W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:24 AM GMT

PDB ID	:	3IBC
Title	:	Crystal Structure of Caspase-7 incomplex with Acetyl-YVAD-CHO
Authors	:	Agniswamy, J.
Deposited on	:	2009-07-15
Resolution	:	2.75 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 ⓘ symbol.

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

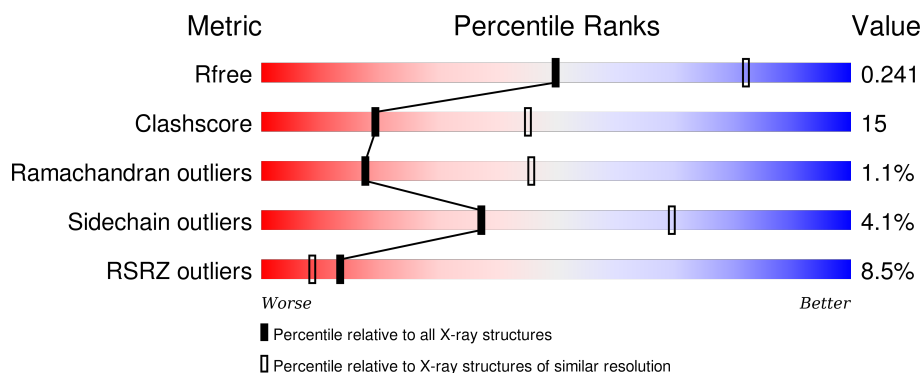|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.75 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	Percentile Ranks	Value
Rfree		0.241
Clashscore		15
Ramachandran outliers		1.1%
Sidechain outliers		4.1%
RSRZ outliers		8.5%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	173	3% 51% 28% • 19%
1	C	173	2% 58% 21% • 19%
2	B	97	14% 54% 41% 5%
2	D	97	16% 63% 30% • •
3	E	5	40% 20% 60% 20%

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Mol	Chain	Length	Quality of chain
3	F	5	60% 20% 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3857 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 Caspase-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total 1100	C 691	N 188	O 210	S 11	0	0	0
1	C	140	Total 1100	C 691	N 188	O 210	S 11	0	0	0

- Molecule 2 is a protein called Caspase-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	92	Total 758	C 487	N 128	O 139	S 4	0	0	0
2	D	93	Total 770	C 496	N 129	O 141	S 4	0	0	0

- Molecule 3 is a protein called Acetyl-YVAD-CHO.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total 35	C 23	N 4	O 8	0	0	0
3	F	5	Total 35	C 23	N 4	O 8	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total 15	O 15	0	0
4	B	8	Total 8	O 8	0	0
4	C	24	Total 24	O 24	0	0
4	D	12	Total 12	O 12	0	0

