



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:20 pm BST

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 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:

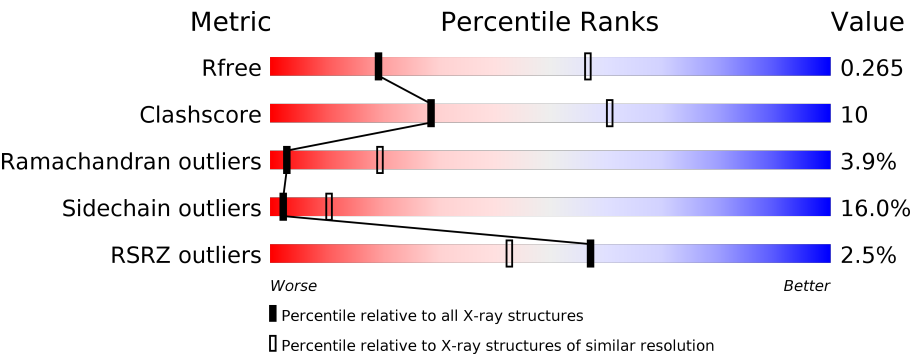
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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









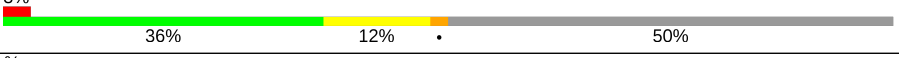


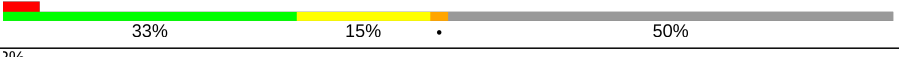


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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 $\leq 5\%$. 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	231	<div><div></div><div><div></div><div>67%</div><div>26%</div><div></div><div></div></div><div></div></div>
1	C	231	<div><div>7%</div><div></div><div><div></div><div>69%</div><div>25%</div><div></div><div></div></div><div></div></div>
1	E	231	<div><div>2%</div><div></div><div><div></div><div>67%</div><div>26%</div><div></div><div></div></div><div></div></div>
1	G	231	<div><div>5%</div><div></div><div><div></div><div>70%</div><div>24%</div><div></div><div></div></div><div></div></div>
1	H	231	<div><div>2%</div><div></div><div><div></div><div>67%</div><div>26%</div><div></div><div></div></div><div></div></div>
1	J	231	<div><div>4%</div><div></div><div><div></div><div>68%</div><div>26%</div><div></div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
2	B	217	
2	D	217	
2	F	217	
2	I	217	
2	K	217	
2	L	217	
3	M	115	
3	N	115	
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 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 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			

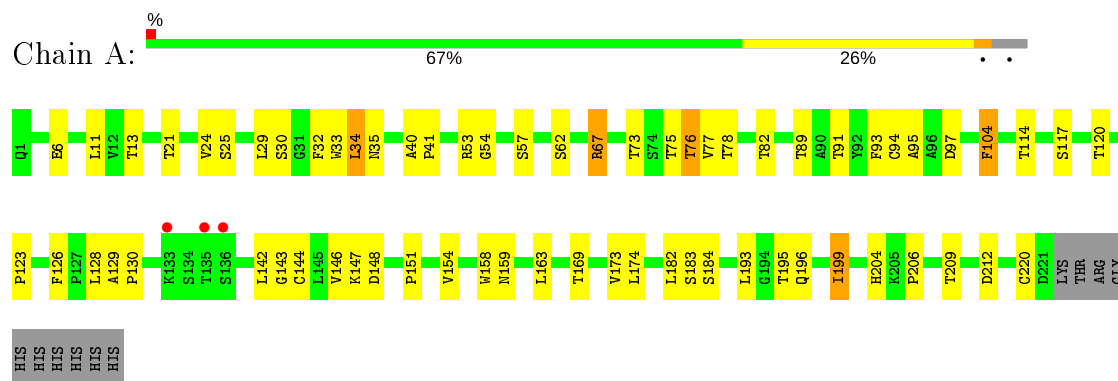
- Molecule 3 is a protein called PROTEIN REV.

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

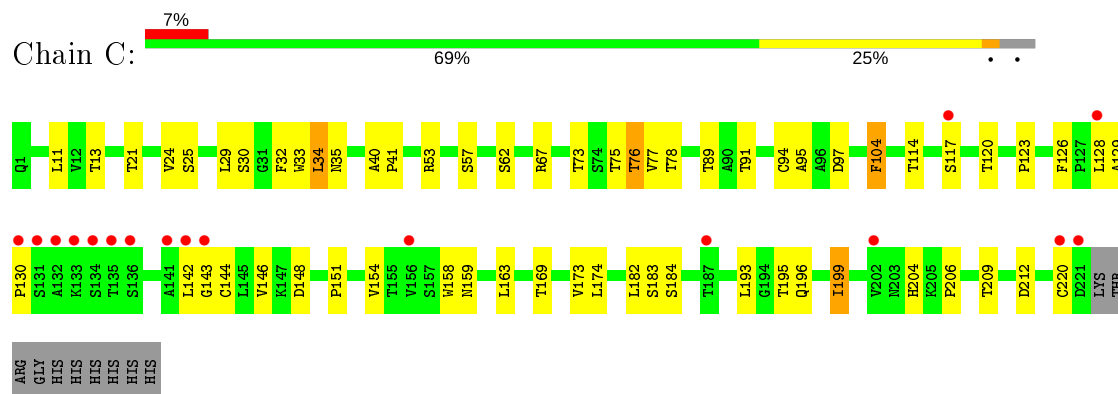
3 Residue-property plots [i](#)

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.

