Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:18 am BST

PDB ID	:	5JER
Title	:	Structure of Rotavirus NSP1 bound to IRF-3
Authors	:	Zhao, B.; Li, P.
Deposited on	:	2016-04-18
Resolution	:	2.91 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 following versions of software and data (see references ⓘ) were used in the production of this report:

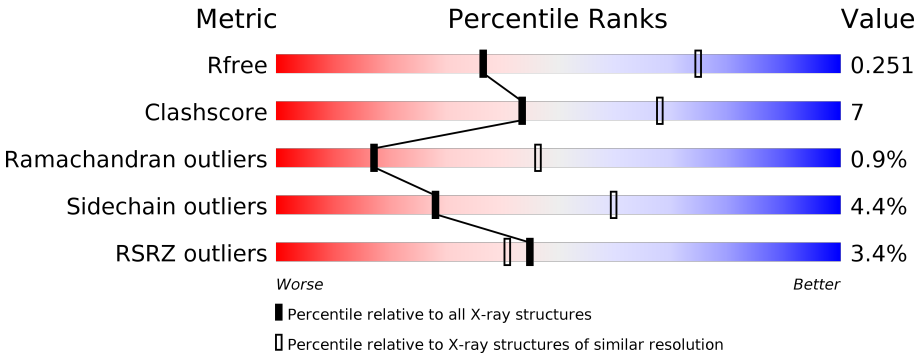
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 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	B	19	5% 32% 16% 5% 47%
1	D	19	11% 42% 11% 47%
1	F	19	11% 47% 5% 47%
1	H	19	11% 32% 21% 47%
2	A	242	3% 79% 15%
2	C	242	2% 78% 17%

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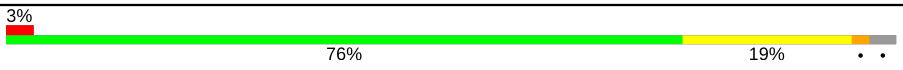
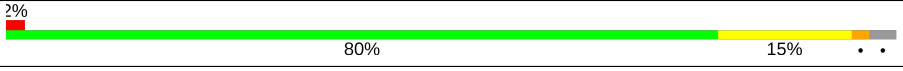
Mol	Chain	Length	Quality of chain
2	E	242	
2	G	242	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7710 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 Rotavirus NSP1 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	B	10	Total	C	N	O	0	0	0
			82	52	11	19			
1	D	10	Total	C	N	O	0	0	0
			82	52	11	19			
1	F	10	Total	C	N	O	0	0	0
			82	52	11	19			
1	H	10	Total	C	N	O	0	0	0
			82	52	11	19			

- Molecule 2 is a protein called Interferon regulatory factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	234	Total	C	N	O	S	6	2	0
			1850	1179	319	342	10			
2	C	234	Total	C	N	O	S	0	1	0
			1844	1176	318	340	10			
2	E	234	Total	C	N	O	S	0	1	0
			1844	1176	318	340	10			
2	G	234	Total	C	N	O	S	0	1	0
			1844	1176	318	340	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	SER	-	expression tag	UNP Q14653
A	187	GLU	-	expression tag	UNP Q14653
A	188	PHE	-	expression tag	UNP Q14653
C	186	SER	-	expression tag	UNP Q14653
C	187	GLU	-	expression tag	UNP Q14653
C	188	PHE	-	expression tag	UNP Q14653
E	186	SER	-	expression tag	UNP Q14653
E	187	GLU	-	expression tag	UNP Q14653

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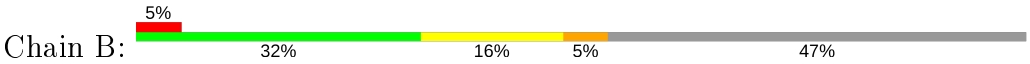
Chain	Residue	Modelled	Actual	Comment	Reference
E	188	PHE	-	expression tag	UNP Q14653
G	186	SER	-	expression tag	UNP Q14653
G	187	GLU	-	expression tag	UNP Q14653
G	188	PHE	-	expression tag	UNP Q14653

