



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2WFF  
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Deposited on : 2009-04-05  
Resolution : 4.00 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](mailto: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.

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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

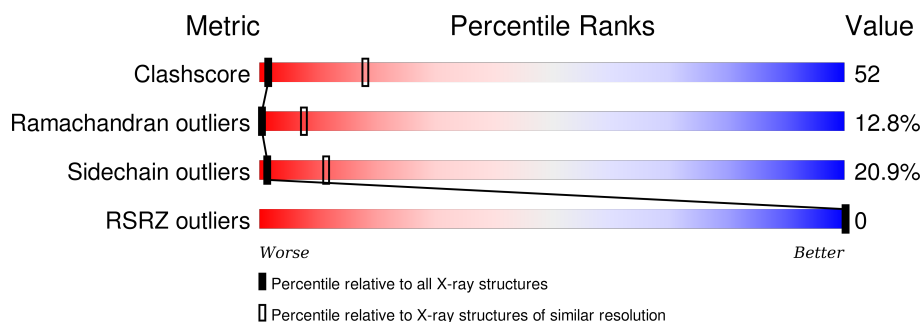
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

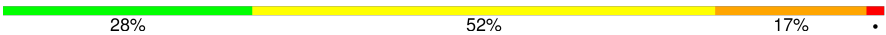
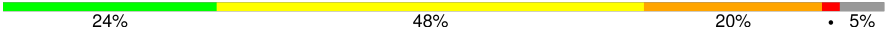


The reported resolution of this entry is 4.00 Å.

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))
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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  $\geq 3$ , 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	1	246	
2	2	230	
3	3	226	
4	4	80	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5506 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 P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	246	Total	C	N	O	S	0	0	0
			1929	1240	329	352	8			

- Molecule 2 is a protein called P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	219	Total	C	N	O	S	0	0	0
			1692	1081	290	314	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	21	VAL	ALA	CONFLICT	UNP B9VV85
2	85	SER	GLY	CONFLICT	UNP B9VV85

- Molecule 3 is a protein called P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	226	Total	C	N	O	S	0	0	0
			1719	1107	280	326	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	59	LYS	ARG	CONFLICT	UNP B9VV85

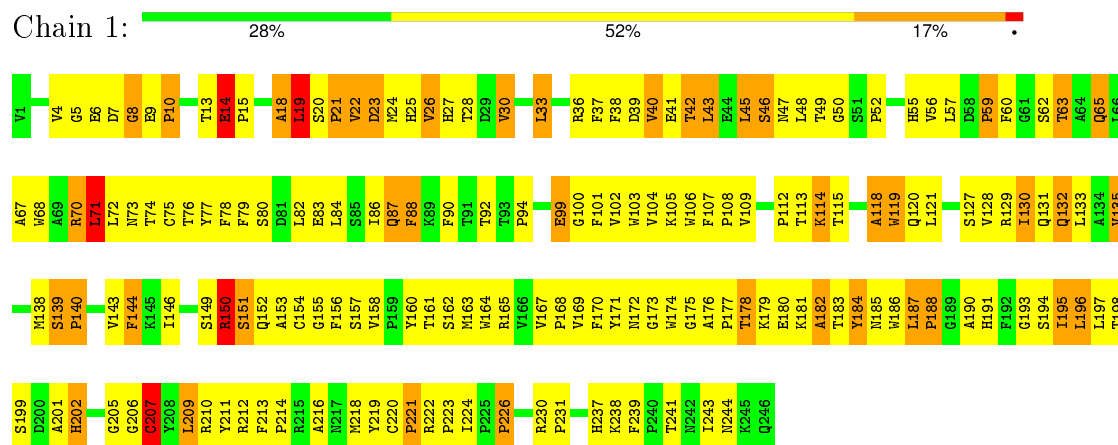
- Molecule 4 is a protein called P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	22	Total	C	N	O	S	0	0	1
			166	101	29	35	1			

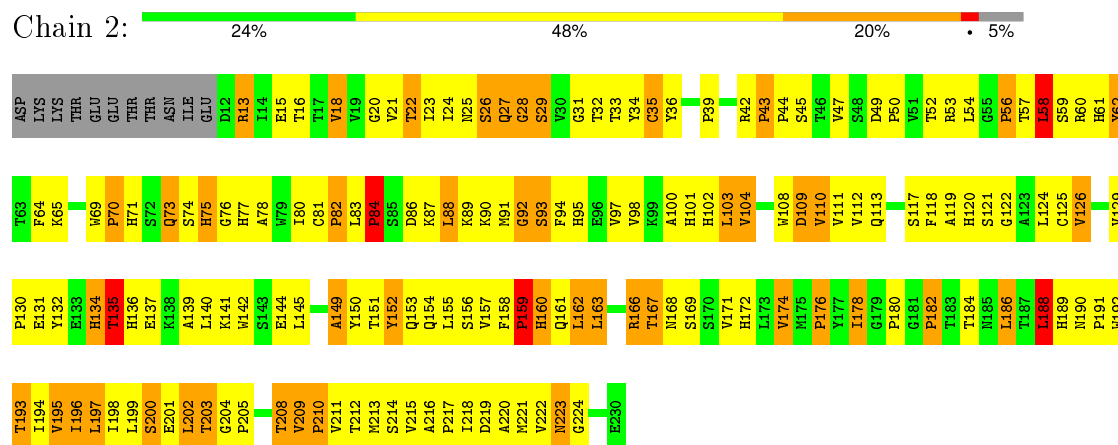
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

