Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2024 – 10:15 AM EDT

PDB ID	:	8ULF
Title	:	Crystal structure of Plasmodium vivax CelTOS in complex with antibody 7g7
Authors	:	Tang, W.K.; Tolia, N.H.
Deposited on	:	2023-10-16
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

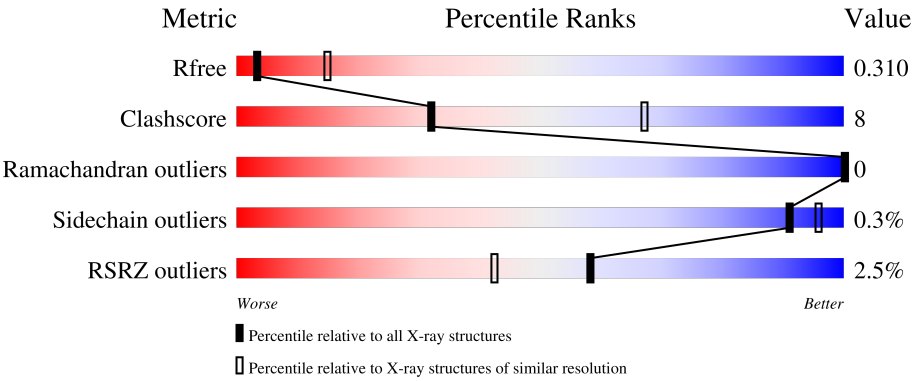
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	171	4% 54% 17% 29%
1	B	171	8% 56% 16% 29%
1	C	171	5% 55% 16% 29%
1	D	171	2% 54% 18% 29%
2	H	240	78% 14% 8%

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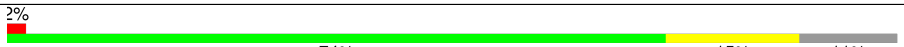
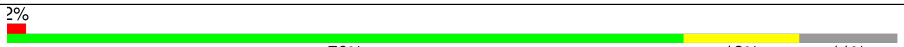
Mol	Chain	Length	Quality of chain
2	I	240	
2	J	240	
2	K	240	
3	L	235	
3	M	235	
3	N	235	
3	O	235	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 33061 atoms, of which 16149 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 Pv cell-traversal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	H	N	O	0	0	0
			1905	605	964	150	186			
1	B	122	Total	C	H	N	O	0	0	0
			1905	605	964	150	186			
1	C	122	Total	C	H	N	O	0	0	0
			1905	605	964	150	186			
1	D	122	Total	C	H	N	O	0	0	0
			1906	605	965	150	186			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	MET	-	initiating methionine	UNP Q53UB7
A	35	GLY	-	expression tag	UNP Q53UB7
A	197	LEU	-	expression tag	UNP Q53UB7
A	198	GLU	-	expression tag	UNP Q53UB7
A	199	HIS	-	expression tag	UNP Q53UB7
A	200	HIS	-	expression tag	UNP Q53UB7
A	201	HIS	-	expression tag	UNP Q53UB7
A	202	HIS	-	expression tag	UNP Q53UB7
A	203	HIS	-	expression tag	UNP Q53UB7
A	204	HIS	-	expression tag	UNP Q53UB7
B	34	MET	-	initiating methionine	UNP Q53UB7
B	35	GLY	-	expression tag	UNP Q53UB7
B	197	LEU	-	expression tag	UNP Q53UB7
B	198	GLU	-	expression tag	UNP Q53UB7
B	199	HIS	-	expression tag	UNP Q53UB7
B	200	HIS	-	expression tag	UNP Q53UB7
B	201	HIS	-	expression tag	UNP Q53UB7
B	202	HIS	-	expression tag	UNP Q53UB7
B	203	HIS	-	expression tag	UNP Q53UB7
B	204	HIS	-	expression tag	UNP Q53UB7
C	34	MET	-	initiating methionine	UNP Q53UB7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	35	GLY	-	expression tag	UNP Q53UB7
C	197	LEU	-	expression tag	UNP Q53UB7
C	198	GLU	-	expression tag	UNP Q53UB7
C	199	HIS	-	expression tag	UNP Q53UB7
C	200	HIS	-	expression tag	UNP Q53UB7
C	201	HIS	-	expression tag	UNP Q53UB7
C	202	HIS	-	expression tag	UNP Q53UB7
C	203	HIS	-	expression tag	UNP Q53UB7
C	204	HIS	-	expression tag	UNP Q53UB7
D	34	MET	-	initiating methionine	UNP Q53UB7
D	35	GLY	-	expression tag	UNP Q53UB7
D	197	LEU	-	expression tag	UNP Q53UB7
D	198	GLU	-	expression tag	UNP Q53UB7
D	199	HIS	-	expression tag	UNP Q53UB7
D	200	HIS	-	expression tag	UNP Q53UB7
D	201	HIS	-	expression tag	UNP Q53UB7
D	202	HIS	-	expression tag	UNP Q53UB7
D	203	HIS	-	expression tag	UNP Q53UB7
D	204	HIS	-	expression tag	UNP Q53UB7

- Molecule 2 is a protein called 7g7 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	221	Total	C	H	N	O	S	0	0	0
			3231	1071	1546	276	331	7			
2	I	221	Total	C	H	N	O	S	0	0	0
			3231	1071	1546	276	331	7			
2	J	221	Total	C	H	N	O	S	0	0	0
			3231	1071	1546	276	331	7			
2	K	221	Total	C	H	N	O	S	0	0	0
			3231	1071	1546	276	331	7			

- Molecule 3 is a protein called 7g7 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	209	Total	C	H	N	O	S	0	2	0
			3128	1000	1527	264	329	8			
3	M	209	Total	C	H	N	O	S	0	2	0
			3128	1000	1527	264	329	8			
3	N	209	Total	C	H	N	O	S	0	2	0
			3128	1000	1527	264	329	8			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	O	209	Total	C	H	N	O	S	0	2	0
			3128	1000	1527	264	329	8			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