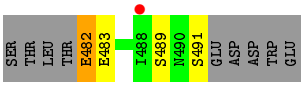
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Rotavirus NSP1 peptide

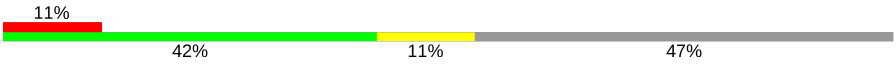
Chain B:

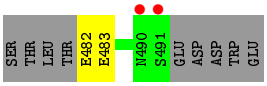




- Molecule 1: Rotavirus NSP1 peptide

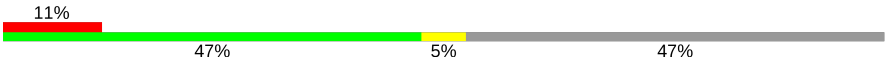
Chain D:

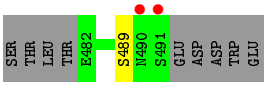




- Molecule 1: Rotavirus NSP1 peptide

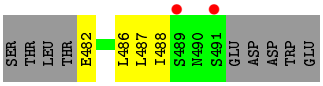
Chain F:





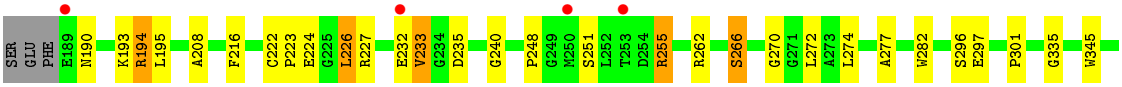
- Molecule 1: Rotavirus NSP1 peptide

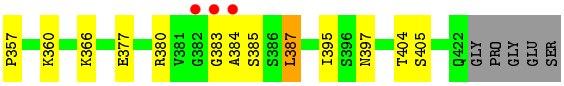
Chain H:



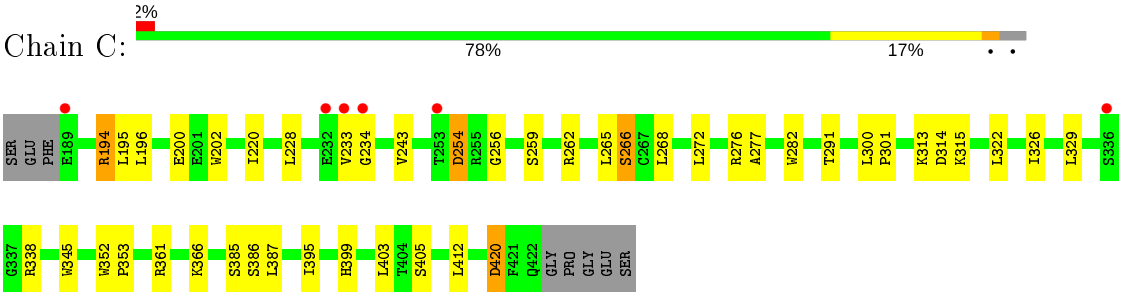
- Molecule 2: Interferon regulatory factor 3

Chain A:

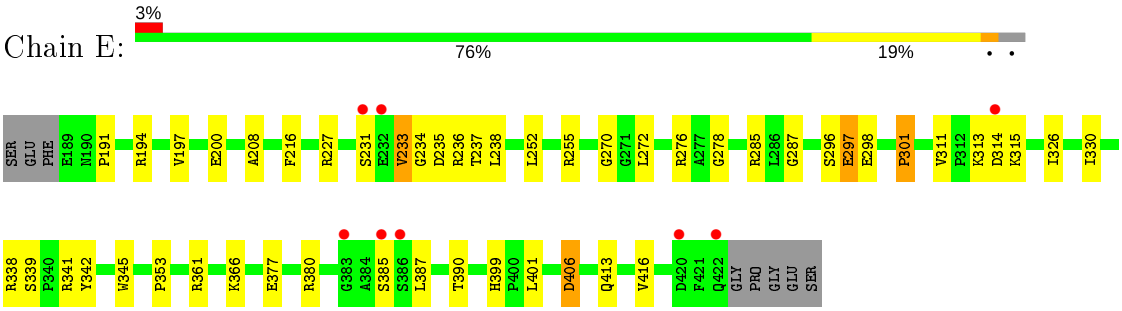




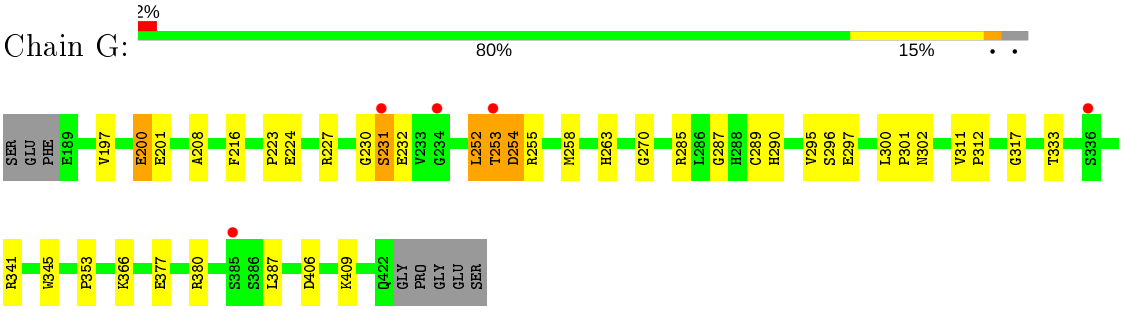
- Molecule 2: Interferon regulatory factor 3



- Molecule 2: Interferon regulatory factor 3



- Molecule 2: Interferon regulatory factor 3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.77Å 107.92Å 135.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.94 – 2.91 47.94 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.94-2.91) 94.8 (47.94-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.210 , 0.250 0.212 , 0.251	Depositor DCC
R_{free} test set	2000 reflections (8.94%)	wwPDB-VP
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 24.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7710	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.49% 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

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	B	0.32	0/82	0.51	0/109
1	D	0.31	0/82	0.43	0/109
1	F	0.29	0/82	0.43	0/109
1	H	0.37	0/82	0.53	0/109
2	A	0.21	0/1903	0.38	0/2593
2	C	0.21	0/1897	0.37	0/2585
2	E	0.21	0/1897	0.37	0/2585
2	G	0.21	0/1897	0.38	0/2585
All	All	0.21	0/7922	0.38	0/10784

