



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:33 PM UTC

PDB ID : 8ULF / pdb_00008ulf
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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

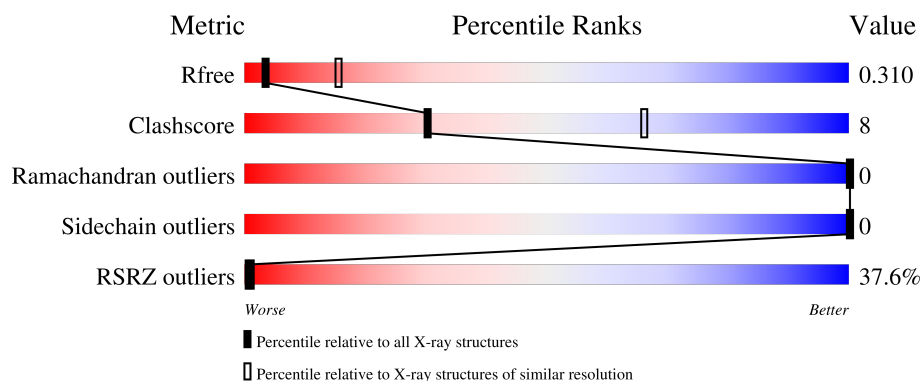
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 $\leq 5\%$. 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	171	19% 54% 18% 29%
1	B	171	24% 56% 16% 29%
1	C	171	20% 54% 17% 29%
1	D	171	22% 54% 18% 29%
2	H	240	36% 77% 15% 8%

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Mol	Chain	Length	Quality of chain
2	I	240	38% 75% 17% 8%
2	J	240	39% 74% 18% 8%
2	K	240	35% 73% 19% 8%
3	L	235	36% 72% 17% 11%
3	M	235	36% 75% 14% 11%
3	N	235	31% 77% 12% 11%
3	O	235	35% 74% 14% 11%

2 Entry composition

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 (CCD ID: 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		

LEU
ASP
LEU
LEU
GLU
GLY
HIS
HIS
HIS
HIS
HIS

• Molecule 1: Pv cell-traversal protein

Chain D: 

MET GLY LEU ARG GLY LYS SER GLY THR ALA SER SER SER LEU GLU GLY GLY SER GLU F54 R57 I58 S61 L62 S67 A70 E73 E78 L79 A80 D81 N82 I83 A84 N85 E86 I87 V88 S89 S90 S95 S101 G102 V105 L109 K110 A113 K114

K115 V116 L117 K122 L125 E126 P127 T128 E129 T130 I131 V132 A133 S134 T135 E140 V141 S142 D144 A145 F147 L148 G150 P151 V152 V153 V160 E161 D162 V163 L164 H165 K166 P167 I168 T171 I172 Y175 GLU SER LYS GLY SER LEU GLU GLU GLU GLU ALA ASP

GLU PHE SER ASP LEU LEU ASP LEU ASP LEU LEU ASP LEU LEU HIS HIS HIS HIS HIS HIS HIS

• Molecule 2: 7g7 heavy chain

Chain H: 

MET GLU TRP TRP ILE PHE LEU PHE LEU LEU SER GLY THR THR VAL HIS SER E19 I20 Q21 Q24 S25 G26 F27 P32 S35 V36 K41 A42 Y45 T50 N51 M52 Y53 W54 V55 K56 Q57 H58 G60 I66 I69 D70 P71 Y72 W73 G74 T76

R77 Y78 F82 K85 A86 T87 L88 T96 A97 F98 N99 H100 L101 S103 V111 Y112 Y113 C114 G117 Y118 Y119 Y120 G121 N122 P123 L124 H125 F126 V128 W129 G132 T133 T134 S138 T142 P145 S146 V147 Y148 P149 L150 P152 G153 S154 A155 A156 Q157 T158

W159 S160 M161 V162 G165 C166 K169 G170 Y171 F172 E174 P175 V176 T177 V178 T179 W180 S184 H190 T191 F192 P193 A194 V195 G197 S198 T202 L203 S204 S205 V207 T208 P210 S211 S212 T213 W214 V219 W222 V223 A227 P230 K231 T232 P238 R239

• Molecule 2: 7g7 heavy chain

Chain I: 

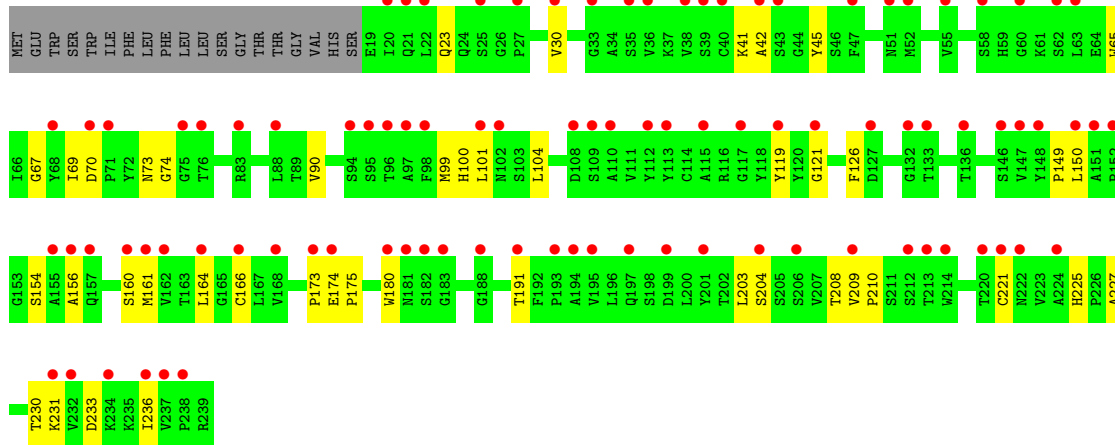
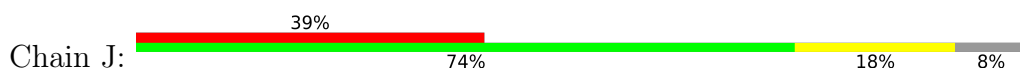
MET GLU TRP TRP ILE PHE LEU PHE LEU LEU SER GLY THR THR VAL HIS SER E19 Q23 Q24 S25 G26 P27 V30 A34 S35 V36 K37 V38 S39 C40 K41 A42 S43 V44 Y45 S46 F47 T48 N51 M52 Y53 W54 V55 S58 S62 L63 E64 W65 I66 G67 Y68