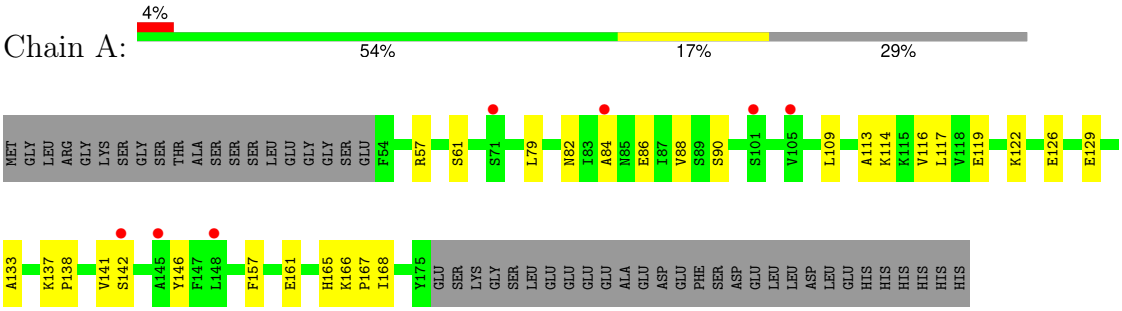
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		
4	D	1	Total	Na	0	0
			1	1		

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.

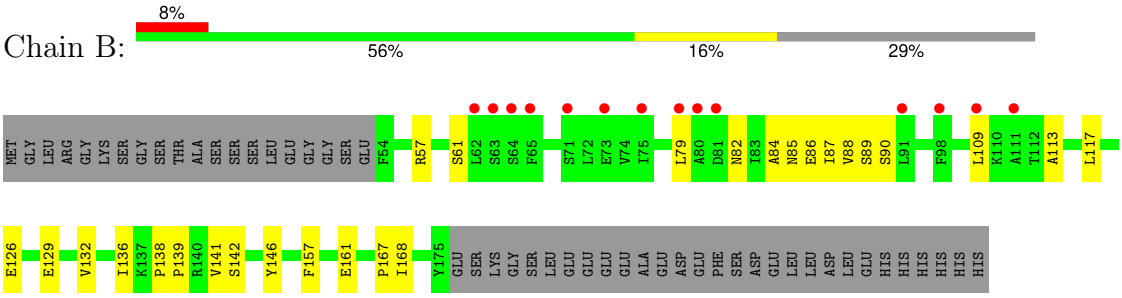
• Molecule 1: Pv cell-traversal protein

Chain A:



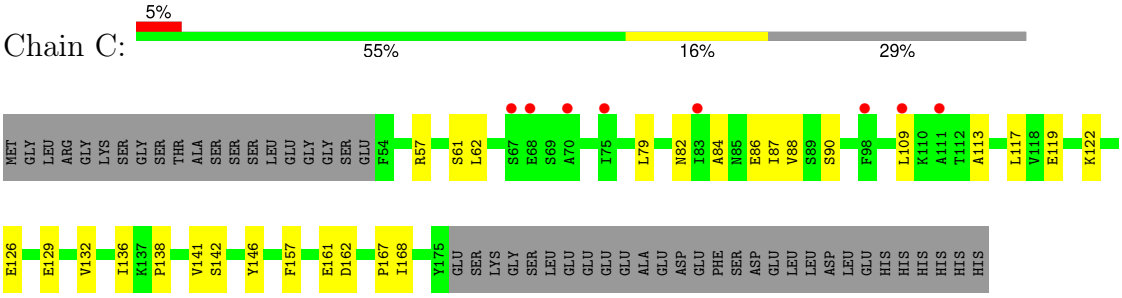
• Molecule 1: Pv cell-traversal protein

Chain B:



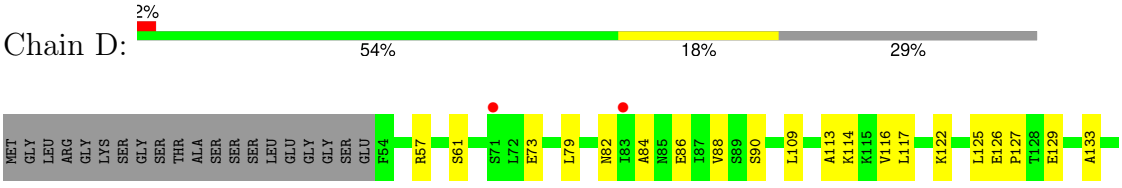
• Molecule 1: Pv cell-traversal protein

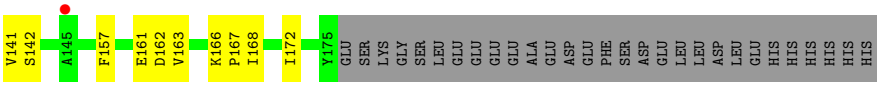
Chain C:



• Molecule 1: Pv cell-traversal protein

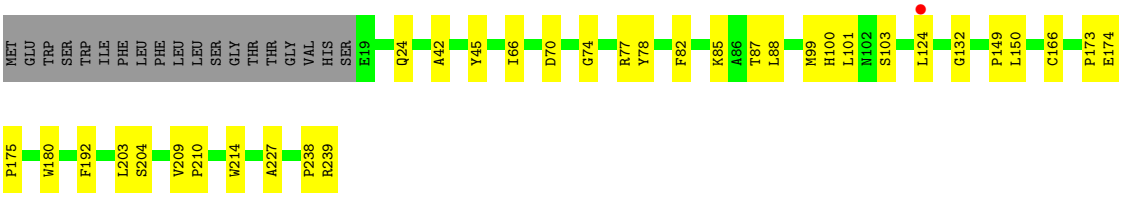
Chain D:





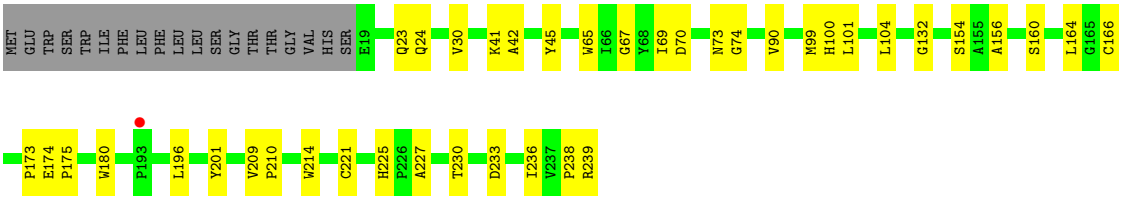
• Molecule 2: 7g7 heavy chain

Chain H:



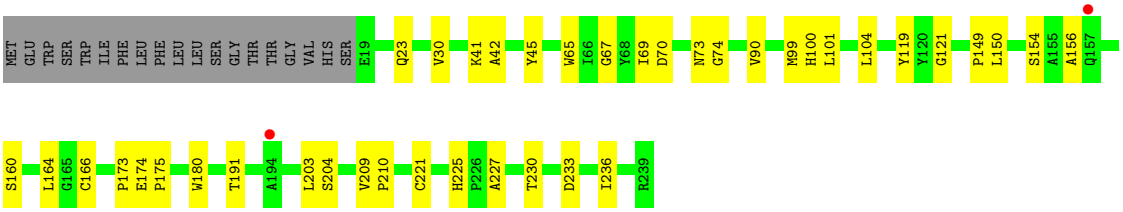
• Molecule 2: 7g7 heavy chain

Chain I:



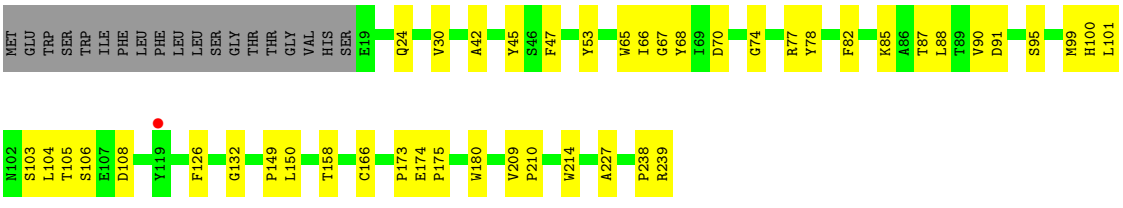
• Molecule 2: 7g7 heavy chain

Chain J:



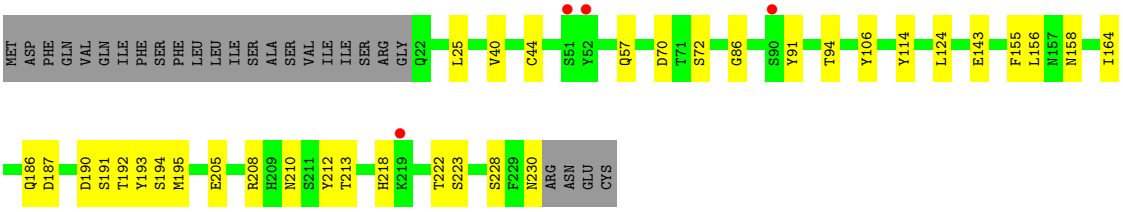
• Molecule 2: 7g7 heavy chain

Chain K:



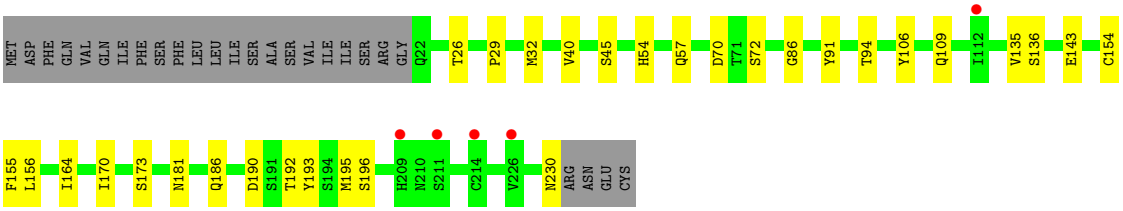
• Molecule 3: 7g7 light chain

Chain L:



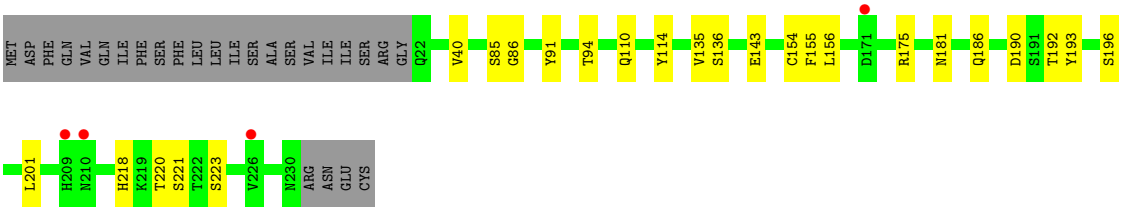
• Molecule 3: 7g7 light chain

Chain M:



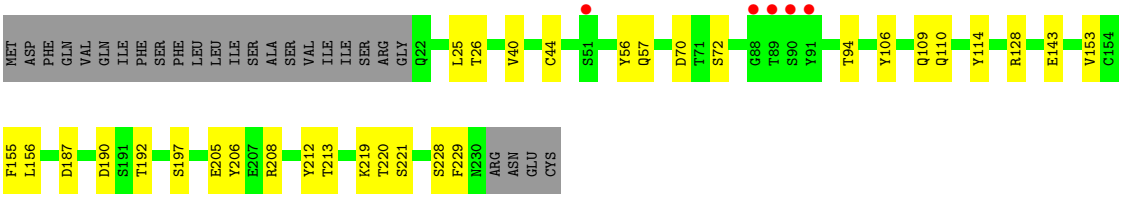
• Molecule 3: 7g7 light chain

Chain N:



• Molecule 3: 7g7 light chain

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	182.89Å 78.62Å 47.32Å 90.03° 95.37° 89.88°	Depositor
Resolution (Å)	48.00 – 3.20 48.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	90.6 (48.00-3.20) 90.1 (48.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.275 , 0.295 0.279 , 0.310	Depositor DCC
R_{free} test set	1962 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	109.8	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 184.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.000 for -h-l,-k,l 0.428 for -h,k,-l 0.000 for h+l,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	33061	wwPDB-VP
Average B, all atoms (Å^2)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 99.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2588e-13. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.27	0/957	0.44	0/1298
1	B	0.27	0/957	0.42	0/1298
1	C	0.27	0/957	0.42	0/1298
1	D	0.27	0/957	0.44	0/1298
2	H	0.29	0/1734	0.49	0/2372
2	I	0.29	0/1734	0.50	0/2372
2	J	0.30	0/1734	0.50	0/2372
2	K	0.29	0/1734	0.49	0/2372
3	L	0.29	0/1640	0.49	0/2229
3	M	0.29	0/1640	0.50	0/2229
3	N	0.29	0/1640	0.49	0/2229
3	O	0.29	0/1640	0.50	0/2229
All	All	0.29	0/17324	0.48	0/23596

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	941	964	963	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	941	964	963	21	0
1	C	941	964	963	23	0
1	D	941	965	963	20	0
2	H	1685	1546	1628	25	0
2	I	1685	1546	1628	28	0
2	J	1685	1546	1628	26	0
2	K	1685	1546	1628	31	0
3	L	1601	1527	1525	25	0
3	M	1601	1527	1525	19	0
3	N	1601	1527	1525	16	0
3	O	1601	1527	1525	22	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	16912	16149	16464	265	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 (265) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ARG:NH2	1:C:86:GLU:OE1	2.15	0.80
1:C:88:VAL:HG22	1:C:109:LEU:HD23	1.65	0.77
2:H:85:LYS:NZ	2:H:103:SER:O	2.18	0.77
3:N:221:SER:OG	3:N:223:SER:O	2.01	0.77
1:B:57:ARG:NH2	1:B:86:GLU:OE1	2.20	0.75
2:K:85:LYS:NZ	2:K:108:ASP:OD2	2.18	0.75
3:M:54:HIS:ND1	3:M:109:GLN:OE1	2.21	0.73
2:I:30:VAL:HG11	2:I:104:LEU:HD13	1.73	0.71
1:D:88:VAL:HG22	1:D:109:LEU:HD23	1.73	0.70
1:A:88:VAL:HG22	1:A:109:LEU:HD23	1.72	0.70
2:K:85:LYS:NZ	2:K:103:SER:O	2.25	0.69
2:J:30:VAL:HG11	2:J:104:LEU:HD13	1.75	0.69
3:M:170:ILE:O	3:M:173:SER:OG	2.03	0.69
2:J:100:HIS:C	2:J:101:LEU:HD12	2.13	0.69
2:I:100:HIS:C	2:I:101:LEU:HD12	2.14	0.67
3:O:190:ASP:OD1	3:O:192:THR:OG1	2.12	0.67
1:B:88:VAL:HG22	1:B:109:LEU:HD23	1.76	0.67
3:O:143:GLU:OE1	3:O:143:GLU:N	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:GLU:O	1:D:90:SER:N	2.29	0.66
2:H:100:HIS:C	2:H:101:LEU:HD12	2.16	0.66
2:K:100:HIS:C	2:K:101:LEU:HD12	2.17	0.66
3:L:143:GLU:OE1	3:L:143:GLU:N	2.27	0.65
1:D:57:ARG:NH2	1:D:86:GLU:OE1	2.29	0.65
1:A:86:GLU:O	1:A:90:SER:N	2.31	0.63
2:H:192:PHE:O	2:H:203:LEU:CD1	2.46	0.62
1:C:167:PRO:O	2:J:73:ASN:ND2	2.32	0.62
1:A:122:LYS:O	1:A:166:LYS:NZ	2.19	0.61
2:K:87:THR:HB	2:K:100:HIS:HB3	1.83	0.61
1:B:139:PRO:HB2	2:J:156:ALA:HA	1.84	0.59
3:O:156:LEU:N	3:O:156:LEU:HD12	2.18	0.59
2:K:149:PRO:O	2:K:150:LEU:HD23	2.04	0.58
2:H:149:PRO:O	2:H:150:LEU:HD23	2.04	0.58
2:H:77:ARG:NH1	2:H:78:TYR:O	2.37	0.57
1:C:86:GLU:O	1:C:90:SER:N	2.35	0.57
1:C:129:GLU:HG2	1:C:157:PHE:CD1	2.38	0.57
