



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:49 PM GMT

PDB ID : 2X7L
Title : Implications of the HIV-1 Rev dimer structure at 3.2Å resolution for multi-
meric binding to the Rev response element
Authors : DiMattia, M.A.; Watts, N.R.; Stahl, S.J.; Rader, C.; Wingfield, P.T.; Stuart,
D.I.; Steven, A.C.; Grimes, J.M.
Deposited on : 2010-03-01
Resolution : 3.17 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

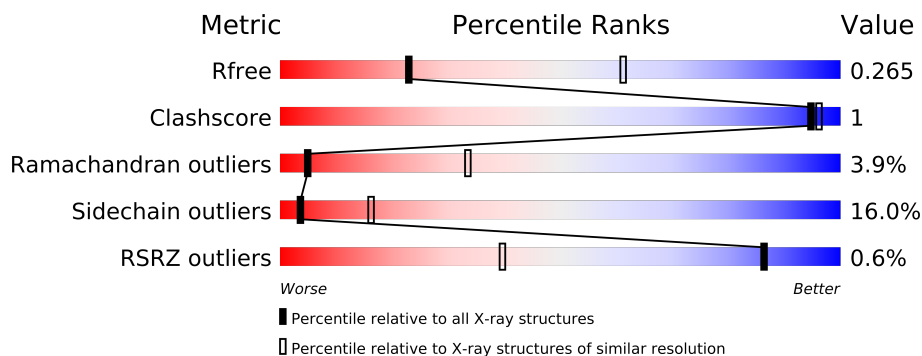
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.17 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}	66092	1472 (3.26-3.10)
Clashscore	79885	1024 (3.24-3.12)
Ramachandran outliers	78287	1002 (3.24-3.12)
Sidechain outliers	78261	1001 (3.24-3.12)
RSRZ outliers	66119	1473 (3.26-3.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	231	
1	C	231	
1	E	231	
1	G	231	
1	H	231	
1	J	231	
2	B	217	
2	D	217	
2	F	217	
2	I	217	
2	K	217	
2	L	217	
3	M	115	
3	N	115	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	O	115	
3	P	115	
3	Q	115	
3	R	115	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22554 atoms, of which 0 are hydrogen and 0 are deuterium.

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 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	1
			1628	1033	267	323	5			
1	C	221	Total	C	N	O	S	0	0	1
			1628	1033	267	323	5			
1	E	221	Total	C	N	O	S	0	0	1
			1628	1033	267	323	5			
1	G	221	Total	C	N	O	S	0	0	1
			1628	1033	267	323	5			
1	H	221	Total	C	N	O	S	0	0	1
			1628	1033	267	323	5			
1	J	221	Total	C	N	O	S	0	0	1
			1628	1033	267	323	5			

- Molecule 2 is a protein called FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1639	1026	269	337	7			
2	D	217	Total	C	N	O	S	0	0	0
			1639	1026	269	337	7			
2	F	217	Total	C	N	O	S	0	0	0
			1639	1026	269	337	7			
2	I	217	Total	C	N	O	S	0	0	0
			1639	1026	269	337	7			
2	K	217	Total	C	N	O	S	0	0	0
			1639	1026	269	337	7			
2	L	217	Total	C	N	O	S	0	0	0
			1639	1026	269	337	7			

- Molecule 3 is a protein called PROTEIN REV.

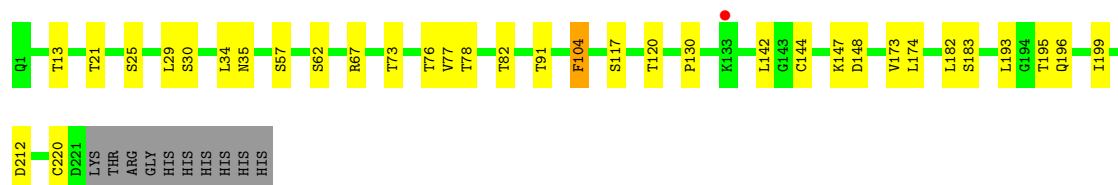
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	57	Total 492	C 303	N 105	O 84	0	0	0
3	N	57	Total 492	C 303	N 105	O 84	0	0	0
3	O	57	Total 492	C 303	N 105	O 84	0	0	0
3	P	57	Total 492	C 303	N 105	O 84	0	0	0
3	Q	57	Total 492	C 303	N 105	O 84	0	0	0
3	R	57	Total 492	C 303	N 105	O 84	0	0	0

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.