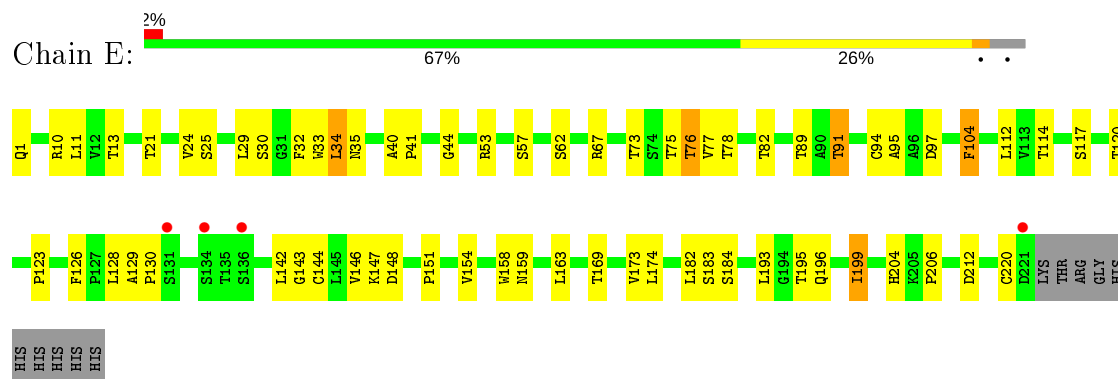
• Molecule 1: FAB HEAVY CHAIN



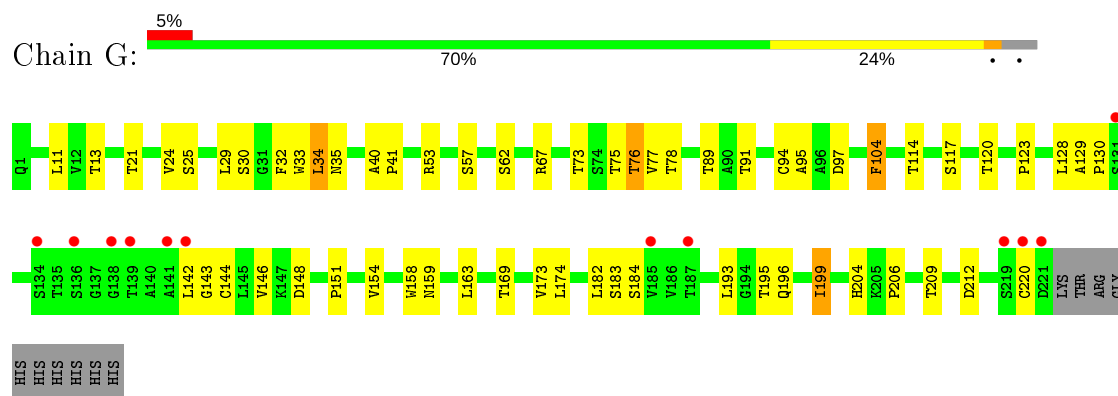
• Molecule 1: FAB HEAVY CHAIN



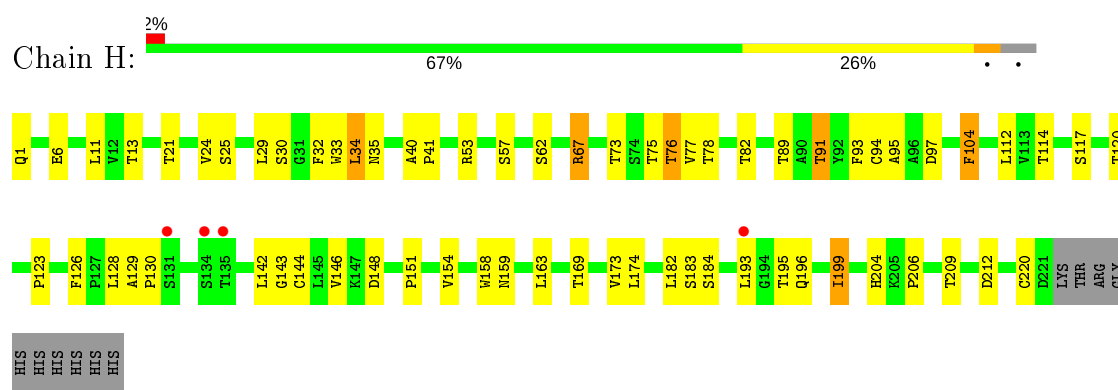
• Molecule 1: FAB HEAVY CHAIN



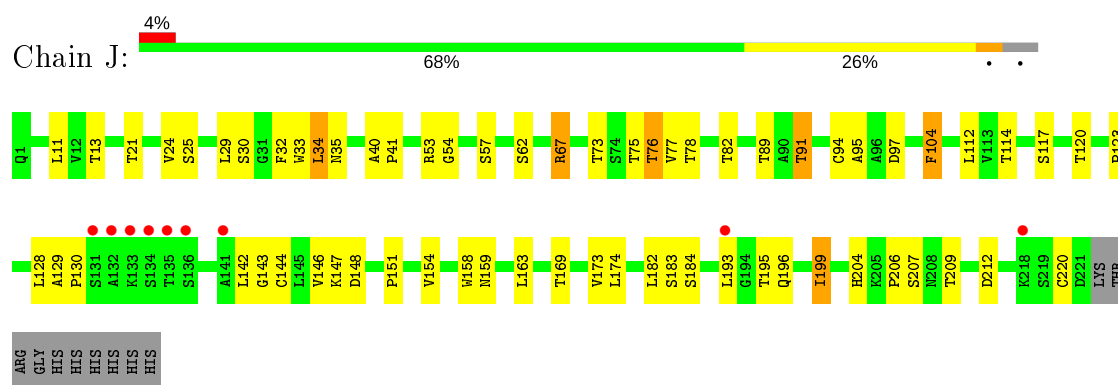
- Molecule 1: FAB HEAVY CHAIN



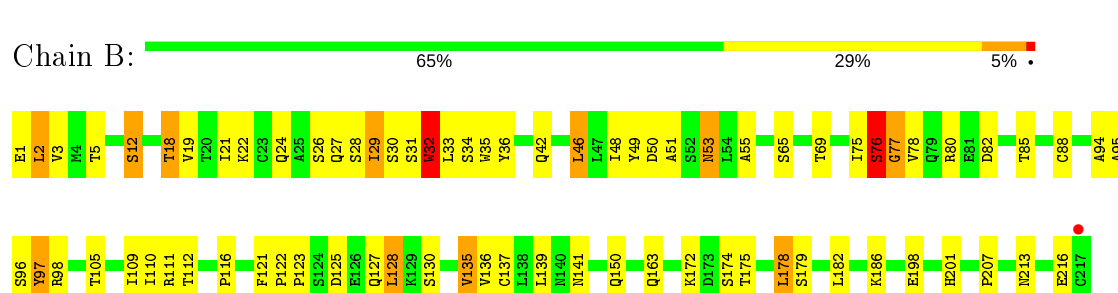
- Molecule 1: FAB HEAVY CHAIN



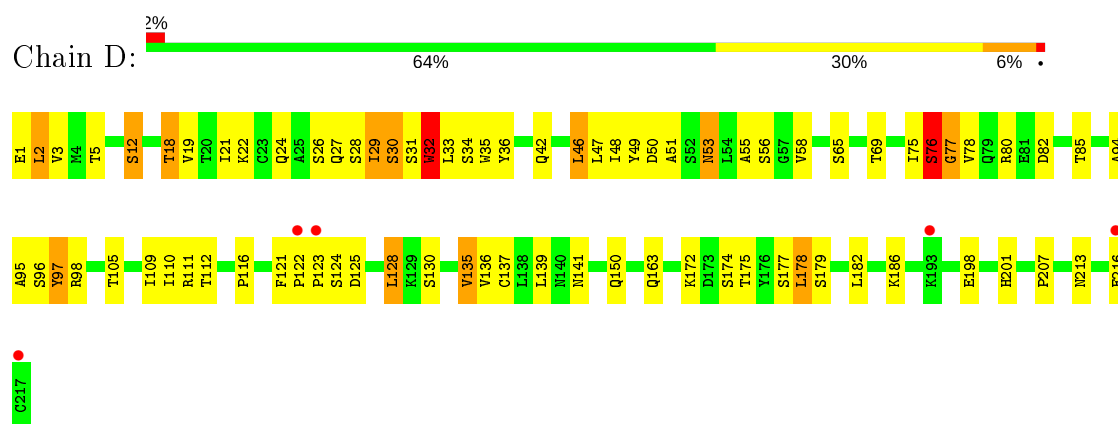
- Molecule 1: FAB HEAVY CHAIN



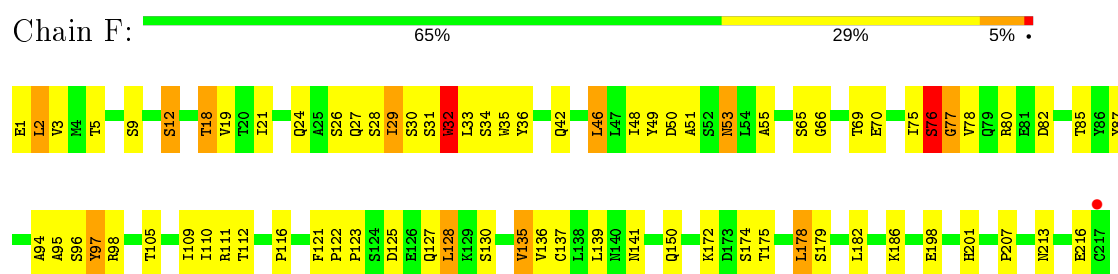
- Molecule 2: FAB LIGHT CHAIN



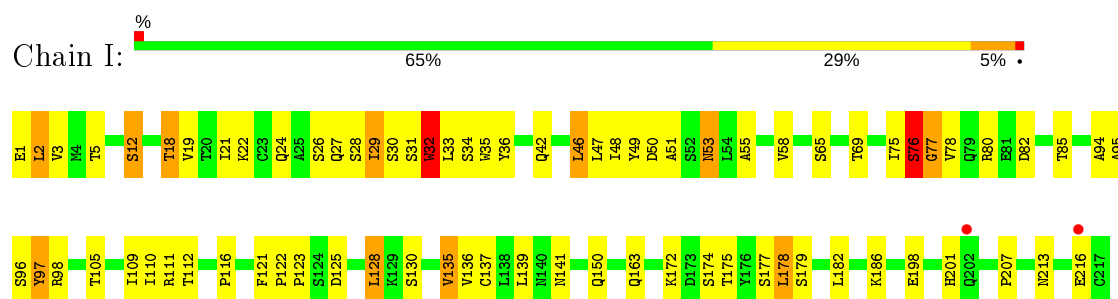
- Molecule 2: FAB LIGHT CHAIN



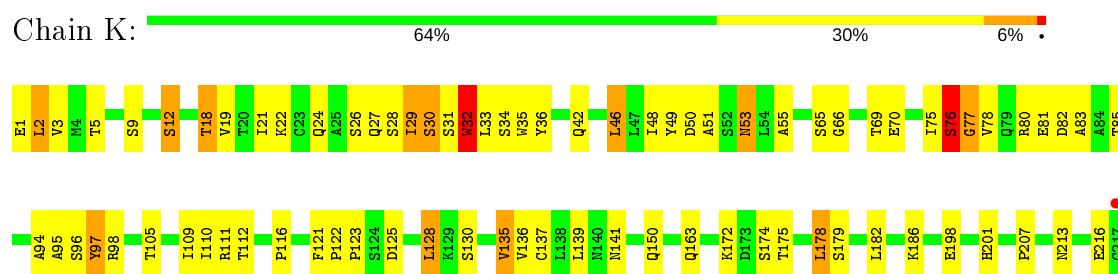
• Molecule 2: FAB LIGHT CHAIN



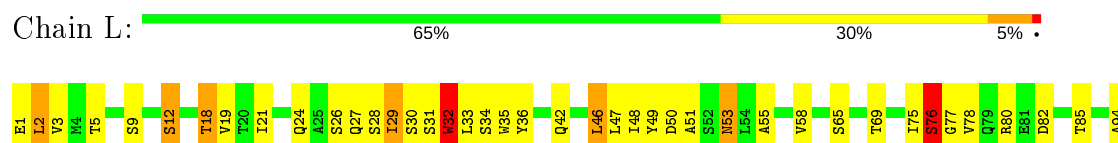
• Molecule 2: FAB LIGHT CHAIN



• Molecule 2: FAB LIGHT CHAIN

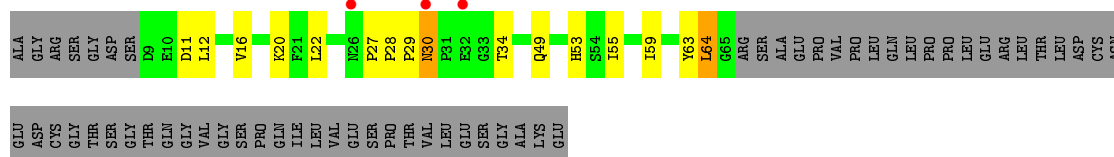
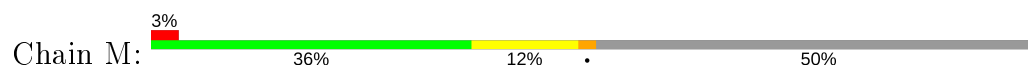