3:L:205:GLU:OE2	3:L:208:ARG:NE	2.37	0.57
2:K:87:THR:O	2:K:100:HIS:N	2.31	0.57
1:D:161:GLU:HB3	1:D:167:PRO:HA	1.86	0.57
3:L:164:ILE:HD11	3:L:195:MET:HE3	1.86	0.57
1:B:129:GLU:HG2	1:B:157:PHE:CD1	2.39	0.57
3:O:219:LYS:O	3:O:220:THR:HG22	2.05	0.56
2:I:154:SER:HB3	2:I:156:ALA:HB2	1.87	0.56
2:J:154:SER:HB3	2:J:156:ALA:HB2	1.86	0.56
1:A:57:ARG:NH2	1:A:86:GLU:OE1	2.37	0.56
3:L:156:LEU:N	3:L:156:LEU:HD12	2.20	0.56
1:B:84:ALA:O	1:B:88:VAL:HG23	2.07	0.55
2:J:23:GLN:O	2:J:41:LYS:N	2.38	0.55
1:B:86:GLU:O	1:B:90:SER:N	2.37	0.55
2:H:87:THR:O	2:H:100:HIS:N	2.34	0.55
1:B:82:ASN:O	1:B:86:GLU:N	2.40	0.55
3:N:86:GLY:HA3	3:N:91:TYR:HA	1.88	0.55
3:L:190:ASP:OD1	3:L:192:THR:OG1	2.16	0.54
1:C:82:ASN:O	1:C:86:GLU:N	2.41	0.54
3:M:190:ASP:OD1	3:M:192:THR:OG1	2.22	0.54
2:K:99:MET:HE2	2:K:101:LEU:HD11	1.87	0.54
1:B:167:PRO:O	2:I:73:ASN:ND2	2.41	0.54
1:A:133:ALA:O	1:A:137:LYS:HB2	2.08	0.53
3:N:135:VAL:HA	3:N:155:PHE:O	2.07	0.53
3:L:155:PHE:C	3:L:156:LEU:HD12	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:88:LEU:HD23	2:K:99:MET:HA	1.91	0.53
2:H:87:THR:HB	2:H:100:HIS:HB3	1.91	0.53
3:O:205:GLU:OE2	3:O:208:ARG:NE	2.42	0.53
2:I:164:LEU:HD13	2:I:236:ILE:HD13	1.90	0.53
3:O:213:THR:OG1	3:O:228:SER:OG	2.20	0.53
3:M:143:GLU:OE1	3:M:143:GLU:N	2.36	0.52
3:N:143:GLU:OE1	3:N:143:GLU:N	2.37	0.52
3:M:135:VAL:HA	3:M:155:PHE:O	2.09	0.52
2:K:87:THR:N	2:K:100:HIS:O	2.39	0.52
1:D:126:GLU:HA	1:D:168:ILE:HD13	1.91	0.52
1:A:161:GLU:HB3	1:A:167:PRO:HA	1.92	0.52
1:C:129:GLU:CG	1:C:157:PHE:CD1	2.92	0.52
3:O:206:TYR:O	3:O:212:TYR:OH	2.26	0.52
3:N:190:ASP:OD1	3:N:192:THR:OG1	2.23	0.52
2:H:192:PHE:O	2:H:203:LEU:HD13	2.10	0.52
2:K:173:PRO:HD2	2:K:227:ALA:CB	2.39	0.51
1:C:126:GLU:HA	1:C:168:ILE:HD13	1.93	0.51
2:H:173:PRO:HD2	2:H:227:ALA:CB	2.41	0.50
1:B:126:GLU:HA	1:B:168:ILE:HD13	1.93	0.50
1:A:82:ASN:O	1:A:86:GLU:N	2.44	0.50
2:H:99:MET:HE2	2:H:101:LEU:HD11	1.92	0.50
2:J:173:PRO:HD2	2:J:227:ALA:CB	2.41	0.50
2:I:23:GLN:O	2:I:41:LYS:N	2.45	0.50
3:O:219:LYS:C	3:O:221:SER:N	2.65	0.50
3:O:155:PHE:C	3:O:156:LEU:HD12	2.33	0.49
2:I:99:MET:SD	2:I:101:LEU:HD11	2.51	0.49
2:J:160:SER:O	2:J:210:PRO:HA	2.12	0.49
2:I:173:PRO:HD2	2:I:227:ALA:CB	2.42	0.49
2:J:30:VAL:HG11	2:J:104:LEU:CD1	2.41	0.49
1:A:116:VAL:HG11	1:B:87:ILE:HG13	1.95	0.49
2:H:66:ILE:HG23	2:H:82:PHE:CG	2.48	0.49
2:H:88:LEU:HD23	2:H:99:MET:HA	1.95	0.49
2:I:30:VAL:HG11	2:I:104:LEU:CD1	2.41	0.49
1:C:62:LEU:HD13	1:D:127:PRO:HG2	1.94	0.49
2:J:164:LEU:HD13	2:J:236:ILE:HD13	1.94	0.49
2:H:203:LEU:HD12	2:H:204:SER:H	1.78	0.48
1:C:88:VAL:HG22	1:C:109:LEU:CD2	2.41	0.48
2:I:209:VAL:HB	2:I:210:PRO:HD2	1.96	0.48
2:I:225:HIS:N	2:I:230:THR:O	2.46	0.48
1:C:84:ALA:O	1:C:88:VAL:HG23	2.14	0.48
3:L:40:VAL:O	3:L:94:THR:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ASN:O	1:D:86:GLU:N	2.45	0.48
3:O:40:VAL:O	3:O:94:THR:HA	2.14	0.48
2:J:209:VAL:HB	2:J:210:PRO:HD2	1.96	0.48
3:O:25:LEU:HB3	3:O:44:CYS:SG	2.54	0.48
1:C:61:SER:HB2	1:C:79:LEU:HD21	1.96	0.48
3:L:86:GLY:HA3	3:L:91:TYR:CG	2.49	0.48
1:D:61:SER:HB2	1:D:79:LEU:HD21	1.94	0.48
2:J:225:HIS:N	2:J:230:THR:O	2.46	0.47
2:I:99:MET:CE	2:I:101:LEU:HD11	2.44	0.47
3:M:156:LEU:N	3:M:156:LEU:HD12	2.29	0.47
2:J:154:SER:CB	2:J:156:ALA:HB2	2.44	0.47
3:N:156:LEU:HD12	3:N:156:LEU:N	2.29	0.47
1:D:73:GLU:HG2	1:D:163:VAL:HG13	1.97	0.47