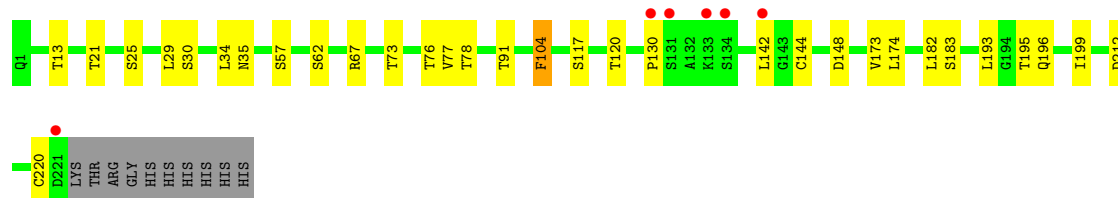
- Molecule 1: FAB HEAVY CHAIN

Chain A: 



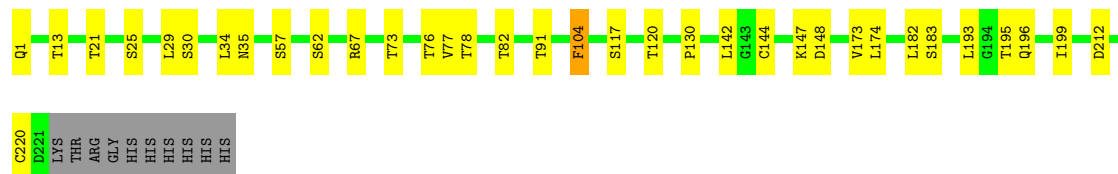
- Molecule 1: FAB HEAVY CHAIN

Chain C: 



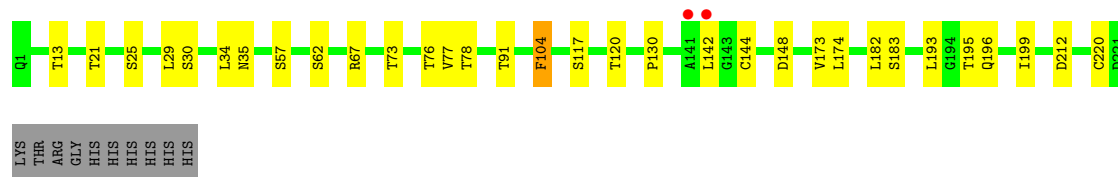
- Molecule 1: FAB HEAVY CHAIN

Chain E: 



- Molecule 1: FAB HEAVY CHAIN

Chain G: 



- Molecule 1: FAB HEAVY CHAIN

Chain H: 



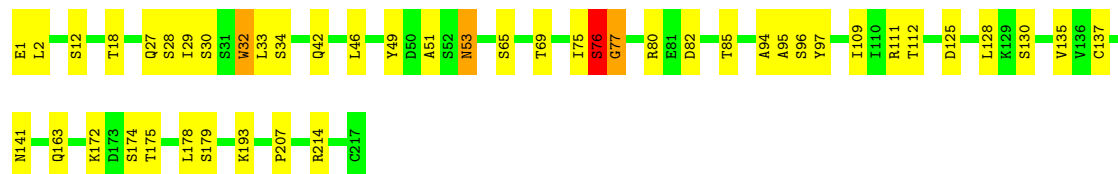
- Molecule 1: FAB HEAVY CHAIN

Chain J: 



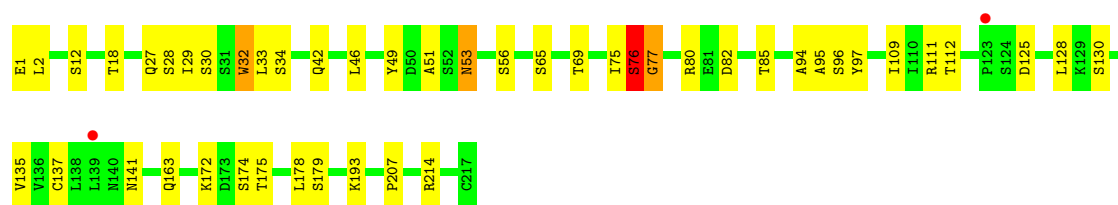
- Molecule 2: FAB LIGHT CHAIN

Chain B: 



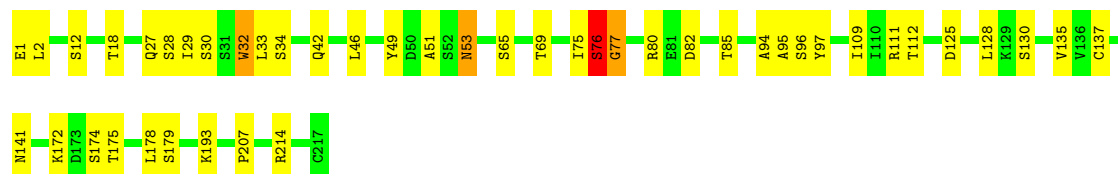
- Molecule 2: FAB LIGHT CHAIN

Chain D: 