• Molecule 2: FAB LIGHT CHAIN

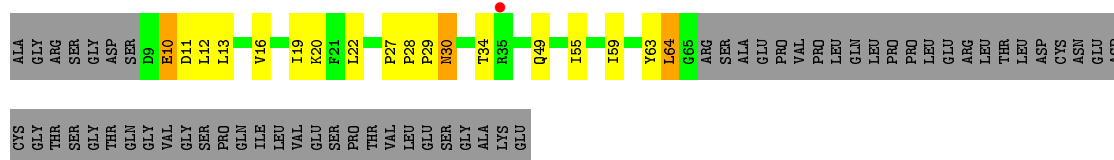
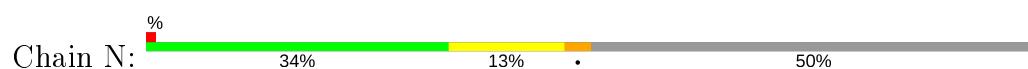




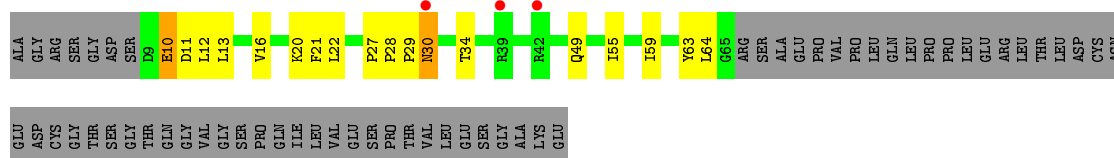
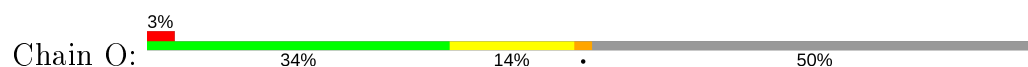
• Molecule 3: PROTEIN REV



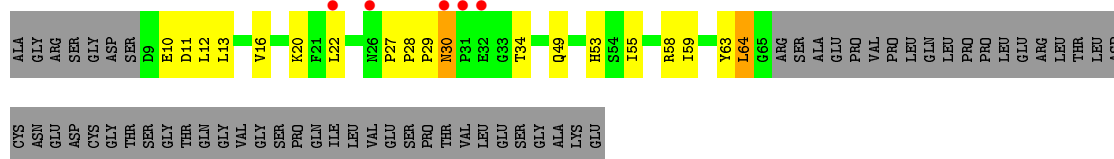
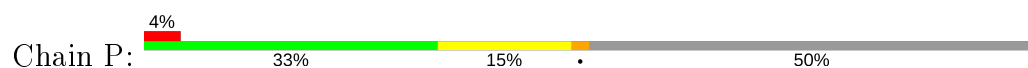
• Molecule 3: PROTEIN REV



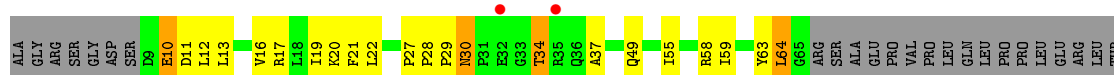
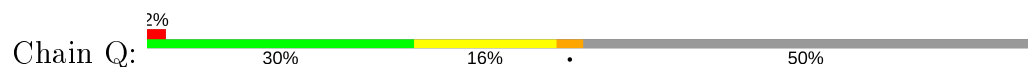
• Molecule 3: PROTEIN REV



• Molecule 3: PROTEIN REV

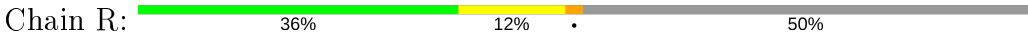


• Molecule 3: PROTEIN REV



LEU
ASP
CYS
ASN
GLU
ASP
CYS
GLY
THR
SER
GLY
THR
GLN
GLY
VAL
GLY
SER
PRO
GLN
TLE
LEU
VAL
GLU
SER
PRO
THR
VAL
LEU
SER
GLY
ALA
LYS
GLU

● Molecule 3: PROTEIN REV



ALA
GLY
ARG
SER
GLY
ASP
SER
D9
E10
D11
L12
L13
V16
K20
F21
L22
F27
F28
P29
N30
T34
Q49
I55
I59
Y63
L64
G65
ARG
SER
SER
ALA
GLU
PRO
VAL
PRO
LEU
GLN
LEU
PRO
PRO
LEU
GLU
ARG
LEU
THR
LEU
ASP
CYS
ASN
GLU
ASP
CYS
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THR
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THR
GLY
GLY
VAL
GLY
SER
PRO
GLU
ILE
LEU
VAL
GLU
SER
PRO
THR
VAL
LEU
GLU
SER
GLY
ALA
LYS
GLU

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 (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	85.2	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.327 for -k,-h,-l	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	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 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	1628	0	1594	29	0
1	C	1628	0	1594	25	0
1	E	1628	0	1594	28	0
1	G	1628	0	1594	24	0
1	H	1628	0	1594	29	0
1	J	1628	0	1594	28	0
2	B	1639	0	1581	40	0
2	D	1639	0	1581	43	0
2	F	1639	0	1581	41	0
2	I	1639	0	1581	40	0
2	K	1639	0	1581	42	0
2	L	1639	0	1581	39	0
3	M	492	0	504	7	0
3	N	492	0	504	9	0
3	O	492	0	504	7	0
3	P	492	0	504	11	0
3	Q	492	0	504	13	0
3	R	492	0	504	7	0
All	All	22554	0	22074	434	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 10.

