



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 02:42 PM BST

PDB ID : 6VI1
Title : Structure of Fab4 bound to P22 TerL(1-33)
Authors : Cingolani, G.; Lokareddy, R.; Ko, Y.
Deposited on : 2020-01-11
Resolution : 2.40 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	:	2.14.2
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)	:	2.14.2

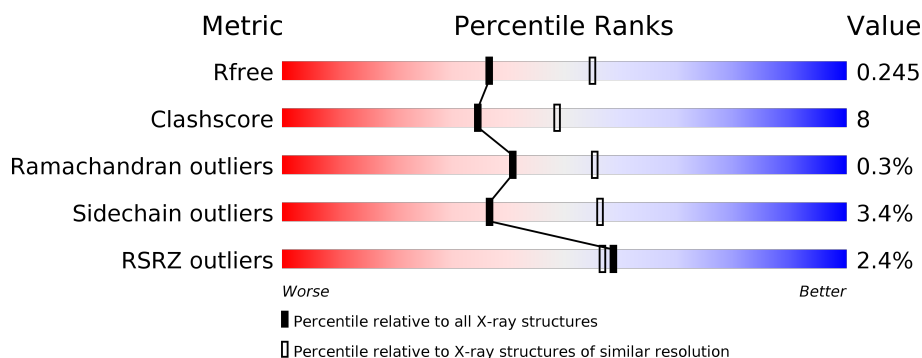
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.





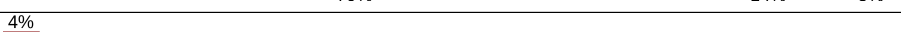

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	215	<div> <div>80%</div> <div>17%</div> <div>•</div> </div>
1	C	215	<div> <div>2%</div> <div>76%</div> <div>21%</div> <div>•</div> </div>
1	D	215	<div> <div>82%</div> <div>17%</div> <div>•</div> </div>
1	G	215	<div> <div>3%</div> <div>77%</div> <div>21%</div> <div>•</div> </div>
1	I	215	<div> <div>3%</div> <div>81%</div> <div>16%</div> <div>•</div> </div>
1	K	215	<div> <div>82%</div> <div>16%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	243	
2	E	243	
2	F	243	
2	H	243	
2	J	243	
2	L	243	
3	M	33	
3	N	33	
3	O	33	
3	P	33	
3	Q	33	
3	R	33	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22166 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 Synthetic Fab4 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	214	Total	C	N	O	S	0	0	0
			1629	1018	274	331	6			
1	A	214	Total	C	N	O	S	0	0	0
			1629	1018	274	331	6			
1	C	214	Total	C	N	O	S	0	0	0
			1629	1018	274	331	6			
1	G	214	Total	C	N	O	S	0	0	0
			1629	1018	274	331	6			
1	I	214	Total	C	N	O	S	0	0	0
			1629	1018	274	331	6			
1	K	214	Total	C	N	O	S	0	0	0
			1629	1018	274	331	6			

- Molecule 2 is a protein called Synthetic Fab4 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	230	Total	C	N	O	S	0	0	0
			1732	1104	284	338	6			
2	B	232	Total	C	N	O	S	0	0	0
			1747	1113	287	341	6			
2	F	231	Total	C	N	O	S	0	0	0
			1741	1110	286	339	6			
2	H	231	Total	C	N	O	S	0	0	0
			1741	1110	286	339	6			
2	J	230	Total	C	N	O	S	0	0	0
			1732	1104	284	338	6			
2	L	232	Total	C	N	O	S	0	0	0
			1747	1113	287	341	6			

- Molecule 3 is a protein called Terminase, large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	23	Total 186	C 116	N 25	O 44	S 1	0	0	0
3	N	23	Total 186	C 116	N 25	O 44	S 1	0	0	0
3	O	23	Total 186	C 116	N 25	O 44	S 1	0	0	0
3	P	23	Total 186	C 116	N 25	O 44	S 1	0	0	0
3	Q	23	Total 186	C 116	N 25	O 44	S 1	0	0	0
3	R	23	Total 186	C 116	N 25	O 44	S 1	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	116	Total 116	O 116	0	0
4	E	74	Total 74	O 74	0	0
4	A	78	Total 78	O 78	0	0
4	B	62	Total 62	O 62	0	0
4	C	79	Total 79	O 79	0	0
4	F	45	Total 45	O 45	0	0
4	G	57	Total 57	O 57	0	0
4	H	27	Total 27	O 27	0	0
4	I	95	Total 95	O 95	0	0
4	J	75	Total 75	O 75	0	0
4	K	65	Total 65	O 65	0	0
4	L	30	Total 30	O 30	0	0
4	M	7	Total 7	O 7	0	0
4	N	3	Total 3	O 3	0	0

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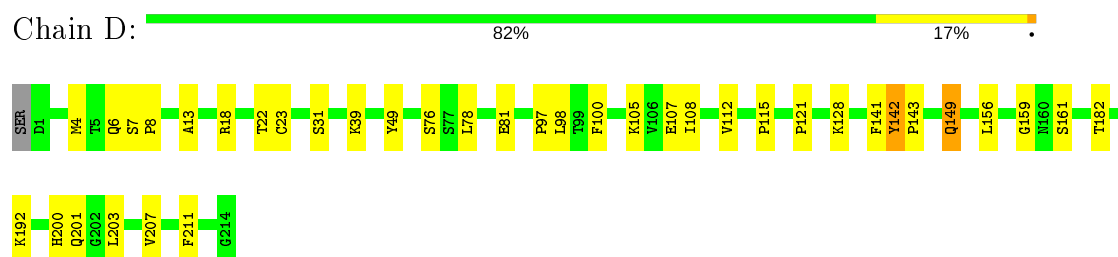
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	2	Total	O	0	0
			2	2		
4	P	5	Total	O	0	0
			5	5		
4	Q	11	Total	O	0	0
			11	11		
4	R	5	Total	O	0	0
			5	5		

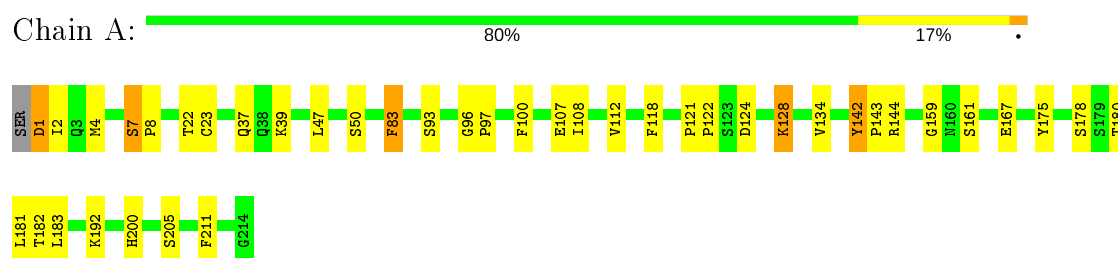
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

