



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:04 AM GMT

PDB ID : 1Z6O
Title : Crystal Structure of Trichoplusia ni secreted ferritin
Authors : Hamburger, A.E.; West Jr., A.P.; Hamburger, Z.A.; Hamburger, P.; Bjorkman, P.J.
Deposited on : 2005-03-22
Resolution : 1.91 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

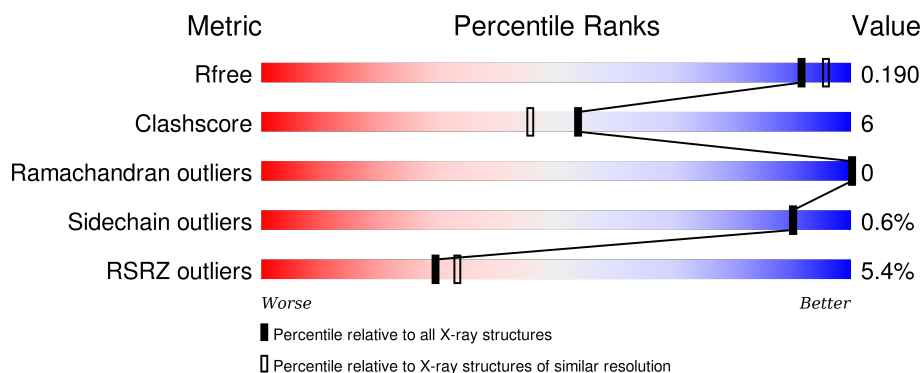
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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}	91344	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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. 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	212	<div> <div>10%</div> <div>88%</div> <div>12%</div> </div>
1	B	212	<div> <div>6%</div> <div>91%</div> <div>9%</div> </div>
1	C	212	<div> <div>7%</div> <div>90%</div> <div>10%</div> </div>
1	D	212	<div> <div>7%</div> <div>91%</div> <div>9%</div> </div>
1	E	212	<div> <div>6%</div> <div>91%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	212	
1	G	212	
1	H	212	
1	I	212	
1	J	212	
1	K	212	
1	L	212	
2	M	191	
2	N	191	
2	O	191	
2	P	191	
2	Q	191	
2	R	191	
2	S	191	
2	T	191	
2	U	191	
2	V	191	
2	W	191	
2	X	191	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 43180 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 Ferritin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1699	1066	294	334	5			
1	B	212	Total	C	N	O	S	0	0	0
			1699	1066	294	334	5			
1	C	212	Total	C	N	O	S	0	0	0
			1699	1066	294	334	5			
1	D	212	Total	C	N	O	S	0	0	0
			1699	1066	294	334	5			
1	E	212	Total	C	N	O	S	0	0	0
			1699	1066	294	334	5			
1	F	212	Total	C	N	O	S	0	0	0
			1699	1066	294	334	5			
1	G	212	Total	C	N	O	S	0	0	0
			1699	1066	294	334	5			
1	H	212	Total	C	N	O	S	0	0	0
			1699	1066	294	334	5			
1	I	212	Total	C	N	O	S	0	0	0
			1699	1066	294	334	5			
1	J	212	Total	C	N	O	S	0	0	0
			1699	1066	294	334	5			
1	K	212	Total	C	N	O	S	0	0	0
			1699	1066	294	334	5			
1	L	212	Total	C	N	O	S	0	0	0
			1699	1066	294	334	5			

- Molecule 2 is a protein called Ferritin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	N	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	P	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	Q	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	R	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	S	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	T	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	U	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	V	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	W	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			
2	X	191	Total	C	N	O	S	0	0	0
			1526	955	267	293	11			

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Fe	0	0
			1	1		
3	Q	1	Total	Fe	0	0
			1	1		
3	B	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	V	1	Total	Fe	0	0
			1	1		
3	W	1	Total	Fe	0	0
			1	1		
3	A	1	Total	Fe	0	0
			1	1		
3	T	1	Total	Fe	0	0
			1	1		
3	N	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	U	1	Total 1	Fe 1	0	0
3	X	1	Total 1	Fe 1	0	0
3	O	1	Total 1	Fe 1	0	0
3	R	1	Total 1	Fe 1	0	0
3	S	1	Total 1	Fe 1	0	0
3	F	1	Total 1	Fe 1	0	0
3	M	1	Total 1	Fe 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Ca 2	0	0
4	A	2	Total 2	Ca 2	0	0
4	C	2	Total 2	Ca 2	0	0
4	F	2	Total 2	Ca 2	0	0

- Molecule 5 is water.

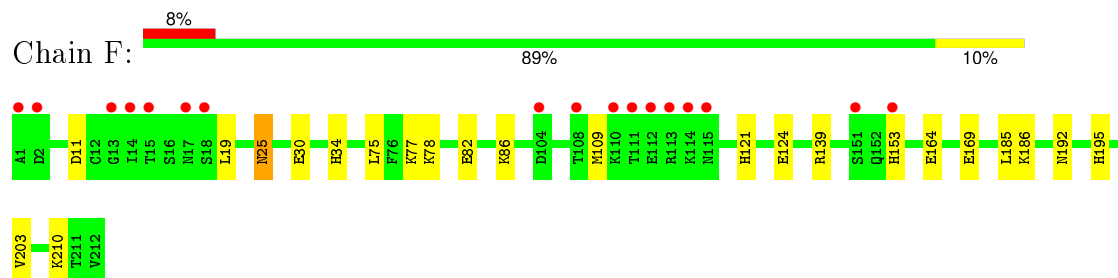
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	155	Total 155	O 155	0	0
5	B	157	Total 157	O 157	0	0
5	C	159	Total 159	O 159	0	0
5	D	158	Total 158	O 158	0	0
5	E	161	Total 161	O 161	0	0
5	F	158	Total 158	O 158	0	0

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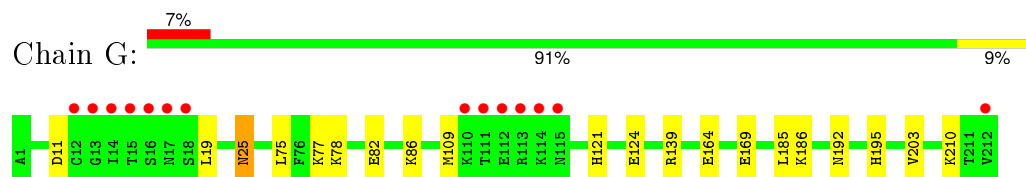
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	157	Total 157	O 157	0	0
5	H	161	Total 161	O 161	0	0
5	I	159	Total 159	O 159	0	0
5	J	158	Total 158	O 158	0	0
5	K	156	Total 156	O 156	0	0
5	L	159	Total 159	O 159	0	0
5	M	215	Total 215	O 215	0	0
5	N	214	Total 214	O 214	0	0
5	O	211	Total 211	O 211	0	0
5	P	215	Total 215	O 215	0	0
5	Q	214	Total 214	O 214	0	0
5	R	211	Total 211	O 211	0	0
5	S	214	Total 214	O 214	0	0
5	T	213	Total 213	O 213	0	0
5	U	211	Total 211	O 211	0	0
5	V	214	Total 214	O 214	0	0
5	W	214	Total 214	O 214	0	0
5	X	212	Total 212	O 212	0	0

