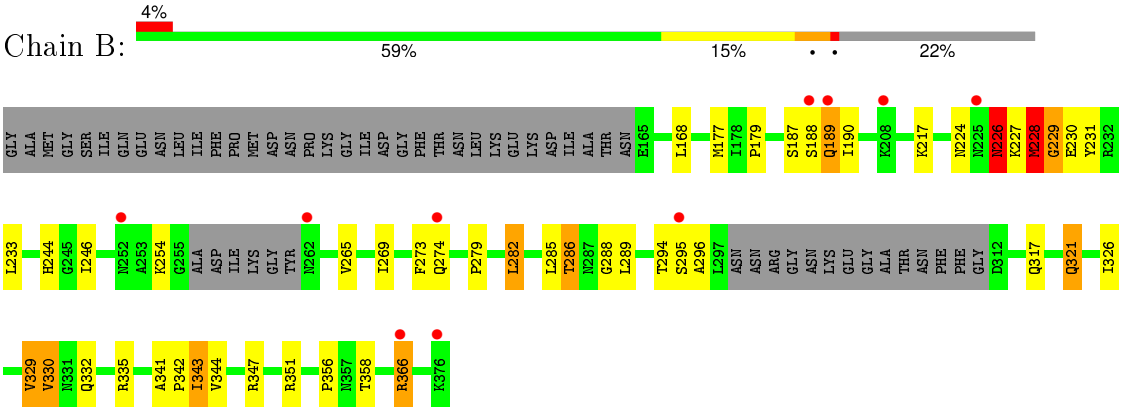
- Molecule 1: COMB10

Chain A:



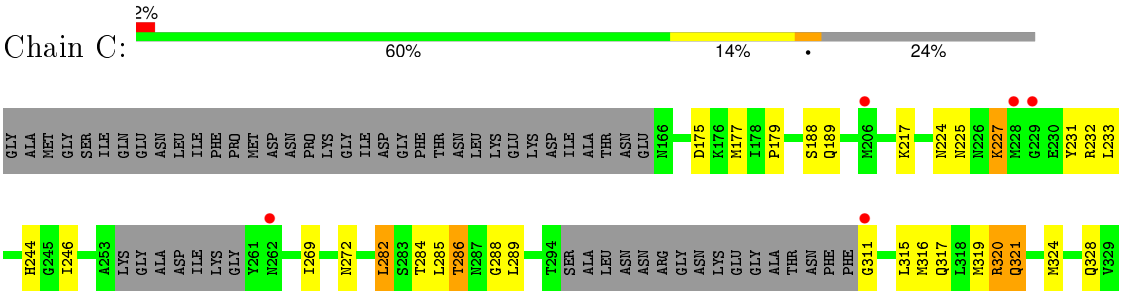
- Molecule 1: COMB10

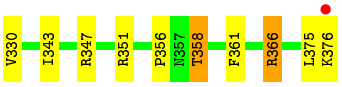
Chain B:



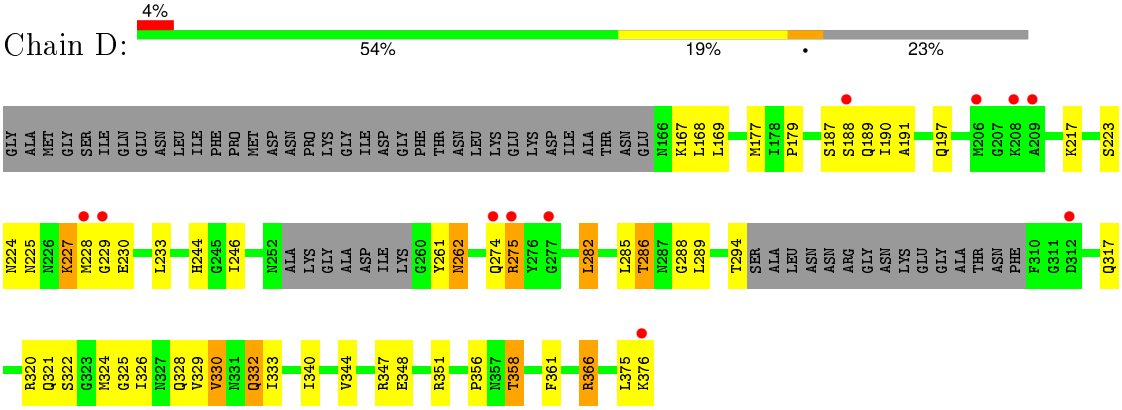
- Molecule 1: COMB10

Chain C:

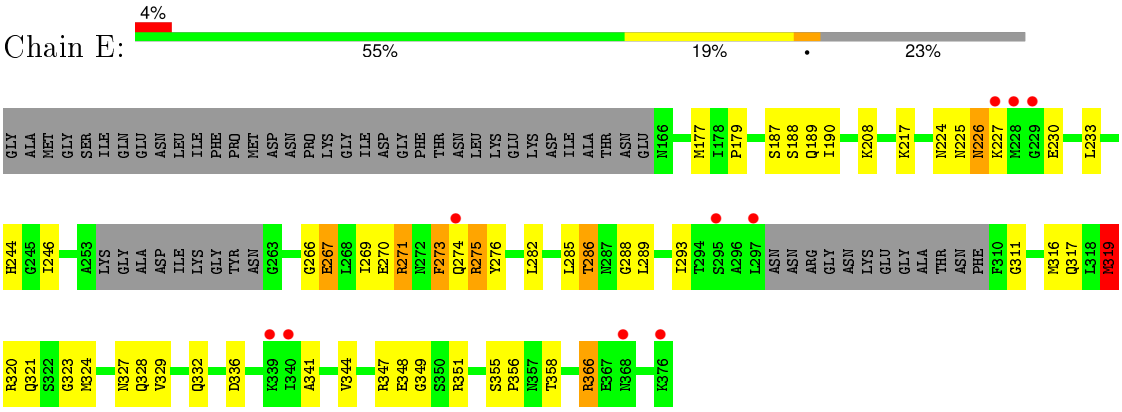




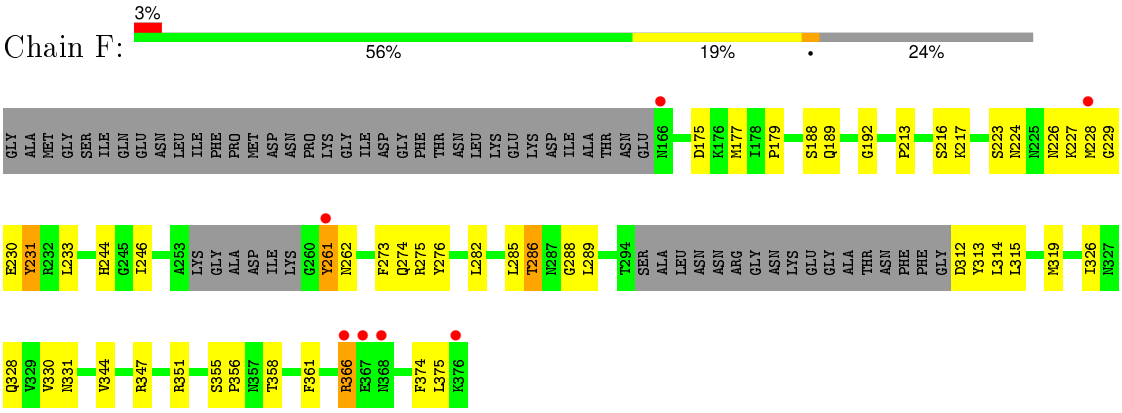
• Molecule 1: COMB10



• Molecule 1: COMB10



• Molecule 1: COMB10



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.73Å 139.41Å 168.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 29.64 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-3.00) 98.3 (29.64-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.257 , 0.293 0.286 , 0.311	Depositor DCC
R_{free} test set	1672 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	74.0	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 25.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 33062 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	8759	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.67	2/1490 (0.1%)	0.64	1/2016 (0.0%)
1	B	0.56	0/1487	0.65	1/2012 (0.0%)
1	C	0.62	1/1480 (0.1%)	0.63	1/2002 (0.0%)
1	D	0.51	0/1487	0.63	1/2011 (0.0%)
1	E	1.14	14/1468 (1.0%)	0.77	3/1986 (0.2%)
1	F	0.49	0/1480	0.61	0/2002
All	All	0.70	17/8892 (0.2%)	0.66	7/12029 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	271	ARG	CZ-NH1	21.26	1.60	1.33
1	E	274	GLN	CD-OE1	16.42	1.60	1.24
1	C	311	GLY	N-CA	12.80	1.65	1.46
1	E	274	GLN	CD-NE2	10.80	1.59	1.32
1	E	319	MET	SD-CE	10.23	2.35	1.77
1	E	271	ARG	CD-NE	9.78	1.63	1.46
1	E	273	PHE	CG-CD2	8.89	1.52	1.38
1	A	322	SER	CB-OG	8.51	1.53	1.42
1	E	273	PHE	CE1-CZ	8.28	1.53	1.37
1	E	273	PHE	CG-CD1	7.93	1.50	1.38
1	E	273	PHE	CE2-CZ	6.93	1.50	1.37
1	E	270	GLU	CD-OE2	6.82	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	271	ARG	CZ-NH2	6.54	1.41	1.33
1	A	318	LEU	C-N	6.09	1.48	1.34
1	E	267	GLU	CD-OE2	5.95	1.32	1.25
1	E	267	GLU	CD-OE1	5.71	1.31	1.25
1	E	270	GLU	CD-OE1	5.28	1.31	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	271	ARG	NE-CZ-NH2	-15.72	112.44	120.30
1	E	271	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	B	282	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	282	LEU	CA-CB-CG	5.22	127.31	115.30
1	D	282	LEU	CA-CB-CG	5.16	127.18	115.30
1	C	282	LEU	CA-CB-CG	5.09	127.00	115.30
1	E	271	ARG	CD-NE-CZ	-5.03	116.56	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	MET	Peptide
1	B	226	ASN	Peptide

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	1468	0	1517	36	3
1	B	1466	0	1519	26	0
1	C	1457	0	1513	26	2
1	D	1464	0	1515	31	0
1	E	1447	0	1493	32	0
1	F	1457	0	1506	29	1
All	All	8759	0	9063	156	3

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 9.