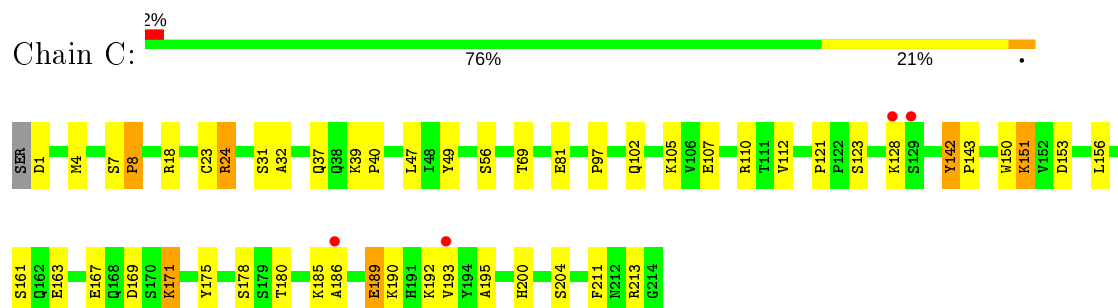
- Molecule 1: Synthetic Fab4 light chain



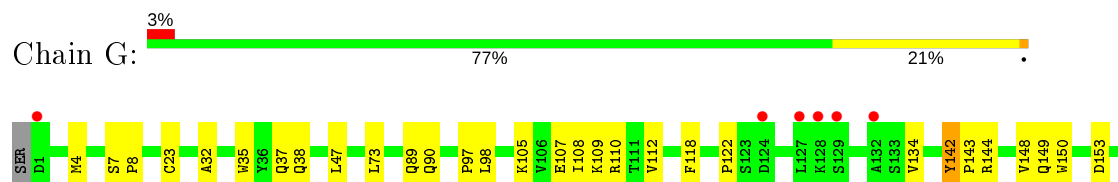
- Molecule 1: Synthetic Fab4 light chain



- Molecule 1: Synthetic Fab4 light chain

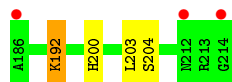
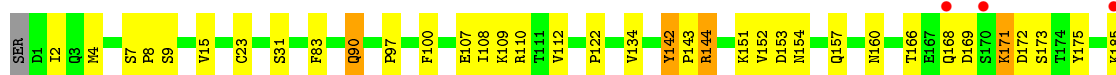
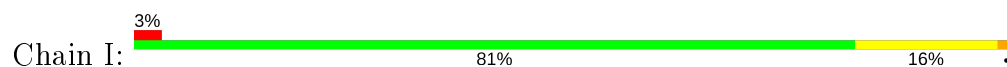


- Molecule 1: Synthetic Fab4 light chain

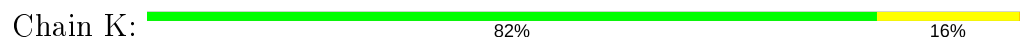




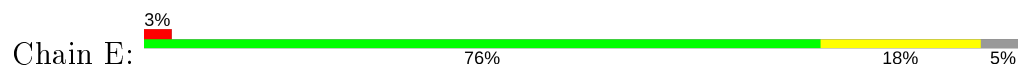
- Molecule 1: Synthetic Fab4 light chain



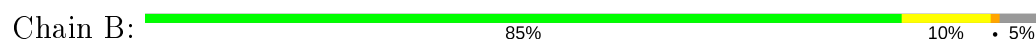
- Molecule 1: Synthetic Fab4 light chain



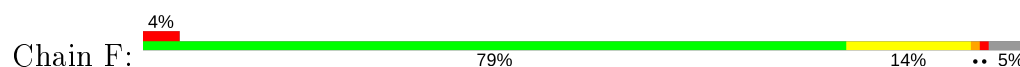
- Molecule 2: Synthetic Fab4 heavy chain



- Molecule 2: Synthetic Fab4 heavy chain

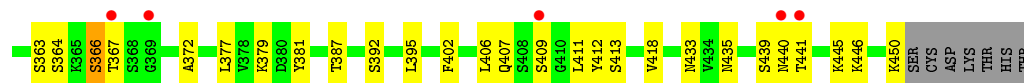
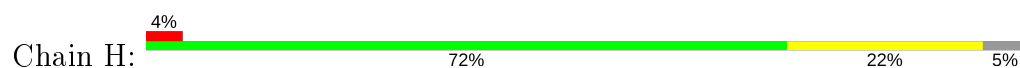


- Molecule 2: Synthetic Fab4 heavy chain

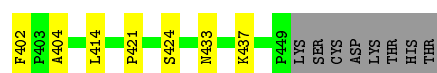
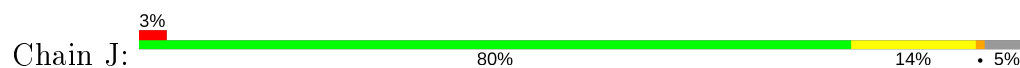




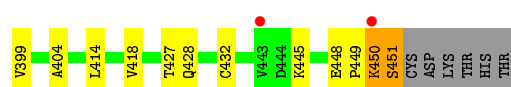
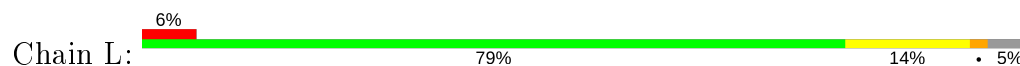
- Molecule 2: Synthetic Fab4 heavy chain



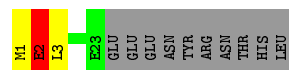
- Molecule 2: Synthetic Fab4 heavy chain



- Molecule 2: Synthetic Fab4 heavy chain



- Molecule 3: Terminase, large subunit



- Molecule 3: Terminase, large subunit



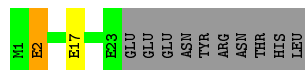
- Molecule 3: Terminase, large subunit

Chain O:  55% 15% 30%



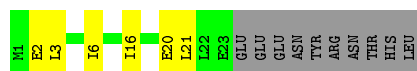
- Molecule 3: Terminase, large subunit

Chain P:  64% 1% 35%



- Molecule 3: Terminase, large subunit

Chain Q:  52% 18% 30%



- Molecule 3: Terminase, large subunit

Chain R:  52% 18% 30%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.75Å 139.33Å 163.76Å 90.00° 98.30° 90.00°	Depositor
Resolution (Å)	14.98 – 2.40 42.69 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.0 (14.98-2.40) 94.0 (42.69-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.189 , 0.239 0.194 , 0.245	Depositor DCC
R_{free} test set	1985 reflections (1.57%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22166	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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	0.53	1/1663 (0.1%)	0.74	2/2257 (0.1%)
1	C	0.56	1/1663 (0.1%)	0.90	6/2257 (0.3%)
1	D	0.54	0/1663	0.71	1/2257 (0.0%)
1	G	0.53	1/1663 (0.1%)	0.75	3/2257 (0.1%)
1	I	0.53	0/1663	0.77	2/2257 (0.1%)
1	K	0.49	0/1663	0.78	3/2257 (0.1%)
2	B	0.49	1/1798 (0.1%)	0.68	2/2455 (0.1%)
2	E	0.53	0/1783	0.72	0/2436
2	F	0.55	1/1792 (0.1%)	0.72	1/2447 (0.0%)
2	H	0.49	0/1792	0.72	1/2447 (0.0%)
2	J	0.51	1/1783 (0.1%)	0.73	3/2436 (0.1%)
2	L	0.51	1/1798 (0.1%)	0.74	5/2455 (0.2%)
3	M	0.48	0/185	0.87	1/249 (0.4%)
3	N	0.59	0/185	0.77	0/249
3	O	0.48	0/185	0.70	0/249
3	P	0.41	0/185	0.60	0/249
3	Q	0.48	0/185	0.67	0/249
3	R	0.44	0/185	0.70	0/249
All	All	0.52	7/21834 (0.0%)	0.75	30/29712 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
1	D	0	2
1	G	0	2
1	I	0	2
1	K	0	2
2	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	13