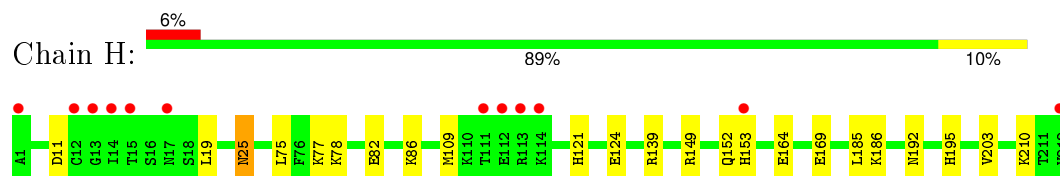
- Molecule 1: Ferritin light chain



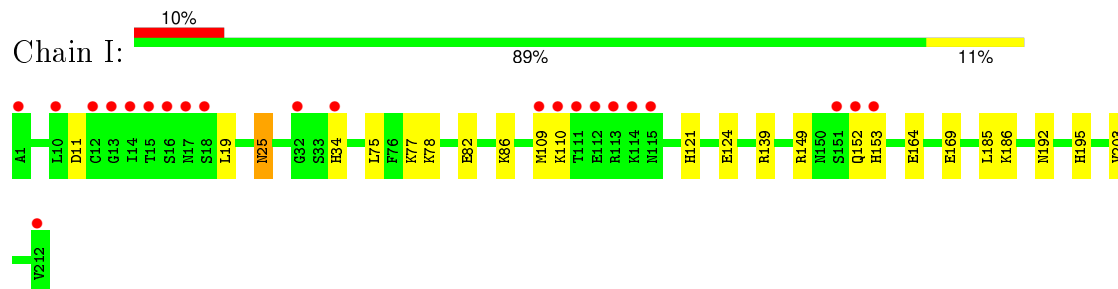
- Molecule 1: Ferritin light chain



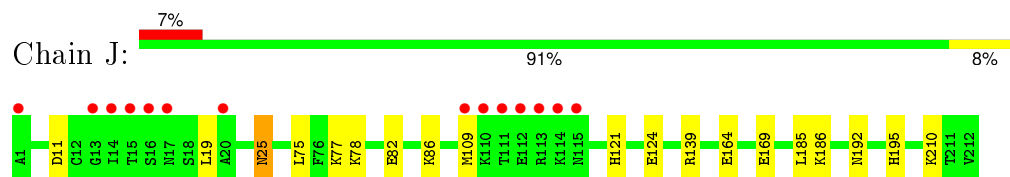
- Molecule 1: Ferritin light chain



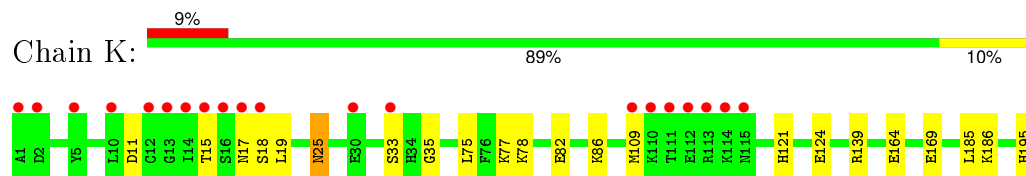
- Molecule 1: Ferritin light chain



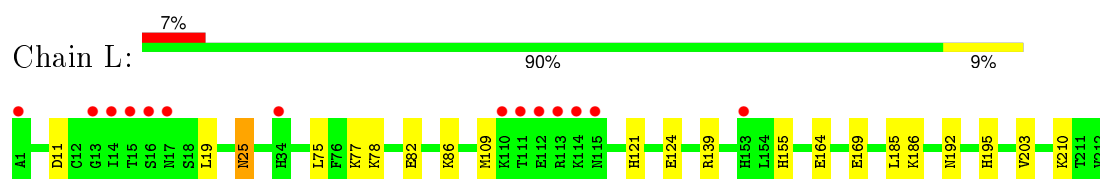
- Molecule 1: Ferritin light chain



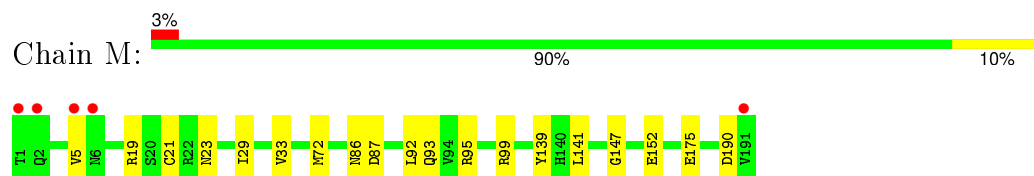
- Molecule 1: Ferritin light chain



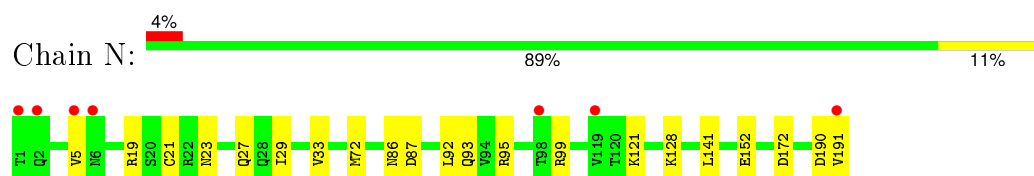
- Molecule 1: Ferritin light chain



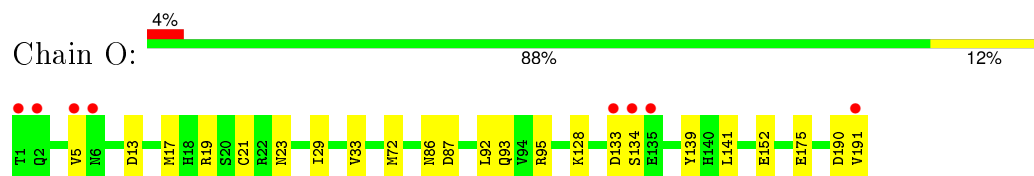
- Molecule 2: Ferritin heavy chain



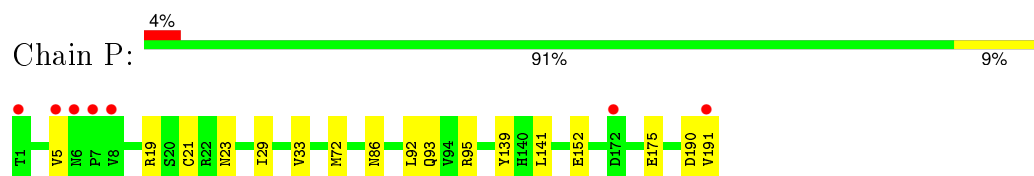
- Molecule 2: Ferritin heavy chain



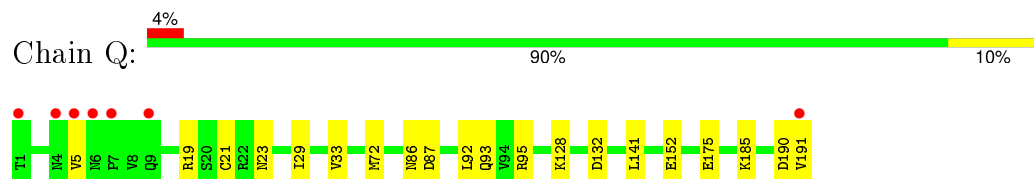
- Molecule 2: Ferritin heavy chain



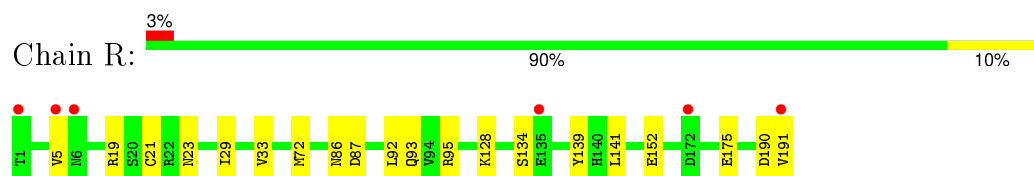
- Molecule 2: Ferritin heavy chain



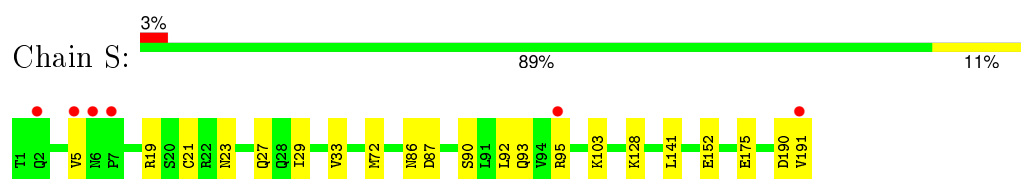
- Molecule 2: Ferritin heavy chain



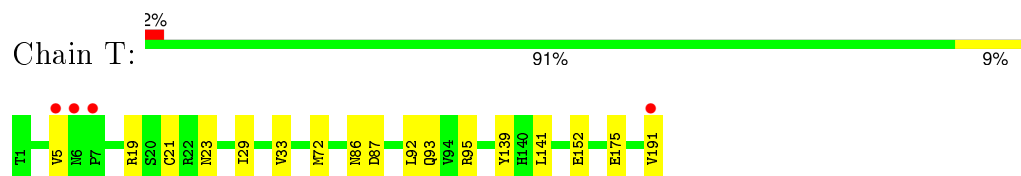
- Molecule 2: Ferritin heavy chain



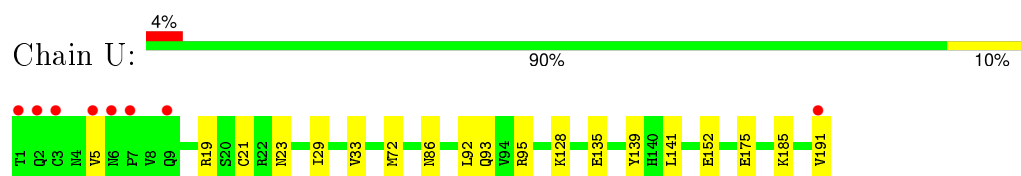
- Molecule 2: Ferritin heavy chain



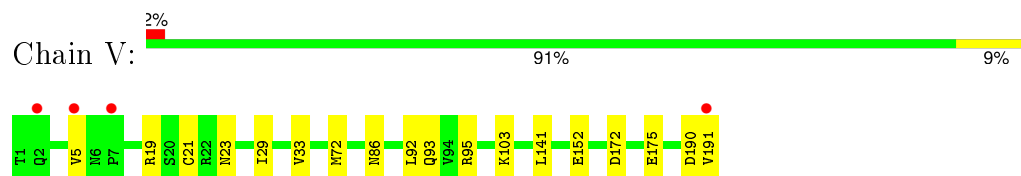
- Molecule 2: Ferritin heavy chain



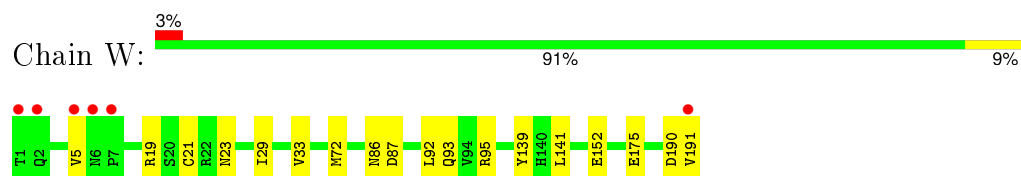
- Molecule 2: Ferritin heavy chain



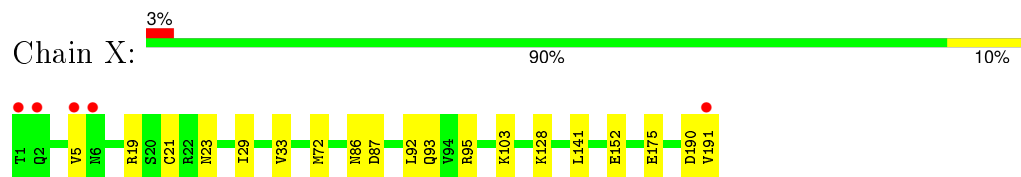
- Molecule 2: Ferritin heavy chain



- Molecule 2: Ferritin heavy chain



- Molecule 2: Ferritin heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	206.88 Å 145.70 Å 209.16 Å 90.00° 94.93° 90.00°	Depositor
Resolution (Å)	19.98 – 1.91 29.85 – 1.91	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.98-1.91) 75.2 (29.85-1.91)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.00 (at 1.91 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.189 , 0.194 0.189 , 0.190	Depositor DCC
R_{free} test set	23175 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	6.3	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.12$	Xtriage
Outliers	0 of 463420 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	43180	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, FE

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	0.45	0/1734	0.60	0/2343
1	B	0.45	0/1734	0.61	0/2343
1	C	0.45	0/1734	0.61	0/2343
1	D	0.45	0/1734	0.60	0/2343
1	E	0.45	0/1734	0.61	0/2343
1	F	0.45	0/1734	0.60	0/2343
1	G	0.45	0/1734	0.60	0/2343
1	H	0.45	0/1734	0.60	0/2343
1	I	0.45	0/1734	0.60	0/2343
1	J	0.45	0/1734	0.60	0/2343
1	K	0.45	0/1734	0.60	0/2343
1	L	0.45	0/1734	0.60	0/2343
2	M	0.48	0/1553	0.60	0/2088
2	N	0.48	0/1553	0.60	0/2088
2	O	0.48	0/1553	0.60	0/2088
2	P	0.48	0/1553	0.60	0/2088
2	Q	0.48	0/1553	0.60	0/2088
2	R	0.48	0/1553	0.60	0/2088
2	S	0.48	0/1553	0.60	0/2088
2	T	0.48	0/1553	0.60	0/2088
2	U	0.48	0/1553	0.60	0/2088
2	V	0.48	0/1553	0.60	0/2088
2	W	0.48	0/1553	0.60	0/2088
2	X	0.48	0/1553	0.60	0/2088
All	All	0.46	0/39444	0.60	0/53172

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	1699	0	1613	28	10
1	B	1699	0	1613	29	0
1	C	1699	0	1613	27	16
1	D	1699	0	1613	23	0
1	E	1699	0	1613	25	0
1	F	1699	0	1613	25	14
1	G	1699	0	1613	25	0
1	H	1699	0	1613	27	18
1	I	1699	0	1613	28	16
1	J	1699	0	1613	27	0
1	K	1699	0	1613	23	10
1	L	1699	0	1613	28	0
2	M	1526	0	1500	23	1
2	N	1526	0	1500	23	18
2	O	1526	0	1500	23	5
2	P	1526	0	1500	21	0
2	Q	1526	0	1500	24	4
2	R	1526	0	1500	22	3
2	S	1526	0	1500	23	6
2	T	1526	0	1500	22	0
2	U	1526	0	1500	23	1
2	V	1526	0	1500	22	5
2	W	1526	0	1500	20	0
2	X	1526	0	1500	22	3
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	F	2	0	0	0	0
5	A	155	0	0	8	2
5	B	157	0	0	7	0
5	C	159	0	0	7	2
5	D	158	0	0	7	0
5	E	161	0	0	7	0
5	F	158	0	0	6	1
5	G	157	0	0	7	0
5	H	161	0	0	8	0
5	I	159	0	0	8	2
5	J	158	0	0	8	0
5	K	156	0	0	7	0
5	L	159	0	0	8	0
5	M	215	0	0	2	0
5	N	214	0	0	4	17
5	O	211	0	0	2	14
5	P	215	0	0	2	0
5	Q	214	0	0	2	1
5	R	211	0	0	2	0
5	S	214	0	0	2	6
5	T	213	0	0	2	0
5	U	211	0	0	2	0
5	V	214	0	0	3	3
5	W	214	0	0	2	0
5	X	212	0	0	2	7
All	All	43180	0	37356	489	99

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 6.

