Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:56 AM GMT

PDB ID	:	2JDQ
Title	:	C-TERMINAL DOMAIN OF INFLUENZA A VIRUS POLYMERASE PB2 SUBUNIT IN COMPLEX WITH HUMAN IMPORTIN ALPHA5
Authors	:	Tarendeau, F.; Guilligay, D.; Mas, P.; Boulo, S.; Baudin, F.; Ruigrok, R.W.H.; Hart, D.J.; Cusack, S.
Deposited on	:	2007-01-11
Resolution	:	2.20 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:

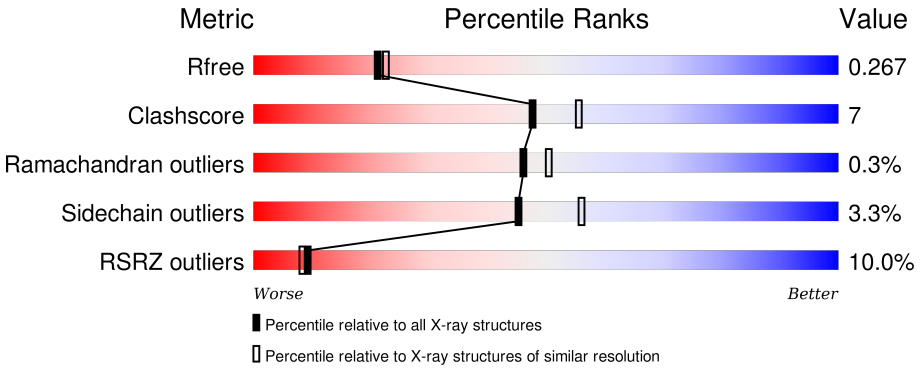
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	450	8% 80% 13% • 6%
1	B	450	10% 79% 14% • 5%
2	D	83	10% 67% 7% • 24%
2	E	83	7% 58% 17% • 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7862 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 IMPORTIN ALPHA-1 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3296	2094	554	630	18			
1	B	426	Total	C	N	O	S	0	0	0
			3313	2103	556	636	18			

- Molecule 2 is a protein called POLYMERASE BASIC PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	63	Total	C	N	O	S	0	0	0
			488	304	95	87	2			
2	E	65	Total	C	N	O	S	0	0	0
			500	312	96	90	2			

- Molecule 3 is water.

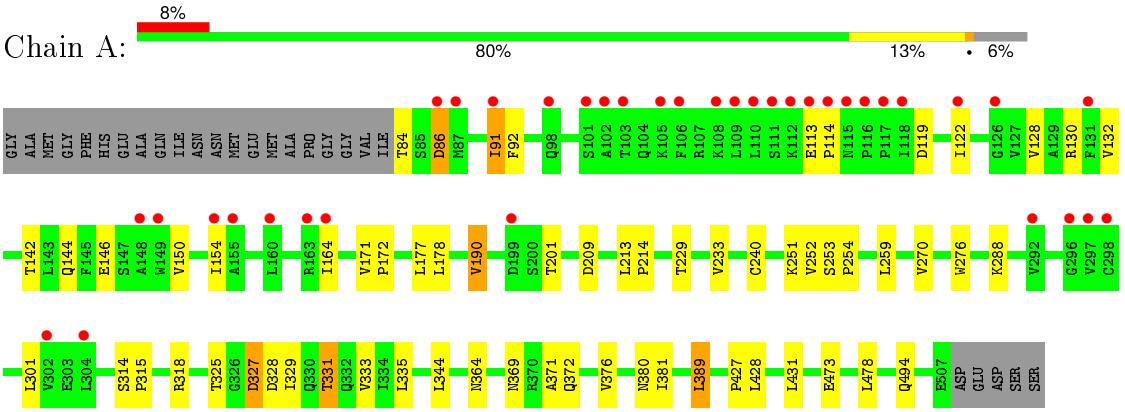
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total	O	0	0
			131	131		
3	B	98	Total	O	0	0
			98	98		
3	D	14	Total	O	0	0
			14	14		
3	E	22	Total	O	0	0
			22	22		

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.