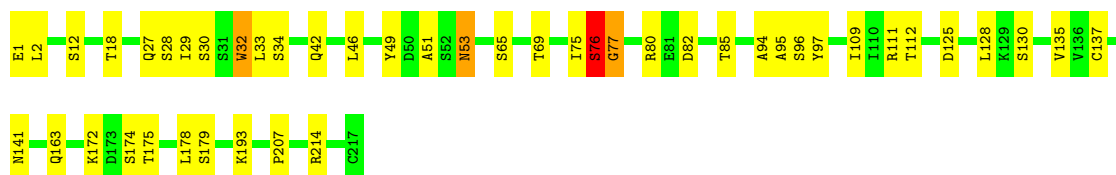
- Molecule 2: FAB LIGHT CHAIN

Chain F: 



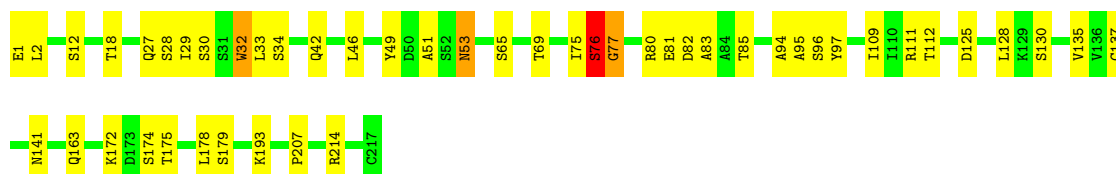
- Molecule 2: FAB LIGHT CHAIN

Chain I: 



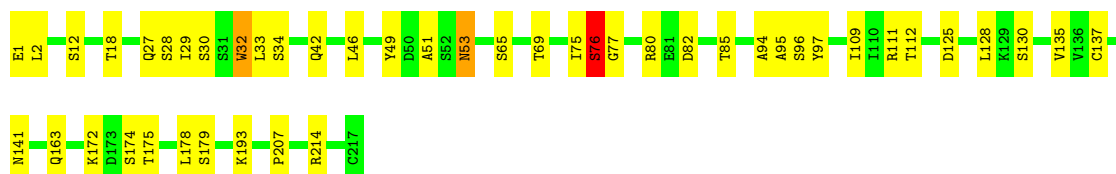
• Molecule 2: FAB LIGHT CHAIN

Chain K:



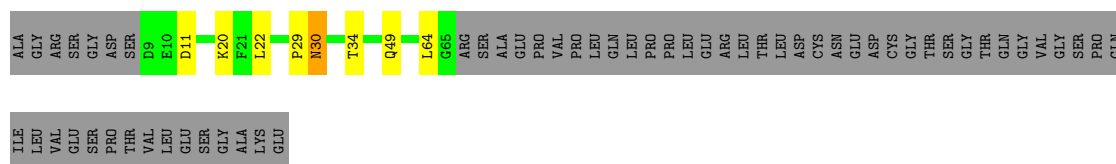
• Molecule 2: FAB LIGHT CHAIN

Chain L:



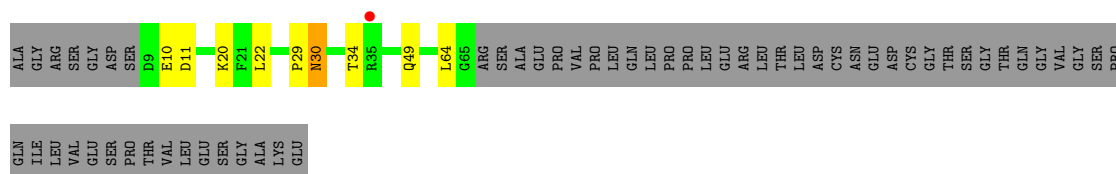
• Molecule 3: PROTEIN REV

Chain M:



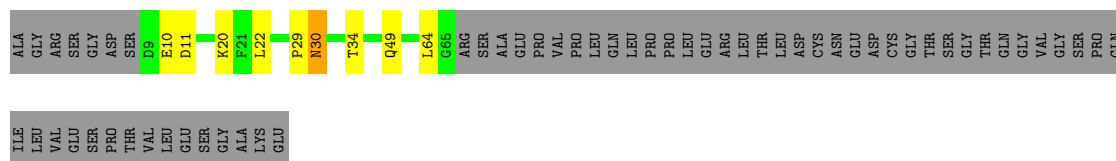
• Molecule 3: PROTEIN REV

Chain N:



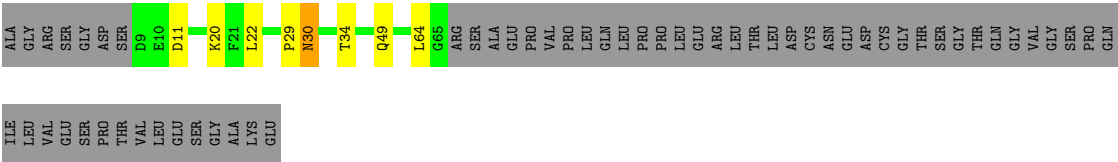
• Molecule 3: PROTEIN REV

Chain O:



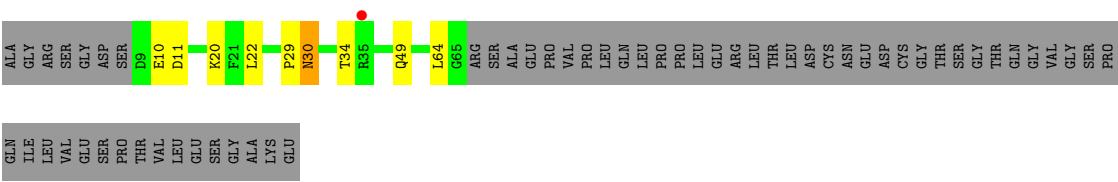
● Molecule 3: PROTEIN REV

Chain P: 



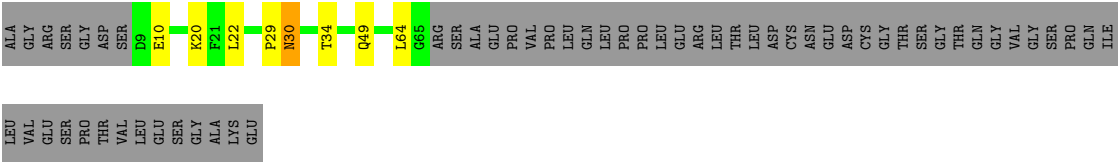
● Molecule 3: PROTEIN REV

Chain Q: 



● Molecule 3: PROTEIN REV

Chain R: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.68Å 87.69Å 176.33Å 94.86° 95.50° 104.60°	Depositor
Resolution (Å)	48.78 – 3.17 48.77 – 3.17	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.78-3.17) 97.6 (48.77-3.17)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.234 , 0.250 0.253 , 0.265	Depositor DCC
R_{free} test set	4187 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	85.2	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 73.3	EDS
Estimated twinning fraction	0.327 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 83636 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22554	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0/1671	0.83	0/2288
1	C	0.46	0/1671	0.78	0/2288
1	E	0.59	0/1671	0.81	0/2288
1	G	0.47	0/1671	0.78	0/2288
1	H	0.56	0/1671	0.81	0/2288
1	J	0.54	0/1671	0.80	0/2288
2	B	0.60	0/1675	0.85	0/2278
2	D	0.50	0/1675	0.81	0/2278
2	F	0.59	0/1675	0.85	0/2278
2	I	0.49	0/1675	0.82	0/2278
2	K	0.57	0/1675	0.84	0/2278
2	L	0.59	0/1675	0.84	0/2278
3	M	0.53	0/501	0.69	0/672
3	N	0.55	0/501	0.68	0/672
3	O	0.60	0/501	0.72	0/672
3	P	0.52	0/501	0.68	0/672
3	Q	0.55	0/501	0.68	0/672
3	R	0.57	0/501	0.70	0/672
All	All	0.55	0/23082	0.80	0/31428