All (489) 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:K:210:LYS:HE2	2:N:190:ASP:O	1.80	0.81
1:L:109:MET:CE	1:L:139:ARG:HE	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:MET:HE1	1:B:139:ARG:HE	1.45	0.81
1:I:109:MET:CE	1:I:139:ARG:HE	1.94	0.81
1:F:109:MET:HE1	1:F:139:ARG:HE	1.45	0.81
1:J:109:MET:CE	1:J:139:ARG:HE	1.94	0.81
1:C:109:MET:CE	1:C:139:ARG:HE	1.94	0.80
1:D:109:MET:CE	1:D:139:ARG:HE	1.94	0.80
1:E:109:MET:CE	1:E:139:ARG:HE	1.94	0.80
1:G:109:MET:CE	1:G:139:ARG:HE	1.94	0.80
1:A:109:MET:CE	1:A:139:ARG:HE	1.94	0.80
1:F:109:MET:CE	1:F:139:ARG:HE	1.94	0.80
1:K:109:MET:CE	1:K:139:ARG:HE	1.94	0.80
1:B:109:MET:CE	1:B:139:ARG:HE	1.94	0.80
1:H:109:MET:CE	1:H:139:ARG:HE	1.94	0.80
1:E:109:MET:HE1	1:E:139:ARG:HE	1.48	0.78
1:G:109:MET:HE1	1:G:139:ARG:HE	1.48	0.78
1:B:195:HIS:HB3	5:B:6441:HOH:O	1.84	0.78
1:C:109:MET:HE1	1:C:139:ARG:HE	1.49	0.78
1:C:192:ASN:HD21	2:U:175:GLU:H	1.29	0.78
1:D:195:HIS:HB3	5:D:1491:HOH:O	1.84	0.78
1:J:195:HIS:HB3	5:J:3718:HOH:O	1.84	0.77
1:F:195:HIS:HB3	5:F:2234:HOH:O	1.84	0.77
1:H:195:HIS:HB3	5:H:2980:HOH:O	1.84	0.77
1:C:195:HIS:HB3	5:C:1119:HOH:O	1.84	0.77
1:E:195:HIS:HB3	5:E:366:HOH:O	1.84	0.77
1:L:195:HIS:HB3	5:L:371:HOH:O	1.84	0.77
1:C:121:HIS:NE2	1:C:124:GLU:HG3	2.00	0.77
1:K:121:HIS:NE2	1:K:124:GLU:HG3	2.00	0.77
1:A:121:HIS:NE2	1:A:124:GLU:HG3	2.00	0.77
1:J:121:HIS:NE2	1:J:124:GLU:HG3	2.00	0.76
1:G:121:HIS:NE2	1:G:124:GLU:HG3	2.00	0.76
1:I:121:HIS:NE2	1:I:124:GLU:HG3	2.00	0.76
1:G:195:HIS:HB3	5:G:2608:HOH:O	1.84	0.76
1:A:195:HIS:HB3	5:A:5438:HOH:O	1.84	0.76
1:L:121:HIS:NE2	1:L:124:GLU:HG3	2.00	0.76
1:H:121:HIS:NE2	1:H:124:GLU:HG3	2.00	0.76
1:K:195:HIS:HB3	5:K:4087:HOH:O	1.84	0.76
1:B:121:HIS:NE2	1:B:124:GLU:HG3	2.00	0.76
1:F:121:HIS:NE2	1:F:124:GLU:HG3	2.00	0.76
1:B:121:HIS:CE1	1:B:124:GLU:HG3	2.21	0.76
1:E:121:HIS:NE2	1:E:124:GLU:HG3	2.00	0.75
1:K:121:HIS:CE1	1:K:124:GLU:HG3	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:HIS:CE1	1:F:124:GLU:HG3	2.21	0.75
1:D:121:HIS:CE1	1:D:124:GLU:HG3	2.21	0.75
1:C:121:HIS:CE1	1:C:124:GLU:HG3	2.21	0.75
1:G:121:HIS:CE1	1:G:124:GLU:HG3	2.21	0.75
1:L:121:HIS:CE1	1:L:124:GLU:HG3	2.21	0.75
1:E:121:HIS:CE1	1:E:124:GLU:HG3	2.21	0.75
1:D:121:HIS:NE2	1:D:124:GLU:HG3	2.00	0.75
1:I:195:HIS:HB3	5:I:3349:HOH:O	1.84	0.75
1:I:121:HIS:CE1	1:I:124:GLU:HG3	2.21	0.75
1:H:121:HIS:CE1	1:H:124:GLU:HG3	2.21	0.75
1:A:121:HIS:CE1	1:A:124:GLU:HG3	2.21	0.75
1:I:192:ASN:HD21	2:T:175:GLU:H	1.34	0.75
1:D:109:MET:HE1	1:D:139:ARG:HE	1.52	0.74
1:J:121:HIS:CE1	1:J:124:GLU:HG3	2.21	0.74
1:K:109:MET:HE1	1:K:139:ARG:HE	1.52	0.73
1:L:109:MET:HE1	1:L:139:ARG:HE	1.55	0.72
1:C:203:VAL:HG13	2:U:191:VAL:HG11	1.72	0.72
1:H:109:MET:HE2	1:H:139:ARG:HE	1.55	0.71
1:J:109:MET:HE2	1:J:139:ARG:HE	1.56	0.70
1:G:19:LEU:O	1:J:186:LYS:HE3	1.92	0.69
1:B:19:LEU:O	1:K:186:LYS:HE3	1.92	0.69
1:A:210:LYS:HE2	2:X:190:ASP:O	1.94	0.68
1:A:109:MET:HE1	1:A:139:ARG:HE	1.56	0.67
1:J:210:LYS:HE2	2:S:190:ASP:O	1.94	0.67
1:I:109:MET:HE2	1:I:139:ARG:HE	1.59	0.67
1:B:210:LYS:HE2	2:P:190:ASP:O	1.95	0.67
1:I:109:MET:HE1	1:I:139:ARG:HE	1.59	0.66
1:H:192:ASN:HD21	2:O:175:GLU:H	1.43	0.65
1:J:109:MET:HE1	1:J:139:ARG:HE	1.61	0.64
1:B:192:ASN:HD21	2:P:175:GLU:H	1.44	0.64
1:I:86:LYS:HE3	5:I:3328:HOH:O	1.97	0.64
1:E:86:LYS:HE3	5:E:355:HOH:O	1.98	0.64
1:H:86:LYS:HE3	5:H:2959:HOH:O	1.98	0.64
1:F:86:LYS:HE3	5:F:2213:HOH:O	1.98	0.64
1:A:86:LYS:HE3	5:A:5427:HOH:O	1.98	0.64
1:A:109:MET:HE2	1:A:139:ARG:HE	1.62	0.64
1:G:210:LYS:HE2	2:R:190:ASP:O	1.98	0.64
1:H:109:MET:HE1	1:H:139:ARG:HE	1.63	0.64
1:J:86:LYS:HE3	5:J:3697:HOH:O	1.98	0.64
1:K:25:ASN:C	1:K:25:ASN:HD22	2.02	0.63
1:L:192:ASN:HD21	2:Q:175:GLU:H	1.44	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ASN:C	1:C:25:ASN:HD22	2.02	0.63
1:E:25:ASN:C	1:E:25:ASN:HD22	2.02	0.63
1:B:25:ASN:C	1:B:25:ASN:HD22	2.02	0.63
1:A:25:ASN:HD22	1:A:25:ASN:C	2.02	0.63
1:G:86:LYS:HE3	5:G:2587:HOH:O	1.97	0.63
1:J:25:ASN:C	1:J:25:ASN:HD22	2.02	0.63
1:G:25:ASN:C	1:G:25:ASN:HD22	2.02	0.63
1:L:86:LYS:HE3	5:L:360:HOH:O	1.97	0.63
1:C:86:LYS:HE3	5:C:1098:HOH:O	1.98	0.63
1:K:86:LYS:HE3	5:K:4066:HOH:O	1.98	0.63
1:D:86:LYS:HE3	5:D:1470:HOH:O	1.98	0.62
1:L:25:ASN:HD22	1:L:25:ASN:C	2.02	0.62
1:F:25:ASN:HD22	1:F:25:ASN:C	2.02	0.62
1:B:86:LYS:HE3	5:B:6430:HOH:O	1.98	0.62
1:I:25:ASN:HD22	1:I:25:ASN:C	2.02	0.61
1:H:25:ASN:HD22	1:H:25:ASN:C	2.02	0.61
2:P:33:VAL:HG21	2:P:92:LEU:HD22	1.83	0.61
5:I:3263:HOH:O	2:U:5:VAL:HG21	2.01	0.61
1:D:25:ASN:HD22	1:D:25:ASN:C	2.02	0.61
2:V:33:VAL:HG21	2:V:92:LEU:HD22	1.83	0.61
1:D:109:MET:HE2	1:D:139:ARG:HE	1.66	0.61
5:J:3632:HOH:O	2:V:5:VAL:HG21	2.01	0.61
5:K:4001:HOH:O	2:W:5:VAL:HG21	2.01	0.61
5:L:331:HOH:O	2:X:5:VAL:HG21	2.01	0.61
1:C:192:ASN:ND2	2:U:175:GLU:H	1.98	0.60
2:N:33:VAL:HG21	2:N:92:LEU:HD22	1.83	0.60
5:F:2148:HOH:O	2:R:5:VAL:HG21	2.01	0.60
5:G:2522:HOH:O	2:S:5:VAL:HG21	2.01	0.60
2:Q:33:VAL:HG21	2:Q:92:LEU:HD22	1.83	0.60
5:C:1033:HOH:O	2:O:5:VAL:HG21	2.01	0.60
5:D:1405:HOH:O	2:P:5:VAL:HG21	2.01	0.60
2:M:33:VAL:HG21	2:M:92:LEU:HD22	1.83	0.60
2:X:33:VAL:HG21	2:X:92:LEU:HD22	1.83	0.60
5:B:6401:HOH:O	2:N:5:VAL:HG21	2.01	0.60
1:L:109:MET:HE2	1:L:139:ARG:HE	1.63	0.60
1:E:192:ASN:HD21	2:M:175:GLU:H	1.49	0.60
2:O:33:VAL:HG21	2:O:92:LEU:HD22	1.83	0.60
5:A:5399:HOH:O	2:M:5:VAL:HG21	2.01	0.60
5:E:325:HOH:O	2:Q:5:VAL:HG21	2.01	0.60
2:W:33:VAL:HG21	2:W:92:LEU:HD22	1.83	0.59
2:N:128:LYS:HG2	2:O:139:TYR:OH	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:LYS:HE3	1:J:19:LEU:O	2.02	0.59
1:E:210:LYS:HE2	2:M:190:ASP:O	2.01	0.59
2:T:33:VAL:HG21	2:T:92:LEU:HD22	1.83	0.59
1:A:186:LYS:HE3	1:L:19:LEU:O	2.03	0.59
1:D:186:LYS:HE3	1:K:19:LEU:O	2.01	0.59
2:S:33:VAL:HG21	2:S:92:LEU:HD22	1.83	0.59
1:F:19:LEU:O	1:G:186:LYS:HE3	2.03	0.59
2:U:33:VAL:HG21	2:U:92:LEU:HD22	1.83	0.59
5:H:2894:HOH:O	2:T:5:VAL:HG21	2.01	0.59
2:R:33:VAL:HG21	2:R:92:LEU:HD22	1.83	0.59
2:O:29:ILE:HG22	2:O:92:LEU:HD21	1.86	0.58
1:G:192:ASN:HD21	2:R:175:GLU:H	1.50	0.58
2:W:29:ILE:HG22	2:W:92:LEU:HD21	1.86	0.58
2:Q:29:ILE:HG22	2:Q:92:LEU:HD21	1.86	0.58
1:B:186:LYS:HE3	1:D:19:LEU:O	2.04	0.58
1:F:192:ASN:HD21	2:V:175:GLU:H	1.49	0.58
2:N:29:ILE:HG22	2:N:92:LEU:HD21	1.86	0.58
1:K:109:MET:HE2	1:K:139:ARG:HE	1.66	0.58
1:F:11:ASP:HB3	1:F:19:LEU:HD12	1.86	0.57
2:X:29:ILE:HG22	2:X:92:LEU:HD21	1.86	0.57
1:D:192:ASN:HD21	2:W:175:GLU:H	1.52	0.57
1:I:11:ASP:HB3	1:I:19:LEU:HD12	1.86	0.57
1:D:210:LYS:HE2	2:W:190:ASP:O	2.04	0.57
2:U:29:ILE:HG22	2:U:92:LEU:HD21	1.86	0.57
1:G:11:ASP:HB3	1:G:19:LEU:HD12	1.86	0.57
1:A:11:ASP:HB3	1:A:19:LEU:HD12	1.86	0.57
2:S:29:ILE:HG22	2:S:92:LEU:HD21	1.86	0.57
2:R:29:ILE:HG22	2:R:92:LEU:HD21	1.86	0.57
1:A:19:LEU:O	1:E:186:LYS:HE3	2.05	0.57
1:C:203:VAL:CG1	2:U:191:VAL:HG11	2.34	0.57
2:V:29:ILE:HG22	2:V:92:LEU:HD21	1.86	0.57
1:E:11:ASP:HB3	1:E:19:LEU:HD12	1.86	0.57
1:E:19:LEU:O	1:L:186:LYS:HE3	2.05	0.57
1:C:109:MET:HE2	1:C:139:ARG:HE	1.69	0.56
2:M:29:ILE:HG22	2:M:92:LEU:HD21	1.86	0.56
2:P:29:ILE:HG22	2:P:92:LEU:HD21	1.86	0.56
1:B:11:ASP:HB3	1:B:19:LEU:HD12	1.86	0.56
2:T:29:ILE:HG22	2:T:92:LEU:HD21	1.86	0.56
1:L:11:ASP:HB3	1:L:19:LEU:HD12	1.86	0.56
1:C:11:ASP:HB3	1:C:19:LEU:HD12	1.86	0.56
1:D:11:ASP:HB3	1:D:19:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:121:HIS:CD2	1:L:124:GLU:H	2.24	0.56
1:D:121:HIS:CD2	1:D:124:GLU:H	2.24	0.56
1:J:11:ASP:HB3	1:J:19:LEU:HD12	1.86	0.56
1:I:121:HIS:CD2	1:I:124:GLU:H	2.24	0.56
1:B:121:HIS:CD2	1:B:124:GLU:H	2.24	0.56
5:J:3632:HOH:O	2:V:5:VAL:HG11	2.06	0.56
1:K:11:ASP:HB3	1:K:19:LEU:HD12	1.86	0.56
1:H:11:ASP:HB3	1:H:19:LEU:HD12	1.86	0.56
1:G:109:MET:HE2	1:G:139:ARG:HE	1.70	0.56
1:G:121:HIS:CD2	1:G:124:GLU:H	2.24	0.56
1:E:109:MET:HE2	1:E:139:ARG:HE	1.70	0.55
1:I:203:VAL:HG13	2:T:191:VAL:HG11	1.89	0.55
5:H:2894:HOH:O	2:T:5:VAL:HG11	2.06	0.55
1:K:121:HIS:CD2	1:K:124:GLU:H	2.24	0.55
1:C:19:LEU:O	1:H:186:LYS:HE3	2.06	0.55
1:A:121:HIS:CD2	1:A:124:GLU:H	2.24	0.55
1:H:121:HIS:CD2	1:H:124:GLU:H	2.24	0.55
1:C:121:HIS:CD2	1:C:124:GLU:H	2.24	0.55
5:F:2148:HOH:O	2:R:5:VAL:HG11	2.06	0.55
5:B:6401:HOH:O	2:N:5:VAL:HG11	2.06	0.55
2:Q:93:GLN:CG	2:Q:95:ARG:HE	2.20	0.55
5:E:325:HOH:O	2:Q:5:VAL:HG11	2.06	0.55
5:I:3263:HOH:O	2:U:5:VAL:HG11	2.06	0.55
1:F:121:HIS:CD2	1:F:124:GLU:H	2.24	0.54
1:L:203:VAL:HG13	2:Q:191:VAL:HG11	1.89	0.54
5:K:4001:HOH:O	2:W:5:VAL:HG11	2.06	0.54
5:L:331:HOH:O	2:X:5:VAL:HG11	2.06	0.54
2:W:93:GLN:CG	2:W:95:ARG:HE	2.20	0.54
2:U:93:GLN:CG	2:U:95:ARG:HE	2.20	0.54
1:J:121:HIS:CD2	1:J:124:GLU:H	2.24	0.54
5:G:2522:HOH:O	2:S:5:VAL:HG11	2.06	0.54
2:S:93:GLN:CG	2:S:95:ARG:HE	2.20	0.54
2:N:93:GLN:CG	2:N:95:ARG:HE	2.20	0.54
2:R:93:GLN:CG	2:R:95:ARG:HE	2.20	0.54
2:M:93:GLN:CG	2:M:95:ARG:HE	2.20	0.54
2:O:93:GLN:CG	2:O:95:ARG:HE	2.20	0.54
2:V:93:GLN:CG	2:V:95:ARG:HE	2.20	0.54
1:K:210:LYS:NZ	2:N:191:VAL:O	2.41	0.54
1:E:121:HIS:CD2	1:E:124:GLU:H	2.24	0.54
5:C:1033:HOH:O	2:O:5:VAL:HG11	2.06	0.54
5:A:5399:HOH:O	2:M:5:VAL:HG11	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1405:HOH:O	2:P:5:VAL:HG11	2.06	0.54
2:P:93:GLN:CG	2:P:95:ARG:HE	2.20	0.54
2:T:93:GLN:CG	2:T:95:ARG:HE	2.20	0.53
1:L:210:LYS:HE2	2:Q:190:ASP:O	2.07	0.53
2:X:93:GLN:CG	2:X:95:ARG:HE	2.20	0.53
1:B:109:MET:HE1	1:B:139:ARG:NE	2.21	0.53
2:S:128:LYS:HG2	2:U:139:TYR:OH	2.09	0.53
1:A:164:GLU:O	1:A:169:GLU:HG3	2.09	0.53
1:B:164:GLU:O	1:B:169:GLU:HG3	2.10	0.52
1:H:164:GLU:O	1:H:169:GLU:HG3	2.09	0.52
1:F:164:GLU:O	1:F:169:GLU:HG3	2.10	0.52
1:E:164:GLU:O	1:E:169:GLU:HG3	2.09	0.52
1:C:164:GLU:O	1:C:169:GLU:HG3	2.10	0.52
1:L:164:GLU:O	1:L:169:GLU:HG3	2.10	0.52
1:H:109:MET:HE1	5:H:2743:HOH:O	2.10	0.52
1:I:164:GLU:O	1:I:169:GLU:HG3	2.09	0.52
1:J:164:GLU:O	1:J:169:GLU:HG3	2.10	0.52
1:K:164:GLU:O	1:K:169:GLU:HG3	2.10	0.52
1:F:109:MET:HE2	1:F:139:ARG:HE	1.73	0.52
1:C:203:VAL:HG13	2:U:191:VAL:CG1	2.39	0.51
1:D:164:GLU:O	1:D:169:GLU:HG3	2.10	0.51
1:G:164:GLU:O	1:G:169:GLU:HG3	2.09	0.51
1:A:192:ASN:HD21	2:X:175:GLU:H	1.57	0.51
1:B:109:MET:HE2	1:B:139:ARG:HE	1.73	0.51
2:Q:93:GLN:HG2	2:Q:95:ARG:HE	1.76	0.51
2:R:93:GLN:HG2	2:R:95:ARG:HE	1.76	0.51
2:O:93:GLN:HG2	2:O:95:ARG:HE	1.76	0.51
1:H:109:MET:HE2	1:H:139:ARG:NE	2.23	0.51
1:F:210:LYS:HE2	2:V:190:ASP:O	2.11	0.51
2:S:93:GLN:HG2	2:S:95:ARG:HE	1.76	0.50
2:W:93:GLN:HG2	2:W:95:ARG:HE	1.76	0.50
2:N:93:GLN:HG2	2:N:95:ARG:HE	1.76	0.50
2:U:93:GLN:HG2	2:U:95:ARG:HE	1.76	0.50
1:H:203:VAL:HG13	2:O:191:VAL:HG11	1.92	0.50
2:P:93:GLN:HG2	2:P:95:ARG:HE	1.76	0.50