All (434) 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:I:21:ILE:HG21	2:I:105:THR:HG21	1.26	1.14
2:L:21:ILE:HG21	2:L:105:THR:HG21	1.28	1.12
2:D:21:ILE:HG21	2:D:105:THR:HG21	1.24	1.11
2:K:21:ILE:HG21	2:K:105:THR:HG21	1.28	1.10
2:B:21:ILE:HG21	2:B:105:THR:HG21	1.27	1.09
2:F:21:ILE:HG21	2:F:105:THR:HG21	1.25	1.08
1:A:75:THR:HA	1:A:76:THR:HG23	1.43	1.00
1:C:75:THR:HA	1:C:76:THR:HG23	1.45	0.97
1:G:75:THR:HA	1:G:76:THR:HG23	1.45	0.96
1:J:75:THR:HA	1:J:76:THR:HG23	1.44	0.96
1:E:75:THR:HA	1:E:76:THR:HG23	1.46	0.96
1:H:75:THR:HA	1:H:76:THR:HG23	1.45	0.95
2:F:46:LEU:HD23	2:F:55:ALA:HB2	1.62	0.81
2:B:46:LEU:HD23	2:B:55:ALA:HB2	1.62	0.80
2:I:128:LEU:HD12	2:I:186:LYS:HG3	1.64	0.79
2:B:21:ILE:CG2	2:B:105:THR:HG21	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:95:ALA:HA	2:F:98:ARG:H	1.48	0.79
2:B:95:ALA:HA	2:B:98:ARG:H	1.47	0.79
2:D:21:ILE:CG2	2:D:105:THR:HG21	2.12	0.79
2:K:95:ALA:HA	2:K:98:ARG:H	1.48	0.79
2:I:95:ALA:HA	2:I:98:ARG:H	1.48	0.78
2:L:128:LEU:HD12	2:L:186:LYS:HG3	1.63	0.78
2:D:128:LEU:HD12	2:D:186:LYS:HG3	1.66	0.77
2:D:95:ALA:HA	2:D:98:ARG:H	1.48	0.77
2:K:128:LEU:HD12	2:K:186:LYS:HG3	1.64	0.77
2:L:95:ALA:HA	2:L:98:ARG:H	1.49	0.77
2:I:21:ILE:CG2	2:I:105:THR:HG21	2.12	0.76
2:F:21:ILE:CG2	2:F:105:THR:HG21	2.11	0.76
2:I:46:LEU:HD23	2:I:55:ALA:HB2	1.67	0.75
2:B:128:LEU:HD12	2:B:186:LYS:HG3	1.67	0.75
2:D:46:LEU:HD23	2:D:55:ALA:HB2	1.68	0.75
2:L:95:ALA:HB1	2:L:96:SER:HA	1.69	0.74
1:E:40:ALA:HB1	1:E:41:PRO:HD2	1.69	0.74
2:L:46:LEU:HD23	2:L:55:ALA:HB2	1.68	0.74
2:B:95:ALA:HB1	2:B:96:SER:HA	1.69	0.74
2:D:95:ALA:HB1	2:D:96:SER:HA	1.69	0.73
2:K:46:LEU:HD23	2:K:55:ALA:HB2	1.70	0.73
2:F:128:LEU:HD12	2:F:186:LYS:HG3	1.68	0.73
2:K:95:ALA:HB1	2:K:96:SER:HA	1.71	0.72
2:F:95:ALA:HB1	2:F:96:SER:HA	1.70	0.72
2:I:95:ALA:HB1	2:I:96:SER:HA	1.70	0.72
1:A:40:ALA:HB1	1:A:41:PRO:HD2	1.73	0.69
3:N:27:PRO:HB2	3:N:28:PRO:HD2	1.75	0.69
2:B:150:GLN:HB2	2:B:198:GLU:HB3	1.75	0.69
1:A:24:VAL:HB	1:A:76:THR:HG21	1.75	0.69
2:L:21:ILE:CG2	2:L:105:THR:HG21	2.16	0.69
2:K:150:GLN:HB2	2:K:198:GLU:HB3	1.75	0.69
2:B:95:ALA:HB1	2:B:96:SER:CA	2.23	0.69
2:D:150:GLN:HB2	2:D:198:GLU:HB3	1.75	0.68
1:J:89:THR:HG23	1:J:114:THR:HA	1.75	0.68
1:J:75:THR:HA	1:J:76:THR:CG2	2.22	0.68
3:P:27:PRO:HB2	3:P:28:PRO:HD2	1.75	0.68
2:L:150:GLN:HB2	2:L:198:GLU:HB3	1.76	0.68
2:L:95:ALA:HB1	2:L:96:SER:CA	2.22	0.68
1:G:24:VAL:HB	1:G:76:THR:HG21	1.74	0.68
2:I:95:ALA:HB1	2:I:96:SER:CA	2.23	0.68
1:J:24:VAL:HB	1:J:76:THR:HG21	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:24:VAL:HB	1:H:76:THR:HG21	1.74	0.68
2:I:150:GLN:HB2	2:I:198:GLU:HB3	1.76	0.67
3:M:27:PRO:HB2	3:M:28:PRO:HD2	1.76	0.67
3:O:27:PRO:HB2	3:O:28:PRO:HD2	1.76	0.67
2:D:95:ALA:HB1	2:D:96:SER:CA	2.23	0.67
1:C:89:THR:HG23	1:C:114:THR:HA	1.77	0.67
3:R:27:PRO:HB2	3:R:28:PRO:HD2	1.76	0.67
1:H:75:THR:HA	1:H:76:THR:CG2	2.24	0.67
1:H:89:THR:HG23	1:H:114:THR:HA	1.76	0.66
2:K:95:ALA:HB1	2:K:96:SER:CA	2.24	0.66
1:E:89:THR:HG23	1:E:114:THR:HA	1.77	0.66
1:E:24:VAL:HB	1:E:76:THR:HG21	1.77	0.66
1:G:75:THR:HA	1:G:76:THR:CG2	2.24	0.66
3:Q:27:PRO:HB2	3:Q:28:PRO:HD2	1.76	0.66
1:C:24:VAL:HB	1:C:76:THR:HG21	1.76	0.66
1:G:89:THR:HG23	1:G:114:THR:HA	1.78	0.66
2:L:116:PRO:HD3	2:L:201:HIS:CD2	2.30	0.66
2:F:150:GLN:HB2	2:F:198:GLU:HB3	1.76	0.66
1:A:75:THR:HA	1:A:76:THR:CG2	2.22	0.66
1:E:129:ALA:HB3	2:F:122:PRO:HD2	1.78	0.66
1:C:75:THR:HA	1:C:76:THR:CG2	2.24	0.65
2:F:95:ALA:HB1	2:F:96:SER:CA	2.24	0.65
2:K:21:ILE:CG2	2:K:105:THR:HG21	2.17	0.65
2:B:95:ALA:HB3	3:O:63:TYR:OH	1.96	0.65
1:A:89:THR:HG23	1:A:114:THR:HA	1.77	0.65
2:K:116:PRO:HD3	2:K:201:HIS:CD2	2.32	0.65
2:D:116:PRO:HD3	2:D:201:HIS:CD2	2.34	0.63
2:B:116:PRO:HD3	2:B:201:HIS:CD2	2.34	0.63
1:G:40:ALA:HB1	1:G:41:PRO:HD2	1.82	0.62
2:I:116:PRO:HD3	2:I:201:HIS:CD2	2.33	0.62
2:D:135:VAL:HG23	2:D:182:LEU:HB3	1.81	0.61
3:N:55:ILE:HG22	3:N:59:ILE:HD11	1.82	0.61
3:R:55:ILE:HG22	3:R:59:ILE:HD11	1.82	0.61
2:K:135:VAL:HG23	2:K:182:LEU:HB3	1.81	0.61
1:E:75:THR:HA	1:E:76:THR:CG2	2.24	0.61
2:L:135:VAL:HG23	2:L:182:LEU:HB3	1.81	0.61
2:F:116:PRO:HD3	2:F:201:HIS:CD2	2.35	0.61
2:B:135:VAL:HG23	2:B:182:LEU:HB3	1.83	0.60
2:L:95:ALA:HB3	3:N:63:TYR:OH	2.00	0.60
1:E:123:PRO:HD3	1:E:204:HIS:HD2	1.66	0.60
2:I:135:VAL:HG23	2:I:182:LEU:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:135:VAL:HG23	2:F:182:LEU:HB3	1.84	0.59
2:I:76:SER:OG	2:I:77:GLY:N	2.32	0.59
1:C:40:ALA:HB1	1:C:41:PRO:HD2	1.84	0.58
1:A:123:PRO:HD3	1:A:204:HIS:HD2	1.67	0.58
2:I:95:ALA:HB3	3:M:63:TYR:OH	2.04	0.58
2:D:76:SER:OG	2:D:77:GLY:N	2.30	0.58
1:C:104:PHE:CD1	1:C:104:PHE:N	2.71	0.58
1:G:104:PHE:N	1:G:104:PHE:CD1	2.70	0.58
1:A:104:PHE:N	1:A:104:PHE:CD1	2.70	0.58
1:A:33:TRP:HB2	1:A:97:ASP:HB3	1.86	0.58
2:K:95:ALA:HB3	3:Q:63:TYR:OH	2.03	0.58
2:B:95:ALA:CB	2:B:96:SER:HA	2.35	0.57
1:J:123:PRO:HD3	1:J:204:HIS:HD2	1.69	0.57
2:D:95:ALA:HB3	3:P:63:TYR:OH	2.04	0.57
1:E:104:PHE:CD1	1:E:104:PHE:N	2.71	0.57
2:F:36:TYR:CE2	2:F:46:LEU:HD12	2.39	0.57
2:F:3:VAL:H	2:F:26:SER:HB3	1.69	0.57
2:K:76:SER:OG	2:K:77:GLY:N	2.34	0.57
3:Q:55:ILE:HG22	3:Q:59:ILE:HD11	1.85	0.57
1:G:123:PRO:HD3	1:G:204:HIS:HD2	1.68	0.57
1:H:104:PHE:N	1:H:104:PHE:CD1	2.71	0.57
1:H:123:PRO:HD3	1:H:204:HIS:HD2	1.69	0.57
3:O:55:ILE:HG22	3:O:59:ILE:HD11	1.87	0.57
1:C:33:TRP:HB2	1:C:97:ASP:HB3	1.87	0.57
1:A:123:PRO:HD3	1:A:204:HIS:CD2	2.40	0.57
2:L:95:ALA:CB	2:L:96:SER:HA	2.34	0.57
1:E:123:PRO:HD3	1:E:204:HIS:CD2	2.40	0.56
2:F:95:ALA:CB	2:F:96:SER:HA	2.34	0.56
1:E:33:TRP:HB2	1:E:97:ASP:HB3	1.85	0.56
1:A:158:TRP:HB3	1:A:163:LEU:HD23	1.88	0.56
2:B:76:SER:OG	2:B:77:GLY:N	2.34	0.56
3:M:53:HIS:CE1	3:N:64:LEU:HB2	2.39	0.56
2:B:36:TYR:CE2	2:B:46:LEU:HD12	2.40	0.56
1:J:104:PHE:CD1	1:J:104:PHE:N	2.71	0.56
1:J:40:ALA:HB1	1:J:41:PRO:HD2	1.87	0.56
1:C:123:PRO:HD3	1:C:204:HIS:HD2	1.69	0.56
2:I:32:TRP:HA	2:I:32:TRP:CE3	2.41	0.56
1:H:40:ALA:HB1	1:H:41:PRO:HD2	1.87	0.56
2:K:32:TRP:HE3	2:K:32:TRP:HA	1.71	0.56
2:D:32:TRP:HA	2:D:32:TRP:HE3	1.71	0.56
1:H:129:ALA:HB3	2:L:122:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:32:TRP:HA	2:I:32:TRP:HE3	1.71	0.56
2:K:36:TYR:CE2	2:K:46:LEU:HD12	2.41	0.56
2:L:19:VAL:HG23	2:L:78:VAL:HG11	1.87	0.56
2:B:3:VAL:H	2:B:26:SER:HB3	1.71	0.55
1:E:158:TRP:HB3	1:E:163:LEU:HD23	1.88	0.55
1:A:129:ALA:HB3	2:B:122:PRO:HD2	1.89	0.55
1:H:33:TRP:HB2	1:H:97:ASP:HB3	1.89	0.55
1:J:33:TRP:HB2	1:J:97:ASP:HB3	1.89	0.55
2:K:32:TRP:HA	2:K:32:TRP:CE3	2.42	0.55
2:D:3:VAL:H	2:D:26:SER:HB3	1.72	0.55
1:G:33:TRP:HB2	1:G:97:ASP:HB3	1.88	0.55
2:K:3:VAL:H	2:K:26:SER:HB3	1.71	0.55
2:L:32:TRP:HA	2:L:32:TRP:HE3	1.71	0.55