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	315	CYS	CB-SG	-6.79	1.70	1.82
2	L	315	CYS	CB-SG	-6.52	1.71	1.82
2	F	249	TYR	CE2-CZ	-6.41	1.30	1.38
1	C	189	GLU	CB-CG	6.29	1.64	1.52
1	G	38	GLN	C-N	-5.80	1.20	1.34
1	A	128	LYS	CG-CD	5.77	1.72	1.52
2	J	315	CYS	CB-SG	-5.37	1.73	1.81

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	189	GLU	CA-CB-CG	11.38	138.44	113.40
2	J	365	LYS	CD-CE-NZ	9.18	132.82	111.70
2	L	306	ARG	NE-CZ-NH1	8.80	124.70	120.30
2	J	365	LYS	CG-CD-CE	-8.64	85.98	111.90
2	L	306	ARG	CG-CD-NE	8.28	129.19	111.80
1	C	105	LYS	CD-CE-NZ	-8.26	92.70	111.70
3	M	2	GLU	CA-CB-CG	8.18	131.40	113.40
1	G	109	LYS	CA-CB-CG	7.49	129.88	113.40
1	K	187	ASP	CB-CG-OD2	-7.22	111.80	118.30
2	B	446	LYS	CD-CE-NZ	-7.10	95.38	111.70
2	J	220	GLU	N-CA-C	-7.05	91.97	111.00
1	C	189	GLU	N-CA-CB	6.77	122.79	110.60
1	I	100	PHE	C-N-CA	-6.75	108.12	122.30
2	L	306	ARG	CD-NE-CZ	6.35	132.49	123.60
1	A	100	PHE	C-N-CA	-6.26	109.16	122.30
1	D	100	PHE	C-N-CA	-6.13	109.43	122.30
1	K	187	ASP	CB-CG-OD1	6.12	123.80	118.30
2	H	232	GLN	CB-CA-C	-6.05	98.31	110.40
1	G	109	LYS	CD-CE-NZ	-5.91	98.11	111.70
2	L	220	GLU	N-CA-C	-5.84	95.23	111.00
2	B	332	HIS	N-CA-CB	-5.60	100.52	110.60
1	C	128	LYS	CD-CE-NZ	-5.50	99.05	111.70
1	K	204	SER	C-N-CA	5.42	135.26	121.70
1	I	192	LYS	CG-CD-CE	-5.37	95.79	111.90
1	C	171	LYS	CB-CG-CD	-5.33	97.75	111.60
2	F	249	TYR	CG-CD1-CE1	-5.32	117.04	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	LYS	N-CA-CB	-5.32	101.03	110.60
1	G	109	LYS	CB-CG-CD	-5.31	97.79	111.60
2	L	365	LYS	CD-CE-NZ	5.14	123.52	111.70
1	C	193	VAL	CG1-CB-CG2	5.12	119.08	110.90

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	TYR	Peptide
1	A	7	SER	Peptide
1	C	142	TYR	Peptide
1	C	7	SER	Peptide
1	D	142	TYR	Peptide
1	D	7	SER	Peptide
2	E	365	LYS	Peptide
1	G	142	TYR	Peptide
1	G	7	SER	Peptide
1	I	142	TYR	Peptide
1	I	7	SER	Peptide
1	K	142	TYR	Peptide
1	K	7	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1629	0	1596	23	0
1	C	1629	0	1596	36	0
1	D	1629	0	1596	26	0
1	G	1629	0	1595	30	0
1	I	1629	0	1596	31	0
1	K	1629	0	1596	25	0
2	B	1747	0	1687	18	0
2	E	1732	0	1669	48	0
2	F	1741	0	1682	52	0
2	H	1741	0	1682	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1732	0	1669	17	0
2	L	1747	0	1687	29	0
3	M	186	0	182	3	0
3	N	186	0	182	1	0
3	O	186	0	182	3	0
3	P	186	0	182	2	0
3	Q	186	0	182	3	0
3	R	186	0	182	3	0
4	A	78	0	0	1	0
4	B	62	0	0	1	0
4	C	79	0	0	2	0
4	D	116	0	0	3	0
4	E	74	0	0	2	0
4	F	45	0	0	0	0
4	G	57	0	0	2	0
4	H	27	0	0	0	0
4	I	95	0	0	5	0
4	J	75	0	0	1	0
4	K	65	0	0	0	0
4	L	30	0	0	1	0
4	M	7	0	0	0	0
4	N	3	0	0	0	0
4	O	2	0	0	0	0
4	P	5	0	0	0	0
4	Q	11	0	0	0	0
4	R	5	0	0	0	0
All	All	22166	0	20743	348	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 8.