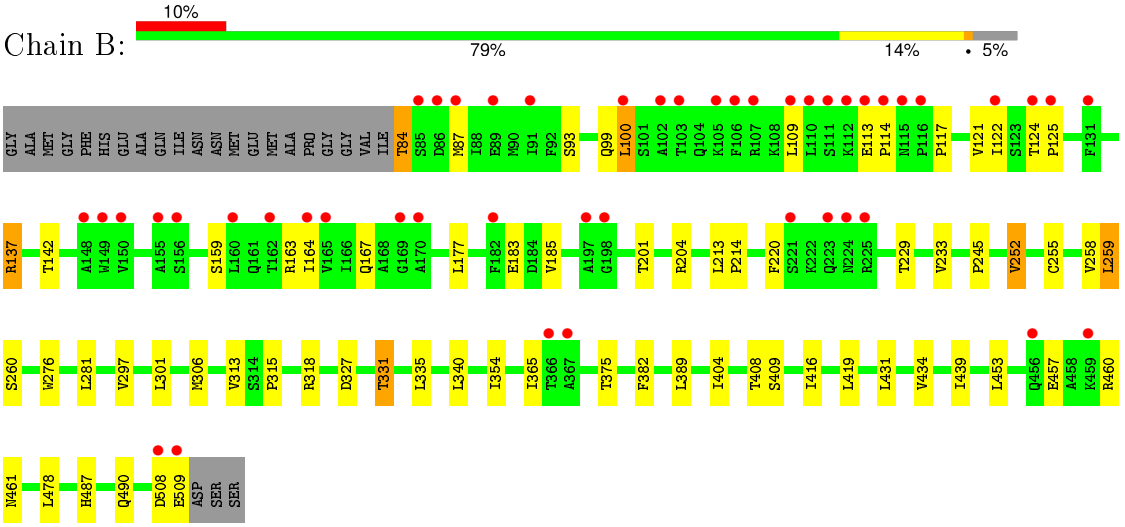
- Molecule 1: IMPORTIN ALPHA-1 SUBUNIT

Chain A:



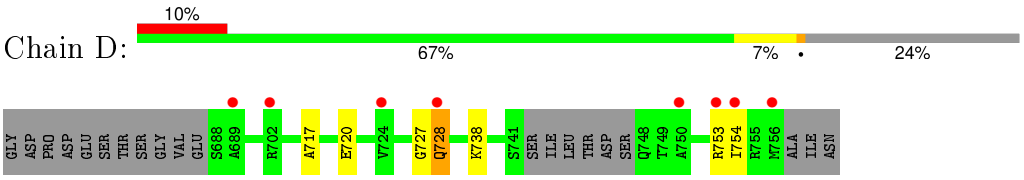
- Molecule 1: IMPORTIN ALPHA-1 SUBUNIT

Chain B:



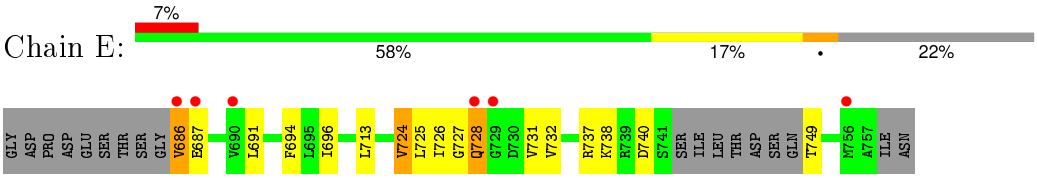
- Molecule 2: POLYMERASE BASIC PROTEIN 2

Chain D:



- Molecule 2: POLYMERASE BASIC PROTEIN 2

Chain E:


7%
58%
17%
22%
GLY ASP PRO ASP GLU SER THR SER GLY V686 E687 V690 L691 F694 L695 I696 L713 V724 L725 I726 G727 Q728 G729 D730 V731 V732 R737 K738 R739 D740 S741 SER ILE LEU THR ASP SER GLN T749 M756 A757 ILE ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.97Å 100.55Å 151.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 47.73 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.20) 99.5 (47.73-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.247 0.241 , 0.267	Depositor DCC
R_{free} test set	2969 reflections (4.01%)	DCC
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 74103 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7862	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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	0.62	1/3354 (0.0%)	0.66	1/4558 (0.0%)
1	B	0.53	0/3371	0.60	0/4581
2	D	0.43	0/489	0.71	0/649
2	E	0.48	0/501	0.71	0/666
All	All	0.56	1/7715 (0.0%)	0.64	1/10454 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	VAL	CB-CG2	7.17	1.68	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	328	ASP	CB-CG-OD1	5.42	123.17	118.30

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	3296	0	3331	40	0
1	B	3313	0	3341	56	0
2	D	488	0	528	4	0
2	E	500	0	540	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	131	0	0	5	0
3	B	98	0	0	1	0
3	D	14	0	0	0	0
3	E	22	0	0	5	0
All	All	7862	0	7740	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 7.