I69 D70 P71 Y72 W73 G75 T76 W79 Q80 R83 T89 V90 S94 S95 T96 F98 H100 L101 L104 D108 S109 Y112 Y113 C114 A115 R116 G117 Y118 Y119 Y120 G121 F126 D127 A131 G132 V137 V147 Y148 P149 L150 A151 S154 A155 A156 Q157

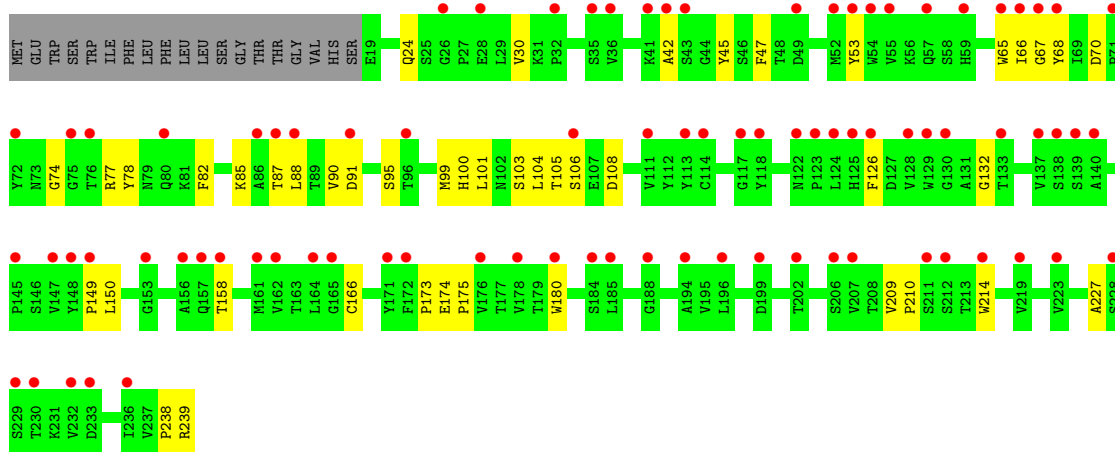
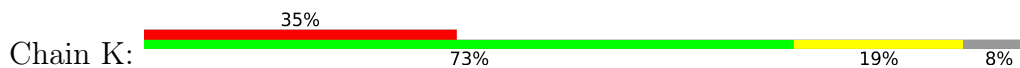
S160 M161 V162 L164 G165 C166 L167 V168 P173 E174 P175 W180 N181 S182 G183 S184 S187 T191 F192 P193 A194 V195 L196 D199 L200 Y201 T202 L203 S204 S205 V207 T208 P209 V210 W214 T220 C221 A224 H225 P226 A227 T230 K231 V232 D233 I236 V237

P238 R239

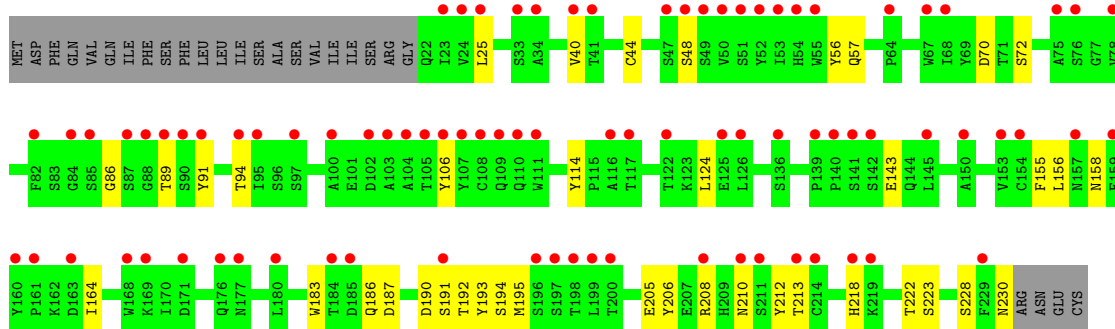
• Molecule 2: 7g7 heavy chain



• Molecule 2: 7g7 heavy chain

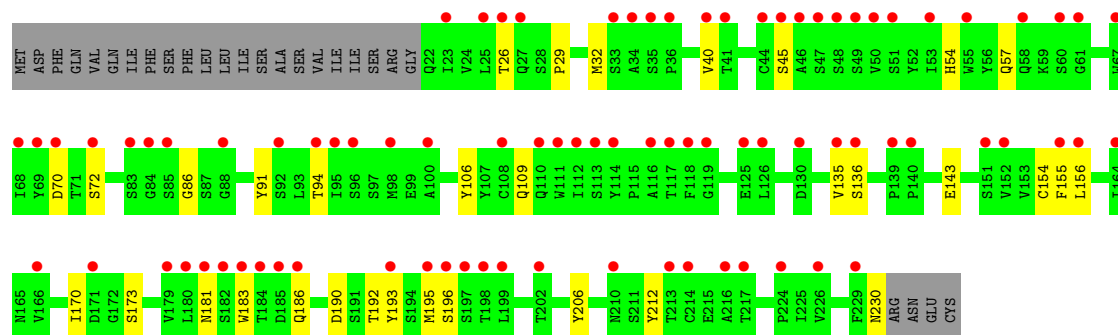


• Molecule 3: 7g7 light chain



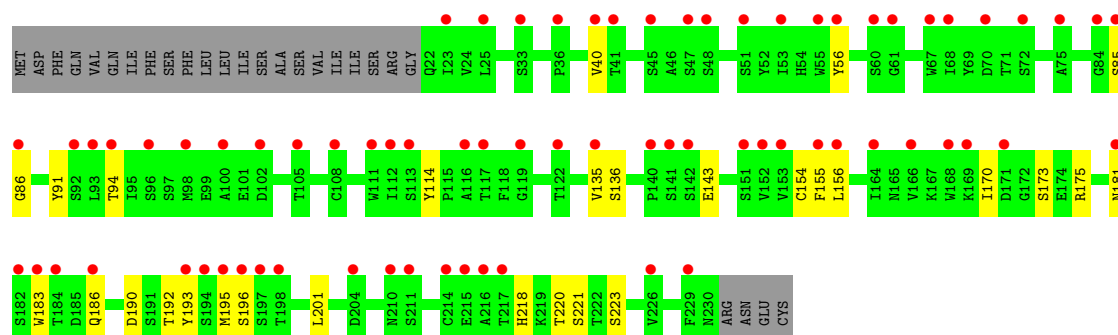
• Molecule 3: 7g7 light chain

Chain M: 