All (348) 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:F:353:LYS:HZ2	2:F:380:ASP:CB	1.24	1.48
2:F:353:LYS:NZ	2:F:380:ASP:CB	1.82	1.38
2:F:353:LYS:NZ	2:F:380:ASP:HB3	1.31	1.37
1:C:24:ARG:NH1	1:C:69:THR:OG1	1.63	1.31
2:E:446:LYS:HE2	2:E:448:GLU:CD	1.63	1.19
2:E:446:LYS:HE2	2:E:448:GLU:OE2	1.41	1.17
2:F:353:LYS:NZ	2:F:380:ASP:O	1.85	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:446:LYS:HE2	2:E:448:GLU:CG	1.85	1.07
2:F:353:LYS:NZ	2:F:380:ASP:HB2	1.75	0.99
2:E:446:LYS:CE	2:E:448:GLU:HG3	1.94	0.97
2:E:446:LYS:CE	2:E:448:GLU:CG	2.44	0.96
2:F:249:TYR:CE1	2:F:273:TYR:CG	2.55	0.95
1:K:49:TYR:HE2	2:L:332:HIS:CE1	1.87	0.93
1:C:24:ARG:NH1	1:C:69:THR:HG1	1.69	0.89
1:G:122:PRO:HD3	1:G:134:VAL:HG12	1.52	0.89
1:C:189:GLU:HB3	1:C:213:ARG:HH21	1.40	0.86
1:C:153:ASP:OD2	1:C:192:LYS:HB3	1.77	0.84
1:K:49:TYR:CE2	2:L:332:HIS:CE1	2.67	0.83
1:C:189:GLU:HB3	1:C:213:ARG:NH2	1.94	0.82
2:F:249:TYR:OH	2:F:273:TYR:CD2	2.32	0.82
1:K:49:TYR:CE2	2:L:332:HIS:HE1	1.98	0.82
1:G:134:VAL:HG22	1:G:181:LEU:HB3	1.62	0.81
1:D:149:GLN:OE1	1:D:156:LEU:HD23	1.82	0.79
1:C:24:ARG:HH12	1:C:69:THR:HG1	1.28	0.79
2:L:448:GLU:HG3	2:L:449:PRO:HD2	1.65	0.79
1:G:190:LYS:O	1:G:191:HIS:ND1	2.18	0.77
1:K:147:LYS:HB3	1:K:199:THR:HG23	1.64	0.77
2:F:249:TYR:CE1	2:F:273:TYR:CB	2.68	0.76
1:C:189:GLU:HA	1:C:213:ARG:HE	1.49	0.76
2:F:353:LYS:HZ1	2:F:380:ASP:CB	1.93	0.76
2:F:353:LYS:HZ2	2:F:380:ASP:CA	1.99	0.75
2:E:446:LYS:CE	2:E:448:GLU:OE2	2.29	0.75
2:F:353:LYS:CD	2:F:380:ASP:O	2.35	0.74
2:F:353:LYS:HZ2	2:F:380:ASP:HB3	0.57	0.74
1:I:143:PRO:HD2	1:I:200:HIS:CE1	2.22	0.74
2:F:249:TYR:OH	2:F:273:TYR:HD2	1.70	0.73
2:J:252:TYR:HB2	2:J:318:TYR:HB2	1.71	0.72
1:C:49:TYR:CE2	2:F:332:HIS:CE1	2.78	0.72
2:F:249:TYR:HE1	2:F:273:TYR:CG	2.04	0.71
1:D:49:TYR:HE2	2:E:332:HIS:NE2	1.89	0.71
2:F:353:LYS:HZ3	2:F:380:ASP:C	1.93	0.71
2:F:353:LYS:NZ	2:F:380:ASP:C	2.43	0.71
1:I:2:ILE:CG2	1:I:90:GLN:OE1	2.40	0.69
2:L:448:GLU:HG3	2:L:449:PRO:CD	2.22	0.69
2:F:353:LYS:CE	2:F:380:ASP:O	2.40	0.69
2:H:252:TYR:HB2	2:H:318:TYR:HB2	1.73	0.69
2:H:445:LYS:HD2	2:H:446:LYS:N	2.07	0.69
1:I:151:LYS:NZ	4:I:301:HOH:O	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:GLN:HB2	1:G:197:GLU:HB3	1.75	0.69
1:K:147:LYS:HB3	1:K:199:THR:CG2	2.22	0.69
1:C:49:TYR:HE2	2:F:332:HIS:CE1	2.10	0.69
2:F:249:TYR:CE1	2:F:273:TYR:HB2	2.28	0.68
2:F:249:TYR:C	2:F:249:TYR:CD2	2.67	0.68
1:I:144:ARG:NH1	4:I:302:HOH:O	2.26	0.68
1:C:151:LYS:HG3	1:C:195:ALA:HB3	1.75	0.68
2:F:353:LYS:NZ	2:F:380:ASP:CA	2.55	0.67
2:F:249:TYR:CZ	2:F:273:TYR:CB	2.77	0.67
2:E:220:GLU:HG3	2:E:221:VAL:H	1.58	0.67
2:E:326:LYS:NZ	4:E:502:HOH:O	2.27	0.66
1:D:143:PRO:HD2	1:D:200:HIS:CE1	2.30	0.66
2:F:249:TYR:O	2:F:249:TYR:CD2	2.49	0.66
1:G:143:PRO:HD2	1:G:200:HIS:CE1	2.31	0.66
1:A:143:PRO:HD2	1:A:200:HIS:CE1	2.31	0.65
1:C:189:GLU:HA	1:C:213:ARG:NE	2.12	0.65
1:C:189:GLU:CB	1:C:213:ARG:HH21	2.08	0.65
2:H:355:PRO:HB3	2:H:381:TYR:HB3	1.79	0.64
1:C:163:GLU:OE2	4:C:301:HOH:O	2.14	0.64
1:C:39:LYS:NZ	1:C:81:GLU:O	2.30	0.64
2:E:359:PRO:HD3	2:E:445:LYS:HE3	1.80	0.64
2:E:446:LYS:HE3	2:E:448:GLU:HG3	1.76	0.64
2:H:392:SER:H	2:H:433:ASN:ND2	1.96	0.64
2:J:221:VAL:HG22	2:J:246:PHE:HB3	1.78	0.63
2:E:446:LYS:CD	2:E:448:GLU:HG3	2.27	0.63
2:B:252:TYR:HB2	2:B:318:TYR:HB2	1.79	0.63
2:B:430:TYR:H	2:B:446:LYS:NZ	1.96	0.63
1:I:2:ILE:HG22	1:I:90:GLN:OE1	1.97	0.63
2:L:308:GLU:N	2:L:308:GLU:OE1	2.31	0.62
1:C:143:PRO:HD2	1:C:200:HIS:CE1	2.34	0.62
2:F:249:TYR:C	2:F:249:TYR:HD2	2.00	0.62
2:H:392:SER:H	2:H:433:ASN:HD21	1.45	0.62
2:F:249:TYR:CE1	2:F:273:TYR:CD2	2.87	0.62
2:F:359:PRO:HD3	2:F:445:LYS:HE3	1.82	0.61
2:J:437:LYS:NZ	4:J:504:HOH:O	2.32	0.61
2:E:399:VAL:HG22	2:E:418:VAL:HG12	1.82	0.61
1:C:185:LYS:HD3	1:C:189:GLU:OE2	2.00	0.61
2:F:353:LYS:HZ3	2:F:380:ASP:CB	2.07	0.61
2:H:407:GLN:HB2	2:H:409:SER:HB3	1.83	0.60
2:F:249:TYR:CZ	2:F:273:TYR:CD2	2.89	0.60
1:I:122:PRO:HD3	1:I:134:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:97:PRO:HA	2:L:266:TRP:CZ3	2.37	0.60
2:F:353:LYS:HZ1	2:F:380:ASP:HB2	1.57	0.60
2:B:430:TYR:H	2:B:446:LYS:HZ1	1.48	0.60
1:C:110:ARG:HB2	4:C:307:HOH:O	2.02	0.59
2:L:448:GLU:HG3	2:L:449:PRO:N	2.17	0.59
1:K:122:PRO:HD3	1:K:134:VAL:HG22	1.83	0.59
1:A:107:GLU:HG2	1:A:108:ILE:N	2.18	0.59
2:J:355:PRO:HB3	2:J:381:TYR:HB3	1.83	0.59
1:G:185:LYS:NZ	1:G:189:GLU:OE1	2.36	0.59
1:I:168:GLN:HG3	1:I:175:TYR:CE2	2.37	0.59
2:E:325:TYR:O	3:M:1:MET:N	2.34	0.59
1:D:18:ARG:NH2	4:D:307:HOH:O	2.35	0.59
2:F:249:TYR:O	2:F:249:TYR:HD2	1.86	0.59
2:F:353:LYS:HD3	2:F:354:GLY:O	2.03	0.59
1:K:107:GLU:HG3	1:K:175:TYR:OH	2.03	0.59
2:E:349:SER:OG	1:C:18:ARG:NH2	2.36	0.58
2:H:395:LEU:HD21	2:H:418:VAL:HG21	1.85	0.58
2:H:295:LYS:NZ	2:H:299:TYR:OH	2.18	0.58
2:F:325:TYR:O	3:O:1:MET:N	2.37	0.58
1:K:143:PRO:HD2	1:K:200:HIS:CE1	2.37	0.58
2:L:450:LYS:HE2	2:L:451:SER:H	1.68	0.58
1:K:144:ARG:HB2	1:K:175:TYR:CE2	2.39	0.58
1:A:112:VAL:HA	1:A:142:TYR:O	2.04	0.58
1:I:185:LYS:NZ	4:I:308:HOH:O	2.37	0.57
2:F:252:TYR:HB2	2:F:318:TYR:HB2	1.86	0.57
2:H:310:THR:HG23	2:H:346:THR:HA	1.85	0.57
1:I:168:GLN:HG3	1:I:175:TYR:CZ	2.39	0.57
2:F:220:GLU:OE1	2:F:221:VAL:N	2.36	0.57
1:I:83:PHE:CE1	1:I:168:GLN:HB3	2.39	0.57
2:L:363:SER:OG	2:L:365:LYS:HG3	2.04	0.57
3:R:16:ILE:O	3:R:20:GLU:HG3	2.04	0.57
2:E:446:LYS:HD3	2:E:448:GLU:HG3	1.86	0.57
1:I:109:LYS:NZ	4:I:309:HOH:O	2.38	0.56
2:J:222:GLN:HB2	2:J:244:SER:OG	2.05	0.56
2:E:399:VAL:HG22	2:E:418:VAL:CG1	2.35	0.56
1:D:49:TYR:CE2	2:E:332:HIS:CE1	2.94	0.56
1:G:167:GLU:HA	4:G:325:HOH:O	2.04	0.56
2:E:445:LYS:HE2	4:E:524:HOH:O	2.05	0.56
2:E:256:VAL:HG21	2:E:336:MET:HE1	1.87	0.56
2:J:281:ASP:HA	2:J:284:LYS:HG3	1.87	0.56
1:A:144:ARG:HB2	1:A:175:TYR:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:VAL:HG12	1:G:198:VAL:HG22	1.87	0.56
2:B:302:MET:HB3	2:B:305:LEU:HD21	1.86	0.55
1:A:124:ASP:O	1:A:128:LYS:HB2	2.06	0.55
1:D:39:LYS:NZ	1:D:81:GLU:O	2.34	0.55
1:I:154:ASN:HB3	4:I:301:HOH:O	2.06	0.55
1:A:97:PRO:HA	2:B:266:TRP:CZ3	2.42	0.55
3:Q:3:LEU:HA	3:Q:6:ILE:HD12	1.88	0.55
1:G:97:PRO:HA	2:H:266:TRP:CZ3	2.42	0.55
2:E:367:THR:HG22	2:E:368:SER:H	1.72	0.55
2:F:249:TYR:CZ	2:F:273:TYR:HB3	2.41	0.55
2:J:231:VAL:HG21	2:J:237:LEU:HG	1.89	0.55
2:E:252:TYR:HB2	2:E:318:TYR:HB2	1.89	0.55
1:A:7:SER:OG	1:A:22:THR:HB	2.08	0.54
2:H:409:SER:OG	2:H:411:LEU:HD13	2.08	0.54
2:E:446:LYS:HE3	2:E:448:GLU:CG	2.31	0.54
1:G:118:PHE:HD1	2:H:366:SER:HA	1.72	0.54
2:L:404:ALA:HA	2:L:414:LEU:HB3	1.90	0.54
2:E:316:ALA:HB3	2:E:336:MET:CE	2.38	0.54
2:F:353:LYS:HD2	2:F:380:ASP:O	2.07	0.54
1:D:49:TYR:HE2	2:E:332:HIS:CE1	2.25	0.54
2:E:390:TRP:CH2	2:E:432:CYS:HB3	2.43	0.53
2:F:249:TYR:CZ	2:F:273:TYR:CG	2.95	0.53
2:H:222:GLN:HB2	2:H:244:SER:HB2	1.90	0.53
1:I:4:MET:HB3	1:I:23:CYS:SG	2.49	0.53
2:E:259:ALA:HB3	2:E:262:LYS:HE3	1.90	0.53
2:B:446:LYS:HD2	2:B:447:VAL:N	2.24	0.53
1:C:4:MET:HB3	1:C:23:CYS:SG	2.49	0.53
1:I:90:GLN:O	1:I:90:GLN:HG3	2.09	0.53
2:F:366:SER:O	2:F:368:SER:N	2.42	0.53
2:J:310:THR:HG23	2:J:346:THR:HA	1.91	0.53
2:E:220:GLU:CG	2:E:221:VAL:H	2.20	0.53
2:H:286:ARG:NE	2:H:306:ARG:HH21	2.07	0.53
1:I:153:ASP:OD2	1:I:192:LYS:N	2.42	0.53
1:A:39:LYS:HE3	1:A:83:PHE:O	2.09	0.52
1:G:110:ARG:HG3	1:G:142:TYR:CD2	2.45	0.52
1:G:89:GLN:NE2	1:G:98:LEU:HD23	2.24	0.52
3:N:6:ILE:HD12	3:N:6:ILE:H	1.75	0.52
1:D:4:MET:HB3	1:D:23:CYS:SG	2.50	0.51
2:H:221:VAL:HG11	2:H:338:TYR:CD1	2.46	0.51
1:G:185:LYS:HD3	1:G:189:GLU:HG3	1.92	0.51
1:G:107:GLU:HG3	1:G:175:TYR:OH	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:220:GLU:OE2	2:E:220:GLU:HA	2.10	0.51
1:G:107:GLU:HG2	1:G:108:ILE:N	2.26	0.51
1:A:167:GLU:HA	4:A:330:HOH:O	2.11	0.50
2:E:320:TRP:CZ2	3:M:2:GLU:HG2	2.47	0.50
2:E:249:TYR:CE2	2:E:293:THR:HB	2.47	0.50
2:H:445:LYS:HD2	2:H:446:LYS:H	1.76	0.50
1:D:143:PRO:HG3	1:D:201:GLN:NE2	2.27	0.49
1:K:12:SER:OG	1:K:107:GLU:OE1	2.29	0.49
1:D:115:PRO:HB3	1:D:141:PHE:CD1	2.48	0.49
1:G:134:VAL:CG2	1:G:181:LEU:HB3	2.38	0.49
1:K:169:ASP:OD1	1:K:171:LYS:HB2	2.12	0.49
2:E:316:ALA:HB3	2:E:336:MET:HE2	1.94	0.49
1:C:40:PRO:CB	1:C:167:GLU:HG3	2.43	0.49
2:L:355:PRO:HB3	2:L:381:TYR:HB3	1.95	0.49
2:F:246:PHE:HE2	2:F:251:SER:HG	1.57	0.49
2:H:439:SER:OG	2:H:441:THR:OG1	2.27	0.49
2:L:367:THR:O	2:L:370:GLY:N	2.46	0.49
1:I:107:GLU:HG3	1:I:175:TYR:OH	2.13	0.49
1:D:31:SER:HG	2:E:333:PHE:HE2	1.60	0.48
1:G:32:ALA:O	1:G:90:GLN:HA	2.13	0.48
1:K:112:VAL:HA	1:K:142:TYR:O	2.13	0.48
1:C:112:VAL:HA	1:C:142:TYR:O	2.13	0.48
1:D:112:VAL:HA	1:D:142:TYR:O	2.14	0.48
2:L:390:TRP:CH2	2:L:432:CYS:HB3	2.48	0.48
2:E:323:VAL:HG13	3:M:3:LEU:HB2	1.95	0.48
1:C:107:GLU:HG3	1:C:175:TYR:OH	2.13	0.48