3 Residue-property plots ⓘ

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 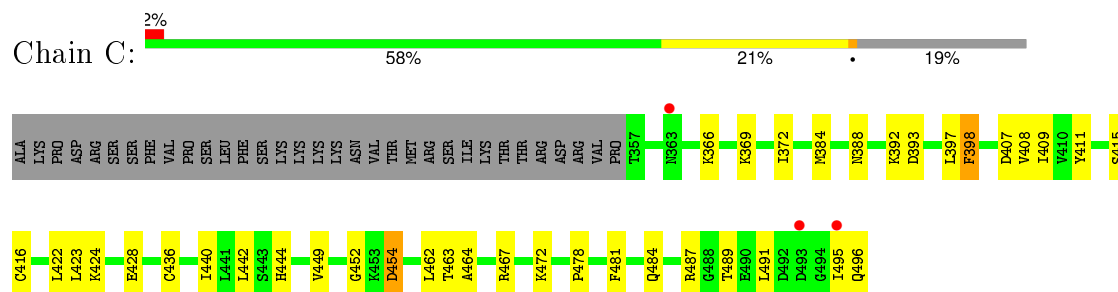least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Caspase-7
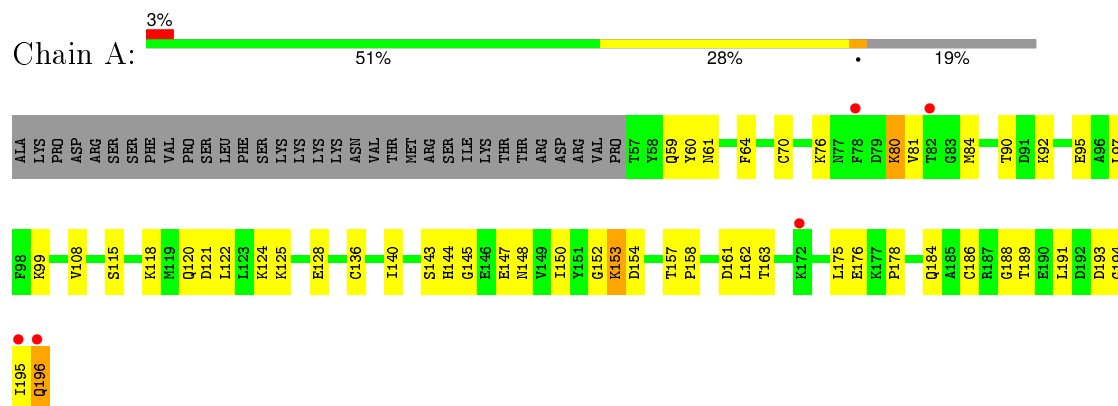
- Molecule 1: Caspase-7
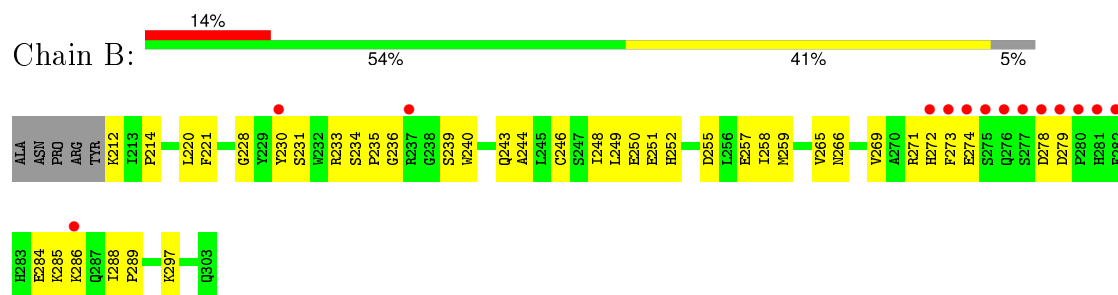
- Molecule 2: Caspase-7

- Molecule 2: Caspase-7

ALA ASN PRO ARG Y511 K512 I513 P514 V515 E516 L520 P527 Y530 R533 S534 P535 S539 V542 Q543 C546 E550 K554 E557 I558 M559 Q560 R564 V565 N566 D567 R571 H572 F573 E574 S575 Q576 S577 D578 D579 P580 H581 F582 H583 E584 K585 K586 Q587 I588

P589 Q603

• Molecule 3: Acetyl-YVAD-CHO

Chain E:

?701 Y702 V703 A704 D705

• Molecule 3: Acetyl-YVAD-CHO

Chain F:

?801 Y802 D805
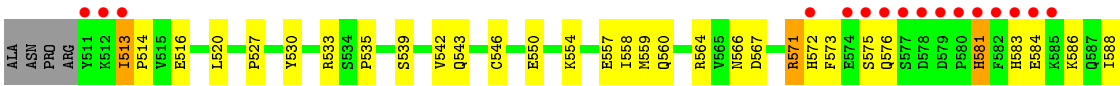
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	88.25Å 88.25Å 188.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.75 48.48 – 2.75	Depositor EDS
% Data completeness (in resolution range)	83.5 (50.00-2.75) 83.8 (48.48-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 2.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.203 , 0.242 0.203 , 0.241	Depositor DCC
R_{free} test set	915 reflections (4.81%)	DCC
Wilson B-factor (Å^2)	58.8	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 60.2	EDS
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	0 of 20517 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3857	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.39	0/1117	0.61	1/1496 (0.1%)
1	C	0.41	0/1117	0.62	1/1496 (0.1%)
2	B	0.39	0/780	0.59	0/1054
2	D	0.40	0/793	0.62	0/1072
3	E	2.01	1/33 (3.0%)	1.07	0/45
3	F	2.10	1/33 (3.0%)	0.99	0/45
All	All	0.48	2/3873 (0.1%)	0.62	2/5208 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	805	ASP	C-O	11.67	1.45	1.23
3	E	705	ASP	C-O	11.14	1.44	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	452	GLY	N-CA-C	-5.99	98.14	113.10
1	A	152	GLY	N-CA-C	-5.96	98.20	113.10

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	1100	0	1085	45	0
1	C	1100	0	1085	33	0
2	B	758	0	731	29	0
2	D	770	0	740	28	0
3	E	35	0	30	3	0
3	F	35	0	30	2	0
4	A	15	0	0	0	0
4	B	8	0	0	0	0
4	C	24	0	0	0	0
4	D	12	0	0	0	0
All	All	3857	0	3701	113	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 15.