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1628	0	0	1	0
1	C	1628	0	0	1	0
1	E	1628	0	0	1	0
1	G	1628	0	0	1	0
1	H	1628	0	0	1	0
1	J	1628	0	0	1	0
2	B	1639	0	0	4	0
2	D	1639	0	0	4	0
2	F	1639	0	0	4	0
2	I	1639	0	0	4	0
2	K	1639	0	0	5	0
2	L	1639	0	0	4	0
3	M	492	0	0	0	0
3	N	492	0	0	0	0
3	O	492	0	0	0	0
3	P	492	0	0	0	0
3	Q	492	0	0	0	0
3	R	492	0	0	0	0
All	All	22554	0	0	31	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (31) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:76:SER:OG	2:D:77:GLY:N	2.30	0.65
2:I:76:SER:OG	2:I:77:GLY:N	2.32	0.62
2:B:76:SER:OG	2:B:77:GLY:N	2.34	0.60
2:L:76:SER:OG	2:L:77:GLY:N	2.35	0.60
2:K:76:SER:OG	2:K:77:GLY:N	2.34	0.59
1:C:104:PHE:CD1	1:C:104:PHE:N	2.71	0.58
1:G:104:PHE:CD1	1:G:104:PHE:N	2.70	0.58
1:A:104:PHE:CD1	1:A:104:PHE:N	2.70	0.58
1:E:104:PHE:CD1	1:E:104:PHE:N	2.71	0.57
2:F:76:SER:OG	2:F:77:GLY:N	2.37	0.57
1:H:104:PHE:CD1	1:H:104:PHE:N	2.71	0.57
1:J:104:PHE:CD1	1:J:104:PHE:N	2.71	0.56
2:B:49:TYR:O	2:B:53:ASN:ND2	2.40	0.55
2:K:49:TYR:O	2:K:53:ASN:ND2	2.41	0.54
2:L:49:TYR:O	2:L:53:ASN:ND2	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:49:TYR:O	2:D:53:ASN:ND2	2.43	0.52
2:F:49:TYR:O	2:F:53:ASN:ND2	2.43	0.51
2:I:49:TYR:O	2:I:53:ASN:ND2	2.44	0.50
2:L:95:ALA:CB	2:L:96:SER:CA	2.91	0.48
2:F:95:ALA:CB	2:F:96:SER:CA	2.93	0.47
2:B:95:ALA:CB	2:B:96:SER:CA	2.92	0.47
2:I:95:ALA:CB	2:I:96:SER:CA	2.93	0.47
2:D:95:ALA:CB	2:D:96:SER:CA	2.94	0.46
2:K:95:ALA:CB	2:K:96:SER:CA	2.93	0.46
2:B:193:LYS:O	2:B:214:ARG:N	2.50	0.45
2:F:193:LYS:O	2:F:214:ARG:N	2.51	0.44
2:L:193:LYS:O	2:L:214:ARG:N	2.51	0.43
2:K:193:LYS:O	2:K:214:ARG:N	2.52	0.43
2:I:193:LYS:O	2:I:214:ARG:N	2.53	0.42
2:D:193:LYS:O	2:D:214:ARG:N	2.52	0.41
2:K:81:GLU:O	2:K:83:ALA:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	219/231 (95%)	187 (85%)	28 (13%)	4 (2%)	13	60
1	C	219/231 (95%)	189 (86%)	26 (12%)	4 (2%)	13	60
1	E	219/231 (95%)	187 (85%)	28 (13%)	4 (2%)	13	60
1	G	219/231 (95%)	190 (87%)	25 (11%)	4 (2%)	13	60
1	H	219/231 (95%)	187 (85%)	28 (13%)	4 (2%)	13	60
1	J	219/231 (95%)	190 (87%)	25 (11%)	4 (2%)	13	60
2	B	215/217 (99%)	188 (87%)	14 (6%)	13 (6%)	2	20
2	D	215/217 (99%)	188 (87%)	14 (6%)	13 (6%)	2	20
2	F	215/217 (99%)	188 (87%)	14 (6%)	13 (6%)	2	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	215/217 (99%)	188 (87%)	14 (6%)	13 (6%)	2	20
2	K	215/217 (99%)	188 (87%)	14 (6%)	13 (6%)	2	20
2	L	215/217 (99%)	188 (87%)	15 (7%)	12 (6%)	3	23
3	M	55/115 (48%)	46 (84%)	7 (13%)	2 (4%)	5	36
3	N	55/115 (48%)	48 (87%)	5 (9%)	2 (4%)	5	36
3	O	55/115 (48%)	47 (86%)	6 (11%)	2 (4%)	5	36
3	P	55/115 (48%)	46 (84%)	7 (13%)	2 (4%)	5	36
3	Q	55/115 (48%)	46 (84%)	7 (13%)	2 (4%)	5	36
3	R	55/115 (48%)	47 (86%)	6 (11%)	2 (4%)	5	36
All	All	2934/3378 (87%)	2538 (86%)	283 (10%)	113 (4%)	5	33

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	174	SER
2	D	174	SER
2	F	174	SER
2	I	174	SER
2	K	174	SER
2	L	174	SER
3	M	29	PRO
3	N	29	PRO
3	O	29	PRO
3	P	29	PRO
3	Q	29	PRO
3	R	29	PRO
1	A	130	PRO
2	B	28	SER
2	B	32	TRP
2	B	76	SER
2	B	141	ASN
1	C	130	PRO
1	C	148	ASP
2	D	28	SER
2	D	76	SER
2	D	141	ASN
1	E	130	PRO
1	E	148	ASP
2	F	28	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	76	SER
2	F	94	ALA
2	F	141	ASN
1	G	130	PRO
1	H	130	PRO
1	H	148	ASP
2	I	28	SER
2	I	76	SER
2	I	141	ASN
1	J	130	PRO
1	J	148	ASP
2	K	28	SER
2	K	76	SER
2	K	94	ALA
2	K	141	ASN
2	L	28	SER
2	L	76	SER
2	L	141	ASN
1	A	148	ASP
1	A	220	CYS
2	B	30	SER
2	B	51	ALA
2	B	82	ASP
2	B	130	SER
2	B	207	PRO
2	D	30	SER
2	D	32	TRP
2	D	82	ASP
2	D	94	ALA
2	D	130	SER
1	E	220	CYS
2	F	30	SER
2	F	32	TRP
2	F	82	ASP
2	F	130	SER
2	F	207	PRO
1	G	148	ASP
2	I	30	SER
2	I	32	TRP
2	I	82	ASP
2	I	94	ALA
2	I	130	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	220	CYS
2	K	30	SER
2	K	32	TRP
2	K	51	ALA
2	K	82	ASP
2	K	130	SER
2	L	30	SER
2	L	32	TRP
2	L	51	ALA
2	L	82	ASP
2	L	94	ALA
2	L	130	SER
2	L	207	PRO
1	A	30	SER
2	B	29	ILE
2	B	94	ALA
1	C	30	SER
1	C	220	CYS
2	D	29	ILE
2	D	207	PRO
1	E	30	SER
2	F	29	ILE
2	F	51	ALA
1	G	220	CYS
1	H	30	SER
1	H	220	CYS
2	I	29	ILE
2	I	207	PRO
1	J	30	SER
2	K	29	ILE
2	K	207	PRO
2	L	29	ILE
3	M	30	ASN
3	N	30	ASN
3	O	30	ASN
3	P	30	ASN
3	Q	30	ASN
3	R	30	ASN
2	D	51	ALA
2	I	51	ALA
1	G	30	SER
2	F	77	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	77	GLY
2	I	77	GLY
2	D	77	GLY
2	K	77	GLY