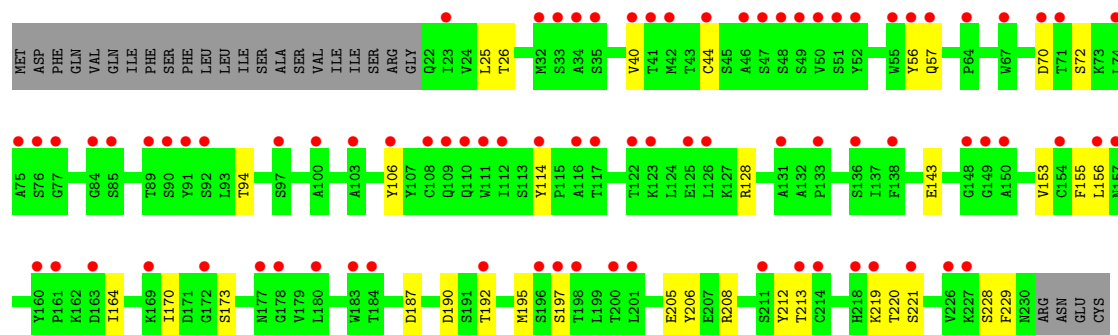
• Molecule 3: 7g7 light chain

Chain N: 



• Molecule 3: 7g7 light chain

Chain O: 



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (4.58%)	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)	0.37 , 600.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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	0.82	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.16	0/957	0.34	0/1298
1	B	0.16	0/957	0.33	0/1298
1	C	0.17	0/957	0.33	0/1298
1	D	0.16	0/957	0.33	0/1298
2	H	0.17	0/1734	0.34	0/2372
2	I	0.17	0/1734	0.37	0/2372
2	J	0.17	0/1734	0.39	0/2372
2	K	0.17	0/1734	0.35	0/2372
3	L	0.17	0/1640	0.35	0/2229
3	M	0.17	0/1640	0.35	0/2229
3	N	0.16	0/1640	0.32	0/2229
3	O	0.18	0/1640	0.35	0/2229
All	All	0.17	0/17324	0.35	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 [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	941	964	963	21	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	24	0
1	D	941	965	963	21	0
2	H	1685	1546	1628	28	0
2	I	1685	1546	1628	29	0
2	J	1685	1546	1628	30	0
2	K	1685	1546	1628	30	0
3	L	1601	1527	1525	28	0
3	M	1601	1527	1525	20	0
3	N	1601	1527	1525	19	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	280	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 (280) 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
3:M:54:HIS:ND1	3:M:109:GLN:OE1	2.21	0.73
2:J:100:HIS:C	2:J:101:LEU:HD12	2.13	0.73
1:A:122:LYS:O	1:A:166:LYS:NZ	2.19	0.72
2:I:100:HIS:C	2:I:101:LEU:HD12	2.14	0.71
3:M:170:ILE:O	3:M:173:SER:OG	2.03	0.71
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:H:100:HIS:C	2:H:101:LEU:HD12	2.16	0.70
2:K:100:HIS:C	2:K:101:LEU:HD12	2.17	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
1:B:88:VAL:HG22	1:B:109:LEU:HD23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:143:GLU:OE1	3:O:143:GLU:N	2.26	0.66
1:D:86:GLU:O	1:D:90:SER:N	2.29	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
3:O:170:ILE:O	3:O:173:SER:OG	2.13	0.65
1:A:86:GLU:O	1:A:90:SER:N	2.31	0.63
2:K:99:MET:HE2	2:K:101:LEU:HD11	1.81	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
2:K:85:LYS:NZ	2:K:108:ASP:OD2	2.18	0.61
2:K:87:THR:HB	2:K:100:HIS:HB3	1.83	0.61
2:I:99:MET:HE2	2:I:101:LEU:HD11	1.82	0.60
3:N:183:TRP:CE2	3:N:195:MET:HE2	2.37	0.59
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:99:MET:HE2	2:H:101:LEU:HD11	1.84	0.58
3:L:155:PHE:C	3:L:156:LEU:HD12	2.29	0.58
2:J:99:MET:HE2	2:J:101:LEU:HD11	1.85	0.58
3:M:183:TRP:CE2	3:M:195:MET:HE2	2.38	0.57
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:O:190:ASP:OD1	3:O:192:THR:OG1	2.12	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:HD12	3:L:156:LEU:N	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
3:N:170:ILE:O	3:N:173:SER:OG	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:155:PHE:C	3:O:156:LEU:HD12	2.33	0.54
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
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
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
2:H:161:MET:HE2	2:H:208:THR:CG2	2.40	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
3:O:219:LYS:C	3:O:221:SER:N	2.65	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: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:L:213:THR:OG1	3:L:228:SER:OG	2.30	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:J:119:TYR:OH	2:J:121:GLY:O	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:H:161:MET:HE2	2:H:208:THR:HG22	1.96	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
3:L:183:TRP:CD1	3:L:195:MET:HE2	2.49	0.47
2:J:126:PHE:HD2	3:N:56:TYR:HH	1.62	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:C:166:LYS:NZ	2:J:70:ASP:OD2	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:214:TRP:CH2	2:H:238:PRO:HB3	2.51	0.46
2:I:154:SER:CB	2:I:156:ALA:HB2	2.45	0.46
3:O:164:ILE:HD11	3:O:195:MET:HE3	1.97	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
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
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
3:L:206:TYR:O	3:L:212:TYR:OH	2.34	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
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:D:162:ASP:O	3:O:114:TYR:OH	2.34	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:J:161:MET:HE2	2:J:208:THR:CG2	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:D:171:THR:O	1:D:172:ILE:C	2.61	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
1:A:171:THR:O	1:A:172:ILE:C	2.62	0.42
3:L:48:SER:C	3:L:89:THR:HG22	2.45	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
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
2:H:126:PHE:HD2	3:L:56:TYR:HH	1.61	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
2:I:66:ILE:HD13	2:I:99:MET:HE1	2.01	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
3:L:70:ASP:O	3:L:72:SER:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O:26:THR:O	3:O:26:THR:HG23	2.20	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:M:206:TYR:O	3:M:212:TYR:OH	2.33	0.41
3:N:40:VAL:O	3:N:94:THR:HA	2.21	0.41
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
3:L:164:ILE:HD11	3:L:195:MET:HE3	2.03	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:171:THR:O	1:B:172:ILE:C	2.64	0.40
2:I:70:ASP:O	2:I:74:GLY:N	2.40	0.40
2:J:230:THR:C	2:J:231:LYS:HD3	2.46	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	107 (100%)	0	100	100
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%)	107 (100%)	0	100	100
2	H	191/208 (92%)	191 (100%)	0	100	100
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%)	182 (100%)	0	100	100
3	O	182/206 (88%)	182 (100%)	0	100	100
All	All	1920/2248 (85%)	1920 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	218	HIS
1	B	77	ASN
1	B	165	HIS
1	C	77	ASN
2	J	125	HIS
3	N	54	HIS
3	N	230	ASN
1	D	165	HIS
2	K	190	HIS
3	O	218	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 ⓘ