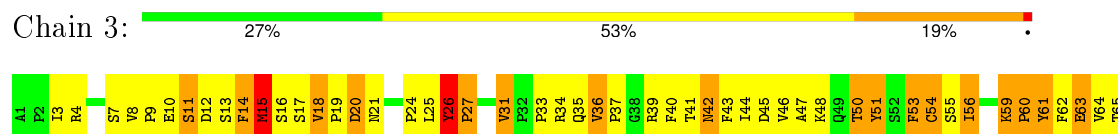
#### • Molecule 1: P1

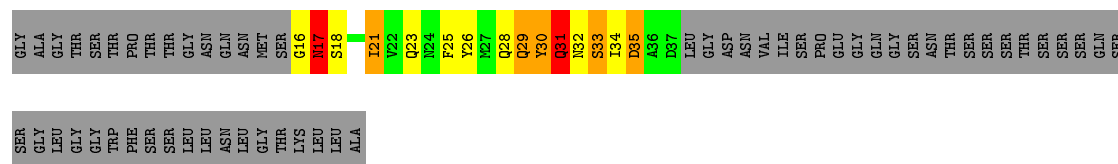


#### • Molecule 2: P1



#### • Molecule 3: P1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	314.00Å 497.80Å 556.50Å 90.00° 92.35° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 49.85 – 3.49	Depositor EDS
% Data completeness (in resolution range)	35.0 (20.00-4.00) 22.9 (49.85-3.49)	Depositor EDS
$R_{merge}$	0.44	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 3.48Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.462 , (Not available) 0.448 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 104.1	EDS
Estimated twinning fraction	0.095 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 491857 reflections	Xtriage
$F_o, F_c$ correlation	0.22	EDS
Total number of atoms	5506	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	1	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
2	2	0.86	1/1746 (0.1%)	1.17	8/2397 (0.3%)
3	3	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
4	4	0.78	0/168	1.03	0/226
All	All	0.85	7/5676 (0.1%)	1.12	21/7764 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	3	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	119	LYS	CE-NZ	7.39	1.67	1.49
3	3	120	PHE	N-CA	6.32	1.58	1.46
3	3	141	CYS	CB-SG	-5.87	1.72	1.81
3	3	12	ASP	CB-CG	5.58	1.63	1.51
2	2	35	CYS	CB-SG	-5.28	1.73	1.81
1	1	207	CYS	CB-SG	-5.14	1.73	1.81
3	3	119	LYS	CD-CE	5.08	1.64	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	58	LEU	CA-CB-CG	9.43	136.99	115.30
3	3	149	GLY	N-CA-C	-9.01	90.58	113.10
3	3	120	PHE	CB-CA-C	-8.33	93.74	110.40
3	3	119	LYS	CD-CE-NZ	7.53	129.02	111.70
2	2	92	GLY	N-CA-C	7.40	131.60	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	188	LEU	CA-CB-CG	6.99	131.38	115.30
2	2	162	LEU	CA-CB-CG	6.68	130.66	115.30
3	3	119	LYS	CB-CA-C	6.52	123.43	110.40
1	1	71	LEU	CA-CB-CG	6.45	130.13	115.30
1	1	70	ARG	N-CA-C	-6.11	94.52	111.00
3	3	120	PHE	CB-CG-CD1	-5.98	116.61	120.80
3	3	119	LYS	CB-CG-CD	5.82	126.73	111.60
1	1	18	ALA	N-CA-C	5.53	125.93	111.00
3	3	119	LYS	CA-C-N	5.52	129.35	117.20
2	2	62	TYR	N-CA-C	-5.51	96.13	111.00
1	1	207	CYS	N-CA-C	5.41	125.60	111.00
2	2	65	LYS	N-CA-C	-5.26	96.80	111.00
1	1	139	SER	C-N-CD	-5.24	109.06	120.60
2	2	163	LEU	CA-CB-CG	5.13	127.10	115.30
2	2	109	ASP	N-CA-C	-5.05	97.37	111.00
1	1	33	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	26	TYR	Sidechain
3	3	53	PHE	Sidechain

## 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	1	1929	0	1864	213	0
2	2	1692	0	1666	221	0
3	3	1719	0	1677	191	0
4	4	166	0	146	17	0
All	All	5506	0	5353	560	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 52.