5.3.2 Protein sidechains ⓘ

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	182/192 (95%)	152 (84%)	30 (16%)	3	15
1	C	182/192 (95%)	154 (85%)	28 (15%)	4	18
1	E	182/192 (95%)	151 (83%)	31 (17%)	3	14
1	G	182/192 (95%)	154 (85%)	28 (15%)	4	18
1	H	182/192 (95%)	152 (84%)	30 (16%)	3	15
1	J	182/192 (95%)	152 (84%)	30 (16%)	3	15
2	B	184/185 (100%)	154 (84%)	30 (16%)	3	15
2	D	184/185 (100%)	153 (83%)	31 (17%)	3	14
2	F	184/185 (100%)	155 (84%)	29 (16%)	4	17
2	I	184/185 (100%)	154 (84%)	30 (16%)	3	15
2	K	184/185 (100%)	154 (84%)	30 (16%)	3	15
2	L	184/185 (100%)	154 (84%)	30 (16%)	3	15
3	M	53/101 (52%)	46 (87%)	7 (13%)	6	27
3	N	53/101 (52%)	45 (85%)	8 (15%)	4	19
3	O	53/101 (52%)	45 (85%)	8 (15%)	4	19
3	P	53/101 (52%)	46 (87%)	7 (13%)	6	27
3	Q	53/101 (52%)	45 (85%)	8 (15%)	4	19
3	R	53/101 (52%)	46 (87%)	7 (13%)	6	27
All	All	2514/2868 (88%)	2112 (84%)	402 (16%)	3	16