1:B:88:VAL:HG22	1:B:109:LEU:CD2	2.44	0.47
3:M:181:ASN:HA	3:M:196:SER:O	2.15	0.47
1:A:61:SER:HB2	1:A:79:LEU:HD21	1.94	0.47
2:H:87:THR:N	2:H:100:HIS:O	2.43	0.47
2:K:42:ALA:HB1	2:K:45:TYR:CE1	2.49	0.47
2:K:66:ILE:HG23	2:K:82:PHE:CG	2.50	0.47
2:H:42:ALA:HB1	2:H:45:TYR:CE1	2.49	0.47
3:L:164:ILE:HG21	3:L:218:HIS:CE1	2.50	0.47
1:B:61:SER:HB2	1:B:79:LEU:HD21	1.97	0.46
2:I:69:ILE:HD13	2:I:90:VAL:HG13	1.97	0.46
2:K:70:ASP:O	2:K:74:GLY:N	2.42	0.46
2:K:77:ARG:NH1	2:K:78:TYR:O	2.48	0.46
1:A:88:VAL:HG22	1:A:109:LEU:CD2	2.42	0.46
1:B:129:GLU:CG	1:B:157:PHE:CD1	2.98	0.46
3:N:181:ASN:HA	3:N:196:SER:O	2.16	0.46
3:L:213:THR:HG23	3:L:228:SER:OG	2.16	0.46
2:H:214:TRP:CH2	2:H:238:PRO:HB3	2.51	0.46
2:J:119:TYR:OH	2:J:121:GLY:O	2.24	0.46
2:I:154:SER:CB	2:I:156:ALA:HB2	2.45	0.46
2:K:214:TRP:CH2	2:K:238:PRO:HB3	2.51	0.46
2:H:209:VAL:HB	2:H:210:PRO:HD2	1.97	0.46
2:I:65:TRP:CZ2	2:I:67:GLY:HA2	2.51	0.46
2:J:99:MET:HE2	2:J:101:LEU:HD11	1.98	0.46
1:C:161:GLU:HB3	1:C:167:PRO:HA	1.98	0.46
1:B:138:PRO:HD3	1:B:146:TYR:CG	2.51	0.45
1:C:138:PRO:HD3	1:C:146:TYR:CG	2.51	0.45
2:H:166:CYS:HB2	2:H:180:TRP:CH2	2.52	0.45
1:A:129:GLU:OE1	1:A:168:ILE:HG21	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:70:ASP:O	2:H:74:GLY:N	2.43	0.45
3:M:26:THR:O	3:M:45:SER:N	2.45	0.45
2:J:69:ILE:HD13	2:J:90:VAL:HG13	1.99	0.45
2:K:126:PHE:N	3:O:56:TYR:OH	2.40	0.45
2:K:90:VAL:HG22	2:K:91:ASP:N	2.31	0.45
1:C:87:ILE:HG13	1:D:116:VAL:HG11	1.99	0.45
3:O:187:ASP:HB3	3:O:190:ASP:OD1	2.17	0.45
3:L:25:LEU:HB3	3:L:44:CYS:SG	2.56	0.45
2:K:166:CYS:HB2	2:K:180:TRP:CH2	2.52	0.45
1:D:88:VAL:HG22	1:D:109:LEU:CD2	2.44	0.45
1:D:133:ALA:CB	1:D:172:ILE:HG22	2.47	0.45
3:L:210:ASN:O	3:L:230:ASN:HA	2.17	0.44
2:K:53:TYR:CD2	2:K:68:TYR:HB3	2.53	0.44
3:O:213:THR:CB	3:O:228:SER:HG	2.24	0.44
2:I:99:MET:HE2	2:I:101:LEU:HD11	1.98	0.44
1:C:119:GLU:HA	1:C:122:LYS:HD3	1.99	0.44
1:A:113:ALA:O	1:A:117:LEU:HG	2.18	0.44
2:K:209:VAL:HB	2:K:210:PRO:HD2	1.99	0.44
3:N:186:GLN:NE2	3:N:193:TYR:OH	2.50	0.44
1:A:84:ALA:O	1:A:88:VAL:HG23	2.18	0.44
1:A:126:GLU:HA	1:A:168:ILE:HD13	2.00	0.44
3:O:57:GLN:HB2	3:O:106:TYR:CE1	2.53	0.44
1:B:136:ILE:HG13	1:B:146:TYR:HE1	1.83	0.43
2:J:101:LEU:HD12	2:J:101:LEU:N	2.32	0.43
2:H:174:GLU:N	2:H:175:PRO:HD2	2.33	0.43
2:I:160:SER:O	2:I:210:PRO:HA	2.18	0.43
2:H:24:GLN:OE1	2:H:132:GLY:N	2.51	0.43
2:I:24:GLN:OE1	2:I:132:GLY:N	2.51	0.43
2:K:174:GLU:N	2:K:175:PRO:HD2	2.33	0.43
3:L:158:ASN:N	3:L:193:TYR:O	2.50	0.43
2:H:238:PRO:O	2:H:239:ARG:HG3	2.18	0.43
3:L:57:GLN:HB2	3:L:106:TYR:CE1	2.54	0.43
3:M:86:GLY:HA2	3:M:91:TYR:HA	2.00	0.43
2:J:65:TRP:CZ2	2:J:67:GLY:HA2	2.54	0.43
2:J:203:LEU:HD12	2:J:204:SER:H	1.83	0.43
2:K:24:GLN:OE1	2:K:132:GLY:N	2.51	0.43
1:B:161:GLU:HB3	1:B:167:PRO:HA	1.99	0.43
3:L:213:THR:CB	3:L:228:SER:HG	2.32	0.43
2:I:196:LEU:HD13	2:I:201:TYR:CZ	2.54	0.43
3:M:40:VAL:O	3:M:94:THR:HA	2.19	0.43
3:N:220:THR:O	3:N:220:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:238:PRO:O	2:K:239:ARG:HG3	2.18	0.43
2:H:66:ILE:HG23	2:H:82:PHE:CD2	2.53	0.43
3:M:186:GLN:NE2	3:M:193:TYR:OH	2.51	0.43
2:I:42:ALA:HB1	2:I:45:TYR:CE1	2.54	0.43
2:J:42:ALA:HB1	2:J:45:TYR:CE1	2.54	0.43
2:J:174:GLU:N	2:J:175:PRO:HD2	2.34	0.43
2:K:105:THR:HG22	2:K:106:SER:N	2.33	0.43
1:C:157:PHE:O	1:C:161:GLU:HG3	2.19	0.42
2:J:221:CYS:O	2:J:233:ASP:HA	2.19	0.42