All (560) 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)
3:3:119:LYS:CE	3:3:119:LYS:NZ	1.67	1.56
1:1:13:THR:HB	3:3:157:ASN:HB2	1.27	1.11
2:2:104:VAL:HG13	2:2:222:VAL:HG22	1.15	1.09
2:2:44:PRO:HB2	2:2:47:VAL:HG22	1.36	1.06
3:3:42:ASN:ND2	3:3:44:ILE:HG22	1.73	1.02
3:3:116:THR:HG23	3:3:191:LEU:HD21	1.44	0.98
3:3:191:LEU:HD22	3:3:192:THR:H	1.29	0.95
2:2:121:SER:HB2	2:2:203:THR:HG22	1.47	0.95
2:2:209:VAL:H	2:2:210:PRO:HD3	1.32	0.94
1:1:187:LEU:HD22	1:1:188:PRO:HD2	1.47	0.94
1:1:88:PHE:CE1	1:1:205:GLY:HA3	2.05	0.92
3:3:117:LYS:HB3	3:3:119:LYS:HE3	1.50	0.91
1:1:164:TRP:CZ2	1:1:187:LEU:HD21	2.07	0.90
1:1:164:TRP:NE1	1:1:187:LEU:HD11	1.88	0.89
3:3:103:SER:HB3	3:3:159:PRO:HA	1.52	0.88
2:2:156:SER:HB3	3:3:51:TYR:HE1	1.40	0.87
1:1:82:LEU:HD11	1:1:211:TYR:HD2	1.37	0.87
3:3:8:VAL:HG12	3:3:9:PRO:HD2	1.56	0.87
3:3:222:LEU:HD13	3:3:223:PRO:HD2	1.56	0.87
2:2:82:PRO:HA	2:2:193:THR:HB	1.54	0.86
1:1:48:LEU:HD22	1:1:130:ILE:HA	1.56	0.86
2:2:73:GLN:HE21	2:2:73:GLN:HA	1.41	0.85
1:1:102:VAL:HG22	1:1:199:SER:HB2	1.58	0.85
2:2:58:LEU:HD13	2:2:94:PHE:HA	1.56	0.85
1:1:187:LEU:HD22	1:1:188:PRO:CD	2.06	0.84
1:1:83:GLU:HB2	1:1:212:ARG:HB3	1.60	0.83
3:3:191:LEU:HD22	3:3:192:THR:N	1.93	0.83
3:3:103:SER:O	3:3:211:GLY:HA3	1.79	0.83
1:1:13:THR:HB	3:3:157:ASN:CB	2.09	0.83
2:2:120:HIS:NE2	2:2:205:PRO:HD2	1.94	0.83
1:1:157:SER:HB2	3:3:24:PRO:HA	1.58	0.82
1:1:130:ILE:HD11	1:1:135:VAL:HG12	1.59	0.82
1:1:70:ARG:O	1:1:71:LEU:HB2	1.79	0.82
2:2:15:GLU:HG3	2:2:29:SER:HB3	1.61	0.82
1:1:75:CYS:HB3	1:1:218:MET:SD	2.20	0.81
3:3:53:PHE:HE1	3:3:205:LEU:HB3	1.43	0.81
2:2:156:SER:HB3	3:3:51:TYR:CE1	2.15	0.81
3:3:63:GLU:HG2	3:3:201:LYS:HD3	1.63	0.81
2:2:13:ARG:O	2:2:27:GLN:HA	1.80	0.81
2:2:122:GLY:HA2	2:2:200:SER:O	1.79	0.81
2:2:161:GLN:HB3	2:2:171:VAL:HG13	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:109:ASP:HB2	2:2:218:ILE:HD11	1.64	0.79
1:1:115:THR:HG23	1:1:133:LEU:H	1.45	0.79
1:1:170:PHE:HD1	1:1:222:ARG:CZ	1.96	0.79
3:3:103:SER:CB	3:3:159:PRO:HA	2.12	0.79
2:2:154:GLN:O	2:2:157:VAL:HG12	1.83	0.79
1:1:174:TRP:HB2	2:2:188:LEU:HD23	1.65	0.79
2:2:213:MET:HE3	2:2:215:VAL:HG22	1.63	0.79
2:2:44:PRO:HB2	2:2:47:VAL:CG2	2.13	0.79
2:2:104:VAL:CG1	2:2:222:VAL:HG22	2.06	0.79
2:2:124:LEU:HD22	2:2:196:ILE:HG22	1.66	0.78
1:1:60:PHE:CE1	1:1:167:VAL:HG11	2.18	0.78
1:1:62:SER:HB2	1:1:73:ASN:HD21	1.49	0.77
1:1:86:ILE:HD12	1:1:86:ILE:N	2.00	0.77
2:2:121:SER:O	2:2:202:LEU:HD22	1.85	0.76
2:2:180:PRO:HD2	2:2:189:HIS:CE1	2.19	0.76
1:1:223:PRO:HB3	2:2:154:GLN:HB3	1.69	0.75
2:2:58:LEU:CD1	2:2:94:PHE:HA	2.17	0.75
1:1:219:TYR:CD1	3:3:39:ARG:HB2	2.22	0.75
1:1:101:PHE:HD1	1:1:143:VAL:CG1	2.00	0.74
2:2:209:VAL:N	2:2:210:PRO:HD3	2.02	0.74
1:1:164:TRP:HE1	1:1:187:LEU:HD11	1.52	0.73
1:1:119:TRP:HB3	1:1:130:ILE:HG23	1.70	0.73
1:1:75:CYS:O	1:1:222:ARG:HD2	1.88	0.73
3:3:116:THR:HG23	3:3:191:LEU:CD2	2.17	0.73
1:1:15:PRO:HG3	3:3:157:ASN:ND2	2.03	0.73
1:1:106:TRP:HZ3	3:3:26:TYR:CD1	2.08	0.72
3:3:24:PRO:HB3	4:4:30:TYR:O	1.89	0.72
3:3:106:PHE:CE2	3:3:208:VAL:HG22	2.25	0.71
2:2:101:HIS:HB3	2:2:222:VAL:HG12	1.72	0.71
1:1:101:PHE:HD1	1:1:143:VAL:HG11	1.56	0.71
3:3:117:LYS:HB3	3:3:119:LYS:CE	2.20	0.71
3:3:19:PRO:HG3	4:4:17:ASN:HD21	1.56	0.71