1:J:109:MET:HE1	5:J:3481:HOH:O	2.11	0.50
2:V:93:GLN:HG2	2:V:95:ARG:HE	1.76	0.49
2:T:93:GLN:HG2	2:T:95:ARG:HE	1.76	0.49
1:G:77:LYS:HZ3	2:S:72:MET:CE	2.25	0.49
2:X:93:GLN:HG2	2:X:95:ARG:HE	1.76	0.49
2:M:93:GLN:HG2	2:M:95:ARG:HE	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:192:ASN:ND2	2:T:175:GLU:H	2.05	0.49
1:C:78:LYS:O	1:C:82:GLU:HG3	2.13	0.49
1:J:77:LYS:HZ3	2:V:72:MET:CE	2.26	0.49
2:Q:19:ARG:HH11	2:Q:23:ASN:HD21	1.61	0.49
1:E:78:LYS:O	1:E:82:GLU:HG3	2.13	0.49
1:F:78:LYS:O	1:F:82:GLU:HG3	2.13	0.49
1:A:77:LYS:HZ3	2:M:72:MET:CE	2.25	0.49
2:X:19:ARG:HH11	2:X:23:ASN:HD21	1.61	0.49
1:I:78:LYS:O	1:I:82:GLU:HG3	2.13	0.49
1:B:78:LYS:O	1:B:82:GLU:HG3	2.13	0.48
1:J:78:LYS:O	1:J:82:GLU:HG3	2.13	0.48
2:M:19:ARG:HH11	2:M:23:ASN:HD21	1.61	0.48
1:E:77:LYS:HZ3	2:Q:72:MET:CE	2.26	0.48
1:H:210:LYS:HE2	2:O:190:ASP:O	2.13	0.48
1:K:78:LYS:O	1:K:82:GLU:HG3	2.13	0.48
2:W:19:ARG:HH11	2:W:23:ASN:HD21	1.61	0.48
2:R:19:ARG:HH11	2:R:23:ASN:HD21	1.61	0.48
1:E:109:MET:HE1	1:E:139:ARG:NE	2.24	0.48
1:H:19:LEU:O	1:I:186:LYS:HE3	2.13	0.48
2:O:19:ARG:HH11	2:O:23:ASN:HD21	1.61	0.48
2:V:19:ARG:HH11	2:V:23:ASN:HD21	1.61	0.48
1:G:78:LYS:O	1:G:82:GLU:HG3	2.13	0.48
1:H:78:LYS:O	1:H:82:GLU:HG3	2.13	0.48
1:I:109:MET:HE2	1:I:139:ARG:NE	2.28	0.48
2:P:19:ARG:HH11	2:P:23:ASN:HD21	1.61	0.48
2:M:147:GLY:HA3	5:N:405:HOH:O	2.14	0.48
1:I:109:MET:HE1	5:I:3112:HOH:O	2.14	0.48
1:J:210:LYS:NZ	2:S:191:VAL:O	2.46	0.48
1:L:192:ASN:ND2	2:Q:175:GLU:H	2.11	0.48
1:L:78:LYS:O	1:L:82:GLU:HG3	2.13	0.48
1:A:78:LYS:O	1:A:82:GLU:HG3	2.13	0.48
1:B:109:MET:HB3	1:B:109:MET:HE2	1.78	0.47
1:G:77:LYS:NZ	2:S:72:MET:SD	2.87	0.47
1:F:77:LYS:HZ3	2:R:72:MET:CE	2.27	0.47
1:J:77:LYS:NZ	2:V:72:MET:SD	2.87	0.47
1:D:77:LYS:NZ	2:P:72:MET:SD	2.87	0.47
1:D:78:LYS:O	1:D:82:GLU:HG3	2.13	0.47
2:T:19:ARG:HH11	2:T:23:ASN:HD21	1.61	0.47
1:L:77:LYS:NZ	2:X:72:MET:SD	2.87	0.47
1:B:203:VAL:O	2:P:191:VAL:HG11	2.14	0.47
1:B:77:LYS:NZ	2:N:72:MET:SD	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:77:LYS:HZ3	2:U:72:MET:CE	2.27	0.47
1:C:77:LYS:NZ	2:O:72:MET:SD	2.87	0.47
1:E:109:MET:HB3	1:E:109:MET:HE2	1.78	0.47
1:E:77:LYS:NZ	2:Q:72:MET:SD	2.88	0.47
1:F:77:LYS:NZ	2:R:72:MET:SD	2.88	0.47
2:O:21:CYS:SG	2:O:141:LEU:HD23	2.55	0.47
1:C:109:MET:HB3	1:C:109:MET:HE2	1.79	0.47
2:U:21:CYS:SG	2:U:141:LEU:HD23	2.55	0.47
2:V:21:CYS:SG	2:V:141:LEU:HD23	2.55	0.47
2:P:21:CYS:SG	2:P:141:LEU:HD23	2.55	0.47
2:S:19:ARG:HH11	2:S:23:ASN:HD21	1.61	0.47
1:F:109:MET:HE1	1:F:139:ARG:NE	2.21	0.47
2:Q:21:CYS:SG	2:Q:141:LEU:HD23	2.55	0.47
2:N:21:CYS:SG	2:N:141:LEU:HD23	2.55	0.47
1:J:109:MET:HE2	1:J:139:ARG:NE	2.25	0.47
1:H:192:ASN:ND2	2:O:175:GLU:H	2.12	0.47
2:S:21:CYS:SG	2:S:141:LEU:HD23	2.55	0.47
1:F:203:VAL:HG13	2:V:191:VAL:HG11	1.96	0.47
1:H:77:LYS:NZ	2:T:72:MET:SD	2.87	0.47
2:N:172:ASP:OD1	5:N:496:HOH:O	2.20	0.47
2:U:19:ARG:HH11	2:U:23:ASN:HD21	1.61	0.47
2:O:86:ASN:HB2	5:O:452:HOH:O	2.15	0.47
1:B:192:ASN:ND2	2:P:175:GLU:H	2.11	0.47
1:L:77:LYS:HZ3	2:X:72:MET:CE	2.28	0.47
2:R:86:ASN:HB2	5:R:2118:HOH:O	2.15	0.47
1:I:77:LYS:NZ	2:U:72:MET:SD	2.87	0.47
2:M:21:CYS:SG	2:M:141:LEU:HD23	2.55	0.47
2:Q:86:ASN:HB2	5:Q:1746:HOH:O	2.15	0.47
1:L:75:LEU:HD23	1:L:75:LEU:C	2.36	0.47
2:N:19:ARG:HH11	2:N:23:ASN:HD21	1.61	0.46
2:T:21:CYS:SG	2:T:141:LEU:HD23	2.55	0.46
1:I:75:LEU:C	1:I:75:LEU:HD23	2.36	0.46
2:X:21:CYS:SG	2:X:141:LEU:HD23	2.55	0.46
1:C:75:LEU:HD23	1:C:75:LEU:C	2.36	0.46
2:T:86:ASN:HB2	5:T:2864:HOH:O	2.15	0.46
1:A:77:LYS:NZ	2:M:72:MET:SD	2.87	0.46
1:A:75:LEU:C	1:A:75:LEU:HD23	2.36	0.46
2:P:86:ASN:HB2	5:P:437:HOH:O	2.15	0.46
1:F:75:LEU:HD23	1:F:75:LEU:C	2.36	0.46
1:C:109:MET:HE1	1:C:139:ARG:NE	2.25	0.46
1:K:77:LYS:NZ	2:W:72:MET:SD	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:21:CYS:SG	2:W:141:LEU:HD23	2.55	0.46
1:K:75:LEU:HD23	1:K:75:LEU:C	2.36	0.46
2:R:21:CYS:SG	2:R:141:LEU:HD23	2.55	0.46
1:B:77:LYS:HZ3	2:N:72:MET:CE	2.27	0.46
1:E:75:LEU:C	1:E:75:LEU:HD23	2.36	0.46
2:N:86:ASN:HB2	5:N:435:HOH:O	2.15	0.46
2:U:86:ASN:HB2	5:U:3233:HOH:O	2.15	0.46
1:F:109:MET:HE2	1:F:109:MET:HB3	1.78	0.46
1:B:75:LEU:C	1:B:75:LEU:HD23	2.36	0.46
1:G:75:LEU:C	1:G:75:LEU:HD23	2.36	0.46
1:L:109:MET:CE	1:L:139:ARG:NE	2.73	0.46
2:V:172:ASP:OD1	5:V:4137:HOH:O	2.20	0.46
2:S:86:ASN:HB2	5:S:2492:HOH:O	2.15	0.46
2:X:86:ASN:HB2	5:X:455:HOH:O	2.15	0.46
1:J:75:LEU:C	1:J:75:LEU:HD23	2.36	0.46
2:N:191:VAL:O	2:U:185:LYS:NZ	2.39	0.45
1:A:109:MET:HE2	1:A:139:ARG:NE	2.31	0.45
1:H:75:LEU:C	1:H:75:LEU:HD23	2.36	0.45
1:D:75:LEU:HD23	1:D:75:LEU:C	2.36	0.45
2:M:86:ASN:HB2	5:M:433:HOH:O	2.15	0.45
2:V:86:ASN:HB2	5:V:3602:HOH:O	2.15	0.45
2:W:86:ASN:HB2	5:W:3971:HOH:O	2.15	0.45
1:I:109:MET:CE	1:I:139:ARG:NE	2.73	0.45
1:C:186:LYS:HE3	1:I:19:LEU:O	2.17	0.45
2:M:139:TYR:OH	2:O:128:LYS:HG2	2.16	0.45
1:A:109:MET:HE1	5:A:5346:HOH:O	2.17	0.45
5:I:3313:HOH:O	2:U:5:VAL:HG22	2.17	0.45
5:D:1455:HOH:O	2:P:5:VAL:HG22	2.17	0.45
5:K:4051:HOH:O	2:W:5:VAL:HG22	2.17	0.44
5:B:6425:HOH:O	2:N:5:VAL:HG22	2.17	0.44
5:C:1083:HOH:O	2:O:5:VAL:HG22	2.17	0.44
1:B:203:VAL:HG13	2:P:191:VAL:HG11	1.99	0.44
1:G:192:ASN:ND2	2:R:175:GLU:H	2.16	0.44
1:G:109:MET:HE1	1:G:139:ARG:NE	2.24	0.44
1:C:109:MET:CE	5:C:882:HOH:O	2.66	0.44
5:G:2572:HOH:O	2:S:5:VAL:HG22	2.17	0.44
1:E:109:MET:CE	5:E:270:HOH:O	2.66	0.44
5:H:2944:HOH:O	2:T:5:VAL:HG22	2.17	0.44
1:I:109:MET:CE	5:I:3112:HOH:O	2.66	0.43
1:B:109:MET:CE	1:B:139:ARG:NE	2.73	0.43
5:J:3682:HOH:O	2:V:5:VAL:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:ASN:ND2	2:M:175:GLU:H	2.13	0.43
5:E:349:HOH:O	2:Q:5:VAL:HG22	2.17	0.43
1:I:203:VAL:CG1	2:T:191:VAL:HG11	2.48	0.43
1:J:109:MET:CE	5:J:3481:HOH:O	2.66	0.43
5:L:355:HOH:O	2:X:5:VAL:HG22	2.17	0.43
1:G:109:MET:CE	5:G:2371:HOH:O	2.66	0.43
1:L:109:MET:HE2	1:L:139:ARG:NE	2.32	0.43
1:A:109:MET:HB3	1:A:109:MET:HE2	1.81	0.43
2:P:33:VAL:HG21	2:P:92:LEU:CD2	2.49	0.43
1:B:109:MET:CE	5:B:6348:HOH:O	2.66	0.43
2:T:19:ARG:NH1	2:T:23:ASN:HD21	2.17	0.43
5:F:2198:HOH:O	2:R:5:VAL:HG22	2.17	0.43
2:W:19:ARG:NH1	2:W:23:ASN:HD21	2.17	0.43
2:U:19:ARG:NH1	2:U:23:ASN:HD21	2.17	0.43
1:L:109:MET:CE	5:L:276:HOH:O	2.66	0.43
1:D:109:MET:HE2	1:D:109:MET:HB3	1.79	0.43
2:V:19:ARG:NH1	2:V:23:ASN:HD21	2.17	0.43
1:K:77:LYS:HZ3	2:W:72:MET:CE	2.32	0.43
1:L:109:MET:HE2	1:L:109:MET:HB3	1.80	0.43
1:F:109:MET:CE	5:F:1997:HOH:O	2.66	0.43
1:D:109:MET:CE	5:D:1254:HOH:O	2.66	0.43
1:K:109:MET:CE	5:K:3850:HOH:O	2.66	0.43
2:Q:33:VAL:HG21	2:Q:92:LEU:CD2	2.49	0.43
5:A:5422:HOH:O	2:M:5:VAL:HG22	2.17	0.43
2:S:33:VAL:HG21	2:S:92:LEU:CD2	2.49	0.43
2:N:19:ARG:NH1	2:N:23:ASN:HD21	2.17	0.43
1:B:25:ASN:C	1:B:25:ASN:ND2	2.72	0.42
2:O:19:ARG:NH1	2:O:23:ASN:HD21	2.17	0.42
2:W:33:VAL:HG21	2:W:92:LEU:CD2	2.49	0.42
2:S:19:ARG:NH1	2:S:23:ASN:HD21	2.17	0.42
1:A:109:MET:CE	5:A:5346:HOH:O	2.66	0.42
2:N:33:VAL:HG21	2:N:92:LEU:CD2	2.49	0.42
1:L:109:MET:HE1	5:L:276:HOH:O	2.19	0.42
1:I:109:MET:HB3	1:I:109:MET:HE2	1.82	0.42
1:A:109:MET:CE	1:A:139:ARG:NE	2.73	0.42
2:R:19:ARG:NH1	2:R:23:ASN:HD21	2.17	0.42
1:H:109:MET:CE	1:H:139:ARG:NE	2.73	0.42
2:R:33:VAL:HG21	2:R:92:LEU:CD2	2.49	0.42
1:D:203:VAL:HG13	2:W:191:VAL:HG11	2.01	0.42
1:F:109:MET:CE	1:F:139:ARG:NE	2.73	0.42
1:D:77:LYS:HD3	5:D:1486:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:77:LYS:HD3	5:I:3344:HOH:O	2.20	0.42
1:C:77:LYS:HD3	5:C:1114:HOH:O	2.20	0.42
2:Q:185:LYS:NZ	2:V:191:VAL:O	2.42	0.42
2:P:139:TYR:OH	2:R:128:LYS:HG2	2.20	0.42
1:G:203:VAL:HG13	2:R:191:VAL:HG11	2.02	0.42
2:V:33:VAL:HG21	2:V:92:LEU:CD2	2.49	0.42
2:X:33:VAL:HG21	2:X:92:LEU:CD2	2.49	0.42
2:X:19:ARG:NH1	2:X:23:ASN:HD21	2.17	0.42
2:V:152:GLU:HG2	5:V:3596:HOH:O	2.20	0.42
1:H:25:ASN:ND2	1:H:25:ASN:C	2.72	0.42
1:E:77:LYS:HD3	5:E:362:HOH:O	2.20	0.42
1:K:77:LYS:HD3	5:K:4082:HOH:O	2.20	0.42
2:S:152:GLU:HG2	5:S:2486:HOH:O	2.20	0.42
1:L:77:LYS:HD3	5:L:367:HOH:O	2.20	0.41
2:W:152:GLU:HG2	5:W:3965:HOH:O	2.20	0.41
1:H:77:LYS:HD3	5:H:2975:HOH:O	2.20	0.41
1:J:192:ASN:HD21	2:S:175:GLU:H	1.68	0.41
1:A:145:ARG:HB2	1:L:155:HIS:CD2	2.55	0.41
2:M:152:GLU:HG2	5:M:431:HOH:O	2.20	0.41
1:K:109:MET:HE1	1:K:139:ARG:NE	2.28	0.41
2:O:93:GLN:HG2	2:O:95:ARG:HH21	1.86	0.41
2:Q:19:ARG:NH1	2:Q:23:ASN:HD21	2.17	0.41
2:U:152:GLU:HG2	5:U:3227:HOH:O	2.20	0.41
2:T:152:GLU:HG2	5:T:2858:HOH:O	2.20	0.41
2:N:152:GLU:HG2	5:N:433:HOH:O	2.20	0.41
2:T:33:VAL:HG21	2:T:92:LEU:CD2	2.49	0.41
1:G:77:LYS:HD3	5:G:2603:HOH:O	2.20	0.41
1:A:77:LYS:HD3	5:A:5434:HOH:O	2.20	0.41
1:B:77:LYS:HD3	5:B:6437:HOH:O	2.20	0.41
1:F:25:ASN:ND2	1:F:25:ASN:C	2.72	0.41
2:S:93:GLN:HG2	2:S:95:ARG:HH21	1.86	0.41
2:X:93:GLN:HG2	2:X:95:ARG:HH21	1.86	0.41
2:M:19:ARG:NH1	2:M:23:ASN:HD21	2.17	0.41
1:C:25:ASN:ND2	1:C:25:ASN:C	2.72	0.41
2:Q:93:GLN:HG2	2:Q:95:ARG:HH21	1.86	0.41
2:O:152:GLU:HG2	5:O:450:HOH:O	2.20	0.41
2:P:19:ARG:NH1	2:P:23:ASN:HD21	2.17	0.41
2:Q:86:ASN:ND2	2:Q:87:ASP:OD1	2.54	0.41
2:Q:128:LYS:HG2	2:R:139:TYR:OH	2.21	0.41
2:M:93:GLN:HG2	2:M:95:ARG:HH21	1.85	0.41
2:P:93:GLN:HG2	2:P:95:ARG:HH21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:93:GLN:HG2	2:T:95:ARG:HH21	1.86	0.41
2:O:86:ASN:ND2	2:O:87:ASP:OD1	2.54	0.41
2:M:86:ASN:ND2	2:M:87:ASP:OD1	2.54	0.41
2:P:152:GLU:HG2	5:P:435:HOH:O	2.20	0.41
2:R:152:GLU:HG2	5:R:2112:HOH:O	2.20	0.41
1:J:109:MET:HE2	1:J:109:MET:HB3	1.83	0.41
1:H:109:MET:CE	5:H:2743:HOH:O	2.66	0.41
2:X:93:GLN:HG3	2:X:95:ARG:HE	1.86	0.41
1:J:77:LYS:HD3	5:J:3713:HOH:O	2.20	0.41
2:R:86:ASN:ND2	2:R:87:ASP:OD1	2.54	0.41
2:T:86:ASN:ND2	2:T:87:ASP:OD1	2.54	0.41
1:E:77:LYS:NZ	2:Q:72:MET:CE	2.84	0.41
2:W:86:ASN:ND2	2:W:87:ASP:OD1	2.54	0.41
1:J:109:MET:CE	1:J:139:ARG:NE	2.73	0.40
2:S:93:GLN:HG3	2:S:95:ARG:HE	1.86	0.40
2:S:86:ASN:ND2	2:S:87:ASP:OD1	2.54	0.40
2:X:86:ASN:ND2	2:X:87:ASP:OD1	2.54	0.40
2:T:139:TYR:OH	2:X:128:LYS:HG2	2.21	0.40
2:N:93:GLN:HG2	2:N:95:ARG:HH21	1.86	0.40
1:G:77:LYS:NZ	2:S:72:MET:CE	2.84	0.40
1:J:77:LYS:NZ	2:V:72:MET:CE	2.84	0.40
1:C:77:LYS:NZ	2:O:72:MET:CE	2.84	0.40
2:U:128:LYS:HG2	2:W:139:TYR:OH	2.21	0.40
2:V:93:GLN:HG3	2:V:95:ARG:HE	1.86	0.40
2:Q:152:GLU:HG2	5:Q:1740:HOH:O	2.20	0.40
1:D:109:MET:CE	1:D:139:ARG:NE	2.73	0.40
1:K:109:MET:CE	1:K:139:ARG:NE	2.73	0.40
2:M:33:VAL:HG21	2:M:92:LEU:CD2	2.49	0.40
1:B:77:LYS:NZ	2:N:72:MET:CE	2.84	0.40
1:H:77:LYS:NZ	2:T:72:MET:CE	2.84	0.40
2:N:86:ASN:ND2	2:N:87:ASP:OD1	2.54	0.40
2:X:152:GLU:HG2	5:X:453:HOH:O	2.20	0.40
1:A:210:LYS:NZ	2:X:191:VAL:O	2.53	0.40
2:O:93:GLN:HG3	2:O:95:ARG:HE	1.86	0.40
1:A:77:LYS:NZ	2:M:72:MET:CE	2.84	0.40
1:I:77:LYS:NZ	2:U:72:MET:CE	2.84	0.40