3:N:12:LEU:O	3:N:16:VAL:HG23	2.07	0.55
2:B:49:TYR:O	2:B:53:ASN:ND2	2.40	0.55
2:L:36:TYR:CE2	2:L:46:LEU:HD12	2.41	0.55
2:B:32:TRP:HA	2:B:32:TRP:HE3	1.72	0.55
2:L:32:TRP:HA	2:L:32:TRP:CE3	2.42	0.55
3:O:55:ILE:O	3:O:59:ILE:HG13	2.07	0.55
1:A:11:LEU:HB2	1:A:151:PRO:HG3	1.89	0.54
1:G:123:PRO:HD3	1:G:204:HIS:CD2	2.42	0.54
2:L:3:VAL:H	2:L:26:SER:HB3	1.72	0.54
1:G:129:ALA:HB3	2:I:122:PRO:HD2	1.89	0.54
2:F:19:VAL:HG23	2:F:78:VAL:HG11	1.90	0.54
1:H:158:TRP:HB3	1:H:163:LEU:HD23	1.89	0.54
2:F:32:TRP:HA	2:F:32:TRP:CE3	2.43	0.54
2:I:3:VAL:H	2:I:26:SER:HB3	1.73	0.54
2:I:95:ALA:CB	2:I:96:SER:HA	2.37	0.54
3:R:12:LEU:O	3:R:16:VAL:HG23	2.07	0.54
2:D:32:TRP:HA	2:D:32:TRP:CE3	2.42	0.54
2:F:32:TRP:HA	2:F:32:TRP:HE3	1.72	0.54
1:J:158:TRP:HB3	1:J:163:LEU:HD23	1.89	0.54
2:B:32:TRP:HA	2:B:32:TRP:CE3	2.42	0.54
1:H:34:LEU:HD21	1:H:94:CYS:HB2	1.90	0.54
3:P:55:ILE:HG22	3:P:59:ILE:HD11	1.90	0.54
2:K:49:TYR:O	2:K:53:ASN:ND2	2.41	0.54
2:D:95:ALA:CB	2:D:96:SER:HA	2.37	0.53
1:E:11:LEU:HB2	1:E:151:PRO:HG3	1.90	0.53
1:C:123:PRO:HD3	1:C:204:HIS:CD2	2.43	0.53
2:K:19:VAL:HG23	2:K:78:VAL:HG11	1.89	0.53
1:E:32:PHE:H	1:E:53:ARG:HB2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:55:ILE:O	3:M:59:ILE:HG13	2.09	0.53
3:R:55:ILE:O	3:R:59:ILE:HG13	2.08	0.53
2:F:76:SER:OG	2:F:77:GLY:N	2.37	0.53
1:A:32:PHE:H	1:A:53:ARG:HB2	1.74	0.52
1:H:123:PRO:HD3	1:H:204:HIS:CD2	2.44	0.52
1:C:158:TRP:HB3	1:C:163:LEU:HD23	1.90	0.52
1:J:123:PRO:HD3	1:J:204:HIS:CD2	2.44	0.52
2:K:95:ALA:CB	2:K:96:SER:HA	2.37	0.52
3:P:64:LEU:HD22	3:Q:19:ILE:HG22	1.92	0.52
1:A:34:LEU:HD21	1:A:94:CYS:HB2	1.91	0.52
2:I:36:TYR:CE2	2:I:46:LEU:HD12	2.45	0.52
2:D:12:SER:CB	2:D:110:ILE:HD11	2.40	0.52
2:L:12:SER:CB	2:L:110:ILE:HD11	2.40	0.52
3:P:12:LEU:O	3:P:16:VAL:HG23	2.10	0.52
2:D:36:TYR:CE2	2:D:46:LEU:HD12	2.44	0.52
2:F:123:PRO:HD3	2:F:135:VAL:HG13	1.92	0.52
2:L:49:TYR:O	2:L:53:ASN:ND2	2.43	0.52
2:K:12:SER:CB	2:K:110:ILE:HD11	2.40	0.52
2:B:123:PRO:HD3	2:B:135:VAL:HG13	1.92	0.51
1:H:32:PHE:H	1:H:53:ARG:HB2	1.76	0.51
1:G:158:TRP:HB3	1:G:163:LEU:HD23	1.90	0.51
1:G:95:ALA:HB1	1:G:104:PHE:HB3	1.92	0.51
1:J:32:PHE:H	1:J:53:ARG:HB2	1.76	0.51
3:M:12:LEU:O	3:M:16:VAL:HG23	2.10	0.51
3:M:55:ILE:HG22	3:M:59:ILE:HD11	1.91	0.51
1:E:34:LEU:HD21	1:E:94:CYS:HB2	1.92	0.51
2:F:49:TYR:O	2:F:53:ASN:ND2	2.43	0.51
2:I:12:SER:CB	2:I:110:ILE:HD11	2.41	0.51
2:L:76:SER:OG	2:L:77:GLY:N	2.35	0.51
1:J:34:LEU:HD21	1:J:94:CYS:HB2	1.92	0.51
3:P:55:ILE:O	3:P:59:ILE:HG13	2.11	0.51
2:F:12:SER:CB	2:F:110:ILE:HD11	2.41	0.51
3:N:55:ILE:O	3:N:59:ILE:HG13	2.10	0.51
3:Q:12:LEU:O	3:Q:16:VAL:HG23	2.10	0.51
1:C:32:PHE:H	1:C:53:ARG:HB2	1.76	0.50
3:M:64:LEU:HD22	3:N:19:ILE:HG22	1.93	0.50
1:G:34:LEU:HD21	1:G:94:CYS:HB2	1.93	0.50
3:O:12:LEU:O	3:O:16:VAL:HG23	2.12	0.50
2:B:19:VAL:HG23	2:B:78:VAL:HG11	1.93	0.50
2:D:49:TYR:O	2:D:53:ASN:ND2	2.43	0.50
2:L:12:SER:HB3	2:L:110:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LEU:HD21	1:C:94:CYS:HB2	1.94	0.50
2:I:2:LEU:HB2	2:I:97:TYR:HB2	1.94	0.50
2:K:123:PRO:HD3	2:K:135:VAL:HG13	1.94	0.50
1:A:95:ALA:HB1	1:A:104:PHE:HB3	1.94	0.50
2:L:123:PRO:HD3	2:L:135:VAL:HG13	1.93	0.50
2:B:12:SER:CB	2:B:110:ILE:HD11	2.42	0.50
1:J:11:LEU:HB2	1:J:151:PRO:HG3	1.93	0.50
1:H:128:LEU:HD12	1:H:143:GLY:HA3	1.94	0.50
1:J:128:LEU:HD12	1:J:143:GLY:HA3	1.93	0.50
1:E:95:ALA:HB1	1:E:104:PHE:HB3	1.94	0.49
1:G:32:PHE:H	1:G:53:ARG:HB2	1.76	0.49
1:A:146:VAL:HG11	1:A:154:VAL:HG11	1.94	0.49
1:C:95:ALA:HB1	1:C:104:PHE:HB3	1.94	0.49
1:H:11:LEU:HB2	1:H:151:PRO:HG3	1.94	0.49
1:G:11:LEU:HB2	1:G:151:PRO:HG3	1.95	0.49
3:Q:55:ILE:O	3:Q:59:ILE:HG13	2.12	0.49
2:F:95:ALA:HA	2:F:98:ARG:N	2.24	0.49
2:I:49:TYR:O	2:I:53:ASN:ND2	2.44	0.49
2:B:213:ASN:HB2	2:B:216:GLU:HB2	1.94	0.49
1:H:146:VAL:O	1:H:146:VAL:HG12	2.12	0.49
2:L:213:ASN:HB2	2:L:216:GLU:HB2	1.95	0.49
2:F:95:ALA:HB3	3:R:63:TYR:OH	2.12	0.48
1:A:146:VAL:O	1:A:146:VAL:HG12	2.14	0.48
2:I:19:VAL:HG23	2:I:78:VAL:HG11	1.95	0.48
1:G:128:LEU:HD12	1:G:143:GLY:HA3	1.96	0.48
2:D:2:LEU:HB2	2:D:97:TYR:HB2	1.95	0.48
1:J:95:ALA:HB1	1:J:104:PHE:HB3	1.96	0.48
1:C:128:LEU:HD12	1:C:143:GLY:HA3	1.95	0.48
2:D:18:THR:HB	2:D:76:SER:HA	1.94	0.48
2:L:95:ALA:CB	2:L:96:SER:CA	2.91	0.48
2:B:121:PHE:HD2	2:B:136:VAL:HG12	1.78	0.48
1:C:11:LEU:HB2	1:C:151:PRO:HG3	1.96	0.48
1:G:146:VAL:HG11	1:G:154:VAL:HG11	1.96	0.48
2:I:5:THR:HB	2:I:24:GLN:HB3	1.94	0.48
1:A:54:GLY:HA3	3:O:21:PHE:HZ	1.79	0.48
2:D:123:PRO:HD3	2:D:135:VAL:HG13	1.95	0.47
2:D:19:VAL:HG23	2:D:78:VAL:HG11	1.95	0.47
1:E:146:VAL:HG11	1:E:154:VAL:HG11	1.96	0.47
1:E:126:PHE:CE2	2:F:127:GLN:HG3	2.49	0.47
1:G:159:ASN:HA	1:G:199:ILE:HD12	1.96	0.47
2:I:123:PRO:HD3	2:I:135:VAL:HG13	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:12:SER:HB3	2:K:110:ILE:HD11	1.96	0.47
2:B:95:ALA:CB	2:B:96:SER:CA	2.92	0.47
1:C:159:ASN:HA	1:C:199:ILE:HD12	1.97	0.47
2:F:2:LEU:HD11	2:F:29:ILE:HD11	1.97	0.47
1:J:146:VAL:HG11	1:J:154:VAL:HG11	1.95	0.47
1:E:128:LEU:HD12	1:E:143:GLY:HA3	1.97	0.47
2:D:5:THR:HB	2:D:24:GLN:HB3	1.95	0.47
2:I:213:ASN:HB2	2:I:216:GLU:HB2	1.96	0.47
1:J:151:PRO:HD2	1:J:206:PRO:HB2	1.97	0.47
3:P:53:HIS:CE1	3:Q:64:LEU:HB2	2.49	0.47
2:K:121:PHE:HD2	2:K:136:VAL:HG12	1.80	0.47
2:L:2:LEU:HD11	2:L:29:ILE:HD11	1.96	0.47
2:B:95:ALA:HB1	2:B:96:SER:C	2.36	0.47
2:I:18:THR:HB	2:I:76:SER:HA	1.97	0.47
2:L:121:PHE:HD2	2:L:136:VAL:HG12	1.80	0.46
2:F:213:ASN:HB2	2:F:216:GLU:HB2	1.97	0.46
2:K:139:LEU:HD13	2:K:178:LEU:HB3	1.97	0.46
1:C:146:VAL:HG11	1:C:154:VAL:HG11	1.96	0.46
2:D:139:LEU:HD13	2:D:178:LEU:HB3	1.96	0.46
1:G:53:ARG:HH12	1:G:76:THR:HG22	1.80	0.46
1:H:151:PRO:HD2	1:H:206:PRO:HB2	1.98	0.46
2:K:213:ASN:HB2	2:K:216:GLU:HB2	1.96	0.46
1:H:95:ALA:HB1	1:H:104:PHE:HB3	1.98	0.46
2:I:139:LEU:HD13	2:I:178:LEU:HB3	1.97	0.46
2:D:213:ASN:HB2	2:D:216:GLU:HB2	1.95	0.46
2:I:95:ALA:HA	2:I:98:ARG:N	2.24	0.46
2:F:121:PHE:HD2	2:F:136:VAL:HG12	1.80	0.46
1:H:146:VAL:HG11	1:H:154:VAL:HG11	1.97	0.46
1:J:159:ASN:HA	1:J:199:ILE:HD12	1.98	0.46
1:A:128:LEU:HD12	1:A:143:GLY:HA3	1.98	0.46
1:A:169:THR:HG23	1:A:184:SER:HB2	1.98	0.46
1:A:53:ARG:HH12	1:A:76:THR:HG22	1.81	0.46
1:E:146:VAL:HG12	1:E:146:VAL:O	2.16	0.46
1:G:204:HIS:ND1	1:G:206:PRO:HD2	2.31	0.46
1:J:204:HIS:ND1	1:J:206:PRO:HD2	2.30	0.46
2:L:139:LEU:HD13	2:L:178:LEU:HB3	1.97	0.46
2:L:95:ALA:HB1	2:L:96:SER:C	2.36	0.46
2:D:121:PHE:HD2	2:D:136:VAL:HG12	1.81	0.46
2:D:95:ALA:CB	2:D:96:SER:CA	2.94	0.46
1:H:159:ASN:HA	1:H:199:ILE:HD12	1.98	0.46
1:J:146:VAL:HG12	1:J:146:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2:LEU:HD11	2:K:29:ILE:HD11	1.97	0.46