2:2:88:LEU:HD23	2:2:91:MET:SD	2.30	0.70
2:2:112:VAL:HG21	2:2:126:VAL:HG21	1.72	0.70
2:2:62:TYR:CD2	2:2:91:MET:HA	2.27	0.70
2:2:13:ARG:HG3	2:2:29:SER:O	1.91	0.70
3:3:116:THR:CG2	3:3:191:LEU:HD21	2.21	0.70
2:2:119:ALA:O	2:2:204:GLY:HA3	1.92	0.70
2:2:208:THR:OG1	2:2:210:PRO:HD3	1.92	0.70
1:1:186:TRP:CZ2	1:1:188:PRO:HA	2.27	0.70
1:1:239:PHE:CD1	3:3:170:TYR:HD2	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:42:ASN:ND2	3:3:44:ILE:H	1.90	0.69
1:1:104:VAL:HG22	1:1:197:LEU:CD2	2.22	0.69
2:2:54:LEU:HD12	2:2:220:ALA:HB1	1.74	0.69
2:2:26:SER:O	2:2:28:GLY:N	2.25	0.69
2:2:58:LEU:HD13	2:2:94:PHE:CA	2.23	0.69
3:3:119:LYS:HG2	3:3:147:ASP:OD2	1.93	0.68
1:1:103:TRP:HB2	1:1:198:THR:CG2	2.23	0.68
1:1:88:PHE:CE2	1:1:146:ILE:HD13	2.28	0.68
3:3:99:GLN:OE1	3:3:217:ARG:HD2	1.93	0.68
1:1:88:PHE:HA	1:1:207:CYS:HA	1.74	0.68
1:1:82:LEU:HD11	1:1:211:TYR:CD2	2.26	0.68
1:1:76:THR:HB	1:1:220:CYS:HB2	1.74	0.68
2:2:20:GLY:HA2	2:2:56:PRO:O	1.94	0.68
1:1:43:LEU:HD23	1:1:43:LEU:N	2.07	0.68
2:2:152:TYR:CZ	3:3:60:PRO:HD3	2.28	0.68
2:2:209:VAL:H	2:2:210:PRO:CD	2.07	0.68
1:1:83:GLU:HG2	1:1:157:SER:HA	1.76	0.68
3:3:56:ILE:O	3:3:59:LYS:HG2	1.94	0.67
2:2:13:ARG:HB3	2:2:27:GLN:OE1	1.95	0.67
1:1:88:PHE:HE2	1:1:146:ILE:HG21	1.58	0.67
2:2:223:ASN:H	2:2:223:ASN:HD22	1.41	0.67
1:1:164:TRP:HZ2	1:1:187:LEU:HD21	1.58	0.67
3:3:8:VAL:HB	3:3:10:GLU:HG2	1.77	0.67
2:2:209:VAL:O	2:2:209:VAL:HG12	1.94	0.67
1:1:130:ILE:CD1	1:1:135:VAL:HG12	2.24	0.67
2:2:120:HIS:CD2	2:2:205:PRO:HD2	2.29	0.67
3:3:56:ILE:HG13	3:3:74:PHE:CE1	2.29	0.67
1:1:40:VAL:HB	1:1:68:TRP:CZ2	2.30	0.67
1:1:210:ARG:NH1	3:3:14:PHE:CE1	2.63	0.67
2:2:101:HIS:HB3	2:2:222:VAL:CG1	2.25	0.66
1:1:77:TYR:HD1	1:1:168:PRO:HA	1.60	0.66
1:1:88:PHE:CZ	1:1:205:GLY:HA3	2.30	0.66
3:3:83:ALA:O	3:3:86:HIS:HB3	1.96	0.66
2:2:126:VAL:CG1	2:2:171:VAL:HG21	2.25	0.66
3:3:19:PRO:O	3:3:20:ASP:HB2	1.94	0.66
1:1:187:LEU:CD2	1:1:188:PRO:HD2	2.25	0.65
1:1:57:LEU:HD21	1:1:195:ILE:HG12	1.76	0.65
2:2:58:LEU:HD22	2:2:93:SER:HB3	1.78	0.65
2:2:135:THR:HB	2:2:139:ALA:HA	1.78	0.65
3:3:66:ASN:HA	3:3:190:ALA:HB1	1.77	0.65
3:3:42:ASN:O	3:3:45:ASP:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:59:PRO:O	1:1:72:LEU:HD13	1.97	0.65
1:1:78:PHE:O	1:1:167:VAL:HB	1.96	0.65
3:3:132:PRO:HG2	3:3:184:GLN:HE22	1.62	0.64
2:2:120:HIS:HA	2:2:203:THR:O	1.98	0.64
1:1:209:LEU:HD13	1:1:210:ARG:H	1.61	0.64
1:1:87:GLN:O	1:1:88:PHE:HB3	1.98	0.64
3:3:115:ALA:HB1	3:3:194:THR:OG1	1.98	0.64
2:2:22:THR:HG21	2:2:61:HIS:N	2.13	0.64
3:3:101:ARG:NH1	3:3:165:ASP:HB3	2.13	0.64
3:3:119:LYS:HA	3:3:147:ASP:HA	1.79	0.63
3:3:110:PHE:CB	3:3:148:VAL:HG11	2.29	0.63
2:2:32:THR:HG23	2:2:172:HIS:CE1	2.33	0.63
3:3:66:ASN:HB3	3:3:191:LEU:O	1.99	0.63
3:3:27:PRO:HB3	4:4:30:TYR:HA	1.82	0.62
2:2:15:GLU:HG3	2:2:29:SER:CB	2.30	0.62
1:1:19:LEU:CD1	3:3:160:TYR:HB3	2.29	0.62
1:1:104:VAL:HG22	1:1:197:LEU:HD23	1.80	0.62
1:1:230:ARG:NH2	3:3:83:ALA:HB1	2.14	0.62
3:3:42:ASN:HD22	3:3:44:ILE:H	1.46	0.62
3:3:53:PHE:CE1	3:3:205:LEU:HB3	2.31	0.62
2:2:208:THR:O	2:2:209:VAL:HG23	1.99	0.62
1:1:74:THR:HG21	3:3:43:PHE:CZ	2.35	0.62
1:1:88:PHE:CE1	1:1:205:GLY:CA	2.81	0.62
2:2:213:MET:CE	2:2:215:VAL:HG22	2.30	0.62
2:2:69:TRP:CZ3	2:2:124:LEU:HG	2.34	0.61
2:2:113:GLN:HA	2:2:169:SER:O	2.01	0.61