All (99) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:132:ASP:OD1	2:V:103:LYS:CE[4_546]	0.54	1.66
1:K:17:ASN:ND2	5:X:411:HOH:O[3_545]	0.55	1.65
1:C:153:HIS:CE1	5:N:483:HOH:O[4_555]	0.55	1.65
1:F:34:HIS:ND1	1:F:34:HIS:NE2[2_656]	0.59	1.61
1:K:35:GLY:O	2:X:103:LYS:NZ[3_545]	0.61	1.59
1:I:149:ARG:O	2:N:121:LYS:NZ[4_555]	0.67	1.53
1:F:34:HIS:ND1	1:F:34:HIS:CE1[2_656]	0.73	1.47
1:C:152:GLN:CG	5:N:440:HOH:O[4_555]	0.86	1.34
1:A:15:THR:CG2	2:S:90:SER:CB[3_445]	0.88	1.32
1:H:153:HIS:CE1	5:O:432:HOH:O[4_555]	0.94	1.26
1:C:110:LYS:CD	2:N:95:ARG:CD[4_555]	0.95	1.25
1:F:34:HIS:CG	1:F:34:HIS:CE1[2_656]	0.98	1.22
1:H:153:HIS:ND1	5:O:432:HOH:O[4_555]	1.01	1.19
1:I:110:LYS:NZ	5:O:379:HOH:O[4_555]	1.13	1.07
1:H:152:GLN:CB	5:O:475:HOH:O[4_555]	1.13	1.07
1:H:153:HIS:NE2	5:O:432:HOH:O[4_555]	1.16	1.04
1:I:153:HIS:CG	2:N:27:GLN:NE2[4_555]	1.17	1.03
1:I:152:GLN:N	5:N:398:HOH:O[4_555]	1.20	1.00
1:C:153:HIS:NE2	5:N:349:HOH:O[4_555]	1.24	0.96
1:F:34:HIS:CE1	1:F:34:HIS:CE1[2_656]	1.25	0.95
1:H:153:HIS:CG	5:O:432:HOH:O[4_555]	1.32	0.88
2:R:134:SER:CA	5:V:3629:HOH:O[4_546]	1.32	0.88
1:F:153:HIS:CG	1:F:153:HIS:ND1[2_656]	1.35	0.85
1:K:33:SER:O	5:X:490:HOH:O[3_545]	1.38	0.82
1:C:152:GLN:CB	5:N:440:HOH:O[4_555]	1.38	0.82
1:H:153:HIS:CD2	5:O:432:HOH:O[4_555]	1.38	0.82
2:Q:132:ASP:CG	2:V:103:LYS:CE[4_546]	1.40	0.80
1:C:153:HIS:ND1	5:N:483:HOH:O[4_555]	1.48	0.72
1:F:34:HIS:CD2	1:F:34:HIS:CE1[2_656]	1.48	0.72
2:Q:132:ASP:OD1	2:V:103:LYS:NZ[4_546]	1.48	0.72
1:A:17:ASN:ND2	5:S:2501:HOH:O[3_445]	1.50	0.70
5:I:3261:HOH:O	5:N:461:HOH:O[4_555]	1.51	0.69
1:F:153:HIS:ND1	1:F:153:HIS:CE1[2_656]	1.53	0.67
1:K:18:SER:CB	5:X:467:HOH:O[3_545]	1.54	0.66
1:K:15:THR:CG2	5:X:466:HOH:O[3_545]	1.54	0.66
1:I:153:HIS:CB	2:N:27:GLN:NE2[4_555]	1.54	0.66
2:R:134:SER:CB	5:V:3629:HOH:O[4_546]	1.54	0.66
1:F:34:HIS:CE1	1:F:34:HIS:NE2[2_656]	1.59	0.61
1:H:152:GLN:CG	5:O:422:HOH:O[4_555]	1.61	0.59
1:I:110:LYS:CD	2:O:134:SER:CA[4_555]	1.62	0.58
1:H:152:GLN:NE2	5:O:471:HOH:O[4_555]	1.63	0.57
1:C:110:LYS:CE	2:N:95:ARG:CD[4_555]	1.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:18:SER:OG	5:X:467:HOH:O[3_545]	1.64	0.56
1:K:17:ASN:CG	5:X:411:HOH:O[3_545]	1.64	0.56
1:H:152:GLN:OE1	5:N:491:HOH:O[4_555]	1.65	0.55
1:C:153:HIS:NE2	5:N:483:HOH:O[4_555]	1.65	0.55
1:C:153:HIS:CD2	5:N:349:HOH:O[4_555]	1.66	0.54
1:I:110:LYS:CB	2:O:134:SER:CB[4_555]	1.67	0.53
1:A:34:HIS:ND1	5:S:2550:HOH:O[3_445]	1.67	0.53
5:A:5398:HOH:O	5:S:2550:HOH:O[3_445]	1.68	0.52
1:K:35:GLY:C	2:X:103:LYS:NZ[3_545]	1.68	0.52
1:H:152:GLN:OE1	5:O:390:HOH:O[4_555]	1.68	0.52
2:M:99:ARG:NH1	2:U:135:GLU:OE2[3_445]	1.68	0.52
1:F:34:HIS:ND1	1:F:34:HIS:CD2[2_656]	1.69	0.51
1:A:15:THR:CG2	2:S:90:SER:OG[3_445]	1.69	0.51
1:F:34:HIS:ND1	1:F:34:HIS:ND1[2_656]	1.73	0.47
1:F:153:HIS:CG	1:F:153:HIS:CG[2_656]	1.75	0.45
1:H:152:GLN:CA	5:O:475:HOH:O[4_555]	1.75	0.45
1:A:17:ASN:CG	5:S:2501:HOH:O[3_445]	1.76	0.44
2:V:103:LYS:NZ	5:Q:1827:HOH:O[4_556]	1.78	0.42
1:A:10:LEU:CD1	2:S:95:ARG:CZ[3_445]	1.80	0.40
1:A:10:LEU:CD1	2:S:95:ARG:NH2[3_445]	1.81	0.39
1:C:110:LYS:CE	2:N:95:ARG:CB[4_555]	1.81	0.39
1:I:110:LYS:NZ	2:O:133:ASP:O[4_555]	1.82	0.38
1:I:152:GLN:OE1	5:N:350:HOH:O[4_555]	1.84	0.36
1:F:34:HIS:CG	1:F:34:HIS:NE2[2_656]	1.87	0.33
1:I:149:ARG:C	2:N:121:LYS:NZ[4_555]	1.89	0.31
1:A:18:SER:CB	2:S:27:GLN:OE1[3_445]	1.92	0.28
1:H:149:ARG:O	2:O:13:ASP:OD1[4_555]	1.92	0.28
2:Q:132:ASP:OD1	2:V:103:LYS:CD[4_546]	1.93	0.27
2:N:99:ARG:NH2	5:C:1031:HOH:O[4_545]	1.93	0.27
5:I:3261:HOH:O	5:N:383:HOH:O[4_555]	1.93	0.27
1:I:149:ARG:O	2:N:121:LYS:CE[4_555]	1.93	0.27
1:I:153:HIS:CD2	2:N:27:GLN:NE2[4_555]	1.95	0.25
1:H:152:GLN:CB	5:O:390:HOH:O[4_555]	1.95	0.25
1:A:35:GLY:CA	2:S:103:LYS:NZ[3_445]	1.96	0.24
1:C:110:LYS:CD	2:N:95:ARG:NE[4_555]	1.97	0.23
5:A:5398:HOH:O	5:S:2389:HOH:O[3_445]	1.99	0.21
1:I:152:GLN:CB	5:N:350:HOH:O[4_555]	2.01	0.19
1:H:152:GLN:N	5:O:475:HOH:O[4_555]	2.01	0.19
1:C:110:LYS:CE	2:N:95:ARG:CG[4_555]	2.02	0.18
1:A:17:ASN:CB	5:S:2501:HOH:O[3_445]	2.03	0.17
2:R:134:SER:C	5:V:3629:HOH:O[4_546]	2.03	0.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:153:HIS:ND1	2:N:27:GLN:NE2[4_555]	2.06	0.14
1:K:35:GLY:O	2:X:103:LYS:CE[3_545]	2.07	0.13
2:N:99:ARG:CZ	5:C:1031:HOH:O[4_545]	2.09	0.11
1:F:34:HIS:CG	1:F:34:HIS:ND1[2_656]	2.13	0.07
1:C:152:GLN:CD	5:N:440:HOH:O[4_555]	2.13	0.07
1:H:152:GLN:CD	5:N:491:HOH:O[4_555]	2.14	0.06
1:I:34:HIS:CE1	5:N:437:HOH:O[4_555]	2.15	0.05
1:K:15:THR:O	5:X:486:HOH:O[3_545]	2.15	0.05
1:H:152:GLN:NE2	5:N:491:HOH:O[4_555]	2.15	0.05
1:F:30:GLU:OE1	5:F:2146:HOH:O[2_656]	2.15	0.05
1:C:110:LYS:CD	2:N:95:ARG:CG[4_555]	2.16	0.04
1:C:110:LYS:NZ	2:N:95:ARG:CD[4_555]	2.16	0.04
1:H:152:GLN:CB	5:O:422:HOH:O[4_555]	2.17	0.03
1:C:110:LYS:NZ	2:N:95:ARG:CB[4_555]	2.17	0.03
1:H:153:HIS:NE2	2:O:17:MET:O[4_555]	2.19	0.01
1:I:34:HIS:CE1	2:N:27:GLN:OE1[4_555]	2.19	0.01