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	122/171 (71%)	1.41	33 (27%) 1 1	126, 190, 246, 292	0
1	B	122/171 (71%)	1.72	41 (33%) 1 1	129, 186, 315, 337	0
1	C	122/171 (71%)	1.64	35 (28%) 1 1	129, 188, 312, 346	0
1	D	122/171 (71%)	1.54	38 (31%) 1 1	130, 188, 252, 284	0
2	H	221/240 (92%)	1.78	87 (39%) 1 1	86, 127, 185, 202	0
2	I	221/240 (92%)	1.86	92 (41%) 0 1	86, 122, 170, 209	0
2	J	221/240 (92%)	1.88	94 (42%) 0 1	83, 120, 170, 200	0
2	K	221/240 (92%)	1.78	85 (38%) 1 1	87, 127, 183, 200	0
3	L	209/235 (88%)	1.82	85 (40%) 0 1	88, 144, 195, 242	0
3	M	209/235 (88%)	1.85	85 (40%) 0 1	95, 148, 217, 240	1 (0%)
3	N	209/235 (88%)	1.74	73 (34%) 1 1	93, 150, 216, 239	1 (0%)
3	O	209/235 (88%)	1.89	83 (39%) 1 1	89, 143, 194, 233	0
All	All	2208/2584 (85%)	1.77	831 (37%) 1 1	83, 145, 229, 346	2 (0%)

All (831) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	90	SER	9.6
3	O	122	THR	8.8
2	H	86	ALA	7.3
3	L	89	THR	7.3
3	O	90	SER	6.9
1	D	145	ALA	6.4
3	N	41	THR	6.2
2	I	156	ALA	6.2
3	O	51	SER	5.9
1	A	145	ALA	5.8
3	M	181	ASN	5.6

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Mol	Chain	Res	Type	RSRZ
3	L	91	TYR	5.6
3	N	197	SER	5.5
3	M	226	VAL	5.3
3	M	41	THR	5.2
3	M	217	THR	5.2
3	L	213	THR	5.2
3	O	89	THR	5.2
3	N	151	SER	5.2
2	K	114	CYS	5.1
1	C	68	GLU	5.1
2	K	86	ALA	5.1
2	K	55	VAL	5.0
1	B	63	SER	5.0
3	L	122	THR	5.0
3	N	85	SER	4.9
1	C	113	ALA	4.9
1	B	84	ALA	4.8
2	J	109	SER	4.8
3	M	113	SER	4.7
3	N	226	VAL	4.7
3	M	196	SER	4.7
1	B	95	SER	4.6
2	K	125	HIS	4.6
3	O	91	TYR	4.6
1	A	142	SER	4.6
3	O	52	TYR	4.5
2	I	220	THR	4.5
2	I	155	ALA	4.4
2	I	201	TYR	4.4
2	H	55	VAL	4.4
3	O	49	SER	4.4
1	D	82	ASN	4.4
3	L	150	ALA	4.4
3	M	67	TRP	4.4
3	N	184	THR	4.4
3	N	61	GLY	4.3
1	D	102	GLY	4.3
2	H	165	GLY	4.3
2	K	26	GLY	4.3
3	N	112	ILE	4.3
3	O	41	THR	4.2
2	K	122	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
3	L	51	SER	4.2
2	J	38	VAL	4.2
1	C	65	PHE	4.2
3	L	75	ALA	4.2
3	N	216	ALA	4.2
3	M	84	GLY	4.2
2	I	147	VAL	4.2
1	B	75	ILE	4.2
2	J	40	CYS	4.2
1	B	111	ALA	4.1
3	M	116	ALA	4.1
2	I	183	GLY	4.1
2	K	140	ALA	4.1
2	I	95	SER	4.1
3	M	179	VAL	4.1
3	L	52	TYR	4.1
2	K	157	GLN	4.1
3	N	51	SER	4.1
3	N	96	SER	4.1
2	I	195	VAL	4.1
1	D	113	ALA	4.1
3	L	33	SER	4.1
1	A	105	VAL	4.1
2	J	147	VAL	4.1
3	M	164	ILE	4.1
2	I	209	VAL	4.0
2	I	154	SER	4.0
2	J	182	SER	4.0
1	A	148	LEU	4.0
3	N	181	ASN	4.0
3	M	68	ILE	4.0
3	O	116	ALA	4.0
2	I	63	LEU	4.0
1	D	101	SER	4.0
2	I	40	CYS	4.0
3	L	154	CYS	4.0
2	J	97	ALA	4.0
2	K	67	GLY	3.9
3	O	169	LYS	3.9
3	L	88	GLY	3.9
2	H	70	ASP	3.9
3	N	217	THR	3.9