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)
2:E:691:LEU:HD11	2:E:726:ILE:HD12	1.46	0.97
1:A:122:ILE:HG21	1:A:164:ILE:HD13	1.48	0.92
2:E:694:PHE:O	3:E:2007:HOH:O	1.90	0.88
1:B:201:THR:HG21	1:B:245:PRO:HD2	1.55	0.86
1:B:100:LEU:HD21	1:B:142:THR:HG22	1.59	0.85
1:B:340:LEU:HD12	1:B:375:THR:HG22	1.60	0.83
1:B:122:ILE:HG21	1:B:164:ILE:HD13	1.60	0.83
1:A:229:THR:O	1:A:233:VAL:HG23	1.81	0.81
1:A:389:LEU:HD13	1:A:427:PRO:HB2	1.65	0.77
1:B:461:ASN:HB3	3:B:2085:HOH:O	1.84	0.77
1:A:209:ASP:OD1	1:A:251:LYS:NZ	2.13	0.76
1:A:122:ILE:HD11	1:A:154:ILE:HG23	1.68	0.75
1:B:331:THR:HG21	2:D:738:LYS:NZ	2.02	0.75
1:B:122:ILE:CG2	1:B:164:ILE:HD13	2.17	0.74
1:A:122:ILE:CG2	1:A:164:ILE:HD13	2.19	0.73
1:B:327:ASP:O	1:B:331:THR:HG23	1.90	0.71
1:B:229:THR:O	1:B:233:VAL:HG23	1.91	0.71
1:B:416:ILE:HG12	1:B:453:LEU:HD12	1.74	0.69
2:E:694:PHE:C	3:E:2007:HOH:O	2.26	0.69
1:A:473:GLU:OE2	1:A:478:LEU:HD13	1.93	0.68
2:E:713:LEU:HD13	2:E:724:VAL:CG1	2.24	0.67
1:A:327:ASP:O	1:A:331:THR:HG23	1.94	0.66
2:E:696:ILE:HG23	2:E:732:VAL:CG1	2.26	0.66
2:E:713:LEU:HD13	2:E:724:VAL:HG13	1.78	0.66
2:E:696:ILE:HG23	2:E:732:VAL:HG13	1.77	0.66
1:B:434:VAL:HG21	1:B:439:ILE:HG21	1.77	0.65
1:B:431:LEU:O	1:B:434:VAL:HG22	1.98	0.64
1:B:331:THR:HG21	2:D:738:LYS:HZ1	1.63	0.64
1:B:340:LEU:CD1	1:B:375:THR:HG22	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:LEU:HD11	1:B:431:LEU:HD11	1.83	0.61
2:E:737:ARG:NE	3:E:2007:HOH:O	2.35	0.58
1:B:408:THR:HA	1:B:416:ILE:HD11	1.85	0.58
1:A:84:THR:HG22	1:A:86:ASP:H	1.69	0.58
1:B:460:ARG:HH12	1:B:461:ASN:HB2	1.69	0.57
1:A:240:CYS:SG	1:A:252:VAL:CG1	2.93	0.57
1:B:201:THR:HG23	1:B:204:ARG:NH2	2.20	0.57
1:B:404:ILE:O	1:B:408:THR:HG23	2.04	0.56
1:A:233:VAL:HG21	1:A:270:VAL:HG13	1.86	0.56
1:B:508:ASP:O	1:B:509:GLU:HB2	2.06	0.56
1:B:382:PHE:CD2	1:B:419:LEU:HD21	2.40	0.56
1:B:416:ILE:HG12	1:B:453:LEU:CD1	2.36	0.55
1:A:344:LEU:HB2	1:A:381:ILE:HD13	1.88	0.54
1:B:335:LEU:HD21	1:B:365:ILE:HD13	1.90	0.54
1:B:117:PRO:O	1:B:121:VAL:HG23	2.08	0.53
1:A:288:LYS:NZ	3:A:2037:HOH:O	2.42	0.53
2:E:686:VAL:HG23	2:E:687:GLU:H	1.74	0.52
1:B:201:THR:HG21	1:B:245:PRO:CD	2.35	0.51
1:A:318:ARG:NE	3:A:2054:HOH:O	2.42	0.51
1:A:91:ILE:HG23	1:A:130:ARG:HG2	1.92	0.51
1:B:306:MET:HA	1:B:306:MET:CE	2.40	0.51
1:A:329:ILE:CD1	1:B:478:LEU:HD21	2.40	0.51
1:B:260:SER:HA	1:B:297:VAL:HG12	1.93	0.50
1:A:331:THR:HG21	2:E:738:LYS:NZ	2.27	0.50
1:B:100:LEU:HD11	1:B:142:THR:CG2	2.42	0.49
1:A:329:ILE:HD11	1:B:478:LEU:HD21	1.94	0.49
1:A:335:LEU:HD12	1:A:372:GLN:HG2	1.95	0.49
1:A:171:VAL:HB	1:A:172:PRO:HD3	1.94	0.48
1:B:122:ILE:HD13	1:B:164:ILE:CD1	2.43	0.48
1:A:318:ARG:HD3	3:A:2054:HOH:O	2.14	0.48
1:A:327:ASP:O	1:A:331:THR:CG2	2.61	0.48
1:A:318:ARG:CD	3:A:2054:HOH:O	2.62	0.47
2:E:725:LEU:HD12	2:E:731:VAL:HG22	1.97	0.47
1:B:508:ASP:O	1:B:509:GLU:CB	2.61	0.47
1:B:122:ILE:HD13	1:B:164:ILE:HD13	1.97	0.47
1:B:177:LEU:HD22	1:B:185:VAL:HG11	1.97	0.46
1:B:109:LEU:HD22	1:B:117:PRO:HG3	1.97	0.46
1:A:288:LYS:HD3	3:A:2038:HOH:O	2.16	0.46
1:B:340:LEU:HD12	1:B:375:THR:CG2	2.39	0.46
1:B:434:VAL:CG2	1:B:439:ILE:HG21	2.44	0.46
1:A:325:THR:HG22	1:A:364:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:HB3	1:A:214:PRO:HD3	1.98	0.45
2:E:713:LEU:HD13	2:E:724:VAL:HG11	1.95	0.45
1:B:124:THR:HG23	1:B:125:PRO:HD2	1.98	0.45
1:B:100:LEU:HD11	1:B:142:THR:HB	1.98	0.45
1:A:473:GLU:OE2	1:A:478:LEU:CD1	2.64	0.45
1:A:91:ILE:HG22	1:A:92:PHE:N	2.31	0.45
1:B:113:GLU:N	1:B:114:PRO:HD2	2.32	0.45
2:E:737:ARG:CZ	3:E:2007:HOH:O	2.63	0.45
1:B:252:VAL:HG13	1:B:281:LEU:HD21	1.99	0.45
1:B:213:LEU:HB3	1:B:214:PRO:HD3	1.99	0.44
1:B:434:VAL:CG2	1:B:439:ILE:CG2	2.95	0.44
1:A:144:GLN:NE2	1:A:177:LEU:HD21	2.32	0.44
2:D:717:ALA:HB3	2:D:720:GLU:CG	2.47	0.44
1:A:128:VAL:O	1:A:132:VAL:HG23	2.18	0.44
1:A:253:SER:N	1:A:254:PRO:CD	2.81	0.44
1:B:276:TRP:CD2	1:B:315:PRO:HB3	2.53	0.43
1:A:178:LEU:CD2	1:A:190:VAL:HG23	2.47	0.43
1:A:146:GLU:O	1:A:150:VAL:HG23	2.18	0.43
1:B:163:ARG:HG2	1:B:167:GLN:HE21	1.84	0.43
2:E:694:PHE:CZ	2:E:713:LEU:HG	2.54	0.42
1:A:389:LEU:HD21	1:A:431:LEU:HD11	2.00	0.42
1:B:457:GLU:OE2	1:B:460:ARG:NH1	2.52	0.42
1:B:177:LEU:HD22	1:B:185:VAL:CG1	2.48	0.42
1:B:487:HIS:HD2	1:B:490:GLN:HE21	1.65	0.42
2:E:713:LEU:HD22	2:E:724:VAL:HG11	2.00	0.42
1:A:376:VAL:HG13	1:A:381:ILE:HG13	2.01	0.42
1:A:240:CYS:SG	1:A:252:VAL:HG11	2.58	0.42
1:A:113:GLU:N	1:A:114:PRO:CD	2.83	0.42
1:A:314:SER:HB2	1:A:315:PRO:CD	2.50	0.42
1:B:84:THR:N	1:B:87:MET:SD	2.93	0.41
1:B:99:GLN:OE1	1:B:137:ARG:NH2	2.53	0.41
2:E:740:ASP:HB2	3:E:2022:HOH:O	2.20	0.41
1:B:93:SER:O	1:B:99:GLN:NE2	2.46	0.41
1:B:124:THR:CG2	1:B:125:PRO:HD2	2.51	0.41
1:B:220:PHE:CD1	1:B:258:VAL:HG11	2.56	0.41
2:E:691:LEU:CD1	2:E:726:ILE:HD12	2.33	0.41
1:B:460:ARG:NH1	1:B:461:ASN:HB2	2.35	0.41
2:D:727:GLY:O	2:D:728:GLN:C	2.59	0.41
1:A:369:ASN:OD1	1:A:371:ALA:HB3	2.21	0.40
1:A:276:TRP:NE1	2:E:749:THR:HG21	2.36	0.40
2:E:727:GLY:O	2:E:728:GLN:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:VAL:CG1	1:B:354:ILE:HD13	2.51	0.40
1:B:255:CYS:SG	1:B:259:LEU:HD22	2.62	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	422/450 (94%)	414 (98%)	7 (2%)	1 (0%)	52 59
1	B	424/450 (94%)	414 (98%)	10 (2%)	0	100 100
2	D	59/83 (71%)	57 (97%)	1 (2%)	1 (2%)	11 7
2	E	61/83 (74%)	60 (98%)	0	1 (2%)	12 8
All	All	966/1066 (91%)	945 (98%)	18 (2%)	3 (0%)	46 50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ASP
2	E	728	GLN
2	D	728	GLN