All (156) 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:C:175:ASP:OD2	1:E:208:LYS:HE3	1.30	1.26
1:A:226:ASN:HB3	1:A:228:MET:HG3	1.21	1.19
1:E:319:MET:SD	1:E:319:MET:CE	2.35	1.15
1:B:326:ILE:O	1:B:330:VAL:HG12	1.78	0.84
1:D:325:GLY:O	1:D:329:VAL:HG23	1.78	0.82
1:C:286:THR:HG22	1:C:288:GLY:H	1.47	0.79
1:C:366:ARG:HH11	1:C:366:ARG:HB2	1.48	0.78
1:B:366:ARG:HB2	1:B:366:ARG:HH11	1.49	0.78
1:B:286:THR:HG22	1:B:288:GLY:H	1.51	0.76
1:D:366:ARG:HB2	1:D:366:ARG:HH11	1.51	0.76
1:A:319:MET:HA	1:A:319:MET:CE	2.16	0.76
1:C:175:ASP:CG	1:E:208:LYS:HE3	2.06	0.75
1:A:286:THR:HG22	1:A:288:GLY:H	1.53	0.73
1:F:286:THR:HG23	1:F:289:LEU:HG	1.72	0.72
1:A:319:MET:HA	1:A:319:MET:HE2	1.72	0.72
1:F:286:THR:HG22	1:F:288:GLY:H	1.54	0.72
1:A:226:ASN:HB3	1:A:228:MET:CG	2.13	0.71
1:D:286:THR:HG23	1:D:289:LEU:HG	1.74	0.70
1:E:286:THR:HG22	1:E:288:GLY:H	1.56	0.69
1:D:225:ASN:ND2	1:D:227:LYS:HE2	2.06	0.69
1:B:286:THR:HG23	1:B:289:LEU:HG	1.75	0.69
1:F:228:MET:O	1:F:230:GLU:N	2.22	0.69
1:E:332:GLN:O	1:E:336:ASP:HB2	1.92	0.69
1:D:286:THR:HG22	1:D:288:GLY:H	1.58	0.69
1:C:286:THR:HG23	1:C:289:LEU:HG	1.75	0.67
1:F:366:ARG:HB2	1:F:366:ARG:HH11	1.59	0.67
1:F:226:ASN:O	1:F:227:LYS:HD2	1.94	0.67
1:F:312:ASP:CG	1:F:313:TYR:H	1.98	0.67
1:E:286:THR:HG23	1:E:289:LEU:HG	1.76	0.66
1:B:265:VAL:O	1:B:269:ILE:HG12	1.95	0.66
1:E:366:ARG:HB2	1:E:366:ARG:HH11	1.60	0.66
1:A:366:ARG:HB2	1:A:366:ARG:HH11	1.61	0.65
1:A:319:MET:HE2	1:A:319:MET:CA	2.27	0.65
1:B:286:THR:HG21	1:C:317:GLN:OE1	1.98	0.64
1:D:317:GLN:OE1	1:F:286:THR:HG21	1.98	0.64
1:C:175:ASP:OD2	1:E:208:LYS:CE	2.25	0.64
1:A:286:THR:HG23	1:A:289:LEU:HG	1.78	0.64
1:C:225:ASN:HB3	1:C:232:ARG:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:ASN:OD1	1:C:227:LYS:HB2	2.00	0.62
1:B:228:MET:O	1:B:230:GLU:N	2.33	0.61
1:A:286:THR:HG21	1:E:317:GLN:OE1	2.00	0.60
1:B:188:SER:HA	1:B:224:ASN:OD1	2.02	0.59
1:B:326:ILE:HG12	1:C:284:THR:O	2.02	0.58
1:A:188:SER:HA	1:A:224:ASN:OD1	2.02	0.58
1:B:228:MET:O	1:B:229:GLY:C	2.41	0.58
1:E:324:MET:HE2	1:E:328:GLN:HB3	1.84	0.58
1:E:227:LYS:HG2	1:E:230:GLU:HB3	1.86	0.58
1:B:286:THR:CG2	1:C:317:GLN:OE1	2.52	0.57
1:F:228:MET:C	1:F:230:GLU:H	2.06	0.57
1:E:317:GLN:HA	1:E:321:GLN:HG2	1.87	0.57
1:A:286:THR:CG2	1:E:317:GLN:OE1	2.53	0.56
1:E:225:ASN:O	1:E:226:ASN:HB3	2.06	0.56