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Mol	Chain	Res	Type	RSRZ
2	I	214	TRP	3.9
2	H	114	CYS	3.9
3	N	214	CYS	3.9
2	J	21	GLN	3.8
3	M	96	SER	3.8
2	I	25	SER	3.8
3	O	33	SER	3.8
3	N	171	ASP	3.8
2	H	156	ALA	3.8
3	O	103	ALA	3.8
3	O	221	SER	3.8
2	K	87	THR	3.8
3	M	198	THR	3.7
2	J	193	PRO	3.7
2	K	53	TYR	3.7
3	O	213	THR	3.7
3	N	25	LEU	3.7
3	L	219	LYS	3.7
1	D	142	SER	3.6
3	L	197	SER	3.6
2	J	83	ARG	3.6
1	A	147	PHE	3.6
2	H	149	PRO	3.6
3	M	112	ILE	3.6
3	N	140	PRO	3.6
3	O	44	CYS	3.6
2	K	138	SER	3.6
3	O	112	ILE	3.6
2	I	71	PRO	3.6
3	O	131	ALA	3.6
1	A	73	GLU	3.6
2	I	55	VAL	3.6
1	C	66	LEU	3.6
2	K	118	TYR	3.6
3	O	85	SER	3.6
2	J	151	ALA	3.5
1	B	68	GLU	3.5
3	L	41	THR	3.5
3	L	180	LEU	3.5
2	J	148	TYR	3.5
3	M	108	CYS	3.5
3	M	136	SER	3.5