2:2:23:ILE:N	2:2:23:ILE:HD12	2.15	0.61
2:2:61:HIS:HA	2:2:216:ALA:HB2	1.81	0.61
4:4:25:PHE:HD2	4:4:26:TYR:CE1	2.19	0.60
3:3:121:LEU:HD23	3:3:121:LEU:C	2.22	0.60
2:2:100:ALA:O	2:2:101:HIS:CD2	2.54	0.60
2:2:18:VAL:HG13	2:2:23:ILE:HG13	1.82	0.60
2:2:54:LEU:HD12	2:2:220:ALA:CB	2.31	0.60
1:1:102:VAL:HG22	1:1:199:SER:CB	2.30	0.60
1:1:86:ILE:N	1:1:86:ILE:CD1	2.65	0.60
1:1:209:LEU:CD1	1:1:210:ARG:H	2.15	0.60
2:2:110:VAL:HG12	2:2:215:VAL:HA	1.83	0.60
3:3:160:TYR:OH	3:3:167:MET:HG2	2.01	0.60
3:3:42:ASN:HD22	3:3:44:ILE:HG22	1.65	0.60
1:1:223:PRO:HD3	2:2:158:PHE:CZ	2.37	0.60
1:1:5:GLY:O	1:1:6:GLU:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:209:LEU:O	1:1:210:ARG:HG2	2.01	0.59
2:2:27:GLN:HG3	2:2:28:GLY:N	2.17	0.59
1:1:224:ILE:HG13	3:3:89:TYR:CE2	2.37	0.59
3:3:56:ILE:N	3:3:56:ILE:HD12	2.18	0.59
1:1:115:THR:HG22	1:1:131:GLN:OE1	2.02	0.59
1:1:88:PHE:CE2	1:1:146:ILE:HG21	2.37	0.59
1:1:173:GLY:HA3	2:2:188:LEU:O	2.03	0.59
2:2:78:ALA:HA	2:2:196:ILE:O	2.02	0.59
1:1:156:PHE:CD2	3:3:25:LEU:HD12	2.38	0.59
1:1:173:GLY:CA	2:2:188:LEU:O	2.50	0.59
2:2:161:GLN:OE1	2:2:171:VAL:HA	2.03	0.58
2:2:126:VAL:HG11	2:2:171:VAL:HG21	1.84	0.58
3:3:14:PHE:O	3:3:15:MET:HB2	2.02	0.58
3:3:17:SER:O	3:3:19:PRO:HD3	2.03	0.58
3:3:100:TYR:CE1	3:3:167:MET:HB2	2.37	0.58
2:2:35:CYS:O	2:2:36:TYR:HB2	2.03	0.58
2:2:36:TYR:HE2	2:2:130:PRO:CG	2.15	0.58
1:1:130:ILE:HD11	1:1:135:VAL:CG1	2.30	0.58
3:3:80:LEU:HD12	3:3:80:LEU:N	2.18	0.58
2:2:176:PRO:O	2:2:192:TRP:NE1	2.36	0.58
3:3:94:SER:HB3	3:3:169:VAL:HG13	1.85	0.58
1:1:84:LEU:O	1:1:155:GLY:HA2	2.04	0.58
2:2:223:ASN:ND2	2:2:223:ASN:H	2.01	0.58
1:1:40:VAL:O	1:1:41:GLU:HB2	2.03	0.58
2:2:98:VAL:O	2:2:98:VAL:HG12	2.04	0.57
1:1:170:PHE:O	2:2:131:GLU:HB3	2.04	0.57
2:2:151:THR:O	2:2:155:LEU:N	2.36	0.57
2:2:153:GLN:NE2	3:3:55:SER:HB2	2.19	0.57
3:3:61:TYR:HB3	3:3:205:LEU:HD23	1.87	0.57
1:1:178:THR:O	1:1:180:GLU:N	2.36	0.57
2:2:209:VAL:N	2:2:210:PRO:CD	2.68	0.57
1:1:206:GLY:O	1:1:207:CYS:SG	2.62	0.56
1:1:218:MET:HB3	3:3:40:PHE:CE1	2.39	0.56
1:1:165:ARG:O	3:3:34:ARG:HG2	2.05	0.56
2:2:36:TYR:HE2	2:2:130:PRO:HG3	1.71	0.56
3:3:122:VAL:O	3:3:143:HIS:HB2	2.05	0.56
2:2:218:ILE:O	2:2:219:ASP:HB2	2.06	0.56
3:3:99:GLN:HB2	3:3:217:ARG:HG3	1.87	0.56
2:2:119:ALA:O	2:2:205:PRO:HD3	2.06	0.56
2:2:126:VAL:HG13	2:2:161:GLN:O	2.06	0.56
2:2:75:HIS:HE2	3:3:59:LYS:HB3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:202:LEU:HD11	2:2:209:VAL:HG21	1.88	0.55
3:3:86:HIS:ND1	3:3:87:GLY:N	2.54	0.55
1:1:19:LEU:HD12	3:3:160:TYR:HB3	1.89	0.55
3:3:179:VAL:HG12	3:3:181:GLY:H	1.71	0.55
1:1:165:ARG:HB2	3:3:33:PRO:O	2.07	0.55
3:3:53:PHE:CE1	3:3:205:LEU:HD13	2.41	0.55
1:1:244:ASN:OD1	3:3:172:ALA:HB1	2.06	0.55
1:1:49:THR:HG22	1:1:50:GLY:N	2.21	0.55
3:3:74:PHE:O	3:3:184:GLN:HA	2.07	0.55
3:3:56:ILE:HG13	3:3:74:PHE:HE1	1.72	0.55
3:3:121:LEU:HD22	3:3:186:TYR:HB2	1.89	0.55
4:4:28:GLN:O	4:4:29:GLN:HG3	2.07	0.55
2:2:84:PRO:HD3	2:2:108:TRP:HZ2	1.71	0.55
2:2:84:PRO:HG3	2:2:108:TRP:HH2	1.72	0.55
1:1:80:SER:HB3	1:1:216:ALA:HA	1.88	0.55
1:1:181:LYS:HA	2:2:137:GLU:HG3	1.89	0.55
2:2:36:TYR:CE2	2:2:130:PRO:HG2	2.42	0.55
2:2:27:GLN:CG	2:2:28:GLY:N	2.70	0.54
1:1:239:PHE:HD2	3:3:226:GLN:NE2	2.05	0.54
2:2:69:TRP:CH2	2:2:124:LEU:HG	2.42	0.54