2:E:221:VAL:HG13	2:E:246:PHE:CD1	2.49	0.48
1:I:2:ILE:HB	1:I:90:GLN:OE1	2.12	0.48
2:F:355:PRO:HB3	2:F:381:TYR:HB3	1.96	0.47
1:I:112:VAL:HA	1:I:142:TYR:O	2.14	0.47
2:B:446:LYS:HZ2	2:B:447:VAL:C	2.16	0.47
1:K:107:GLU:HG2	1:K:108:ILE:N	2.29	0.47
1:A:4:MET:HB3	1:A:23:CYS:SG	2.55	0.47
1:G:112:VAL:HA	1:G:142:TYR:O	2.14	0.47
1:G:37:GLN:HB2	1:G:47:LEU:HD11	1.96	0.47
2:J:225:GLU:HA	2:J:240:SER:O	2.14	0.47
1:C:24:ARG:CZ	1:C:69:THR:OG1	2.54	0.47
2:H:387:THR:CG2	2:H:435:ASN:HB3	2.44	0.47
1:C:32:ALA:HB2	2:F:333:PHE:CD1	2.50	0.47
2:H:379:LYS:HG3	2:H:413:SER:HB2	1.97	0.47
1:I:15:VAL:HA	1:I:108:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:SER:OG	2:B:250:SER:O	2.29	0.47
2:E:221:VAL:HG13	2:E:246:PHE:HD1	1.78	0.47
2:E:249:TYR:HD2	2:E:249:TYR:N	2.13	0.47
2:F:302:MET:HB3	2:F:305:LEU:HD21	1.95	0.47
2:B:286:ARG:HB3	2:B:303:ASN:O	2.15	0.47
1:K:210:SER:O	2:L:365:LYS:HE3	2.15	0.47
1:D:161:SER:HB3	4:D:350:HOH:O	2.16	0.46
1:G:190:LYS:NZ	4:G:308:HOH:O	2.48	0.46
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.97	0.46
1:G:4:MET:HB3	1:G:23:CYS:SG	2.55	0.46
1:D:159:GLY:O	1:C:8:PRO:HA	2.15	0.46
2:L:363:SER:OG	2:L:364:SER:N	2.48	0.46
2:H:320:TRP:CH2	3:P:2:GLU:HG2	2.50	0.46
1:A:1:ASP:CG	1:A:2:ILE:H	2.19	0.46
1:I:110:ARG:HD2	1:I:173:SER:HB2	1.97	0.46
1:A:121:PRO:HB3	1:A:211:PHE:CE2	2.50	0.46
1:C:123:SER:OG	2:F:358:PHE:HB3	2.16	0.46
1:G:134:VAL:HG23	1:G:150:TRP:CH2	2.51	0.46
1:G:153:ASP:HA	1:G:193:VAL:HG12	1.98	0.46
1:K:144:ARG:HH12	1:K:165:VAL:HG21	1.80	0.46
2:B:237:LEU:HD22	4:B:528:HOH:O	2.16	0.46
2:H:363:SER:O	2:H:367:THR:HG23	2.16	0.46
3:Q:16:ILE:O	3:Q:20:GLU:HG3	2.15	0.46
1:D:107:GLU:HG2	1:D:108:ILE:N	2.30	0.46
1:I:97:PRO:HA	2:J:266:TRP:CZ3	2.51	0.46
1:K:177:LEU:HD23	1:K:178:SER:N	2.31	0.46
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.98	0.45
2:H:450:LYS:HE2	2:H:450:LYS:HA	1.97	0.45
2:L:399:VAL:HG22	2:L:418:VAL:HG22	1.98	0.45
1:C:150:TRP:O	1:C:156:LEU:HD12	2.17	0.45
2:L:302:MET:HB3	2:L:305:LEU:HD21	1.98	0.45
1:A:107:GLU:HG3	1:A:175:TYR:OH	2.17	0.45
2:H:250:SER:OG	2:H:250:SER:O	2.26	0.45
2:L:364:SER:C	2:L:366:SER:H	2.19	0.45
1:C:97:PRO:HA	2:F:266:TRP:CZ3	2.52	0.45
1:K:210:SER:O	2:L:365:LYS:CE	2.64	0.45
2:B:221:VAL:HG13	2:B:246:PHE:CD1	2.52	0.45
1:C:49:TYR:CD2	2:F:332:HIS:CE1	3.05	0.45
1:K:37:GLN:HB2	1:K:47:LEU:HD11	1.99	0.45
1:A:122:PRO:HD3	1:A:134:VAL:HG22	1.99	0.45
2:E:379:LYS:HE2	2:E:379:LYS:HB2	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2:ILE:CB	1:I:90:GLN:OE1	2.66	0.44
2:L:427:THR:OG1	2:L:428:GLN:N	2.50	0.44
2:H:221:VAL:HG11	2:H:338:TYR:CE1	2.53	0.44
2:H:240:SER:HB3	2:H:299:TYR:CE1	2.52	0.44
2:B:237:LEU:HA	2:B:237:LEU:HD23	1.74	0.44
1:I:168:GLN:HB2	1:I:175:TYR:CE1	2.52	0.44
2:J:306:ARG:NH2	3:P:17:GLU:OE1	2.49	0.44
2:E:420:VAL:HG11	2:E:430:TYR:CE1	2.52	0.44
2:H:406:LEU:HD23	2:H:412:TYR:CE1	2.52	0.44
1:A:118:PHE:CD1	2:B:366:SER:HA	2.51	0.44
1:C:143:PRO:HD2	1:C:200:HIS:NE2	2.32	0.44
2:J:255:TRP:HD1	2:J:289:ILE:HD12	1.83	0.44
3:R:6:ILE:HG22	3:R:10:LEU:HD11	1.99	0.44
2:H:302:MET:HB3	2:H:305:LEU:HD21	2.00	0.44
2:H:379:LYS:HE2	2:H:407:GLN:OE1	2.18	0.43
2:L:246:PHE:HB2	2:L:317:ARG:NH2	2.33	0.43
1:C:186:ALA:HB1	1:C:190:LYS:HE3	1.99	0.43
1:I:168:GLN:HB2	1:I:175:TYR:CZ	2.53	0.43
1:D:49:TYR:HE2	2:E:332:HIS:HE2	1.62	0.43
2:E:249:TYR:CD2	2:E:249:TYR:N	2.86	0.43
1:G:188:TYR:CZ	1:G:213:ARG:HG3	2.53	0.43
1:I:203:LEU:HD23	1:I:203:LEU:HA	1.81	0.43
2:E:368:SER:O	2:E:423:SER:OG	2.35	0.43
1:I:166:THR:HG23	2:J:402:PHE:CE1	2.52	0.43
2:F:249:TYR:HE1	2:F:273:TYR:CD2	2.31	0.43
2:H:231:VAL:HG11	2:H:305:LEU:HD13	1.99	0.43
1:D:182:THR:OG1	4:D:301:HOH:O	2.18	0.43
2:H:237:LEU:HA	2:H:237:LEU:HD23	1.83	0.43
1:I:143:PRO:HD2	1:I:200:HIS:NE2	2.32	0.43
1:A:181:LEU:HG	1:A:183:LEU:CD1	2.49	0.43
3:O:3:LEU:HA	3:O:6:ILE:HD12	2.00	0.42
2:B:367:THR:HA	2:B:372:ALA:HA	2.01	0.42
2:B:446:LYS:HD2	2:B:447:VAL:H	1.84	0.42
2:L:308:GLU:H	2:L:308:GLU:CD	2.18	0.42
1:A:93:SER:OG	1:A:96:GLY:HA3	2.19	0.42
2:B:446:LYS:NZ	2:B:447:VAL:O	2.43	0.42
1:A:182:THR:C	1:A:183:LEU:HD12	2.39	0.42
1:K:210:SER:O	2:L:365:LYS:NZ	2.52	0.42
1:K:4:MET:HB3	1:K:23:CYS:SG	2.58	0.42
3:R:20:GLU:HA	3:R:23:GLU:HG3	2.01	0.42
1:A:143:PRO:HD2	1:A:200:HIS:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:TYR:CE2	2:E:332:HIS:NE2	2.79	0.42
2:H:252:TYR:CE1	2:H:272:PRO:HD2	2.54	0.42
3:Q:21:LEU:HD23	3:Q:21:LEU:HA	1.92	0.42
1:A:161:SER:HA	1:A:180:THR:O	2.19	0.42
2:B:355:PRO:HB3	2:B:381:TYR:HB3	2.01	0.42
1:D:203:LEU:HD22	1:D:207:VAL:HG21	2.01	0.42
2:F:446:LYS:HE3	2:F:448:GLU:OE1	2.20	0.42
1:G:144:ARG:HB2	1:G:175:TYR:CE2	2.55	0.42
2:J:421:PRO:O	2:J:424:SER:OG	2.34	0.42
1:C:121:PRO:HB3	1:C:211:PHE:CE2	2.55	0.42
1:C:189:GLU:CG	1:C:213:ARG:HH21	2.33	0.42
2:E:316:ALA:CB	2:E:336:MET:HE2	2.49	0.42
2:J:256:VAL:HG21	2:J:336:MET:HE1	2.01	0.42
1:D:97:PRO:HA	2:E:266:TRP:CZ3	2.55	0.41
2:F:367:THR:O	2:F:367:THR:CG2	2.68	0.41
1:G:35:TRP:CD2	1:G:73:LEU:HB2	2.54	0.41
1:I:160:ASN:OD1	1:I:160:ASN:N	2.53	0.41
1:C:161:SER:HA	1:C:180:THR:O	2.20	0.41
2:E:372:ALA:O	2:E:419:THR:HA	2.20	0.41
2:H:357:VAL:HA	2:H:377:LEU:O	2.20	0.41
1:K:127:LEU:O	1:K:185:LYS:HD3	2.20	0.41
2:L:255:TRP:O	2:L:267:VAL:HG22	2.21	0.41
1:D:203:LEU:HD13	1:D:207:VAL:HG23	2.01	0.41
2:H:367:THR:HG22	2:H:372:ALA:HB2	2.01	0.41
1:D:98:LEU:HD12	2:E:266:TRP:CD1	2.55	0.41
1:A:159:GLY:HA3	3:O:11:SER:HB2	2.02	0.41
1:G:98:LEU:HB2	2:H:266:TRP:CG	2.55	0.41
1:K:144:ARG:NH1	1:K:165:VAL:HG21	2.35	0.41
1:K:78:LEU:HD21	1:K:108:ILE:HD13	2.02	0.41
2:L:225:GLU:H	2:L:341:GLN:HE22	1.69	0.41
1:D:121:PRO:HB3	1:D:211:PHE:CE2	2.55	0.41
2:H:292:ASP:OD2	2:H:295:LYS:HE3	2.20	0.41
1:I:110:ARG:HG3	1:I:142:TYR:CD2	2.56	0.41
2:J:404:ALA:HA	2:J:414:LEU:HB3	2.03	0.41
1:D:6:GLN:HA	1:D:22:THR:O	2.21	0.41
2:H:364:SER:HA	2:H:367:THR:OG1	2.20	0.41
2:F:429:THR:HG22	2:F:446:LYS:NZ	2.36	0.41
2:J:231:VAL:O	2:J:347:VAL:HA	2.21	0.41
1:A:7:SER:HG	1:A:22:THR:HB	1.85	0.41
1:G:165:VAL:HG22	1:G:177:LEU:HD12	2.03	0.41
2:L:264:LEU:N	4:L:504:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:ALA:HB3	1:D:78:LEU:HD22	2.03	0.40
2:F:388:VAL:HG22	2:F:434:VAL:HG22	2.01	0.40
1:I:169:ASP:OD1	1:I:171:LYS:N	2.46	0.40
2:B:247:ASN:HB3	2:B:250:SER:HB3	2.03	0.40
1:G:32:ALA:HB2	2:H:333:PHE:CD1	2.56	0.40
1:I:152:VAL:HG23	1:I:157:GLN:HG3	2.03	0.40
1:C:169:ASP:OD1	1:C:171:LYS:HD3	2.22	0.40
2:F:231:VAL:HG11	2:F:305:LEU:HD13	2.02	0.40
2:L:395:LEU:HD21	2:L:418:VAL:HG11	2.02	0.40
1:D:18:ARG:HG3	1:D:76:SER:HA	2.04	0.40
2:E:355:PRO:HD2	2:E:441:THR:HG21	2.02	0.40
1:G:178:SER:HB2	2:H:402:PHE:CZ	2.56	0.40
1:K:32:ALA:HB2	2:L:333:PHE:CD1	2.57	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	212/215 (99%)	201 (95%)	10 (5%)	1 (0%)	29	41
1	C	212/215 (99%)	198 (93%)	13 (6%)	1 (0%)	29	41
1	D	212/215 (99%)	205 (97%)	6 (3%)	1 (0%)	29	41
1	G	212/215 (99%)	204 (96%)	7 (3%)	1 (0%)	29	41
1	I	212/215 (99%)	203 (96%)	8 (4%)	1 (0%)	29	41
1	K	212/215 (99%)	201 (95%)	10 (5%)	1 (0%)	29	41
2	B	230/243 (95%)	220 (96%)	10 (4%)	0	100	100
2	E	228/243 (94%)	223 (98%)	5 (2%)	0	100	100
2	F	229/243 (94%)	219 (96%)	9 (4%)	1 (0%)	34	48
2	H	229/243 (94%)	222 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	228/243 (94%)	221 (97%)	6 (3%)	1 (0%)	34	48
2	L	230/243 (95%)	224 (97%)	6 (3%)	0	100	100
3	M	21/33 (64%)	21 (100%)	0	0	100	100
3	N	21/33 (64%)	21 (100%)	0	0	100	100
3	O	21/33 (64%)	21 (100%)	0	0	100	100
3	P	21/33 (64%)	21 (100%)	0	0	100	100
3	Q	21/33 (64%)	21 (100%)	0	0	100	100
3	R	21/33 (64%)	21 (100%)	0	0	100	100
All	All	2772/2946 (94%)	2667 (96%)	97 (4%)	8 (0%)	41	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	8	PRO
1	D	8	PRO
1	A	8	PRO
1	C	8	PRO
1	G	8	PRO
1	K	8	PRO
2	F	367	THR
2	J	245	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	188/189 (100%)	182 (97%)	6 (3%)	39	59
1	C	188/189 (100%)	180 (96%)	8 (4%)	29	46
1	D	188/189 (100%)	184 (98%)	4 (2%)	53	72
1	G	188/189 (100%)	183 (97%)	5 (3%)	44	65
1	I	188/189 (100%)	181 (96%)	7 (4%)	34	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	188/189 (100%)	182 (97%)	6 (3%)	39	59
2	B	194/205 (95%)	189 (97%)	5 (3%)	46	66
2	E	192/205 (94%)	185 (96%)	7 (4%)	35	54
2	F	193/205 (94%)	182 (94%)	11 (6%)	20	33
2	H	193/205 (94%)	189 (98%)	4 (2%)	53	72
2	J	192/205 (94%)	187 (97%)	5 (3%)	46	66
2	L	194/205 (95%)	186 (96%)	8 (4%)	30	48
3	M	22/32 (69%)	21 (96%)	1 (4%)	27	44
3	N	22/32 (69%)	21 (96%)	1 (4%)	27	44
3	O	22/32 (69%)	21 (96%)	1 (4%)	27	44
3	P	22/32 (69%)	21 (96%)	1 (4%)	27	44
3	Q	22/32 (69%)	21 (96%)	1 (4%)	27	44
3	R	22/32 (69%)	21 (96%)	1 (4%)	27	44
All	All	2418/2556 (95%)	2336 (97%)	82 (3%)	37	56