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Mol	Chain	Res	Type	RSRZ
2	K	223	VAL	3.5
3	N	210	ASN	3.5
2	H	169	LYS	3.5
2	H	129	TRP	3.5
2	H	223	VAL	3.5
3	M	180	LEU	3.5
3	N	211	SER	3.5
2	K	126	PHE	3.4
2	H	53	TYR	3.4
2	J	232	VAL	3.4
2	J	117	GLY	3.4
3	N	45	SER	3.4
2	K	54	TRP	3.4
1	C	116	VAL	3.4
1	A	117	LEU	3.4
3	O	100	ALA	3.4
2	J	96	THR	3.4
2	K	184	SER	3.4
1	C	73	GLU	3.4
2	I	39	SER	3.4
3	M	88	GLY	3.4
3	L	23	ILE	3.4
2	J	76	THR	3.4
3	M	110	GLN	3.4
1	A	164	LEU	3.3
1	D	148	LEU	3.3
3	O	197	SER	3.3
3	O	75	ALA	3.3
1	B	109	LEU	3.3
3	M	152	VAL	3.3
1	A	113	ALA	3.3
2	H	206	SER	3.3
2	J	183	GLY	3.3
2	K	194	ALA	3.3
2	H	180	TRP	3.3
3	M	216	ALA	3.3
2	H	113	TYR	3.3
1	B	65	PHE	3.3
2	H	158	THR	3.3
3	M	94	THR	3.3
3	N	93	LEU	3.3
1	C	70	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
3	O	92[A]	SER	3.2
2	J	98	PHE	3.2
2	J	51	ASN	3.2
1	B	169	PRO	3.2
1	D	95	SER	3.2
3	M	151	SER	3.2
2	J	55	VAL	3.2
3	O	109	GLN	3.2
2	J	214	TRP	3.2
2	J	121	GLY	3.2
1	C	117	LEU	3.2
2	K	124	LEU	3.2
2	I	23	GLN	3.2
3	O	46	ALA	3.2
3	N	168	TRP	3.2
3	O	56	TYR	3.2
3	N	152	VAL	3.2
2	K	211	SER	3.2
3	M	125	GLU	3.2
1	D	153	VAL	3.2
2	H	190	HIS	3.2
2	J	62	SER	3.2
2	J	95	SER	3.2
2	J	161	MET	3.2
1	D	84	ALA	3.2
2	I	202	THR	3.2
3	L	116	ALA	3.2
3	N	84	GLY	3.1
3	N	215	GLU	3.1
2	H	122	ASN	3.1
2	H	147	VAL	3.1
2	J	36	VAL	3.1
1	D	109	LEU	3.1
3	M	44	CYS	3.1
3	M	214	CYS	3.1
3	O	183	TRP	3.1
3	L	104	ALA	3.1
2	J	94	SER	3.1
3	M	182	SER	3.1
1	C	162	ASP	3.1
1	C	160	VAL	3.1
2	K	156	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
3	O	218	HIS	3.1
2	H	184	SER	3.1
3	N	48	SER	3.1
2	I	168	VAL	3.1
3	L	67	TRP	3.1
2	I	120	TYR	3.1
3	O	126	LEU	3.1
2	I	96	THR	3.1
3	N	86	GLY	3.1
3	M	72	SER	3.1
3	O	50	VAL	3.1
2	H	54	TRP	3.1
2	J	127	ASP	3.1
3	O	154	CYS	3.1
3	M	210	ASN	3.0
2	H	195	VAL	3.0
2	I	36	VAL	3.0
3	M	48	SER	3.0
1	D	131	ILE	3.0
2	H	150	LEU	3.0
2	I	224	ALA	3.0
2	J	209	VAL	3.0
3	N	153	VAL	3.0
3	M	55	TRP	3.0
2	H	52	MET	3.0
2	J	234	LYS	3.0
3	M	118	PHE	3.0
2	K	229	SER	3.0
2	H	120	TYR	3.0
1	B	162	ASP	3.0
2	J	60	GLY	3.0
1	A	82	ASN	3.0
3	O	23	ILE	3.0
2	H	32	PRO	3.0
2	H	124	LEU	3.0
3	O	211	SER	3.0
3	N	204	ASP	3.0
2	J	168	VAL	3.0
3	M	27	GLN	3.0
3	O	157	ASN	3.0
3	N	117	THR	3.0
1	A	140	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	143	GLU	2.9
2	J	238	PRO	2.9
2	J	206	SER	2.9
2	K	35	SER	2.9
2	J	33	GLY	2.9
1	C	135	THR	2.9
3	L	198	THR	2.9
3	O	200	THR	2.9
1	A	106	LYS	2.9
1	C	143	GLU	2.9
2	H	151	ALA	2.9
2	H	194	ALA	2.9
1	B	71	SER	2.9
1	C	64	SER	2.9
1	C	71	SER	2.9
2	I	232	VAL	2.9
2	K	188	GLY	2.9
3	M	171	ASP	2.9
2	K	66	ILE	2.9
1	B	155	THR	2.9
2	H	87	THR	2.9
3	O	198	THR	2.9
1	C	139	PRO	2.9
2	H	123	PRO	2.9
3	L	139	PRO	2.9
1	B	80	ALA	2.9
2	J	224	ALA	2.9
3	M	69	TYR	2.9
2	I	192	PHE	2.9
3	M	33	SER	2.9
3	O	161	PRO	2.9
2	K	129	TRP	2.9
1	A	116	VAL	2.9
2	K	75	GLY	2.9
1	C	101	SER	2.9
2	H	212	SER	2.9
2	J	43	SER	2.9
2	H	41	LYS	2.9
3	M	70	ASP	2.9
2	I	208	THR	2.9
3	L	100	ALA	2.9
3	M	184	THR	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	111	VAL	2.9
3	O	40	VAL	2.9
1	D	147	PHE	2.9
1	C	67	SER	2.8
3	M	45	SER	2.8
3	M	197	SER	2.8
2	H	145	PRO	2.8
3	L	200	THR	2.8
2	J	181	ASN	2.8
2	K	128	VAL	2.8
2	K	147	VAL	2.8
2	K	207	VAL	2.8
2	I	113	TYR	2.8
3	M	23	ILE	2.8
2	I	109	SER	2.8
3	M	49	SER	2.8
2	H	71	PRO	2.8
3	N	36	PRO	2.8
1	C	81	ASP	2.8
3	O	214	CYS	2.8
1	D	165	HIS	2.8
2	I	94	SER	2.8
2	K	32	PRO	2.8
2	I	48	THR	2.8
2	J	191	THR	2.8
1	B	72	LEU	2.8
3	O	67	TRP	2.8
1	C	118	VAL	2.8
2	H	219	VAL	2.8
2	K	202	THR	2.8
3	L	68	ILE	2.8
2	J	132	GLY	2.8
3	O	32	MET	2.8
1	A	70	ALA	2.8
2	J	110	ALA	2.8
3	L	103	ALA	2.8
2	H	36	VAL	2.8
2	K	145	PRO	2.8
3	N	40	VAL	2.8
1	A	62	LEU	2.8
2	J	146	SER	2.8
3	N	47	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	K	96	THR	2.8
2	I	54	TRP	2.7
3	L	157	ASN	2.7
3	L	160	TYR	2.7
1	A	111	ALA	2.7
3	N	116	ALA	2.7
3	M	166	VAL	2.7
3	L	64	PRO	2.7
3	O	180	LEU	2.7
2	J	39	SER	2.7
3	N	72	SER	2.7
2	K	230	THR	2.7
3	N	94	THR	2.7
3	L	84	GLY	2.7
1	C	146	TYR	2.7
2	I	151	ALA	2.7
2	J	42	ALA	2.7
2	J	156	ALA	2.7
2	K	42	ALA	2.7
2	K	59	HIS	2.7
3	N	75	ALA	2.7
1	C	169	PRO	2.7
2	J	166	CYS	2.7
2	K	196	LEU	2.7
2	I	76	THR	2.7
3	M	60	SER	2.7
2	K	171	TYR	2.7
2	H	125	HIS	2.7