3:N:218:HIS:HB3	3:N:221:SER:HB3	2.01	0.42
2:K:47:PHE:CD2	2:K:95:SER:HA	2.54	0.42
2:I:174:GLU:N	2:I:175:PRO:HD2	2.34	0.42
3:M:57:GLN:HB2	3:M:106:TYR:CE1	2.54	0.42
2:J:166:CYS:HB2	2:J:180:TRP:CH2	2.54	0.42
1:D:113:ALA:O	1:D:117:LEU:HG	2.19	0.42
1:D:129:GLU:OE2	1:D:161:GLU:OE2	2.37	0.42
3:L:213:THR:OG1	3:L:228:SER:OG	2.30	0.42
1:A:114:LYS:HA	1:A:117:LEU:HD12	2.00	0.42
2:I:221:CYS:O	2:I:233:ASP:HA	2.20	0.42
3:M:164:ILE:HD11	3:M:195:MET:HE3	2.01	0.42
2:J:70:ASP:O	2:J:74:GLY:N	2.39	0.42
3:L:86:GLY:HA3	3:L:91:TYR:CD2	2.53	0.42
1:B:85:ASN:O	1:B:89:SER:OG	2.32	0.42
2:K:66:ILE:HG23	2:K:82:PHE:CD2	2.54	0.42
1:A:141:VAL:HG12	1:A:142:SER:N	2.34	0.42
3:M:70:ASP:O	3:M:72:SER:N	2.49	0.42
1:C:132:VAL:O	1:C:136:ILE:HG12	2.20	0.42
1:D:162:ASP:O	3:O:114:TYR:OH	2.34	0.42
3:L:70:ASP:O	3:L:72:SER:N	2.47	0.42
2:I:214:TRP:CH2	2:I:238:PRO:HB3	2.54	0.42
2:I:238:PRO:O	2:I:239:ARG:HG3	2.19	0.42
1:C:113:ALA:O	1:C:117:LEU:HG	2.19	0.42
2:J:191:THR:CG2	2:J:203:LEU:HD11	2.49	0.42
1:D:141:VAL:HG12	1:D:142:SER:N	2.35	0.42
3:O:26:THR:HG23	3:O:26:THR:O	2.20	0.42
3:M:86:GLY:HA3	3:M:91:TYR:CE2	2.54	0.42
1:D:84:ALA:O	1:D:88:VAL:HG23	2.20	0.42
1:A:165:HIS:CE1	3:L:114:TYR:OH	2.73	0.41
3:M:230:ASN:OD1	3:M:230:ASN:O	2.38	0.41
2:I:101:LEU:HD12	2:I:101:LEU:N	2.34	0.41
3:N:40:VAL:O	3:N:94:THR:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:30:VAL:HG11	2:K:104:LEU:HD13	2.02	0.41
3:L:186:GLN:NE2	3:L:191:SER:O	2.53	0.41
1:B:132:VAL:O	1:B:136:ILE:HG12	2.19	0.41
3:O:128:ARG:NH1	3:O:190:ASP:HB2	2.35	0.41
2:H:174:GLU:N	2:H:175:PRO:CD	2.84	0.41
1:C:129:GLU:OE1	1:C:168:ILE:HG21	2.20	0.41
3:N:136:SER:O	3:N:154:CYS:HA	2.21	0.41
1:B:113:ALA:O	1:B:117:LEU:HG	2.20	0.41
1:C:162:ASP:O	3:N:114:TYR:OH	2.36	0.41
2:J:149:PRO:O	2:J:150:LEU:HD23	2.21	0.41
3:N:175:ARG:CZ	3:N:201:LEU:HD21	2.50	0.41
1:D:122:LYS:HB3	1:D:166:LYS:HE3	2.02	0.41
2:H:99:MET:SD	2:H:101:LEU:HD11	2.61	0.41
2:I:166:CYS:HB2	2:I:180:TRP:CH2	2.56	0.41
3:M:29:PRO:HG2	3:M:32:MET:HB2	2.02	0.41
3:M:136:SER:O	3:M:154:CYS:HA	2.21	0.41
3:M:136:SER:N	3:M:155:PHE:O	2.46	0.41
1:A:138:PRO:HD3	1:A:146:TYR:CD1	2.55	0.41
3:L:156:LEU:O	3:L:194:SER:HA	2.20	0.41
3:L:222:THR:HG23	3:L:223:SER:N	2.36	0.41
2:K:126:PHE:HD2	3:O:56:TYR:HH	1.67	0.41
2:K:158:THR:O	2:K:158:THR:HG22	2.21	0.41
3:O:212:TYR:HB2	3:O:229:PHE:CE1	2.55	0.41
1:C:141:VAL:HG12	1:C:142:SER:N	2.36	0.41
2:K:174:GLU:N	2:K:175:PRO:CD	2.84	0.41
3:O:70:ASP:O	3:O:72:SER:N	2.47	0.41
3:O:153:VAL:HA	3:O:197:SER:O	2.21	0.41
3:L:187:ASP:HB3	3:L:190:ASP:OD1	2.21	0.40
3:N:136:SER:N	3:N:155:PHE:O	2.45	0.40
2:K:65:TRP:CZ2	2:K:67:GLY:HA2	2.57	0.40
1:A:138:PRO:HD3	1:A:146:TYR:CG	2.56	0.40
3:L:40:VAL:HG11	3:L:124:LEU:HD11	2.03	0.40
1:C:138:PRO:HD3	1:C:146:TYR:CD1	2.55	0.40
1:D:114:LYS:HA	1:D:117:LEU:HD12	2.02	0.40
3:L:212:TYR:O	3:L:228:SER:HB3	2.22	0.40
2:I:70:ASP:O	2:I:74:GLY:N	2.40	0.40
1:B:141:VAL:HG12	1:B:142:SER:N	2.36	0.40
1:D:125:LEU:HG	1:D:168:ILE:CD1	2.50	0.40
1:A:119:GLU:HA	1:A:122:LYS:HD3	2.04	0.40
1:B:138:PRO:HD3	1:B:146:TYR:CD1	2.56	0.40
2:I:196:LEU:HD13	2:I:201:TYR:CE1	2.56	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	120/171 (70%)	116 (97%)	4 (3%)	0	100	100
1	B	120/171 (70%)	115 (96%)	5 (4%)	0	100	100
1	C	120/171 (70%)	115 (96%)	5 (4%)	0	100	100
1	D	120/171 (70%)	118 (98%)	2 (2%)	0	100	100
2	H	219/240 (91%)	211 (96%)	8 (4%)	0	100	100