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	105	LYS
1	D	128	LYS
1	D	149	GLN
1	D	192	LYS
2	E	244	SER
2	E	284	LYS
2	E	295	LYS
2	E	317	ARG
2	E	363	SER
2	E	422	SER
2	E	446	LYS
1	A	1	ASP
1	A	50	SER
1	A	83	PHE
1	A	178	SER
1	A	192	LYS
1	A	205	SER
2	B	236	SER
2	B	317	ARG

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Mol	Chain	Res	Type
2	B	366	SER
2	B	368	SER
2	B	433	ASN
1	C	1	ASP
1	C	24	ARG
1	C	31	SER
1	C	56	SER
1	C	102	GLN
1	C	151	LYS
1	C	178	SER
1	C	204	SER
2	F	247	ASN
2	F	249	TYR
2	F	284	LYS
2	F	306	ARG
2	F	317	ARG
2	F	332	HIS
2	F	366	SER
2	F	367	THR
2	F	397	SER
2	F	422	SER
2	F	433	ASN
1	G	105	LYS
1	G	161	SER
1	G	183	LEU
1	G	190	LYS
1	G	213	ARG
2	H	226	SER
2	H	317	ARG
2	H	366	SER
2	H	440	ASN
1	I	9	SER
1	I	31	SER
1	I	90	GLN
1	I	144	ARG
1	I	171	LYS
1	I	172	ASP
1	I	204	SER
2	J	236	SER
2	J	237	LEU
2	J	306	ARG
2	J	317	ARG