2:L:31:SER:O	2:L:50:ASP:HA	2.16	0.46
2:B:35:TRP:HB2	2:B:48:ILE:HB	1.97	0.46
2:B:2:LEU:HD11	2:B:29:ILE:HD11	1.97	0.45
2:F:95:ALA:HB1	2:F:96:SER:C	2.36	0.45
1:C:204:HIS:ND1	1:C:206:PRO:HD2	2.31	0.45
1:C:151:PRO:HD2	1:C:206:PRO:HB2	1.98	0.45
2:D:12:SER:HB3	2:D:110:ILE:HD11	1.98	0.45
2:K:18:THR:HB	2:K:76:SER:HA	1.99	0.45
1:C:53:ARG:HH12	1:C:76:THR:HG22	1.80	0.45
2:B:5:THR:HB	2:B:24:GLN:HB3	1.97	0.45
2:K:5:THR:HB	2:K:24:GLN:HB3	1.98	0.45
2:K:30:SER:HB2	3:Q:58:ARG:HH21	1.82	0.45
2:B:2:LEU:HB2	2:B:97:TYR:HB2	1.99	0.45
1:C:146:VAL:O	1:C:146:VAL:HG12	2.17	0.45
1:E:159:ASN:HA	1:E:199:ILE:HD12	1.97	0.45
1:E:204:HIS:ND1	1:E:206:PRO:HD2	2.32	0.45
1:E:169:THR:HG23	1:E:184:SER:HB2	1.99	0.45
2:F:2:LEU:HB2	2:F:97:TYR:HB2	1.99	0.45
2:F:35:TRP:HB2	2:F:48:ILE:HB	1.98	0.45
1:J:169:THR:HG23	1:J:184:SER:HB2	1.97	0.45
2:L:5:THR:HB	2:L:24:GLN:HB3	1.98	0.45
2:D:35:TRP:HB2	2:D:48:ILE:HB	1.99	0.45
1:G:146:VAL:HG12	1:G:146:VAL:O	2.16	0.45
1:H:204:HIS:ND1	1:H:206:PRO:HD2	2.32	0.45
1:J:67:ARG:H	1:J:67:ARG:HG2	1.64	0.45
1:A:159:ASN:HA	1:A:199:ILE:HD12	1.98	0.45
2:D:2:LEU:HD11	2:D:29:ILE:HD11	1.98	0.45
2:K:95:ALA:HB1	2:K:96:SER:C	2.37	0.45
1:H:123:PRO:HD2	1:H:209:THR:HG21	1.99	0.45
2:B:95:ALA:HA	2:B:98:ARG:N	2.24	0.45
1:G:151:PRO:HD2	1:G:206:PRO:HB2	1.98	0.45
2:K:2:LEU:HB2	2:K:97:TYR:HB2	1.99	0.45
2:L:2:LEU:HB2	2:L:97:TYR:HB2	1.99	0.44
1:E:91:THR:HG22	1:E:112:LEU:HD13	1.99	0.44
2:B:121:PHE:HA	2:B:122:PRO:HD3	1.86	0.44
2:D:30:SER:HB2	3:P:58:ARG:HH21	1.82	0.44
1:A:204:HIS:ND1	1:A:206:PRO:HD2	2.32	0.44
2:I:121:PHE:HD2	2:I:136:VAL:HG12	1.81	0.44
2:K:31:SER:O	2:K:50:ASP:HA	2.17	0.44
1:H:126:PHE:CE2	2:L:127:GLN:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5:THR:HB	2:F:24:GLN:HB3	1.99	0.44
2:I:2:LEU:HD11	2:I:29:ILE:HD11	1.99	0.44
2:I:35:TRP:HB2	2:I:48:ILE:HB	1.99	0.44
1:J:129:ALA:HB3	2:K:122:PRO:HD2	1.99	0.44
3:O:10:GLU:HA	3:O:13:LEU:HD12	2.00	0.44
2:B:12:SER:HB3	2:B:110:ILE:HD11	1.99	0.43
2:L:95:ALA:HA	2:L:98:ARG:N	2.25	0.43
1:C:129:ALA:HB3	2:D:122:PRO:HD2	1.99	0.43
2:D:128:LEU:HA	2:D:128:LEU:HD13	1.89	0.43
3:P:13:LEU:HD21	3:Q:17:ARG:HH21	1.83	0.43
1:A:67:ARG:H	1:A:67:ARG:HG2	1.65	0.43
2:K:95:ALA:CB	2:K:96:SER:CA	2.93	0.43
1:A:151:PRO:HD2	1:A:206:PRO:HB2	2.00	0.43
2:F:95:ALA:CB	2:F:96:SER:CA	2.93	0.43
1:J:91:THR:HG22	1:J:112:LEU:HD13	2.01	0.43
2:B:139:LEU:HD13	2:B:178:LEU:HB3	1.99	0.43
2:B:18:THR:HB	2:B:76:SER:HA	1.99	0.43
2:F:12:SER:HB3	2:F:110:ILE:HD11	2.00	0.43
2:F:31:SER:O	2:F:50:ASP:HA	2.19	0.43
1:J:53:ARG:HH12	1:J:76:THR:HG22	1.84	0.43
1:A:126:PHE:CE2	2:B:127:GLN:HG3	2.54	0.43
2:F:139:LEU:HD13	2:F:178:LEU:HB3	2.00	0.43
2:L:18:THR:HB	2:L:76:SER:HA	2.01	0.43
2:L:35:TRP:HB2	2:L:48:ILE:HB	2.00	0.43
2:D:31:SER:O	2:D:50:ASP:HA	2.19	0.42
2:F:18:THR:HB	2:F:76:SER:HA	2.00	0.42
2:I:95:ALA:HB1	2:I:96:SER:C	2.40	0.42
3:N:55:ILE:HG22	3:N:59:ILE:CD1	2.48	0.42
3:Q:10:GLU:HA	3:Q:13:LEU:HD12	2.01	0.42
1:J:54:GLY:HA3	3:Q:21:PHE:HZ	1.84	0.42
3:R:10:GLU:HA	3:R:13:LEU:HD12	2.00	0.42
1:E:53:ARG:HH12	1:E:76:THR:HG22	1.84	0.42
1:H:53:ARG:HH12	1:H:76:THR:HG22	1.84	0.42
2:L:47:LEU:HA	2:L:58:VAL:HG21	2.02	0.42
1:A:6:GLU:OE1	1:A:93:PHE:HA	2.19	0.42
2:D:95:ALA:HB1	2:D:96:SER:C	2.40	0.42
1:E:151:PRO:HD2	1:E:206:PRO:HB2	2.00	0.42
1:H:67:ARG:HG2	1:H:67:ARG:H	1.65	0.42
2:I:12:SER:HB3	2:I:110:ILE:HD11	2.00	0.42
2:K:9:SER:O	2:K:105:THR:HA	2.20	0.42
2:K:35:TRP:HB2	2:K:48:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:SER:H	3:P:58:ARG:HH21	1.67	0.42
2:D:95:ALA:HA	2:D:98:ARG:N	2.25	0.42
2:I:121:PHE:HA	2:I:122:PRO:HD3	1.87	0.42
2:B:31:SER:O	2:B:50:ASP:HA	2.20	0.42
1:G:123:PRO:HD2	1:G:209:THR:HG21	2.02	0.42
3:P:10:GLU:HA	3:P:13:LEU:HD12	2.02	0.42
2:B:22:LYS:HE2	2:B:24:GLN:HB2	2.02	0.42
2:D:139:LEU:O	2:D:177:SER:HA	2.20	0.42
1:G:169:THR:HG23	1:G:184:SER:HB2	2.01	0.42
1:H:169:THR:HG23	1:H:184:SER:HB2	2.01	0.42
1:A:75:THR:HA	1:A:76:THR:CB	2.50	0.42
2:I:31:SER:O	2:I:50:ASP:HA	2.20	0.42
2:D:47:LEU:HA	2:D:58:VAL:HG21	2.02	0.41
1:J:123:PRO:HD2	1:J:209:THR:HG21	2.00	0.41
1:A:123:PRO:HD2	1:A:209:THR:HG21	2.02	0.41
2:I:12:SER:HB2	2:I:110:ILE:HD11	2.01	0.41
1:C:123:PRO:HD2	1:C:209:THR:HG21	2.03	0.41
2:D:12:SER:HB2	2:D:110:ILE:HD11	2.02	0.41
1:C:126:PHE:HB3	2:D:124:SER:OG	2.20	0.41
2:F:121:PHE:HA	2:F:122:PRO:HD3	1.83	0.41
2:I:139:LEU:O	2:I:177:SER:HA	2.20	0.41
1:E:10:ARG:HD3	1:J:207:SER:HA	2.02	0.41
2:B:128:LEU:HD13	2:B:128:LEU:HA	1.90	0.41
2:I:47:LEU:HA	2:I:58:VAL:HG21	2.02	0.41
3:N:10:GLU:HA	3:N:13:LEU:HD12	2.02	0.41
3:Q:55:ILE:HG22	3:Q:59:ILE:CD1	2.50	0.41
1:C:169:THR:HG23	1:C:184:SER:HB2	2.00	0.41
2:I:128:LEU:HA	2:I:128:LEU:HD13	1.89	0.41
2:I:22:LYS:HE2	2:I:24:GLN:HB2	2.01	0.41
2:K:66:GLY:HA2	2:K:70:GLU:O	2.21	0.41
2:K:128:LEU:HA	2:K:128:LEU:HD13	1.93	0.41
2:L:9:SER:O	2:L:105:THR:HA	2.21	0.41
2:B:35:TRP:CZ3	2:B:88:CYS:HB3	2.56	0.41
2:K:22:LYS:HE2	2:K:24:GLN:HB2	2.02	0.41
3:Q:34:THR:HB	3:Q:37:ALA:HB3	2.03	0.41
2:F:128:LEU:HA	2:F:128:LEU:HD13	1.91	0.41
1:H:6:GLU:OE1	1:H:93:PHE:HA	2.20	0.41
1:H:75:THR:HA	1:H:76:THR:CB	2.51	0.41
2:K:12:SER:HB2	2:K:110:ILE:HD11	2.03	0.41
2:K:95:ALA:HA	2:K:98:ARG:N	2.24	0.41
2:D:22:LYS:HE2	2:D:24:GLN:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:121:PHE:HA	2:L:122:PRO:HD3	1.87	0.40
1:E:44:GLY:HA2	2:F:87:TYR:OH	2.22	0.40
1:E:75:THR:HA	1:E:76:THR:CB	2.52	0.40
1:H:91:THR:HG22	1:H:112:LEU:HD13	2.03	0.40
2:K:81:GLU:O	2:K:83:ALA:N	2.54	0.40
2:F:9:SER:O	2:F:105:THR:HA	2.21	0.40
3:R:55:ILE:HG22	3:R:59:ILE:CD1	2.51	0.40
2:F:66:GLY:HA2	2:F:70:GLU:O	2.22	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	219/231 (95%)	187 (85%)	28 (13%)	4 (2%)	8	38
1	C	219/231 (95%)	189 (86%)	26 (12%)	4 (2%)	8	38
1	E	219/231 (95%)	187 (85%)	28 (13%)	4 (2%)	8	38
1	G	219/231 (95%)	190 (87%)	25 (11%)	4 (2%)	8	38
1	H	219/231 (95%)	187 (85%)	28 (13%)	4 (2%)	8	38
1	J	219/231 (95%)	190 (87%)	25 (11%)	4 (2%)	8	38
2	B	215/217 (99%)	188 (87%)	14 (6%)	13 (6%)	1	11
2	D	215/217 (99%)	188 (87%)	14 (6%)	13 (6%)	1	11
2	F	215/217 (99%)	188 (87%)	14 (6%)	13 (6%)	1	11
2	I	215/217 (99%)	188 (87%)	14 (6%)	13 (6%)	1	11
2	K	215/217 (99%)	188 (87%)	14 (6%)	13 (6%)	1	11
2	L	215/217 (99%)	188 (87%)	15 (7%)	12 (6%)	2	12
3	M	55/115 (48%)	46 (84%)	7 (13%)	2 (4%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	N	55/115 (48%)	48 (87%)	5 (9%)	2 (4%)	3	21
3	O	55/115 (48%)	47 (86%)	6 (11%)	2 (4%)	3	21
3	P	55/115 (48%)	46 (84%)	7 (13%)	2 (4%)	3	21
3	Q	55/115 (48%)	46 (84%)	7 (13%)	2 (4%)	3	21
3	R	55/115 (48%)	47 (86%)	6 (11%)	2 (4%)	3	21
All	All	2934/3378 (87%)	2538 (86%)	283 (10%)	113 (4%)	3	19