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	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	B	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	C	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	D	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	E	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	F	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	G	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	H	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	I	210/212 (99%)	205 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
1	L	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
2	M	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	N	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	O	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	P	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	Q	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	R	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	S	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	T	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	U	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	V	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	W	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
2	X	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
All	All	4788/4836 (99%)	4704 (98%)	84 (2%)	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	177/181 (98%)	175 (99%)	2 (1%)	80	78
1	B	177/181 (98%)	175 (99%)	2 (1%)	80	78
1	C	177/181 (98%)	175 (99%)	2 (1%)	80	78
1	D	177/181 (98%)	175 (99%)	2 (1%)	80	78
1	E	177/181 (98%)	175 (99%)	2 (1%)	80	78
1	F	177/181 (98%)	175 (99%)	2 (1%)	80	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	177/181 (98%)	175 (99%)	2 (1%)	80	78
1	H	177/181 (98%)	175 (99%)	2 (1%)	80	78
1	I	177/181 (98%)	175 (99%)	2 (1%)	80	78
1	J	177/181 (98%)	175 (99%)	2 (1%)	80	78
1	K	177/181 (98%)	175 (99%)	2 (1%)	80	78
1	L	177/181 (98%)	175 (99%)	2 (1%)	80	78
2	M	167/167 (100%)	167 (100%)	0	100	100
2	N	167/167 (100%)	167 (100%)	0	100	100
2	O	167/167 (100%)	167 (100%)	0	100	100
2	P	167/167 (100%)	167 (100%)	0	100	100
2	Q	167/167 (100%)	167 (100%)	0	100	100
2	R	167/167 (100%)	167 (100%)	0	100	100
2	S	167/167 (100%)	167 (100%)	0	100	100
2	T	167/167 (100%)	167 (100%)	0	100	100
2	U	167/167 (100%)	167 (100%)	0	100	100
2	V	167/167 (100%)	167 (100%)	0	100	100
2	W	167/167 (100%)	167 (100%)	0	100	100
2	X	167/167 (100%)	167 (100%)	0	100	100
All	All	4128/4176 (99%)	4104 (99%)	24 (1%)	90	90