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	B	82	0	75	1	0
1	D	82	0	75	1	0
1	F	82	0	75	0	0
1	H	82	0	75	3	0
2	A	1850	0	1794	22	0
2	C	1844	0	1790	27	0
2	E	1844	0	1790	26	0
2	G	1844	0	1790	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7710	0	7464	101	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 (101) 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:482:GLU:OE2	2:A:360:LYS:NZ	1.95	1.00
2:C:194:ARG:NH1	2:C:200:GLU:OE2	1.94	1.00
2:A:194:ARG:NH1	2:A:397:ASN:O	2.02	0.92
2:A:377:GLU:OE1	2:A:380:ARG:NH1	2.08	0.87
2:G:377:GLU:OE1	2:G:380:ARG:NH1	2.08	0.85
1:H:482:GLU:OE2	2:C:338:ARG:NH2	2.10	0.84
2:C:200:GLU:O	2:C:276:ARG:NH1	2.20	0.73
2:C:385:SER:HB3	2:C:387:LEU:HD22	1.70	0.72
2:G:254:ASP:HB3	2:G:258:MET:HG2	1.72	0.71
2:E:285:ARG:NH1	2:E:287:GLY:O	2.27	0.68
2:G:285:ARG:NH1	2:G:287:GLY:O	2.27	0.67
2:A:384:ALA:HB3	2:A:387:LEU:HD21	1.77	0.66
2:A:262:ARG:O	2:A:266:SER:OG	2.18	0.62
2:A:227:ARG:NH2	2:A:270:GLY:O	2.32	0.62
2:E:377:GLU:OE1	2:E:380:ARG:NH1	2.32	0.61
2:A:383:GLY:O	2:E:252:LEU:N	2.24	0.60
2:C:228:LEU:HD12	2:C:272:LEU:HD23	1.84	0.59
2:A:195:LEU:HD23	2:A:395:ILE:HD13	1.85	0.59
2:E:227:ARG:NH2	2:E:270:GLY:O	2.36	0.58
2:G:301:PRO:HB3	2:G:345:TRP:CD2	2.40	0.57
2:E:252:LEU:HA	2:E:255:ARG:HE	1.69	0.57
2:G:300:LEU:HD12	2:G:301:PRO:HD2	1.87	0.56
2:E:276:ARG:NH2	2:E:278:GLY:O	2.39	0.55
2:E:313:LYS:HG2	2:E:314:ASP:H	1.72	0.54
2:E:191:PRO:HB2	2:E:401:LEU:HD21	1.89	0.54
2:E:301:PRO:HB3	2:E:345:TRP:CD2	2.42	0.54
2:C:353:PRO:HG3	2:C:361:ARG:HG3	1.89	0.54
2:E:338:ARG:NH1	2:E:341:ARG:NH1	2.54	0.54
2:A:226:LEU:HD21	2:A:274:LEU:HD23	1.90	0.54
2:E:313:LYS:O	2:E:315:LYS:N	2.38	0.54
2:E:353:PRO:HG3	2:E:361:ARG:HG3	1.91	0.53
2:C:301:PRO:HB3	2:C:345:TRP:CD2	2.43	0.53
2:A:301:PRO:HB3	2:A:345:TRP:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:387:LEU:H	2:A:387:LEU:HD23	1.75	0.52
2:C:202:TRP:HA	2:C:395:ILE:HG22	1.91	0.52
2:A:251:SER:O	2:A:255:ARG:HB3	2.10	0.51
2:C:262:ARG:O	2:C:266:SER:OG	2.30	0.51
2:E:298:GLU:OE2	2:E:342:TYR:OH	2.18	0.50
2:E:208:ALA:HB3	2:E:216:PHE:HB3	1.93	0.50
2:G:201:GLU:OE2	2:G:223:PRO:HD3	2.11	0.50
2:E:197:VAL:HG23	2:E:200:GLU:HB2	1.92	0.50
2:E:345:TRP:CZ2	2:E:366:LYS:HD3	2.47	0.50
2:C:265:LEU:HA	2:C:268:LEU:HD12	1.93	0.49
2:E:194:ARG:NH2	2:E:200:GLU:OE2	2.45	0.49
1:H:486:LEU:HB3	1:H:488:ILE:HD12	1.95	0.49
2:G:253:THR:O	2:G:253:THR:OG1	2.30	0.49
2:G:252:LEU:HA	2:G:255:ARG:HB2	1.94	0.49
2:C:313:LYS:O	2:C:315:LYS:N	2.46	0.48
2:C:385:SER:OG	2:C:386:SER:N	2.46	0.48
2:C:220:ILE:HG13	2:C:243:VAL:HG22	1.96	0.48
2:C:329:LEU:HD23	2:C:412:LEU:HD11	1.97	0.47