All (113) 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:80:LYS:HD2	1:A:80:LYS:H	1.08	1.18
1:A:175:LEU:HD11	1:C:495:ILE:HG21	1.51	0.93
1:A:191:LEU:HD23	2:B:285:LYS:HG3	1.53	0.90
1:A:80:LYS:N	1:A:80:LYS:HD2	1.93	0.76
1:A:195:ILE:HD11	1:C:472:LYS:HE3	1.65	0.76
2:B:233:ARG:HA	2:B:239:SER:HA	1.68	0.73
1:A:95:GLU:HG2	1:A:99:LYS:NZ	2.05	0.72
1:C:424:LYS:O	1:C:428:GLU:HG3	1.91	0.70
2:D:533:ARG:HA	2:D:539:SER:HA	1.74	0.68
1:A:163:THR:HG21	2:B:221:PHE:HE1	1.59	0.67
2:B:240:TRP:HE1	3:E:702:TYR:HE2	1.44	0.66
1:C:397:LEU:HD13	1:C:440:ILE:HG21	1.77	0.66
2:B:246:CYS:O	2:B:250:GLU:HG2	1.96	0.65
1:C:393:ASP:HB3	2:D:542:VAL:HG11	1.81	0.63
1:A:97:LEU:HD13	1:A:140:ILE:HG21	1.81	0.62
3:E:703:VAL:HG12	3:E:704:ALA:H	1.65	0.62
1:C:436:CYS:HB3	1:C:478:PRO:HG2	1.82	0.61
1:A:147:GLU:HG3	1:A:148:ASN:OD1	2.01	0.60
1:C:411:TYR:CG	1:C:422:LEU:HD11	2.37	0.59
1:A:153:LYS:HB2	1:A:153:LYS:NZ	2.18	0.59
2:D:566:ASN:OD1	2:D:589:PRO:HB2	2.02	0.58
1:C:464:ALA:O	1:C:467:ARG:HG3	2.02	0.58
1:C:436:CYS:CB	1:C:478:PRO:HG2	2.33	0.58
1:A:175:LEU:CD1	1:C:495:ILE:HG21	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:539:SER:O	2:D:543:GLN:HG3	2.04	0.58
1:A:95:GLU:HG2	1:A:99:LYS:HZ3	1.67	0.58
1:C:423:LEU:HD12	1:C:462:LEU:HD22	1.85	0.58
1:A:76:LYS:HB2	1:A:90:THR:HG21	1.86	0.57
1:A:60:TYR:CD1	1:A:178:PRO:HD3	2.38	0.57
2:D:560:GLN:O	2:D:564:ARG:HG3	2.04	0.57
2:D:588:ILE:HD12	2:D:589:PRO:HD2	1.86	0.57
2:B:212:LYS:HA	1:C:495:ILE:O	2.04	0.56
3:E:703:VAL:HG12	3:E:704:ALA:N	2.21	0.56
2:D:576:GLN:H	3:F:802:TYR:HD1	1.52	0.56
1:A:143:SER:HB3	1:A:150:ILE:HD11	1.86	0.56
2:B:257:GLU:OE2	2:B:258:ILE:HG22	2.05	0.56
2:D:571:ARG:O	2:D:573:PHE:N	2.39	0.56
2:B:265:VAL:O	2:B:269:VAL:HG23	2.06	0.56
2:B:271:ARG:O	2:B:273:PHE:N	2.39	0.55
1:A:136:CYS:HB3	1:A:178:PRO:HG2	1.89	0.54
2:D:546:CYS:O	2:D:550:GLU:HG3	2.07	0.54
1:C:384:MET:HB3	1:C:444:HIS:CD2	2.44	0.53
1:C:369:LYS:HE2	1:C:409:ILE:HD11	1.91	0.53
1:A:60:TYR:CD2	2:B:297:LYS:HB2	2.43	0.53
2:D:571:ARG:HH11	2:D:571:ARG:HG2	1.73	0.53
1:A:184:GLN:HE22	2:B:231:SER:HB3	1.75	0.52
1:A:145:GLY:O	1:A:186:CYS:HB2	2.10	0.52
1:A:80:LYS:CD	1:A:80:LYS:H	1.88	0.51
1:A:115:SER:HB2	1:A:154:ASP:OD2	2.11	0.51
1:A:195:ILE:O	1:A:196:GLN:HG3	2.10	0.51
1:A:189:THR:HG22	2:B:230:TYR:OH	2.11	0.50
1:C:398:PHE:C	1:C:398:PHE:CD1	2.84	0.50
2:D:557:GLU:OE2	2:D:558:ILE:HG22	2.11	0.50
1:A:70:CYS:HB3	1:A:108:VAL:HB	1.93	0.50
1:A:158:PRO:HB2	1:A:161:ASP:OD2	2.12	0.50
1:A:163:THR:HG21	2:B:221:PHE:CE1	2.45	0.50
2:B:274:GLU:OE2	2:B:284:GLU:HG2	2.12	0.50
2:B:214:PRO:HG3	2:D:586:LYS:HB3	1.93	0.49
1:C:491:LEU:CD2	2:D:530:TYR:HD2	2.24	0.49
1:A:136:CYS:CB	1:A:178:PRO:HG2	2.42	0.49
2:D:575:SER:HA	3:F:802:TYR:CD1	2.47	0.49
1:A:175:LEU:O	1:A:176:GLU:HB2	2.11	0.49