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	185	LEU
1	B	25	ASN
1	B	185	LEU
1	C	25	ASN
1	C	185	LEU
1	D	25	ASN
1	D	185	LEU
1	E	25	ASN
1	E	185	LEU
1	F	25	ASN
1	F	185	LEU
1	G	25	ASN

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Mol	Chain	Res	Type
1	G	185	LEU
1	H	25	ASN
1	H	185	LEU
1	I	25	ASN
1	I	185	LEU
1	J	25	ASN
1	J	185	LEU
1	K	25	ASN
1	K	185	LEU
1	L	25	ASN
1	L	185	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	121	HIS
1	A	192	ASN
1	A	195	HIS
1	B	25	ASN
1	B	121	HIS
1	B	192	ASN
1	B	195	HIS
1	C	25	ASN
1	C	121	HIS
1	C	192	ASN
1	C	195	HIS
1	D	25	ASN
1	D	121	HIS
1	D	192	ASN
1	D	195	HIS
1	E	25	ASN
1	E	121	HIS
1	E	192	ASN
1	E	195	HIS
1	F	25	ASN
1	F	121	HIS
1	F	192	ASN
1	F	195	HIS
1	G	25	ASN
1	G	121	HIS
1	G	192	ASN

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Mol	Chain	Res	Type
1	G	195	HIS
1	H	25	ASN
1	H	121	HIS
1	H	192	ASN
1	H	195	HIS
1	I	25	ASN
1	I	121	HIS
1	I	192	ASN
1	I	195	HIS
1	J	25	ASN
1	J	121	HIS
1	J	192	ASN
1	K	25	ASN
1	K	121	HIS
1	K	192	ASN
1	K	195	HIS
1	L	25	ASN
1	L	121	HIS
1	L	192	ASN
1	L	195	HIS
2	M	23	ASN
2	M	86	ASN
2	M	157	GLN
2	N	23	ASN
2	N	86	ASN
2	N	157	GLN
2	O	23	ASN
2	O	86	ASN
2	O	157	GLN
2	P	23	ASN
2	P	86	ASN
2	P	157	GLN
2	Q	23	ASN
2	Q	86	ASN
2	Q	157	GLN
2	R	23	ASN
2	R	86	ASN
2	R	157	GLN
2	S	23	ASN
2	S	86	ASN
2	S	157	GLN
2	T	23	ASN

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Mol	Chain	Res	Type
2	T	86	ASN
2	T	157	GLN
2	U	23	ASN
2	U	86	ASN
2	U	157	GLN
2	V	23	ASN
2	V	86	ASN
2	V	157	GLN
2	W	23	ASN
2	W	86	ASN
2	W	157	GLN
2	X	23	ASN
2	X	86	ASN
2	X	157	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 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

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	212/212 (100%)	0.42	21 (9%) 9 11	16, 23, 66, 116	0
1	B	212/212 (100%)	0.25	13 (6%) 25 28	16, 23, 66, 116	0
1	C	212/212 (100%)	0.43	14 (6%) 22 24	16, 23, 66, 116	0
1	D	212/212 (100%)	0.20	14 (6%) 22 24	16, 23, 66, 116	0
1	E	212/212 (100%)	0.16	12 (5%) 27 31	16, 23, 66, 116	0
1	F	212/212 (100%)	0.34	17 (8%) 15 17	16, 23, 66, 116	0
1	G	212/212 (100%)	0.23	14 (6%) 22 24	16, 23, 66, 116	0
1	H	212/212 (100%)	0.27	12 (5%) 27 31	16, 23, 66, 116	0
1	I	212/212 (100%)	0.40	22 (10%) 8 9	16, 23, 66, 116	0
1	J	212/212 (100%)	0.20	14 (6%) 22 24	16, 23, 66, 116	0
1	K	212/212 (100%)	0.43	20 (9%) 11 12	16, 23, 66, 116	0
1	L	212/212 (100%)	0.22	14 (6%) 22 24	16, 23, 66, 116	0
2	M	191/191 (100%)	-0.10	5 (2%) 59 63	15, 21, 51, 81	0
2	N	191/191 (100%)	0.14	7 (3%) 45 49	15, 21, 51, 81	0
2	O	191/191 (100%)	0.14	8 (4%) 40 44	15, 21, 51, 81	0
2	P	191/191 (100%)	-0.07	7 (3%) 45 49	15, 21, 51, 81	0
2	Q	191/191 (100%)	0.02	7 (3%) 45 49	15, 21, 51, 81	0
2	R	191/191 (100%)	-0.04	6 (3%) 52 56	15, 21, 51, 81	0
2	S	191/191 (100%)	-0.03	6 (3%) 52 56	15, 21, 51, 81	0
2	T	191/191 (100%)	-0.11	4 (2%) 67 70	15, 21, 51, 81	0
2	U	191/191 (100%)	-0.01	8 (4%) 40 44	15, 21, 51, 81	0
2	V	191/191 (100%)	-0.09	4 (2%) 67 70	15, 21, 51, 81	0
2	W	191/191 (100%)	-0.04	6 (3%) 52 56	15, 21, 51, 81	0
2	X	191/191 (100%)	-0.04	5 (2%) 59 63	15, 21, 51, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
All	All	4836/4836 (100%)	0.15	260 (5%)	29 33	15, 22, 58, 116	0