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	368/387 (95%)	355 (96%)	13 (4%)	43	53
1	B	370/387 (96%)	359 (97%)	11 (3%)	48	60
2	D	52/69 (75%)	50 (96%)	2 (4%)	40	49
2	E	53/69 (77%)	51 (96%)	2 (4%)	40	49
All	All	843/912 (92%)	815 (97%)	28 (3%)	45	56

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ASP
1	A	91	ILE
1	A	119	ASP
1	A	142	THR
1	A	190	VAL
1	A	201	THR
1	A	259	LEU
1	A	301	LEU
1	A	331	THR
1	A	380	ASN
1	A	389	LEU
1	A	428	LEU
1	A	494	GLN
1	B	84	THR
1	B	100	LEU
1	B	137	ARG
1	B	159	SER
1	B	183	GLU
1	B	252	VAL
1	B	259	LEU
1	B	301	LEU
1	B	318	ARG
1	B	331	THR
1	B	409	SER
2	D	753	ARG
2	D	754	ILE
2	E	686	VAL
2	E	724	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	224	ASN
1	A	257	ASN
1	A	345	HIS
1	A	380	ASN
1	A	390	GLN
1	A	490	GLN
1	A	502	HIS
1	B	167	GLN
1	B	223	GLN
1	B	345	HIS
1	B	487	HIS
1	B	490	GLN
2	D	715	ASN
2	D	728	GLN