2	I	219/240 (91%)	209 (95%)	10 (5%)	0	100	100
2	J	219/240 (91%)	210 (96%)	9 (4%)	0	100	100
2	K	219/240 (91%)	211 (96%)	8 (4%)	0	100	100
3	L	207/235 (88%)	199 (96%)	8 (4%)	0	100	100
3	M	207/235 (88%)	198 (96%)	9 (4%)	0	100	100
3	N	207/235 (88%)	200 (97%)	7 (3%)	0	100	100
3	O	207/235 (88%)	197 (95%)	10 (5%)	0	100	100
All	All	2184/2584 (84%)	2099 (96%)	85 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	107/148 (72%)	106 (99%)	1 (1%)	75 89
1	B	107/148 (72%)	107 (100%)	0	100 100
1	C	107/148 (72%)	107 (100%)	0	100 100
1	D	107/148 (72%)	106 (99%)	1 (1%)	75 89
2	H	191/208 (92%)	190 (100%)	1 (0%)	86 93
2	I	191/208 (92%)	191 (100%)	0	100 100
2	J	191/208 (92%)	191 (100%)	0	100 100
2	K	191/208 (92%)	191 (100%)	0	100 100
3	L	182/206 (88%)	182 (100%)	0	100 100
3	M	182/206 (88%)	182 (100%)	0	100 100
3	N	182/206 (88%)	181 (100%)	1 (0%)	86 93
3	O	182/206 (88%)	180 (99%)	2 (1%)	70 86
All	All	1920/2248 (85%)	1914 (100%)	6 (0%)	91 96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	PHE
2	H	124	LEU
3	N	110	GLN
1	D	157	PHE
3	O	109	GLN
3	O	110	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	218	HIS
3	N	54	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	122/171 (71%)	-0.01	7 (5%) 30 20	126, 190, 246, 292	0
1	B	122/171 (71%)	0.06	14 (11%) 11 8	129, 186, 315, 337	0
1	C	122/171 (71%)	-0.06	8 (6%) 26 17	129, 188, 312, 346	0
1	D	122/171 (71%)	-0.00	3 (2%) 58 42	130, 188, 252, 284	0
2	H	221/240 (92%)	-0.90	1 (0%) 87 78	86, 127, 185, 202	0
2	I	221/240 (92%)	-0.88	1 (0%) 87 78	86, 122, 170, 209	0
2	J	221/240 (92%)	-0.87	2 (0%) 81 68	83, 120, 170, 200	0
2	K	221/240 (92%)	-0.84	1 (0%) 87 78	87, 127, 183, 200	0
3	L	209/235 (88%)	-0.77	4 (1%) 66 50	88, 144, 195, 242	0
3	M	209/235 (88%)	-0.56	5 (2%) 59 44	95, 148, 217, 240	1 (0%)
3	N	209/235 (88%)	-0.57	4 (1%) 66 50	93, 150, 216, 239	1 (0%)
3	O	209/235 (88%)	-0.77	5 (2%) 59 44	89, 143, 194, 233	0
All	All	2208/2584 (85%)	-0.60	55 (2%) 58 42	83, 145, 229, 346	2 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	VAL	6.5
1	B	73	GLU	4.8
3	O	89	THR	4.2
1	B	109	LEU	4.0
1	B	63	SER	3.5
1	C	109	LEU	3.5
1	D	145	ALA	3.4
1	B	64	SER	3.4
1	B	111	ALA	3.3
3	L	90	SER	3.2
2	I	193	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	142	SER	3.2
3	O	90	SER	3.0
1	C	70	ALA	3.0
3	M	226	VAL	3.0
1	C	75	ILE	3.0
1	C	67	SER	2.8
3	L	219	LYS	2.8
3	N	210	ASN	2.8
3	N	226	VAL	2.8
1	B	80	ALA	2.7
3	O	51	SER	2.7
3	M	214	CYS	2.6
1	A	148	LEU	2.6
1	C	111	ALA	2.5
3	L	51	SER	2.5
1	A	71	SER	2.5
3	O	88	GLY	2.5
3	M	209	HIS	2.4
1	B	81	ASP	2.4
1	B	98	PHE	2.4
1	D	83	ILE	2.4
2	J	194	ALA	2.4
1	C	68	GLU	2.4
3	N	171	ASP	2.3
1	B	62	LEU	2.3
1	C	83	ILE	2.3
1	A	84	ALA	2.3
1	C	98	PHE	2.2
1	B	75	ILE	2.2
3	N	209	HIS	2.2
3	O	91	TYR	2.2
1	A	145	ALA	2.2
1	A	101	SER	2.2
3	M	211	SER	2.2
1	B	65	PHE	2.2
1	B	71	SER	2.2
1	D	71	SER	2.2
1	B	79	LEU	2.2
1	B	91	LEU	2.2
3	L	52	TYR	2.1
3	M	112	ILE	2.1
2	K	119	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	J	157	GLN	2.1
2	H	124	LEU	2.1

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	D	301	1/1	0.98	0.04	107,107,107,107	0
4	NA	C	301	1/1	0.99	0.06	101,101,101,101	0
4	NA	A	301	1/1	0.99	0.08	110,110,110,110	0
4	NA	B	301	1/1	1.00	0.04	101,101,101,101	0

6.5 Other polymers (i)

There are no such residues in this entry.