2:C:420:ASP:OD1	2:C:420:ASP:N	2.45	0.47
2:G:312:PRO:HG2	2:G:317:GLY:HA3	1.97	0.47
2:E:406:ASP:OD2	2:E:406:ASP:N	2.48	0.47
2:E:296[B]:SER:OG	2:E:297:GLU:N	2.47	0.46
2:C:196:LEU:HD21	2:C:322:LEU:HD23	1.98	0.46
2:G:296[B]:SER:OG	2:G:297:GLU:N	2.45	0.46
2:C:195:LEU:HD23	2:C:395:ILE:HD13	1.97	0.46
2:A:277:ALA:HB3	2:A:282:TRP:HE1	1.80	0.45
2:A:345:TRP:CZ2	2:A:366:LYS:HD3	2.51	0.45
2:C:254:ASP:OD2	2:C:254:ASP:N	2.49	0.45
2:C:300:LEU:HD12	2:C:301:PRO:HD2	1.99	0.45
2:G:295:VAL:HG12	2:G:341:ARG:HB2	1.98	0.45
2:G:227:ARG:NH2	2:G:270:GLY:O	2.40	0.45
2:G:302:ASN:ND2	2:G:353:PRO:O	2.42	0.45
2:C:352:TRP:HA	2:C:353:PRO:HD3	1.84	0.45
2:E:235:ASP:O	2:E:237:THR:N	2.46	0.44
2:A:232:GLU:HA	2:A:233:VAL:HA	1.62	0.44
2:E:233:VAL:HA	2:E:234:GLY:HA2	1.70	0.44
2:A:387:LEU:O	2:A:404:THR:HA	2.18	0.44
2:G:252:LEU:HB3	2:G:255:ARG:HH11	1.81	0.44
2:A:190:ASN:HB3	2:A:193:LYS:HG3	1.98	0.44
2:C:233:VAL:HA	2:C:234:GLY:HA3	1.69	0.44
2:C:313:LYS:HG2	2:C:314:ASP:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:254:ASP:HB3	2:G:258:MET:CG	2.44	0.43
2:A:296[A]:SER:OG	2:A:297:GLU:N	2.51	0.43
2:C:277:ALA:HB3	2:C:282:TRP:HE1	1.83	0.43
2:E:272:LEU:HD11	2:E:311:VAL:HG11	2.01	0.43
2:E:413:GLN:HA	2:E:416:VAL:HG12	2.01	0.43
2:G:230:GLY:C	2:G:232:GLU:H	2.23	0.43
2:G:333:THR:HB	2:G:409:LYS:HE2	2.01	0.42
2:G:208:ALA:HB3	2:G:216:PHE:HB3	2.00	0.42
2:A:224:GLU:CD	2:A:240:GLY:H	2.23	0.42
2:A:222:CYS:HA	2:A:223:PRO:HD3	1.88	0.42
2:E:235:ASP:HB3	2:E:238:LEU:HG	2.01	0.42
1:H:487:LEU:HB2	2:G:290:HIS:HB2	2.01	0.42
2:G:230:GLY:O	2:G:232:GLU:N	2.52	0.42
2:G:197:VAL:HG23	2:G:200:GLU:HB2	2.01	0.41
2:G:345:TRP:CZ2	2:G:366:LYS:HD3	2.55	0.41
2:A:357:PRO:HG2	2:A:360:LYS:HG2	2.03	0.41
2:G:311:VAL:HA	2:G:312:PRO:HD3	1.90	0.41
2:A:208:ALA:HB3	2:A:216:PHE:HB3	2.01	0.41
2:G:252:LEU:H	2:G:252:LEU:HG	1.60	0.41
2:C:345:TRP:CZ2	2:C:366:LYS:HD3	2.55	0.41
2:E:326:ILE:O	2:E:330:ILE:HG12	2.20	0.41
2:E:235:ASP:C	2:E:237:THR:H	2.21	0.41
2:C:272:LEU:HD22	2:C:291:THR:HG21	2.03	0.41
2:G:252:LEU:CB	2:G:255:ARG:HH11	2.34	0.41
2:C:256:GLY:O	2:C:259:SER:OG	2.35	0.40
1:D:482:GLU:HB2	1:D:483:GLU:H	1.76	0.40
2:C:326:ILE:HG23	2:C:412:LEU:HD12	2.03	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	B	8/19 (42%)	7 (88%)	1 (12%)	0	100 100
1	D	8/19 (42%)	7 (88%)	1 (12%)	0	100 100
1	F	8/19 (42%)	8 (100%)	0	0	100 100
1	H	8/19 (42%)	7 (88%)	1 (12%)	0	100 100
2	A	234/242 (97%)	216 (92%)	14 (6%)	4 (2%)	9 29
2	C	233/242 (96%)	216 (93%)	17 (7%)	0	100 100
2	E	233/242 (96%)	217 (93%)	13 (6%)	3 (1%)	12 36
2	G	233/242 (96%)	215 (92%)	16 (7%)	2 (1%)	17 46
All	All	965/1044 (92%)	893 (92%)	63 (6%)	9 (1%)	17 46