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	ILE	14.0
1	K	14	ILE	14.0
1	K	114	LYS	13.3
1	L	14	ILE	12.9
1	F	113	ARG	12.3
1	H	111	THR	11.5
1	G	113	ARG	11.5
1	L	113	ARG	11.1
1	B	112	GLU	11.1
1	D	14	ILE	10.0
1	B	14	ILE	9.5
1	D	112	GLU	9.4
1	I	111	THR	9.3
1	K	110	LYS	9.3
1	L	112	GLU	9.1
1	F	15	THR	9.1
1	A	113	ARG	9.0
1	E	113	ARG	8.8
1	C	111	THR	8.8
1	I	112	GLU	8.7
1	E	14	ILE	8.4
2	Q	5	VAL	8.3
1	K	1	ALA	8.2
1	B	114	LYS	8.2
1	K	13	GLY	8.0
1	A	111	THR	7.8
1	G	14	ILE	7.7
1	A	1	ALA	7.7
1	K	15	THR	7.6
1	E	112	GLU	7.5
1	D	113	ARG	7.3
1	I	113	ARG	7.2
1	C	112	GLU	7.2
1	H	14	ILE	7.1
1	A	15	THR	7.1
2	O	134	SER	7.1
1	C	15	THR	7.0

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Mol	Chain	Res	Type	RSRZ
2	X	6	ASN	6.7
1	K	112	GLU	6.7
2	Q	6	ASN	6.7
2	S	5	VAL	6.7
2	W	5	VAL	6.5
2	N	191	VAL	6.4
1	G	112	GLU	6.4
1	I	115	ASN	6.4
1	F	14	ILE	6.3
1	F	112	GLU	6.2
2	U	5	VAL	6.2
1	B	1	ALA	6.1
1	E	111	THR	6.1
2	S	6	ASN	6.1
1	A	110	LYS	6.1
1	C	113	ARG	6.0
1	I	14	ILE	5.9
2	P	6	ASN	5.9
2	O	191	VAL	5.8
1	J	110	LYS	5.7
1	C	110	LYS	5.7
1	C	14	ILE	5.7
1	B	113	ARG	5.7
2	M	6	ASN	5.7
1	H	1	ALA	5.6
1	J	111	THR	5.6
1	H	15	THR	5.6
2	Q	1	THR	5.6
1	D	18	SER	5.6
1	K	113	ARG	5.6
1	H	112	GLU	5.5
1	K	17	ASN	5.5
1	A	13	GLY	5.5
1	I	18	SER	5.5
1	G	110	LYS	5.4
2	O	6	ASN	5.4
1	B	15	THR	5.4
2	O	5	VAL	5.4
2	W	191	VAL	5.4
1	L	16	SER	5.3
1	A	16	SER	5.3
1	G	13	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
1	E	17	ASN	5.3
1	J	15	THR	5.3
1	B	115	ASN	5.2
1	F	2	ASP	5.2
1	I	1	ALA	5.1
2	M	5	VAL	5.0
1	L	17	ASN	5.0
1	E	15	THR	5.0
1	J	113	ARG	4.9
1	F	111	THR	4.9
2	T	5	VAL	4.9
1	G	15	THR	4.8
1	J	14	ILE	4.8
1	G	115	ASN	4.8
1	E	114	LYS	4.8
1	A	112	GLU	4.8
1	C	1	ALA	4.7
2	T	6	ASN	4.7
1	A	10	LEU	4.5
1	A	114	LYS	4.5
1	K	2	ASP	4.4
2	Q	7	PRO	4.4
1	L	13	GLY	4.4
1	D	114	LYS	4.4
1	H	17	ASN	4.4
1	J	114	LYS	4.4
1	I	153	HIS	4.4
2	P	191	VAL	4.4
1	J	17	ASN	4.4
1	L	15	THR	4.3
1	A	115	ASN	4.3
1	I	34	HIS	4.2
1	K	111	THR	4.2
1	D	115	ASN	4.2
2	T	191	VAL	4.1
1	C	114	LYS	4.1
1	B	110	LYS	4.1
1	I	15	THR	4.1
1	G	114	LYS	4.1
1	D	110	LYS	4.1
1	H	114	LYS	4.1
1	I	110	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	18	SER	4.1
1	L	111	THR	4.0
1	G	18	SER	4.0
2	N	6	ASN	4.0
2	R	191	VAL	3.9
1	C	17	ASN	3.9
1	K	10	LEU	3.9
2	P	5	VAL	3.8
1	L	1	ALA	3.8
1	I	109	MET	3.8
2	W	6	ASN	3.8
2	S	2	GLN	3.8
2	T	7	PRO	3.8
1	F	110	LYS	3.7
1	K	16	SER	3.7
2	M	1	THR	3.7
1	C	212	VAL	3.7
1	G	17	ASN	3.7
2	R	5	VAL	3.6
1	B	18	SER	3.6
1	E	110	LYS	3.6
1	B	17	ASN	3.6
1	F	13	GLY	3.5
1	D	13	GLY	3.5
2	X	5	VAL	3.5
2	U	6	ASN	3.5
1	F	18	SER	3.5
1	C	30	GLU	3.5
1	B	10	LEU	3.4
2	U	2	GLN	3.4
1	G	16	SER	3.4
1	D	1	ALA	3.3
1	H	13	GLY	3.3
1	J	112	GLU	3.3
1	E	16	SER	3.3
1	B	111	THR	3.3
1	F	1	ALA	3.3
1	D	111	THR	3.3
1	F	104	ASP	3.2
2	S	7	PRO	3.2
1	F	108	THR	3.2
1	K	12	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	J	1	ALA	3.2
2	V	191	VAL	3.2
2	P	1	THR	3.2
1	A	17	ASN	3.2
2	N	5	VAL	3.1
2	W	1	THR	3.1
1	E	18	SER	3.1
1	J	13	GLY	3.1
1	H	153	HIS	3.0
2	X	2	GLN	3.0
1	I	17	ASN	3.0
2	X	191	VAL	3.0
2	S	95	ARG	3.0
1	I	151	SER	2.9
1	A	20	ALA	2.9
1	G	111	THR	2.9
2	U	1	THR	2.9
1	C	109	MET	2.9
1	L	114	LYS	2.9
1	D	17	ASN	2.8
2	R	6	ASN	2.8
1	J	20	ALA	2.8
1	J	16	SER	2.8
1	K	30	GLU	2.8
1	A	2	ASP	2.7
1	I	114	LYS	2.7
1	K	115	ASN	2.7
1	E	211	THR	2.7
2	N	98	THR	2.7
1	I	10	LEU	2.7
1	L	110	LYS	2.7
2	V	5	VAL	2.7
1	H	212	VAL	2.6
1	K	5	TYR	2.6
1	L	34	HIS	2.6
1	L	153	HIS	2.6
1	A	9	ALA	2.5
2	M	191	VAL	2.5
2	U	3	CYS	2.5
2	Q	191	VAL	2.5
2	V	2	GLN	2.5
2	X	1	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	U	7	PRO	2.5
1	D	15	THR	2.5
2	U	191	VAL	2.4
1	C	18	SER	2.4
1	H	113	ARG	2.4
1	A	19	LEU	2.4
1	D	109	MET	2.4
2	M	2	GLN	2.4
2	N	2	GLN	2.4
2	W	2	GLN	2.4
2	O	1	THR	2.4
1	K	18	SER	2.4
1	G	212	VAL	2.4
2	N	1	THR	2.4
1	F	17	ASN	2.3
1	J	115	ASN	2.3
2	P	7	PRO	2.3
1	I	32	GLY	2.3
1	G	12	CYS	2.3
1	F	153	HIS	2.3
1	K	109	MET	2.3
1	I	12	CYS	2.2
1	K	33	SER	2.2
1	F	114	LYS	2.2
1	F	151	SER	2.2
2	V	7	PRO	2.2
1	B	16	SER	2.2
1	I	152	GLN	2.2
2	U	9	GLN	2.2
2	S	191	VAL	2.2
2	R	172	ASP	2.2
2	P	8	VAL	2.2
1	F	115	ASN	2.1
1	E	13	GLY	2.1
2	O	133	ASP	2.1
2	R	1	THR	2.1
1	A	212	VAL	2.1
2	O	2	GLN	2.1
1	I	212	VAL	2.1
2	N	119	VAL	2.1
2	O	135	GLU	2.1
1	J	109	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	12	CYS	2.1
2	P	172	ASP	2.1
2	Q	4	ASN	2.1
1	I	13	GLY	2.1
1	A	22	PRO	2.1
2	W	7	PRO	2.1
2	Q	9	GLN	2.1
1	L	115	ASN	2.0
2	R	135	GLU	2.0
1	C	191	ALA	2.0
1	D	19	LEU	2.0
1	I	16	SER	2.0
1	A	153	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	CA	A	5303	1/1	0.94	0.10	1.99	63,63,63,63	0
4	CA	F	8303	1/1	0.93	0.10	1.46	63,63,63,63	0
4	CA	C	7303	1/1	0.96	0.10	0.34	63,63,63,63	0
4	CA	B	6303	1/1	0.93	0.09	0.09	63,63,63,63	0
4	CA	C	7302	1/1	0.99	0.09	-0.79	18,18,18,18	0
4	CA	B	6302	1/1	1.00	0.08	-1.35	18,18,18,18	0
4	CA	A	5302	1/1	0.99	0.07	-1.83	18,18,18,18	0
3	FE	F	301	1/1	0.95	0.07	-2.06	34,34,34,34	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	FE	A	301	1/1	0.91	0.07	-2.07	34,34,34,34	1
3	FE	C	301	1/1	0.97	0.07	-2.16	34,34,34,34	1
4	CA	F	8302	1/1	1.00	0.06	-3.38	18,18,18,18	0
3	FE	B	301	1/1	0.99	0.04	-3.40	34,34,34,34	1
3	FE	N	300	1/1	0.97	0.08	-	18,18,18,18	0
3	FE	W	300	1/1	1.00	0.07	-	18,18,18,18	0
3	FE	Q	300	1/1	1.00	0.07	-	18,18,18,18	0
3	FE	U	300	1/1	1.00	0.07	-	18,18,18,18	0
3	FE	T	300	1/1	1.00	0.07	-	18,18,18,18	0
3	FE	O	300	1/1	0.99	0.09	-	18,18,18,18	0
3	FE	R	300	1/1	1.00	0.06	-	18,18,18,18	0
3	FE	V	300	1/1	1.00	0.07	-	18,18,18,18	0
3	FE	X	300	1/1	1.00	0.05	-	18,18,18,18	0
3	FE	S	300	1/1	1.00	0.05	-	18,18,18,18	0
3	FE	M	300	1/1	1.00	0.06	-	18,18,18,18	0
3	FE	P	300	1/1	1.00	0.06	-	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.