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Mol	Chain	Res	Type
2	J	433	ASN
1	K	7	SER
1	K	31	SER
1	K	102	GLN
1	K	144	ARG
1	K	158	SER
1	K	196	CYS
2	L	220	GLU
2	L	250	SER
2	L	295	LYS
2	L	317	ARG
2	L	332	HIS
2	L	445	LYS
2	L	450	LYS
2	L	451	SER
3	M	2	GLU
3	N	12	ASP
3	O	2	GLU
3	P	2	GLU
3	Q	2	GLU
3	R	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	201	GLN
2	F	247	ASN
2	F	332	HIS
2	H	433	ASN
2	H	440	ASN
2	L	332	HIS
2	L	435	ASN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	214/215 (99%)	-0.16	0 100 100	27, 42, 71, 81	0
1	C	214/215 (99%)	0.08	4 (1%) 66 64	27, 44, 95, 117	0
1	D	214/215 (99%)	-0.17	0 100 100	28, 41, 61, 83	0
1	G	214/215 (99%)	-0.04	6 (2%) 53 51	31, 53, 87, 109	0
1	I	214/215 (99%)	0.07	6 (2%) 53 51	27, 45, 82, 97	0
1	K	214/215 (99%)	-0.19	1 (0%) 91 89	35, 51, 75, 92	0
2	B	232/243 (95%)	-0.24	1 (0%) 92 91	27, 47, 70, 92	0
2	E	230/243 (94%)	-0.13	8 (3%) 44 43	29, 45, 76, 110	0
2	F	231/243 (95%)	-0.02	10 (4%) 35 33	32, 56, 85, 119	0
2	H	231/243 (95%)	0.10	9 (3%) 39 38	36, 62, 84, 95	0
2	J	230/243 (94%)	-0.12	8 (3%) 44 43	29, 46, 68, 103	0
2	L	232/243 (95%)	0.16	14 (6%) 21 20	39, 65, 92, 125	0
3	M	23/33 (69%)	-0.40	0 100 100	34, 43, 54, 62	0
3	N	23/33 (69%)	-0.42	0 100 100	38, 47, 61, 63	0
3	O	23/33 (69%)	-0.48	0 100 100	34, 42, 54, 59	0
3	P	23/33 (69%)	-0.35	0 100 100	39, 49, 65, 69	0
3	Q	23/33 (69%)	-0.32	0 100 100	33, 42, 52, 62	0
3	R	23/33 (69%)	-0.40	0 100 100	43, 55, 70, 72	0
All	All	2808/2946 (95%)	-0.07	67 (2%) 59 57	27, 50, 82, 125	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	366	SER	10.3
1	I	170	SER	5.8
2	F	249	TYR	5.6