1:A:84:MET:HB3	1:A:144:HIS:CD2	2.48	0.49
1:A:175:LEU:HD11	1:C:495:ILE:CG2	2.34	0.48
2:B:271:ARG:HH11	2:B:271:ARG:HG3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:ASN:OD1	2:B:289:PRO:HB2	2.14	0.48
1:C:496:GLN:HG2	1:C:496:GLN:O	2.14	0.48
1:A:189:THR:HA	2:B:230:TYR:CZ	2.49	0.47
1:C:491:LEU:HD21	2:D:530:TYR:HD2	1.79	0.47
1:A:194:GLY:HA2	2:D:513:ILE:O	2.15	0.47
2:D:571:ARG:NH1	2:D:571:ARG:HG2	2.30	0.47
2:B:220:LEU:HD23	2:B:220:LEU:C	2.35	0.47
2:B:249:LEU:C	2:B:251:GLU:H	2.17	0.46
2:B:257:GLU:OE1	2:B:259:MET:HB2	2.15	0.46
2:D:567:ASP:O	2:D:571:ARG:HG3	2.16	0.46
1:A:124:LYS:O	1:A:128:GLU:HG3	2.16	0.46
2:B:288:ILE:HG21	2:D:516:GLU:HB2	1.97	0.46
2:D:583:HIS:CE1	2:D:584:GLU:HG3	2.51	0.46
2:B:286:LYS:HB3	2:D:514:PRO:HG3	1.97	0.46
1:C:366:LYS:HE3	1:C:407:ASP:OD2	2.16	0.46
1:C:415:SER:HB2	1:C:454:ASP:OD2	2.16	0.46
1:C:436:CYS:HB2	1:C:478:PRO:O	2.17	0.45
1:A:195:ILE:O	1:A:196:GLN:OXT	2.35	0.45
1:C:372:ILE:HG12	1:C:440:ILE:HD12	1.98	0.45
1:A:153:LYS:HB2	1:A:153:LYS:HZ2	1.81	0.45
1:A:118:LYS:HE3	1:A:122:LEU:HD11	1.98	0.45
1:C:487:ARG:CZ	2:D:527:PRO:HG3	2.47	0.44
1:A:143:SER:OG	1:A:144:HIS:N	2.50	0.44
1:C:491:LEU:HD13	2:D:581:HIS:O	2.17	0.44
1:A:136:CYS:HB2	1:A:178:PRO:O	2.18	0.44
2:D:558:ILE:HG23	2:D:559:MET:N	2.33	0.44
2:B:234:SER:O	2:B:236:GLY:N	2.51	0.44
1:C:495:ILE:HG13	1:C:496:GLN:N	2.33	0.44
1:C:388:ASN:O	2:D:535:PRO:HA	2.18	0.43
2:B:244:ALA:O	2:B:248:ILE:HG12	2.18	0.43
1:C:411:TYR:CD2	1:C:422:LEU:HD11	2.54	0.43
1:C:489:THR:HA	2:D:530:TYR:CE1	2.54	0.43
1:A:120:GLN:NE2	1:A:162:LEU:HD23	2.33	0.43
1:C:416:CYS:H	1:C:454:ASP:HB2	1.83	0.43
1:A:121:ASP:O	1:A:125:LYS:HG2	2.19	0.43
2:B:239:SER:O	2:B:243:GLN:HG3	2.18	0.42
1:C:463:THR:HG22	1:C:481:PHE:CE2	2.54	0.42
1:C:495:ILE:HG13	1:C:496:GLN:H	1.85	0.42
1:A:61:ASN:ND2	1:A:64:PHE:CE2	2.87	0.42
2:B:251:GLU:HG2	2:B:252:HIS:CD2	2.54	0.41
1:C:442:LEU:HD23	1:C:484:GLN:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:520:LEU:HD23	2:D:520:LEU:C	2.41	0.41
2:D:588:ILE:HD12	2:D:589:PRO:CD	2.50	0.41
1:A:196:GLN:OE1	1:A:196:GLN:OXT	2.39	0.41
2:B:278:ASP:O	2:B:279:ASP:C	2.59	0.41
1:A:157:THR:HA	1:A:158:PRO:HD3	1.89	0.40
1:A:76:LYS:HB2	1:A:90:THR:CG2	2.51	0.40
1:A:188:GLY:HA3	2:B:228:GLY:HA2	2.04	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	138/173 (80%)	131 (95%)	7 (5%)	0	100	100
1	C	138/173 (80%)	130 (94%)	8 (6%)	0	100	100
2	B	90/97 (93%)	79 (88%)	9 (10%)	2 (2%)	8	24
2	D	91/97 (94%)	85 (93%)	4 (4%)	2 (2%)	8	24
3	E	3/5 (60%)	2 (67%)	0	1 (33%)	0	0
3	F	3/5 (60%)	3 (100%)	0	0	100	100
All	All	463/550 (84%)	430 (93%)	28 (6%)	5 (1%)	17	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	272	HIS
2	D	572	HIS
3	E	702	TYR
2	D	571	ARG
2	B	235	PRO