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
2	F	76	SER
2	F	94	ALA
2	F	141	ASN
1	G	130	PRO
1	H	130	PRO

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Mol	Chain	Res	Type
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
1	J	220	CYS
2	K	30	SER
2	K	32	TRP
2	K	51	ALA
2	K	82	ASP

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Mol	Chain	Res	Type
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
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%)	2	10
1	C	182/192 (95%)	154 (85%)	28 (15%)	2	12
1	E	182/192 (95%)	151 (83%)	31 (17%)	2	9
1	G	182/192 (95%)	154 (85%)	28 (15%)	2	12
1	H	182/192 (95%)	152 (84%)	30 (16%)	2	10
1	J	182/192 (95%)	152 (84%)	30 (16%)	2	10
2	B	184/185 (100%)	154 (84%)	30 (16%)	2	10
2	D	184/185 (100%)	153 (83%)	31 (17%)	2	9
2	F	184/185 (100%)	155 (84%)	29 (16%)	2	11
2	I	184/185 (100%)	154 (84%)	30 (16%)	2	10
2	K	184/185 (100%)	154 (84%)	30 (16%)	2	10
2	L	184/185 (100%)	154 (84%)	30 (16%)	2	10
3	M	53/101 (52%)	46 (87%)	7 (13%)	4	17
3	N	53/101 (52%)	45 (85%)	8 (15%)	3	13
3	O	53/101 (52%)	45 (85%)	8 (15%)	3	13
3	P	53/101 (52%)	46 (87%)	7 (13%)	4	17
3	Q	53/101 (52%)	45 (85%)	8 (15%)	3	13
3	R	53/101 (52%)	46 (87%)	7 (13%)	4	17
All	All	2514/2868 (88%)	2112 (84%)	402 (16%)	2	10