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Mol	Chain	Res	Type	RSRZ
2	L	369	GLY	5.1
2	E	368	SER	4.7
2	E	365	LYS	4.6
2	L	367	THR	4.4
2	E	366	SER	3.9
2	F	366	SER	3.9
2	F	368	SER	3.8
2	J	368	SER	3.8
1	C	193	VAL	3.8
2	J	367	THR	3.6
2	J	365	LYS	3.6
2	L	368	SER	3.5
1	C	186	ALA	3.5
1	G	127	LEU	3.5
2	L	365	LYS	3.5
2	E	367	THR	3.4
1	G	129	SER	3.4
2	F	367	THR	3.3
2	H	440	ASN	3.3
2	F	365	LYS	3.3
2	E	364	SER	3.1
2	B	369	GLY	3.1
2	L	220	GLU	3.1
2	H	369	GLY	3.1
2	L	364	SER	3.0
2	H	367	THR	3.0
1	C	128	LYS	3.0
2	F	220	GLU	2.9
2	L	349	SER	2.9
1	I	214	GLY	2.8
2	E	249	TYR	2.8
2	H	441	THR	2.6
2	J	366	SER	2.6
2	J	220	GLU	2.5
2	F	349	SER	2.5
1	C	129	SER	2.5
2	H	295	LYS	2.5
1	G	128	LYS	2.4
1	K	127	LEU	2.4
2	J	364	SER	2.4
2	F	450	LYS	2.4
1	G	124	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	L	351	SER	2.4
2	L	246	PHE	2.3
2	F	364	SER	2.3
2	L	443	VAL	2.2
2	H	409	SER	2.2
2	E	220	GLU	2.2
1	I	185	LYS	2.2
2	L	450	LYS	2.2
1	G	132	ALA	2.2
1	I	186	ALA	2.2
2	J	369	GLY	2.2
2	F	426	GLY	2.1
1	G	1	ASP	2.1
2	H	328	TYR	2.1
2	H	249	TYR	2.1
2	H	232	GLN	2.1
2	E	294	SER	2.1
2	L	332	HIS	2.1
1	I	212	ASN	2.1
1	I	168	GLN	2.0
2	L	245	GLY	2.0
2	J	336	MET	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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.