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	424/450 (94%)	0.61	37 (8%) 13 12	2, 23, 36, 44	0
1	B	426/450 (94%)	0.64	47 (11%) 7 7	2, 24, 41, 52	0
2	D	63/83 (75%)	0.78	8 (12%) 5 4	15, 22, 56, 62	0
2	E	65/83 (78%)	0.56	6 (9%) 11 10	8, 16, 40, 44	0
All	All	978/1066 (91%)	0.63	98 (10%) 9 8	2, 22, 40, 62	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	LEU	9.0
1	B	87	MET	6.6
1	A	114	PRO	6.4
1	B	103	THR	6.2
1	A	112	LYS	6.1
1	B	113	GLU	5.9
1	B	86	ASP	5.7
1	B	111	SER	5.6
2	D	750	ALA	5.5
1	B	89	GLU	5.2
2	E	686	VAL	5.2
1	A	115	ASN	5.2
1	B	164	ILE	5.1
1	A	113	GLU	5.0
1	B	102	ALA	5.0
1	A	87	MET	5.0
2	E	729	GLY	5.0
1	B	112	LYS	4.9
1	B	105	LYS	4.9
1	B	114	PRO	4.8
1	B	508	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	109	LEU	4.7
1	A	106	PHE	4.5
1	B	148	ALA	4.4
1	A	118	ILE	4.3
1	B	124	THR	4.3
2	D	689	ALA	4.2
1	A	117	PRO	4.1
1	B	149	TRP	4.0
1	A	116	PRO	4.0
1	B	100	LEU	3.9
1	B	115	ASN	3.9
1	B	110	LEU	3.7
2	E	687	GLU	3.6
1	A	163	ARG	3.5
1	A	98	GLN	3.5
1	A	122	ILE	3.4
1	B	125	PRO	3.4
1	A	155	ALA	3.3
1	B	165	VAL	3.3
1	A	101	SER	3.2
1	B	197	ALA	3.2
1	A	111	SER	3.1
1	B	198	GLY	3.1
1	B	182	PHE	3.1
2	D	724	VAL	3.0
2	E	690	VAL	3.0
1	B	162	THR	3.0
1	B	223	GLN	3.0
1	B	155	ALA	3.0
1	A	131	PHE	3.0
1	A	164	ILE	3.0
1	B	116	PRO	2.9
1	A	86	ASP	2.9
2	E	756	MET	2.8
1	B	221	SER	2.8
1	A	298	CYS	2.8
1	A	103	THR	2.8
1	B	156	SER	2.7
1	B	106	PHE	2.7
1	A	126	GLY	2.7
1	B	509	GLU	2.7
1	A	91	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	225	ARG	2.6
1	B	131	PHE	2.6
1	B	459	LYS	2.6
2	D	754	ILE	2.6
1	A	105	LYS	2.5
1	B	107	ARG	2.5
1	B	169	GLY	2.5
2	D	756	MET	2.4
2	D	702	ARG	2.4
1	A	302	VAL	2.4
1	B	91	ILE	2.4
1	A	108	LYS	2.4
1	A	160	LEU	2.3
2	E	728	GLN	2.3
1	A	148	ALA	2.2
1	A	297	VAL	2.2
1	B	150	VAL	2.2
1	B	160	LEU	2.2
1	B	122	ILE	2.1
1	A	296	GLY	2.1
1	B	170	ALA	2.1
1	B	366	THR	2.1
1	B	456	GLN	2.1
1	A	154	ILE	2.1
1	A	199	ASP	2.1
1	A	304	LEU	2.1
2	D	728	GLN	2.1
1	A	102	ALA	2.1
1	A	110	LEU	2.1
1	B	224	ASN	2.1
1	B	367	ALA	2.1
1	A	292	VAL	2.1
1	A	149	TRP	2.0
1	B	85	SER	2.0
2	D	753	ARG	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.