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

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Mol	Chain	Res	Type
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
2	B	75	ILE
2	B	76	SER
2	B	80	ARG
2	B	85	THR
2	B	97	TYR

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Mol	Chain	Res	Type
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
1	C	196	GLN
1	C	199	ILE
1	C	212	ASP
2	D	1	GLU
2	D	2	LEU

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Mol	Chain	Res	Type
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
1	E	62	SER
1	E	67	ARG
1	E	73	THR
1	E	76	THR
1	E	77	VAL

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Mol	Chain	Res	Type
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
2	F	111	ARG
2	F	112	THR
2	F	125	ASP
2	F	128	LEU
2	F	135	VAL

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Mol	Chain	Res	Type
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
1	H	29	LEU
1	H	34	LEU
1	H	35	ASN
1	H	57	SER
1	H	62	SER

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Mol	Chain	Res	Type
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
2	I	85	THR
2	I	97	TYR
2	I	109	ILE
2	I	111	ARG
2	I	112	THR

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Mol	Chain	Res	Type
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
1	J	199	ILE
1	J	212	ASP
2	K	1	GLU
2	K	2	LEU
2	K	12	SER

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Mol	Chain	Res	Type
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
2	L	53	ASN
2	L	65	SER
2	L	69	THR
2	L	75	ILE
2	L	76	SER

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Mol	Chain	Res	Type
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
3	O	64	LEU
3	P	11	ASP
3	P	20	LYS
3	P	22	LEU
3	P	30	ASN

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Mol	Chain	Res	Type
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. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	79	GLN
2	B	127	GLN
2	B	169	GLN
2	B	201	HIS
2	D	53	ASN
2	D	79	GLN
2	D	127	GLN
2	D	169	GLN
2	D	201	HIS
1	E	204	HIS
2	F	53	ASN
2	F	79	GLN
2	F	127	GLN
2	F	169	GLN
2	F	201	HIS
2	I	53	ASN
2	I	79	GLN
2	I	127	GLN
2	I	169	GLN

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Mol	Chain	Res	Type
2	I	201	HIS
2	K	53	ASN
2	K	79	GLN
2	K	127	GLN
2	K	169	GLN
2	K	201	HIS
2	L	53	ASN
2	L	79	GLN
2	L	127	GLN
2	L	169	GLN
2	L	201	HIS
3	M	51	GLN
3	N	51	GLN
3	O	51	GLN
3	P	51	GLN
3	Q	51	GLN
3	R	51	GLN

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 ⓘ

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%)	-0.27	3 (1%) 75 63	75, 114, 192, 246	0
1	C	221/231 (95%)	0.11	17 (7%) 13 7	102, 173, 235, 263	0
1	E	221/231 (95%)	-0.31	4 (1%) 68 55	78, 118, 191, 251	0
1	G	221/231 (95%)	0.14	12 (5%) 25 14	100, 175, 246, 265	0
1	H	221/231 (95%)	-0.29	4 (1%) 68 55	67, 113, 195, 224	0
1	J	221/231 (95%)	-0.23	9 (4%) 37 23	74, 119, 201, 236	0
2	B	217/217 (100%)	-0.45	1 (0%) 91 86	73, 116, 189, 208	0
2	D	217/217 (100%)	-0.23	5 (2%) 60 46	98, 156, 248, 263	0
2	F	217/217 (100%)	-0.39	1 (0%) 91 86	74, 113, 200, 229	0
2	I	217/217 (100%)	-0.29	2 (0%) 84 75	88, 149, 251, 283	0
2	K	217/217 (100%)	-0.48	1 (0%) 91 86	75, 116, 188, 222	0
2	L	217/217 (100%)	-0.45	0 100 100	76, 116, 186, 211	0
3	M	57/115 (49%)	-0.10	3 (5%) 26 14	109, 164, 278, 284	0
3	N	57/115 (49%)	-0.26	1 (1%) 68 55	96, 155, 287, 298	0
3	O	57/115 (49%)	0.04	3 (5%) 26 14	97, 151, 278, 287	0
3	P	57/115 (49%)	0.01	5 (8%) 10 5	119, 165, 276, 280	0
3	Q	57/115 (49%)	0.03	2 (3%) 44 28	98, 151, 275, 277	0
3	R	57/115 (49%)	0.06	0 100 100	95, 156, 274, 280	0
All	All	2970/3378 (87%)	-0.23	73 (2%) 57 43	67, 129, 236, 298	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	134	SER	11.9
1	C	221	ASP	8.0
1	C	134	SER	7.0

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Mol	Chain	Res	Type	RSRZ
2	D	123	PRO	6.8
1	H	134	SER	6.2
1	G	142	LEU	5.2
1	A	133	LYS	5.0
1	C	131	SER	5.0
1	G	136	SER	4.6
1	C	133	LYS	4.5
1	J	135	THR	4.3
1	E	134	SER	4.2
1	J	133	LYS	4.2
1	H	135	THR	4.1
1	G	131	SER	3.8
1	A	136	SER	3.8
3	P	31	PRO	3.5
1	C	136	SER	3.5
1	G	141	ALA	3.5
3	N	35	ARG	3.5
1	G	187	THR	3.5
3	Q	35	ARG	3.4
2	D	217	CYS	3.4
3	M	26	ASN	3.3
1	C	187	THR	3.3
1	A	135	THR	3.3
3	P	26	ASN	3.2
1	C	156	VAL	3.2
1	C	132	ALA	3.2
1	C	220	CYS	3.1
1	H	131	SER	3.1
1	J	193	LEU	2.9
1	C	135	THR	2.9
1	C	202	VAL	2.8
1	G	219	SER	2.8
1	H	193	LEU	2.8
1	J	131	SER	2.8
2	D	122	PRO	2.7
3	O	42	ARG	2.7
1	C	130	PRO	2.7
1	J	132	ALA	2.7
2	B	217	CYS	2.6
3	O	39	ARG	2.6
1	C	142	LEU	2.6
1	E	136	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	Q	32	GLU	2.5
2	F	217	CYS	2.4
3	O	30	ASN	2.4
2	I	202	GLN	2.4
1	G	220	CYS	2.4
1	E	131	SER	2.4
1	G	221	ASP	2.4
3	P	32	GLU	2.4
2	D	216	GLU	2.3
2	K	217	CYS	2.3
1	J	141	ALA	2.3
1	G	134	SER	2.3
1	G	185	VAL	2.3
1	G	139	THR	2.2
1	C	141	ALA	2.2
3	P	30	ASN	2.2
1	E	221	ASP	2.2
1	J	218	LYS	2.2
3	P	22	LEU	2.2
2	D	193	LYS	2.1
2	I	216	GLU	2.1
1	J	136	SER	2.1
1	C	143	GLY	2.1
1	C	117	SER	2.1
1	C	128	LEU	2.1
3	M	30	ASN	2.1
1	G	138	GLY	2.1
3	M	32	GLU	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 ⓘ

There are no such residues in this entry.