All (402) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	21	THR
1	A	25	SER
1	A	29	LEU
1	A	34	LEU
1	A	35	ASN
1	A	57	SER
1	A	62	SER
1	A	67	ARG
1	A	73	THR
1	A	76	THR
1	A	77	VAL
1	A	78	THR
1	A	82	THR
1	A	91	THR
1	A	104	PHE
1	A	117	SER
1	A	120	THR
1	A	142	LEU
1	A	144	CYS
1	A	147	LYS
1	A	173	VAL
1	A	174	LEU
1	A	182	LEU
1	A	183	SER
1	A	193	LEU
1	A	195	THR
1	A	196	GLN
1	A	199	ILE
1	A	212	ASP
2	B	1	GLU
2	B	2	LEU
2	B	12	SER
2	B	18	THR
2	B	27	GLN
2	B	32	TRP
2	B	33	LEU
2	B	34	SER
2	B	42	GLN
2	B	46	LEU
2	B	53	ASN
2	B	65	SER
2	B	69	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	75	ILE
2	B	76	SER
2	B	80	ARG
2	B	85	THR
2	B	97	TYR
2	B	109	ILE
2	B	111	ARG
2	B	112	THR
2	B	125	ASP
2	B	128	LEU
2	B	135	VAL
2	B	137	CYS
2	B	163	GLN
2	B	172	LYS
2	B	175	THR
2	B	178	LEU
2	B	179	SER
1	C	13	THR
1	C	21	THR
1	C	25	SER
1	C	29	LEU
1	C	34	LEU
1	C	35	ASN
1	C	57	SER
1	C	62	SER
1	C	67	ARG
1	C	73	THR
1	C	76	THR
1	C	77	VAL
1	C	78	THR
1	C	91	THR
1	C	104	PHE
1	C	117	SER
1	C	120	THR
1	C	142	LEU
1	C	144	CYS
1	C	173	VAL
1	C	174	LEU
1	C	182	LEU
1	C	183	SER
1	C	193	LEU
1	C	195	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	196	GLN
1	C	199	ILE
1	C	212	ASP
2	D	1	GLU
2	D	2	LEU
2	D	12	SER
2	D	18	THR
2	D	27	GLN
2	D	32	TRP
2	D	33	LEU
2	D	34	SER
2	D	42	GLN
2	D	46	LEU
2	D	53	ASN
2	D	56	SER
2	D	65	SER
2	D	69	THR
2	D	75	ILE
2	D	76	SER
2	D	80	ARG
2	D	85	THR
2	D	97	TYR
2	D	109	ILE
2	D	111	ARG
2	D	112	THR
2	D	125	ASP
2	D	128	LEU
2	D	135	VAL
2	D	137	CYS
2	D	163	GLN
2	D	172	LYS
2	D	175	THR
2	D	178	LEU
2	D	179	SER
1	E	1	GLN
1	E	13	THR
1	E	21	THR
1	E	25	SER
1	E	29	LEU
1	E	34	LEU
1	E	35	ASN
1	E	57	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	62	SER
1	E	67	ARG
1	E	73	THR
1	E	76	THR
1	E	77	VAL
1	E	78	THR
1	E	82	THR
1	E	91	THR
1	E	104	PHE
1	E	117	SER
1	E	120	THR
1	E	142	LEU
1	E	144	CYS
1	E	147	LYS
1	E	173	VAL
1	E	174	LEU
1	E	182	LEU
1	E	183	SER
1	E	193	LEU
1	E	195	THR
1	E	196	GLN
1	E	199	ILE
1	E	212	ASP
2	F	1	GLU
2	F	2	LEU
2	F	12	SER
2	F	18	THR
2	F	27	GLN
2	F	32	TRP
2	F	33	LEU
2	F	34	SER
2	F	42	GLN
2	F	46	LEU
2	F	53	ASN
2	F	65	SER
2	F	69	THR
2	F	75	ILE
2	F	76	SER
2	F	80	ARG
2	F	85	THR
2	F	97	TYR
2	F	109	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	111	ARG
2	F	112	THR
2	F	125	ASP
2	F	128	LEU
2	F	135	VAL
2	F	137	CYS
2	F	172	LYS
2	F	175	THR
2	F	178	LEU
2	F	179	SER
1	G	13	THR
1	G	21	THR
1	G	25	SER
1	G	29	LEU
1	G	34	LEU
1	G	35	ASN
1	G	57	SER
1	G	62	SER
1	G	67	ARG
1	G	73	THR
1	G	76	THR
1	G	77	VAL
1	G	78	THR
1	G	91	THR
1	G	104	PHE
1	G	117	SER
1	G	120	THR
1	G	142	LEU
1	G	144	CYS
1	G	173	VAL
1	G	174	LEU
1	G	182	LEU
1	G	183	SER
1	G	193	LEU
1	G	195	THR
1	G	196	GLN
1	G	199	ILE
1	G	212	ASP
1	H	1	GLN
1	H	13	THR
1	H	21	THR
1	H	25	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	29	LEU
1	H	34	LEU
1	H	35	ASN
1	H	57	SER
1	H	62	SER
1	H	67	ARG
1	H	73	THR
1	H	76	THR
1	H	77	VAL
1	H	78	THR
1	H	82	THR
1	H	91	THR
1	H	104	PHE
1	H	117	SER
1	H	120	THR
1	H	142	LEU
1	H	144	CYS
1	H	173	VAL
1	H	174	LEU
1	H	182	LEU
1	H	183	SER
1	H	193	LEU
1	H	195	THR
1	H	196	GLN
1	H	199	ILE
1	H	212	ASP
2	I	1	GLU
2	I	2	LEU
2	I	12	SER
2	I	18	THR
2	I	27	GLN
2	I	32	TRP
2	I	33	LEU
2	I	34	SER
2	I	42	GLN
2	I	46	LEU
2	I	53	ASN
2	I	65	SER
2	I	69	THR
2	I	75	ILE
2	I	76	SER
2	I	80	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	85	THR
2	I	97	TYR
2	I	109	ILE
2	I	111	ARG
2	I	112	THR
2	I	125	ASP
2	I	128	LEU
2	I	135	VAL
2	I	137	CYS
2	I	163	GLN
2	I	172	LYS