1:D:227:LYS:O	1:D:229:GLY:O	2.22	0.56
1:C:188:SER:HA	1:C:224:ASN:OD1	2.05	0.56
1:D:326:ILE:O	1:D:330:VAL:HG12	2.04	0.56
1:B:227:LYS:O	1:B:229:GLY:N	2.39	0.56
1:A:324:MET:HE2	1:A:328:GLN:HB3	1.88	0.56
1:F:223:SER:HB2	1:F:262:ASN:HD22	1.70	0.55
1:E:316:MET:SD	1:E:320:ARG:HG3	2.47	0.55
1:D:329:VAL:O	1:D:333:ILE:HD12	2.06	0.55
1:A:319:MET:HE1	1:D:197:GLN:HE22	1.72	0.55
1:B:226:ASN:C	1:B:228:MET:N	2.60	0.55
1:D:317:GLN:OE1	1:F:286:THR:CG2	2.55	0.54
1:A:264:LEU:O	1:A:268:LEU:HG	2.08	0.54
1:A:343:ILE:HD12	1:A:343:ILE:H	1.72	0.54
1:B:317:GLN:HA	1:B:321:GLN:HG3	1.89	0.53
1:A:336:ASP:O	1:A:339:LYS:HB2	2.09	0.53
1:F:188:SER:HA	1:F:224:ASN:OD1	2.09	0.53
1:D:230:GLU:HB3	1:F:331:ASN:OD1	2.08	0.53
1:C:315:LEU:O	1:C:319:MET:HG3	2.09	0.53
1:A:317:GLN:HA	1:A:321:GLN:HB2	1.91	0.52
1:A:324:MET:HE1	1:A:329:VAL:HG12	1.90	0.52
1:D:188:SER:HA	1:D:224:ASN:OD1	2.09	0.52
1:B:177:MET:O	1:B:179:PRO:HD3	2.10	0.52
1:E:266:GLY:HA2	1:E:269:ILE:HD12	1.92	0.52
1:C:282:LEU:HD13	1:C:356:PRO:HA	1.92	0.52
1:B:294:THR:C	1:B:296:ALA:H	2.13	0.51
1:B:282:LEU:HD13	1:B:356:PRO:HA	1.91	0.51
1:E:275:ARG:HD3	1:E:276:TYR:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:282:LEU:HD13	1:F:356:PRO:HA	1.94	0.50
1:A:319:MET:CE	1:D:197:GLN:HE22	2.24	0.50
1:A:334:LEU:O	1:A:337:LYS:HB2	2.11	0.50
1:A:315:LEU:HD22	1:D:348:GLU:HG3	1.94	0.49
1:C:225:ASN:O	1:C:227:LYS:HD2	2.12	0.49
1:E:188:SER:HA	1:E:224:ASN:OD1	2.12	0.49
1:B:168:LEU:HD21	1:D:320:ARG:NH2	2.27	0.49
1:D:187:SER:OG	1:D:190:ILE:HB	2.12	0.49
1:E:267:GLU:O	1:E:271:ARG:HG2	2.12	0.49
1:D:289:LEU:HD11	1:F:326:ILE:HG12	1.95	0.49
1:A:326:ILE:HA	1:A:329:VAL:HG22	1.96	0.48
1:B:329:VAL:HG11	1:C:286:THR:OG1	2.13	0.48
1:D:282:LEU:HD13	1:D:356:PRO:HA	1.94	0.48
1:E:282:LEU:HD13	1:E:356:PRO:HA	1.95	0.48
1:D:328:GLN:O	1:D:332:GLN:HB2	2.13	0.48
1:A:317:GLN:OE1	1:E:289:LEU:N	2.40	0.48
1:D:177:MET:O	1:D:179:PRO:HD3	2.14	0.47
1:A:282:LEU:HD13	1:A:356:PRO:HA	1.96	0.47
1:C:317:GLN:HA	1:C:321:GLN:HG3	1.96	0.47
1:F:231:TYR:CD1	1:F:231:TYR:C	2.88	0.47
1:E:225:ASN:O	1:E:226:ASN:CB	2.64	0.46
1:B:189:GLN:HG3	1:B:343:ILE:HD13	1.98	0.46
1:A:315:LEU:O	1:A:319:MET:HG2	2.16	0.46
1:F:177:MET:O	1:F:179:PRO:HD3	2.15	0.46
1:B:188:SER:HB3	1:B:344:VAL:O	2.17	0.45
1:D:167:LYS:C	1:D:169:LEU:H	2.19	0.45
1:D:275:ARG:H	1:D:275:ARG:HD2	1.81	0.45