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	120/152 (79%)	113 (94%)	7 (6%)	25	54
1	C	120/152 (79%)	115 (96%)	5 (4%)	36	68
2	B	84/88 (96%)	83 (99%)	1 (1%)	78	94
2	D	85/88 (97%)	82 (96%)	3 (4%)	43	75
3	E	3/3 (100%)	3 (100%)	0	100	100
3	F	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	415/486 (85%)	398 (96%)	17 (4%)	37	69

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	80	LYS
1	A	81	VAL
1	A	92	LYS
1	A	153	LYS
1	A	193	ASP
1	A	196	GLN
2	B	255	ASP
1	C	392	LYS
1	C	398	PHE
1	C	408	VAL
1	C	449	VAL
1	C	454	ASP
2	D	513	ILE
2	D	554	LYS
2	D	581	HIS
3	F	805	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	A	184	GLN
2	B	252	HIS
2	B	283	HIS
1	C	448	ASN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6   Ligand geometry (i)

There are no ligands in this entry.

5.7   Other polymers (i)

There are no such residues in this entry.

5.8   Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	140/173 (80%)	0.33	5 (3%)	46	40	52, 74, 99, 107	0
1	C	140/173 (80%)	0.41	3 (2%)	67	61	49, 63, 91, 121	0
2	B	92/97 (94%)	0.97	14 (15%)	3	2	47, 69, 134, 144	0
2	D	93/97 (95%)	0.73	16 (17%)	2	1	46, 66, 134, 141	0
3	E	4/5 (80%)	2.18	2 (50%)	0	0	95, 100, 103, 112	0
3	F	4/5 (80%)	0.58	0	100	100	80, 82, 87, 98	0
All	All	473/550 (86%)	0.57	40 (8%)	13	8	46, 68, 114, 144	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	278	ASP	6.1
2	B	280	PRO	5.5
2	B	277	SER	5.5
2	B	282	PHE	5.3
2	D	580	PRO	5.2
2	B	276	GLN	5.2
2	B	281	HIS	4.6
2	D	581	HIS	4.2
2	D	576	GLN	4.1
2	D	511	TYR	4.0
3	E	702	TYR	3.8
3	E	703	VAL	3.7
2	D	575	SER	3.7
2	D	579	ASP	3.6
2	B	279	ASP	3.5
2	B	230	TYR	3.3
2	D	513	ILE	2.8
2	D	578	ASP	2.8
1	A	78	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	585	LYS	2.7
2	B	286	LYS	2.7
2	B	237	ARG	2.7
2	B	275	SER	2.7
2	D	582	PHE	2.6
1	C	363	ASN	2.5
2	B	273	PHE	2.5
2	D	584	GLU	2.5
1	A	196	GLN	2.4
2	D	577	SER	2.4
1	C	495	ILE	2.4
2	D	572	HIS	2.4
1	A	195	ILE	2.4
2	B	274	GLU	2.3
2	B	272	HIS	2.3
2	D	574	GLU	2.2
1	A	172	LYS	2.2
1	C	493	ASP	2.1
1	A	82	THR	2.1
2	D	583	HIS	2.0
2	D	512	LYS	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.