3	M	100	ALA	2.7
1	D	116	VAL	2.7
3	M	40	VAL	2.7
1	C	156	LEU	2.7
2	K	88	LEU	2.7
3	M	25	LEU	2.7
2	K	123	PRO	2.7
1	A	78	GLU	2.7
2	K	117	GLY	2.7
1	D	110	LYS	2.7
3	L	49	SER	2.7
3	N	169	LYS	2.7
3	O	160	TYR	2.7
1	D	105	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	58	ILE	2.7
3	L	53	ILE	2.7
1	B	76	GLY	2.7
2	J	133	THR	2.7
3	N	92[A]	SER	2.7
3	N	196	SER	2.7
2	I	119	TYR	2.7
2	J	112	TYR	2.7
3	O	74	LEU	2.7
3	L	185	ASP	2.7
2	I	210	PRO	2.6
2	J	157	GLN	2.6
2	J	236	ILE	2.6
3	L	95	ILE	2.6
3	L	110	GLN	2.6
3	L	140	PRO	2.6
2	H	174	GLU	2.6
3	O	184	THR	2.6
3	L	34	ALA	2.6
3	L	136	SER	2.6
3	L	141	SER	2.6
3	L	211	SER	2.6
2	H	72	TYR	2.6
3	O	163	ASP	2.6
2	J	27	PRO	2.6
2	H	60	GLY	2.6
2	K	176	VAL	2.6
1	B	64	SER	2.6
2	I	182	SER	2.6
3	L	196	SER	2.6
3	M	47	SER	2.6
3	N	142	SER	2.6
3	N	194	SER	2.6
1	D	146	TYR	2.6
2	J	201	TYR	2.6
3	M	193	TYR	2.6
2	J	231	LYS	2.6
3	N	155	PHE	2.6
3	L	102	ASP	2.6
3	M	34	ALA	2.6
1	D	61	SER	2.6
1	D	67	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	59	HIS	2.6
2	I	68	TYR	2.6
3	M	139	PRO	2.6
2	K	233	ASP	2.6
2	H	75	GLY	2.6
2	K	153	GLY	2.6
3	L	125	GLU	2.6
1	A	155	THR	2.6
1	C	80	ALA	2.6
2	K	219	VAL	2.6
2	K	65	TRP	2.6
3	N	164	ILE	2.6
1	B	165	HIS	2.6
2	I	112	TYR	2.6
3	O	42	MET	2.6
2	I	27	PRO	2.6
2	I	187	SER	2.6
2	I	204	SER	2.6
2	J	204	SER	2.6
3	L	54	HIS	2.6
3	L	76	SER	2.6
3	M	155	PHE	2.6
3	O	125	GLU	2.6
1	B	88	VAL	2.6
2	J	162	VAL	2.6
3	O	34	ALA	2.6
3	M	117	THR	2.6
3	M	202	THR	2.6
3	N	111	TRP	2.5
3	O	111	TRP	2.5
2	I	98	PHE	2.5
2	H	118	TYR	2.5
3	L	108	CYS	2.5
3	L	97	SER	2.5
3	N	113	SER	2.5
2	H	153	GLY	2.5
1	B	148	LEU	2.5
2	K	49	ASP	2.5
2	J	194	ALA	2.5
3	L	218	HIS	2.5
2	K	106	SER	2.5
3	M	35	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	197	GLN	2.5
2	I	41	LYS	2.5
1	D	162	ASP	2.5
2	H	222	ASN	2.5
2	I	194	ALA	2.5
2	J	115	ALA	2.5
2	I	66	ILE	2.5
3	M	195	MET	2.5
3	M	114	TYR	2.5
3	N	56	TYR	2.5
3	O	148	GLY	2.5
2	H	154	SER	2.5
2	J	58	SER	2.5
2	H	162	VAL	2.5
3	N	70	ASP	2.5
2	H	230	THR	2.5
1	D	151	PRO	2.5
1	C	79	LEU	2.5
2	H	196	LEU	2.5
2	J	63	LEU	2.5
2	H	26	GLY	2.5
2	H	121	GLY	2.5
2	K	137	VAL	2.5
2	K	43	SER	2.5
1	A	131	ILE	2.5
3	N	68	ILE	2.5
1	A	144	ASP	2.5
1	C	77	ASN	2.5
2	I	47	PHE	2.5
2	J	108	ASP	2.5
2	K	199	ASP	2.5
3	N	102	ASP	2.5
2	H	202	THR	2.5
3	M	183	TRP	2.5
1	B	66	LEU	2.5
2	K	149	PRO	2.5
3	M	156	LEU	2.5
2	H	119	TYR	2.5
2	J	119	TYR	2.5
2	I	43	SER	2.4
2	K	212	SER	2.4
3	O	136	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	J	174	GLU	2.4
1	A	98	PHE	2.4
3	L	169	LYS	2.4
1	B	135	THR	2.4
1	D	135	THR	2.4
3	L	105	THR	2.4
3	M	199	LEU	2.4
3	L	107	TYR	2.4
2	H	128	VAL	2.4
2	K	165	GLY	2.4
2	I	205	SER	2.4
3	L	87	SER	2.4
2	J	47	PHE	2.4
3	M	126	LEU	2.4
2	I	191	THR	2.4
3	N	183	TRP	2.4
3	N	198	THR	2.4
3	O	70	ASP	2.4
3	O	192	THR	2.4
1	B	138	PRO	2.4
1	D	160	VAL	2.4
2	K	36	VAL	2.4
2	K	72	TYR	2.4
3	M	61	GLY	2.4
3	N	166	VAL	2.4
3	O	106	TYR	2.4
3	O	226	VAL	2.4
2	H	204	SER	2.4
3	O	76	SER	2.4
1	C	109	LEU	2.4
1	C	121	LEU	2.4
2	H	51	ASN	2.4
2	K	158	THR	2.4
3	M	140	PRO	2.4
2	I	127	ASP	2.4
2	K	111	VAL	2.4
3	M	130	ASP	2.4
2	I	117	GLY	2.4
1	B	131	ILE	2.4
3	M	53	ILE	2.4
2	J	197	GLN	2.4
1	D	73	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	I	203	LEU	2.4
3	N	141	SER	2.4
3	N	182	SER	2.4
1	B	118	VAL	2.4
2	H	232	VAL	2.4
2	K	71	PRO	2.4
3	N	122	THR	2.4
2	I	73	ASN	2.4
3	O	177	ASN	2.4
3	N	193	TYR	2.4
1	A	110	LYS	2.4
1	D	140	ARG	2.4
2	K	161	MET	2.4
3	N	195	MET	2.4
3	N	186	GLN	2.4
2	J	101	LEU	2.4
2	K	185	LEU	2.4
2	J	25	SER	2.4
3	O	48	SER	2.4
3	L	50	VAL	2.4
3	L	55	TRP	2.4
2	H	73	ASN	2.3
2	I	42	ALA	2.3
2	I	100	HIS	2.3
3	L	177	ASN	2.3
1	D	81	ASP	2.3
3	L	106	TYR	2.3
1	D	62	LEU	2.3
2	K	164	LEU	2.3
3	L	82	PHE	2.3
3	L	109	GLN	2.3
3	O	156	LEU	2.3
1	B	116	VAL	2.3
1	B	160	VAL	2.3
1	C	88	VAL	2.3
2	I	207	VAL	2.3
3	L	40	VAL	2.3
2	J	180	TRP	2.3
3	N	55	TRP	2.3
2	H	133	THR	2.3
2	J	75	GLY	2.3
2	J	213	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	K	76	THR	2.3
1	A	120	ALA	2.3
1	B	124	ALA	2.3
2	I	114	CYS	2.3
1	D	85	ASN	2.3
2	H	171	TYR	2.3
3	L	126	LEU	2.3
3	O	110	GLN	2.3
1	B	163	VAL	2.3
1	C	74	VAL	2.3
2	K	162	VAL	2.3
2	K	232	VAL	2.3
1	B	154	LYS	2.3
1	A	71	SER	2.3
1	A	75	ILE	2.3
2	H	35	SER	2.3