2:2:62:TYR:CE2	2:2:91:MET:HA	2.43	0.54
1:1:48:LEU:HD21	1:1:103:TRP:CZ3	2.43	0.54
2:2:60:ARG:O	2:2:216:ALA:HB1	2.07	0.54
1:1:86:ILE:H	1:1:86:ILE:HD12	1.72	0.54
2:2:117:SER:OG	2:2:118:PHE:N	2.41	0.54
1:1:103:TRP:HB2	1:1:198:THR:HG22	1.89	0.54
3:3:109:ILE:HB	3:3:205:LEU:HB2	1.88	0.54
2:2:22:THR:HG21	2:2:61:HIS:HB2	1.88	0.54
3:3:15:MET:HB3	3:3:18:VAL:HG13	1.90	0.54
2:2:27:GLN:HG3	2:2:28:GLY:H	1.73	0.54
1:1:118:ALA:HB2	1:1:132:GLN:NE2	2.23	0.54
3:3:107:ASN:HA	3:3:154:PHE:O	2.08	0.53
2:2:69:TRP:HD1	2:2:70:PRO:N	2.07	0.53
1:1:115:THR:OG1	1:1:133:LEU:HB2	2.08	0.53
3:3:101:ARG:HA	3:3:160:TYR:HE1	1.73	0.53
3:3:90:VAL:HG11	3:3:208:VAL:HG12	1.91	0.53
3:3:48:LYS:HA	3:3:210:ALA:HB3	1.90	0.53
1:1:221:PRO:CA	3:3:40:PHE:HE2	2.21	0.53
2:2:69:TRP:CZ3	2:2:124:LEU:CG	2.92	0.53
1:1:157:SER:CB	3:3:24:PRO:HA	2.36	0.53
1:1:30:VAL:HG13	1:1:218:MET:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:165:ARG:HD3	2:2:182:PRO:HG3	1.90	0.53
1:1:48:LEU:HD21	1:1:103:TRP:CE3	2.44	0.53
3:3:145:VAL:HG22	3:3:188:LEU:HD12	1.91	0.53
1:1:186:TRP:O	1:1:187:LEU:HB3	2.09	0.53
1:1:99:GLU:OE2	1:1:101:PHE:HE2	1.92	0.53
1:1:109:VAL:HG23	1:1:161:THR:OG1	2.09	0.53
1:1:109:VAL:H	1:1:161:THR:HB	1.74	0.53
2:2:73:GLN:NE2	2:2:73:GLN:HA	2.17	0.53
2:2:124:LEU:HD12	2:2:163:LEU:HD12	1.91	0.52
1:1:55:HIS:O	1:1:194:SER:CB	2.56	0.52
1:1:184:TYR:HE1	2:2:139:ALA:CB	2.23	0.52
3:3:108:PHE:HA	3:3:205:LEU:O	2.09	0.52
1:1:219:TYR:OH	3:3:34:ARG:HD2	2.08	0.52
3:3:42:ASN:HD22	3:3:44:ILE:N	2.08	0.52
2:2:81:CYS:O	2:2:82:PRO:C	2.46	0.52
1:1:37:PHE:HA	1:1:211:TYR:O	2.10	0.52
2:2:153:GLN:NE2	3:3:55:SER:N	2.58	0.52
2:2:178:ILE:HG22	2:2:191:PRO:CB	2.40	0.52
3:3:56:ILE:HD13	3:3:206:VAL:HG11	1.91	0.52
1:1:212:ARG:O	1:1:214:PRO:HD2	2.09	0.52
2:2:80:ILE:HG23	2:2:82:PRO:HD3	1.91	0.52
1:1:86:ILE:H	1:1:86:ILE:CD1	2.23	0.52
1:1:50:GLY:O	1:1:131:GLN:NE2	2.43	0.52
1:1:48:LEU:O	1:1:131:GLN:NE2	2.43	0.52
2:2:152:TYR:CB	2:2:197:LEU:HD22	2.40	0.52
3:3:100:TYR:CZ	3:3:167:MET:HB2	2.45	0.52
1:1:88:PHE:HE1	1:1:205:GLY:C	2.14	0.52
1:1:76:THR:O	1:1:169:VAL:HG23	2.10	0.51
2:2:186:LEU:HD23	2:2:186:LEU:O	2.11	0.51
3:3:60:PRO:O	3:3:61:TYR:HB3	2.11	0.51
1:1:106:TRP:O	1:1:139:SER:HB2	2.11	0.51
4:4:25:PHE:CD2	4:4:26:TYR:CE1	2.98	0.51
2:2:152:TYR:CE1	3:3:60:PRO:HD3	2.45	0.51
3:3:31:VAL:HB	4:4:34:ILE:O	2.10	0.51
1:1:239:PHE:CD1	3:3:170:TYR:CD2	2.96	0.51
2:2:104:VAL:HG22	2:2:222:VAL:HG13	1.92	0.51
1:1:108:PRO:HA	1:1:161:THR:HG21	1.92	0.51
2:2:80:ILE:HD11	2:2:132:TYR:OH	2.11	0.51
3:3:169:VAL:O	3:3:169:VAL:HG12	2.09	0.51
3:3:19:PRO:HG3	4:4:17:ASN:ND2	2.26	0.51
2:2:87:LYS:HG3	2:2:142:TRP:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:88:PHE:CE1	1:1:205:GLY:C	2.85	0.51
1:1:210:ARG:HD2	3:3:14:PHE:CZ	2.46	0.51
1:1:212:ARG:HG2	1:1:214:PRO:HD3	1.91	0.51
1:1:104:VAL:HG22	1:1:197:LEU:HD21	1.90	0.51
2:2:153:GLN:HA	3:3:53:PHE:HB2	1.94	0.50
3:3:31:VAL:HG12	4:4:35:ASP:HA	1.92	0.50
2:2:16:THR:HA	2:2:24:ILE:O	2.11	0.50
2:2:111:VAL:HG22	2:2:172:HIS:CD2	2.46	0.50
3:3:3:ILE:HG22	3:3:4:ARG:N	2.27	0.50
1:1:40:VAL:HG22	1:1:211:TYR:CE1	2.46	0.50
3:3:75:GLN:HG3	3:3:184:GLN:HG2	1.93	0.50
1:1:48:LEU:HD23	1:1:198:THR:OG1	2.12	0.50
1:1:107:PHE:HE1	1:1:196:LEU:HB2	1.76	0.50
1:1:238:LYS:HA	3:3:171:SER:O	2.12	0.50