1:A:326:ILE:O	1:A:330:VAL:HG23	2.17	0.45
1:D:191:ALA:CB	1:D:262:ASN:HB3	2.47	0.45
1:E:177:MET:O	1:E:179:PRO:HD3	2.17	0.45
1:C:269:ILE:HA	1:C:272:ASN:HD22	1.82	0.44
1:A:232:ARG:HA	1:E:327:ASN:OD1	2.18	0.44
1:A:285:LEU:HG	1:E:323:GLY:O	2.18	0.44
1:E:226:ASN:HD21	1:E:341:ALA:HB2	1.82	0.44
1:F:312:ASP:CG	1:F:313:TYR:N	2.68	0.44
1:C:177:MET:O	1:C:179:PRO:HD3	2.18	0.44
1:B:317:GLN:HA	1:B:321:GLN:CG	2.48	0.44
1:F:315:LEU:O	1:F:319:MET:HG3	2.18	0.44
1:E:293:ILE:HG23	1:E:293:ILE:O	2.17	0.43
1:F:228:MET:C	1:F:230:GLU:N	2.69	0.43
1:C:316:MET:O	1:C:320:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:SER:HB3	1:F:344:VAL:O	2.19	0.43
1:E:188:SER:HB3	1:E:344:VAL:O	2.18	0.43
1:C:324:MET:HE3	1:C:328:GLN:HB3	2.01	0.43
1:B:330:VAL:HG11	1:C:231:TYR:CE2	2.54	0.43
1:F:192:GLY:HA2	1:F:261:TYR:CD1	2.53	0.43
1:D:321:GLN:HG2	1:D:324:MET:SD	2.58	0.43
1:E:348:GLU:HG3	1:F:315:LEU:HD22	2.01	0.43
1:A:252:ASN:HB3	1:A:253:ALA:H	1.48	0.42
1:F:276:TYR:CE2	1:F:374:PHE:CD1	3.07	0.42
1:D:361:PHE:HB2	1:D:375:LEU:HD21	2.01	0.42
1:A:316:MET:SD	1:A:320:ARG:NH2	2.93	0.42
1:F:361:PHE:HB2	1:F:375:LEU:HD21	2.01	0.42
1:B:187:SER:OG	1:B:190:ILE:HB	2.20	0.42
1:D:223:SER:HB2	1:D:262:ASN:HB2	2.01	0.42
1:E:349:GLY:HA3	1:F:314:LEU:HD23	2.01	0.42
1:E:187:SER:OG	1:E:190:ILE:HB	2.20	0.42
1:C:361:PHE:HB2	1:C:375:LEU:HD21	2.01	0.42
1:A:188:SER:HB3	1:A:344:VAL:O	2.19	0.41
1:C:343:ILE:HD12	1:C:343:ILE:N	2.35	0.41
1:A:238:SER:HB2	1:A:251:THR:O	2.20	0.41
1:F:355:SER:HA	1:F:356:PRO:HD3	1.97	0.41
1:A:187:SER:OG	1:A:190:ILE:HB	2.21	0.41
1:B:279:PRO:HB2	1:D:227:LYS:NZ	2.35	0.41
1:F:275:ARG:HG2	1:F:276:TYR:CE2	2.55	0.41
1:C:358:THR:HG21	1:C:376:LYS:HA	2.03	0.41
1:B:341:ALA:HA	1:B:342:PRO:HD3	1.97	0.41
1:A:321:GLN:O	1:A:322:SER:C	2.59	0.41
1:D:223:SER:CB	1:D:262:ASN:HB2	2.50	0.41
1:D:188:SER:HB3	1:D:344:VAL:O	2.21	0.40
1:A:358:THR:HG21	1:A:376:LYS:HA	2.03	0.40
1:F:223:SER:HB2	1:F:262:ASN:ND2	2.35	0.40
1:A:336:ASP:OD1	1:A:339:LYS:HE2	2.22	0.40
1:C:343:ILE:HD12	1:C:343:ILE:H	1.86	0.40
1:E:355:SER:HA	1:E:356:PRO:HD3	1.98	0.40
1:D:358:THR:HG21	1:D:376:LYS:HA	2.03	0.40
1:F:213:PRO:O	1:F:216:SER:OG	2.34	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LYS:CE	1:F:175:ASP:OD2[3_555]	1.95	0.25
1:A:232:ARG:NH1	1:C:366:ARG:CD[4_455]	2.06	0.14
1:A:234:ASP:OD1	1:C:366:ARG:NE[4_455]	2.09	0.11