2	H	134	THR	2.3
2	I	34	ALA	2.3
2	I	58	SER	2.3
2	K	139	SER	2.3
3	L	48	SER	2.3
3	M	111	TRP	2.3
3	M	26	THR	2.3
2	J	52	MET	2.3
3	O	108	CYS	2.3
1	B	62	LEU	2.3
2	I	193	PRO	2.3
2	J	173	PRO	2.3
2	I	132	GLY	2.3
1	B	113	ALA	2.3
1	C	120	ALA	2.3
2	H	97	ALA	2.3
1	A	64	SER	2.3
2	H	208	THR	2.3
2	I	89	THR	2.3
2	J	212	SER	2.3
3	N	156	LEU	2.3
2	I	79	ASN	2.3
2	J	222	ASN	2.3
2	I	108	ASP	2.3
1	D	166	LYS	2.3
2	H	176	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	L	208	ARG	2.3
2	I	173	PRO	2.3
3	M	224	PRO	2.3
1	C	145	ALA	2.3
1	D	70	ALA	2.3
2	K	130	GLY	2.3
3	O	84	GLY	2.3
2	K	180	TRP	2.3
1	D	79	LEU	2.3
2	K	133	THR	2.3
3	L	145	LEU	2.3
2	H	126	PHE	2.3
2	H	138	SER	2.3
3	L	191	SER	2.3
3	M	83	SER	2.3
3	N	60	SER	2.3
2	I	148	TYR	2.3
2	J	113	TYR	2.3
2	J	195	VAL	2.3
2	J	237	VAL	2.3
3	L	153	VAL	2.3
3	L	163	ASP	2.3
3	N	23	ILE	2.2
1	A	151	PRO	2.2
1	D	127	PRO	2.2
1	D	150	GLY	2.2
3	M	36	PRO	2.2
3	M	46	ALA	2.2
3	N	67	TRP	2.2
1	B	146	TYR	2.2
2	H	25	SER	2.2
2	J	35	SER	2.2
2	J	68	TYR	2.2
3	M	85	SER	2.2
3	O	47	SER	2.2
3	O	114	TYR	2.2
1	A	118	VAL	2.2
2	I	51	ASN	2.2
2	J	102	ASN	2.2
3	M	58	GLN	2.2
3	M	135	VAL	2.2
2	I	149	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
3	L	159	PHE	2.2
3	M	229	PHE	2.2
1	A	146	TYR	2.2
2	I	83	ARG	2.2
3	L	142	SER	2.2
2	I	30	VAL	2.2
3	L	78	VAL	2.2
3	O	57	GLN	2.2
2	J	221	CYS	2.2
1	B	94	ASP	2.2
2	J	71	PRO	2.2
3	O	219	LYS	2.2
3	L	117	THR	2.2
3	M	213	THR	2.2
2	H	50	TYR	2.2
2	K	178	VAL	2.2
2	J	160	SER	2.2
2	J	20	ILE	2.2
3	L	25	LEU	2.2
3	L	161	PRO	2.2
3	N	119	GLY	2.2
3	O	178	GLY	2.2
1	C	170	ASP	2.2
3	M	185	ASP	2.2
3	O	138	PHE	2.2
1	A	74	VAL	2.2
2	I	53	TYR	2.2
2	H	57	GLN	2.2
2	H	157	GLN	2.2
2	I	80	GLN	2.2
3	L	176	GLN	2.2
3	O	97	SER	2.2
3	O	201	LEU	2.2
1	A	129	GLU	2.2
1	B	85	ASN	2.2
3	O	123	LYS	2.2
3	O	172	GLY	2.2
2	I	166	CYS	2.2
3	N	108	CYS	2.2
2	H	192	PHE	2.2
3	N	229	PHE	2.2
2	H	142	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	207	VAL	2.1
2	H	78	TYR	2.1
1	D	149	LEU	2.1
1	C	63	SER	2.1
2	K	52	MET	2.1
3	M	92[A]	SER	2.1
3	N	98	MET	2.1
2	I	131	ALA	2.1
3	O	150	ALA	2.1
2	J	70	ASP	2.1
2	J	30	VAL	2.1
2	H	96	THR	2.1
1	A	58	ILE	2.1
1	A	109	LEU	2.1
2	J	22	LEU	2.1
1	B	70	ALA	2.1
1	B	96	ALA	2.1
1	C	90	SER	2.1
2	I	184	SER	2.1
3	L	47	SER	2.1
3	L	85	SER	2.1
3	M	51	SER	2.1
3	M	119	GLY	2.1
2	H	159	ASN	2.1
3	L	210	ASN	2.1
2	I	180	TRP	2.1
2	J	199	ASP	2.1
2	J	136	THR	2.1
2	I	45	TYR	2.1
2	I	164	LEU	2.1
2	K	236	ILE	2.1
2	H	21	GLN	2.1
3	M	186	GLN	2.1
2	I	121	GLY	2.1
2	J	152	PRO	2.1
3	O	149	GLY	2.1
1	C	89	SER	2.1
2	H	198	SER	2.1
2	K	206	SER	2.1
3	N	135	VAL	2.1
2	I	150	LEU	2.1
2	I	199	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	K	113	TYR	2.1
2	I	115	ALA	2.1
2	K	57	GLN	2.1
2	K	80	GLN	2.1
2	H	117	GLY	2.1
3	O	77	GLY	2.1
1	D	78	GLU	2.1
2	H	27	PRO	2.1
2	K	28	GLU	2.1
1	B	90	SER	2.1
2	I	62	SER	2.1
2	I	137	VAL	2.1
2	K	41	LYS	2.1
1	B	149	LEU	2.1
2	H	69	ILE	2.1
2	J	88	LEU	2.1
2	J	164	LEU	2.1
3	L	111	TRP	2.1
1	B	170	ASP	2.1
2	H	166	CYS	2.1
2	I	230	THR	2.1
3	L	184	THR	2.1
3	N	105	THR	2.1
3	O	71	THR	2.1
2	J	155	ALA	2.1
2	J	188	GLY	2.1
2	K	172	PHE	2.1
3	O	64	PRO	2.1
2	I	38	VAL	2.0
2	I	162	VAL	2.0
3	M	50	VAL	2.0
2	K	228	SER	2.0
3	N	33	SER	2.0
3	O	35	SER	2.0
2	J	150	LEU	2.0
3	M	95	ILE	2.0
3	L	168	TRP	2.0
3	O	55	TRP	2.0
3	M	98	MET	2.0
1	B	145	ALA	2.0
2	J	220	THR	2.0
3	O	117	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	I	157	GLN	2.0
3	L	229	PHE	2.0
3	O	133	PRO	2.0
1	B	78	GLU	2.0
2	I	237	VAL	2.0
3	L	199	LEU	2.0
2	H	103	SER	2.0
3	N	53	ILE	2.0
3	O	196	SER	2.0
2	K	214	TRP	2.0
3	N	100	ALA	2.0
2	K	68	TYR	2.0
2	K	148	TYR	2.0
3	L	94	THR	2.0
2	K	91	ASP	2.0
3	L	171	ASP	2.0
2	I	126	PHE	2.0
3	L	214	CYS	2.0
3	O	227	LYS	2.0
2	H	178	VAL	2.0
2	I	174	GLU	2.0
3	L	24	VAL	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 oligosaccharides 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, 95th 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	A	301	1/1	0.94	0.10	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	C	301	1/1	0.94	0.17	101,101,101,101	0
4	NA	D	301	1/1	0.94	0.12	107,107,107,107	0
4	NA	B	301	1/1	0.97	0.22	101,101,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.