3:3:135:ARG:O	3:3:138:ALA:N	2.45	0.50
2:2:140:LEU:HD22	2:2:190:ASN:OD1	2.12	0.50
1:1:79:PHE:CZ	3:3:31:VAL:HG11	2.47	0.50
1:1:150:ARG:HE	1:1:150:ARG:H	1.60	0.50
2:2:124:LEU:HD12	2:2:163:LEU:CD1	2.40	0.50
3:3:97:PHE:CE1	3:3:216:LEU:HD23	2.47	0.50
2:2:21:VAL:H	2:2:60:ARG:HG2	1.75	0.49
2:2:84:PRO:HD2	2:2:186:LEU:HD22	1.95	0.49
1:1:109:VAL:HG22	1:1:191:HIS:CD2	2.46	0.49
1:1:181:LYS:O	1:1:182:ALA:HB2	2.11	0.49
2:2:180:PRO:HD2	2:2:189:HIS:HE1	1.76	0.49
3:3:121:LEU:HD23	3:3:121:LEU:O	2.12	0.49
3:3:102:GLY:HA3	3:3:214:PHE:HA	1.93	0.49
2:2:152:TYR:CE1	3:3:60:PRO:HG3	2.48	0.49
2:2:135:THR:HB	2:2:139:ALA:CA	2.41	0.49
2:2:110:VAL:CG1	2:2:215:VAL:HA	2.43	0.49
3:3:56:ILE:CD1	3:3:56:ILE:N	2.75	0.49
1:1:40:VAL:HG22	1:1:211:TYR:HE1	1.77	0.49
2:2:178:ILE:HG22	2:2:191:PRO:HB2	1.94	0.49
1:1:160:TYR:CE1	1:1:167:VAL:HG23	2.48	0.49
1:1:171:TYR:N	1:1:185:ASN:OD1	2.45	0.49
2:2:195:VAL:C	2:2:196:ILE:HG13	2.33	0.49
3:3:101:ARG:HA	3:3:160:TYR:CE1	2.48	0.49
2:2:167:THR:O	2:2:168:ASN:HB3	2.13	0.48
1:1:237:HIS:O	3:3:171:SER:HB2	2.13	0.48
4:4:30:TYR:CD1	4:4:30:TYR:N	2.81	0.48
1:1:170:PHE:CD1	1:1:222:ARG:CZ	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:32:THR:HG23	2:2:172:HIS:ND1	2.29	0.48
1:1:187:LEU:HD12	1:1:190:ALA:HB2	1.94	0.48
2:2:152:TYR:HE1	3:3:60:PRO:HB3	1.78	0.48
1:1:27:HIS:O	1:1:33:LEU:HD21	2.13	0.48
2:2:125:CYS:HB2	2:2:199:LEU:HD11	1.94	0.48
3:3:101:ARG:HD2	3:3:165:ASP:O	2.14	0.48
2:2:52:THR:O	2:2:221:MET:HA	2.13	0.48
1:1:82:LEU:HD23	1:1:84:LEU:HD11	1.94	0.48
3:3:80:LEU:HD12	3:3:80:LEU:H	1.77	0.48
3:3:130:ALA:O	3:3:131:ALA:HB3	2.13	0.48
3:3:56:ILE:CD1	3:3:206:VAL:HG11	2.43	0.48
2:2:200:SER:HA	3:3:61:TYR:CE2	2.48	0.48
3:3:70:ASP:HA	3:3:135:ARG:HH12	1.79	0.48
1:1:4:VAL:HG22	3:3:151:ASN:O	2.14	0.48
3:3:53:PHE:HB3	3:3:60:PRO:CB	2.44	0.47
2:2:223:ASN:N	2:2:223:ASN:ND2	2.60	0.47
2:2:121:SER:CB	2:2:203:THR:HG22	2.32	0.47
1:1:101:PHE:O	1:1:199:SER:CB	2.62	0.47
2:2:176:PRO:HD2	2:2:192:TRP:CZ2	2.49	0.47
2:2:84:PRO:HD3	2:2:108:TRP:CZ2	2.49	0.47
1:1:113:THR:O	1:1:133:LEU:HD12	2.14	0.47
1:1:156:PHE:CG	3:3:25:LEU:HD12	2.49	0.47
3:3:84:GLU:N	3:3:84:GLU:OE1	2.48	0.47
2:2:84:PRO:HG3	2:2:108:TRP:CH2	2.50	0.47
1:1:224:ILE:HD11	3:3:89:TYR:CZ	2.49	0.47
1:1:237:HIS:HB2	3:3:81:SER:O	2.14	0.47
3:3:75:GLN:HA	3:3:183:LEU:O	2.14	0.47
1:1:84:LEU:CD2	1:1:209:LEU:HD11	2.45	0.47
1:1:105:LYS:HE3	1:1:139:SER:OG	2.13	0.47
3:3:160:TYR:HD2	3:3:161:SER:N	2.13	0.47
2:2:84:PRO:HG2	2:2:88:LEU:HG	1.97	0.47
1:1:103:TRP:HB2	1:1:198:THR:HG23	1.96	0.47
3:3:53:PHE:HB3	3:3:60:PRO:HB2	1.96	0.47
1:1:43:LEU:CD2	1:1:43:LEU:N	2.74	0.47
3:3:157:ASN:O	3:3:159:PRO:HD3	2.14	0.47
3:3:73:LEU:HB3	3:3:185:VAL:O	2.14	0.47
1:1:120:GLN:HB2	1:1:129:ARG:HD3	1.96	0.47
3:3:220:VAL:HG12	3:3:221:ASP:O	2.15	0.47
3:3:117:LYS:O	3:3:191:LEU:HD22	2.15	0.47
3:3:44:ILE:HG23	3:3:45:ASP:N	2.30	0.47
1:1:37:PHE:CD1	1:1:212:ARG:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:76:GLY:HA2	2:2:197:LEU:HD21	1.97	0.47
1:1:46:SER:HB2	1:1:197:LEU:O	2.15	0.47
2:2:152:TYR:C	2:2:152:TYR:CD1	2.88	0.46
1:1:187:LEU:HD22	1:1:188:PRO:N	2.30	0.46
2:2:212:THR:HG22	2:2:213:MET:N	2.30	0.46
3:3:62:PHE:CE1	3:3:204:VAL:HG11	2.50	0.46
1:1:121:LEU:C	1:1:121:LEU:HD13	2.36	0.46