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	185/246 (75%)	166 (90%)	15 (8%)	4 (2%)	8 38
1	B	186/246 (76%)	172 (92%)	8 (4%)	6 (3%)	5 27
1	C	182/246 (74%)	172 (94%)	10 (6%)	0	100 100
1	D	183/246 (74%)	171 (93%)	10 (6%)	2 (1%)	17 58
1	E	184/246 (75%)	166 (90%)	16 (9%)	2 (1%)	17 58
1	F	182/246 (74%)	171 (94%)	10 (6%)	1 (0%)	34 76
All	All	1102/1476 (75%)	1018 (92%)	69 (6%)	15 (1%)	14 51

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	228	MET
1	B	254	LYS
1	A	313	TYR
1	B	229	GLY
1	B	274	GLN
1	F	229	GLY
1	A	252	ASN
1	A	322	SER
1	B	295	SER
1	D	168	LEU
1	D	340	ILE
1	E	226	ASN
1	E	311	GLY

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Mol	Chain	Res	Type
1	A	226	ASN
1	B	273	PHE

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	159/209 (76%)	143 (90%)	16 (10%)	9 34
1	B	158/209 (76%)	138 (87%)	20 (13%)	5 23
1	C	159/209 (76%)	144 (91%)	15 (9%)	11 39
1	D	160/209 (77%)	139 (87%)	21 (13%)	5 22
1	E	155/209 (74%)	140 (90%)	15 (10%)	10 37
1	F	159/209 (76%)	142 (89%)	17 (11%)	8 31
All	All	950/1254 (76%)	846 (89%)	104 (11%)	8 30

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	217	LYS
1	A	225	ASN
1	A	233	LEU
1	A	244	HIS
1	A	246	ILE
1	A	261	TYR
1	A	285	LEU
1	A	286	THR
1	A	319	MET
1	A	328	GLN
1	A	336	ASP
1	A	347	ARG
1	A	351	ARG
1	A	358	THR
1	A	366	ARG