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	254	ASP
2	A	248	PRO
2	A	385	SER
2	E	236	ARG
2	G	231	SER
2	E	385	SER
2	A	235	ASP
2	A	335	GLY
2	E	301	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	B	10/19 (53%)	6 (60%)	4 (40%)	0 0
1	D	10/19 (53%)	10 (100%)	0	100 100
1	F	10/19 (53%)	9 (90%)	1 (10%)	7 22
1	H	10/19 (53%)	10 (100%)	0	100 100
2	A	201/205 (98%)	193 (96%)	8 (4%)	31 63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	200/205 (98%)	193 (96%)	7 (4%)	36 68
2	E	200/205 (98%)	192 (96%)	8 (4%)	31 63
2	G	200/205 (98%)	191 (96%)	9 (4%)	27 59
All	All	841/896 (94%)	804 (96%)	37 (4%)	28 60

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	482	GLU
1	B	483	GLU
1	B	489	SER
1	B	491	SER
1	F	489	SER
2	A	194	ARG
2	A	226	LEU
2	A	233	VAL
2	A	255	ARG
2	A	266	SER
2	A	272	LEU
2	A	387	LEU
2	A	405	SER
2	C	194	ARG
2	C	254	ASP
2	C	266	SER
2	C	399	HIS
2	C	403	LEU
2	C	405	SER
2	C	420	ASP
2	E	231	SER
2	E	233	VAL
2	E	297	GLU
2	E	339	SER
2	E	387	LEU
2	E	390	THR
2	E	399	HIS
2	E	406	ASP
2	G	200	GLU
2	G	224	GLU
2	G	231	SER
2	G	252	LEU
2	G	253	THR

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Mol	Chain	Res	Type
2	G	263	HIS
2	G	289	CYS
2	G	387	LEU
2	G	406	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	263	HIS

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	B	10/19 (52%)	0.46	1 (10%)	7	5	46, 54, 85, 89	0
1	D	10/19 (52%)	1.13	2 (20%)	1	0	43, 52, 80, 92	0
1	F	10/19 (52%)	1.19	2 (20%)	1	0	48, 61, 99, 113	0
1	H	10/19 (52%)	1.03	2 (20%)	1	0	48, 58, 85, 94	0
2	A	234/242 (96%)	0.11	7 (2%)	50	46	21, 44, 77, 100	0
2	C	234/242 (96%)	0.04	6 (2%)	56	53	20, 47, 78, 99	0
2	E	234/242 (96%)	0.02	8 (3%)	45	41	21, 45, 79, 99	0
2	G	234/242 (96%)	0.03	5 (2%)	63	62	19, 43, 73, 83	0
All	All	976/1044 (93%)	0.09	33 (3%)	45	41	19, 45, 78, 113	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	491	SER	5.5
2	A	384	ALA	5.1
1	H	491	SER	4.9
2	A	232	GLU	4.6
1	D	491	SER	4.5
2	A	383	GLY	4.4
2	E	422	GLN	4.3
2	A	250	MET	3.9
2	C	234	GLY	3.8
2	C	232	GLU	3.7
2	E	232	GLU	3.5
2	A	189	GLU	3.5
1	D	490	ASN	3.4
2	G	231	SER	3.3
2	E	386	SER	3.2
2	G	385	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	G	234	GLY	2.8
2	E	385	SER	2.7
2	A	253	THR	2.7
2	E	231	SER	2.7
2	E	383	GLY	2.5
1	F	490	ASN	2.3
2	E	420	ASP	2.3
2	G	253	THR	2.3
2	A	382	GLY	2.3
2	G	336	SER	2.2
1	B	488	ILE	2.2
2	E	314	ASP	2.2
2	C	336	SER	2.2
2	C	189	GLU	2.2
2	C	233	VAL	2.1
1	H	489	SER	2.0
2	C	253	THR	2.0

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 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.