2	I	175	THR
2	I	178	LEU
2	I	179	SER
1	J	13	THR
1	J	21	THR
1	J	25	SER
1	J	29	LEU
1	J	34	LEU
1	J	35	ASN
1	J	57	SER
1	J	62	SER
1	J	67	ARG
1	J	73	THR
1	J	76	THR
1	J	77	VAL
1	J	78	THR
1	J	82	THR
1	J	91	THR
1	J	104	PHE
1	J	117	SER
1	J	120	THR
1	J	142	LEU
1	J	144	CYS
1	J	147	LYS
1	J	173	VAL
1	J	174	LEU
1	J	182	LEU
1	J	183	SER
1	J	193	LEU
1	J	195	THR
1	J	196	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	199	ILE
1	J	212	ASP
2	K	1	GLU
2	K	2	LEU
2	K	12	SER
2	K	18	THR
2	K	27	GLN
2	K	32	TRP
2	K	33	LEU
2	K	34	SER
2	K	42	GLN
2	K	46	LEU
2	K	53	ASN
2	K	65	SER
2	K	69	THR
2	K	75	ILE
2	K	76	SER
2	K	80	ARG
2	K	85	THR
2	K	97	TYR
2	K	109	ILE
2	K	111	ARG
2	K	112	THR
2	K	125	ASP
2	K	128	LEU
2	K	135	VAL
2	K	137	CYS
2	K	163	GLN
2	K	172	LYS
2	K	175	THR
2	K	178	LEU
2	K	179	SER
2	L	1	GLU
2	L	2	LEU
2	L	12	SER
2	L	18	THR
2	L	27	GLN
2	L	32	TRP
2	L	33	LEU
2	L	34	SER
2	L	42	GLN
2	L	46	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	53	ASN
2	L	65	SER
2	L	69	THR
2	L	75	ILE
2	L	76	SER
2	L	80	ARG
2	L	85	THR
2	L	97	TYR
2	L	109	ILE
2	L	111	ARG
2	L	112	THR
2	L	125	ASP
2	L	128	LEU
2	L	135	VAL
2	L	137	CYS
2	L	163	GLN
2	L	172	LYS
2	L	175	THR
2	L	178	LEU
2	L	179	SER
3	M	11	ASP
3	M	20	LYS
3	M	22	LEU
3	M	30	ASN
3	M	34	THR
3	M	49	GLN
3	M	64	LEU
3	N	10	GLU
3	N	11	ASP
3	N	20	LYS
3	N	22	LEU
3	N	30	ASN
3	N	34	THR
3	N	49	GLN
3	N	64	LEU
3	O	10	GLU
3	O	11	ASP
3	O	20	LYS
3	O	22	LEU
3	O	30	ASN
3	O	34	THR
3	O	49	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	O	64	LEU
3	P	11	ASP
3	P	20	LYS
3	P	22	LEU
3	P	30	ASN
3	P	34	THR
3	P	49	GLN
3	P	64	LEU
3	Q	10	GLU
3	Q	11	ASP
3	Q	20	LYS
3	Q	22	LEU
3	Q	30	ASN
3	Q	34	THR
3	Q	49	GLN
3	Q	64	LEU
3	R	10	GLU
3	R	20	LYS
3	R	22	LEU
3	R	30	ASN
3	R	34	THR
3	R	49	GLN
3	R	64	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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, 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	221/231 (95%)	0.04	1 (0%) 88 43	75, 114, 192, 246	0
1	C	221/231 (95%)	0.19	6 (2%) 52 9	102, 173, 235, 263	0
1	E	221/231 (95%)	0.01	0 100 100	78, 118, 191, 251	0
1	G	221/231 (95%)	0.17	2 (0%) 81 30	100, 175, 246, 265	0
1	H	221/231 (95%)	0.03	2 (0%) 81 30	67, 113, 195, 224	0
1	J	221/231 (95%)	0.05	4 (1%) 65 16	74, 119, 201, 236	0
2	B	217/217 (100%)	-0.07	0 100 100	73, 116, 189, 208	0
2	D	217/217 (100%)	0.01	2 (0%) 81 30	98, 156, 248, 263	0
2	F	217/217 (100%)	-0.05	0 100 100	74, 113, 200, 229	0
2	I	217/217 (100%)	-0.03	0 100 100	88, 149, 251, 283	0
2	K	217/217 (100%)	-0.11	0 100 100	75, 116, 188, 222	0
2	L	217/217 (100%)	-0.08	0 100 100	76, 116, 186, 211	0
3	M	57/115 (49%)	0.00	0 100 100	109, 164, 278, 284	0
3	N	57/115 (49%)	-0.08	1 (1%) 65 16	96, 155, 287, 298	0
3	O	57/115 (49%)	0.12	0 100 100	97, 151, 278, 287	0
3	P	57/115 (49%)	0.06	0 100 100	119, 165, 276, 280	0
3	Q	57/115 (49%)	0.09	1 (1%) 65 16	98, 151, 275, 277	0
3	R	57/115 (49%)	0.13	0 100 100	95, 156, 274, 280	0
All	All	2970/3378 (87%)	0.02	19 (0%) 86 40	67, 129, 236, 298	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	134	SER	4.9
2	D	123	PRO	4.5
1	G	142	LEU	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	221	ASP	3.8
1	C	133	LYS	3.8
1	J	133	LYS	3.2
1	C	134	SER	3.2
1	A	133	LYS	3.0
1	G	141	ALA	3.0
1	C	142	LEU	2.7
1	J	193	LEU	2.6
1	C	131	SER	2.5
1	H	134	SER	2.4
1	H	193	LEU	2.3
2	D	139	LEU	2.2
1	J	135	THR	2.1
1	C	130	PRO	2.1
3	Q	35	ARG	2.1
3	N	35	ARG	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.