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Mol	Chain	Res	Type
1	B	189	GLN
1	B	217	LYS
1	B	226	ASN
1	B	228	MET
1	B	231	TYR
1	B	233	LEU
1	B	244	HIS
1	B	246	ILE
1	B	285	LEU
1	B	286	THR
1	B	321	GLN
1	B	329	VAL
1	B	330	VAL
1	B	332	GLN
1	B	335	ARG
1	B	343	ILE
1	B	347	ARG
1	B	351	ARG
1	B	358	THR
1	B	366	ARG
1	C	189	GLN
1	C	217	LYS
1	C	227	LYS
1	C	233	LEU
1	C	244	HIS
1	C	246	ILE
1	C	285	LEU
1	C	286	THR
1	C	320	ARG
1	C	321	GLN
1	C	330	VAL
1	C	347	ARG
1	C	351	ARG
1	C	358	THR
1	C	366	ARG
1	D	189	GLN
1	D	217	LYS
1	D	227	LYS
1	D	228	MET
1	D	233	LEU
1	D	244	HIS
1	D	246	ILE

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Mol	Chain	Res	Type
1	D	261	TYR
1	D	262	ASN
1	D	274	GLN
1	D	275	ARG
1	D	285	LEU
1	D	286	THR
1	D	294	THR
1	D	322	SER
1	D	330	VAL
1	D	332	GLN
1	D	347	ARG
1	D	351	ARG
1	D	358	THR
1	D	366	ARG
1	E	189	GLN
1	E	217	LYS
1	E	233	LEU
1	E	244	HIS
1	E	246	ILE
1	E	273	PHE
1	E	275	ARG
1	E	285	LEU
1	E	286	THR
1	E	319	MET
1	E	329	VAL
1	E	347	ARG
1	E	351	ARG
1	E	358	THR
1	E	366	ARG
1	F	189	GLN
1	F	217	LYS
1	F	231	TYR
1	F	233	LEU
1	F	244	HIS
1	F	246	ILE
1	F	261	TYR
1	F	273	PHE
1	F	274	GLN
1	F	285	LEU
1	F	286	THR
1	F	328	GLN
1	F	330	VAL

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Mol	Chain	Res	Type
1	F	347	ARG
1	F	351	ARG
1	F	358	THR
1	F	366	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	A	262	ASN
1	A	274	GLN
1	A	328	GLN
1	B	321	GLN
1	C	272	ASN
1	D	197	GLN
1	D	274	GLN
1	E	226	ASN
1	F	262	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	191/246 (77%)	0.13	2 (1%) 84 60	33, 47, 56, 68	0
1	B	192/246 (78%)	0.20	10 (5%) 31 12	28, 47, 57, 68	0
1	C	188/246 (76%)	0.28	6 (3%) 51 23	32, 47, 54, 67	0
1	D	189/246 (76%)	0.17	11 (5%) 26 10	34, 47, 57, 62	0
1	E	190/246 (77%)	0.31	10 (5%) 30 12	25, 47, 56, 63	0
1	F	188/246 (76%)	0.24	7 (3%) 45 19	35, 47, 54, 67	0
All	All	1138/1476 (77%)	0.22	46 (4%) 42 17	25, 47, 56, 68	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	229	GLY	6.9
1	E	228	MET	5.5
1	C	229	GLY	5.3
1	F	376	LYS	4.8
1	A	368	ASN	4.6
1	B	188	SER	4.2
1	D	208	LYS	3.6
1	D	228	MET	3.4
1	E	368	ASN	3.2
1	C	376	LYS	3.2
1	D	188	SER	3.2
1	B	262	ASN	3.0
1	C	228	MET	3.0
1	F	166	ASN	3.0
1	E	295	SER	2.8
1	B	225	ASN	2.8
1	E	274	GLN	2.8
1	D	312	ASP	2.7
1	B	274	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	368	ASN	2.6
1	C	262	ASN	2.6
1	D	277	GLY	2.6
1	B	189	GLN	2.6
1	F	367	GLU	2.5
1	B	376	LYS	2.5
1	D	209	ALA	2.4
1	E	227	LYS	2.4
1	E	297	LEU	2.3
1	D	275	ARG	2.3
1	E	376	LYS	2.3
1	D	229	GLY	2.3
1	F	228	MET	2.3
1	B	252	ASN	2.3
1	C	311	GLY	2.3
1	C	206	MET	2.3
1	D	274	GLN	2.2
1	D	206	MET	2.2
1	F	366	ARG	2.1
1	F	261	TYR	2.1
1	B	208	LYS	2.1
1	E	339	LYS	2.1
1	A	228	MET	2.0
1	B	366	ARG	2.0
1	D	376	LYS	2.0
1	B	295	SER	2.0
1	E	340	ILE	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 carbohydrates 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.