2:2:163:LEU:HD21	2:2:169:SER:C	2.36	0.46
1:1:101:PHE:CD1	1:1:143:VAL:HG11	2.44	0.46
3:3:108:PHE:O	3:3:153:ALA:HA	2.15	0.46
3:3:122:VAL:HG22	3:3:123:ALA:N	2.30	0.46
2:2:23:ILE:H	2:2:23:ILE:HD12	1.80	0.46
2:2:160:HIS:HE2	3:3:51:TYR:HE1	1.64	0.46
2:2:75:HIS:NE2	3:3:59:LYS:HB3	2.30	0.46
3:3:195:ASP:HB2	3:3:198:VAL:HG22	1.98	0.46
1:1:22:VAL:CG1	1:1:23:ASP:N	2.79	0.46
1:1:183:THR:HA	1:1:186:TRP:HB3	1.98	0.46
3:3:120:PHE:HD1	3:3:146:TRP:CH2	2.34	0.46
1:1:149:SER:C	1:1:151:SER:H	2.18	0.46
1:1:22:VAL:C	1:1:24:MET:H	2.18	0.46
3:3:85:LEU:O	3:3:91:ALA:CB	2.64	0.46
3:3:56:ILE:CG1	3:3:74:PHE:CE1	2.98	0.45
1:1:82:LEU:CD2	1:1:84:LEU:HD11	2.46	0.45
1:1:113:THR:O	1:1:114:LYS:C	2.55	0.45
1:1:184:TYR:CE1	2:2:139:ALA:HB2	2.51	0.45
2:2:22:THR:HG21	2:2:61:HIS:CB	2.46	0.45
1:1:151:SER:C	1:1:153:ALA:H	2.19	0.45
2:2:81:CYS:O	2:2:83:LEU:N	2.49	0.45
2:2:152:TYR:HB2	2:2:197:LEU:HD22	1.98	0.45
2:2:211:VAL:HG12	2:2:212:THR:N	2.30	0.45
3:3:103:SER:HB3	3:3:159:PRO:CA	2.35	0.45
3:3:110:PHE:HB3	3:3:148:VAL:HG11	1.96	0.45
3:3:172:ALA:O	3:3:178:ASN:OD1	2.34	0.45
2:2:135:THR:HG23	2:2:145:LEU:HD11	1.99	0.45
1:1:165:ARG:HG2	2:2:180:PRO:O	2.16	0.45
1:1:107:PHE:HB2	1:1:194:SER:OG	2.16	0.45
2:2:163:LEU:HG	2:2:171:VAL:HG23	1.99	0.45
2:2:75:HIS:HA	2:2:198:ILE:O	2.17	0.45
3:3:101:ARG:O	3:3:101:ARG:HG2	2.17	0.45
1:1:219:TYR:HD1	3:3:39:ARG:HB2	1.79	0.45
3:3:198:VAL:HG23	3:3:199:ASN:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:49:ASP:HA	2:2:50:PRO:HD2	1.80	0.45
3:3:13:SER:OG	3:3:15:MET:CE	2.64	0.45
1:1:170:PHE:CD1	1:1:222:ARG:NH1	2.85	0.45
1:1:109:VAL:HG22	1:1:191:HIS:HD2	1.82	0.45
3:3:77:ASP:O	3:3:79:SER:N	2.50	0.45
2:2:158:PHE:O	2:2:159:PRO:C	2.55	0.45
2:2:156:SER:HA	2:2:160:HIS:CD2	2.52	0.45
2:2:125:CYS:SG	2:2:160:HIS:HD2	2.40	0.45
2:2:54:LEU:HD21	2:2:97:VAL:HG11	1.99	0.45
2:2:39:PRO:HB3	2:2:176:PRO:HA	1.99	0.45
3:3:122:VAL:HA	3:3:185:VAL:HA	1.97	0.44
3:3:7:SER:OG	3:3:11:SER:HB3	2.17	0.44
2:2:108:TRP:O	2:2:218:ILE:HD12	2.17	0.44
3:3:154:PHE:CG	3:3:155:SER:N	2.84	0.44
3:3:103:SER:HB2	3:3:159:PRO:HA	1.95	0.44
3:3:97:PHE:CD1	3:3:216:LEU:HD23	2.51	0.44
3:3:175:THR:OG1	3:3:178:ASN:ND2	2.51	0.44
1:1:146:ILE:O	1:1:146:ILE:HG22	2.17	0.44
2:2:78:ALA:HB1	2:2:195:VAL:HG12	1.99	0.44
2:2:153:GLN:NE2	3:3:55:SER:CB	2.80	0.44
2:2:157:VAL:HG23	3:3:50:THR:HG21	1.99	0.44
1:1:201:ALA:O	1:1:202:HIS:CD2	2.71	0.44
1:1:45:LEU:HB2	1:1:202:HIS:HA	1.98	0.44
1:1:13:THR:C	1:1:14:GLU:HG3	2.38	0.44
2:2:84:PRO:HD2	2:2:186:LEU:CD2	2.48	0.44
2:2:152:TYR:OH	3:3:60:PRO:HD3	2.17	0.44
2:2:34:TYR:HA	2:2:174:VAL:O	2.18	0.44
4:4:16:GLY:O	4:4:18:SER:N	2.50	0.44
3:3:134:THR:OG1	3:3:137:GLU:HG3	2.17	0.44
1:1:174:TRP:HB2	2:2:188:LEU:CD2	2.44	0.44
1:1:201:ALA:O	1:1:202:HIS:HD2	2.01	0.44
3:3:36:VAL:HA	3:3:37:PRO:HD3	1.53	0.44
3:3:97:PHE:HB3	3:3:218:HIS:O	2.17	0.44
2:2:36:TYR:CE2	2:2:130:PRO:CG	2.98	0.44
2:2:54:LEU:HB2	2:2:220:ALA:HB3	1.99	0.44
3:3:179:VAL:HG12	3:3:181:GLY:N	2.32	0.43
2:2:69:TRP:CZ3	2:2:124:LEU:HD11	2.52	0.43
1:1:40:VAL:HB	1:1:68:TRP:CH2	2.53	0.43
2:2:57:THR:HG22	2:2:58:LEU:H	1.82	0.43
1:1:62:SER:O	1:1:63:THR:CB	2.66	0.43
1:1:49:THR:HG22	1:1:50:GLY:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:13:ARG:HD3	2:2:13:ARG:HA	1.72	0.43
1:1:176:ALA:C	1:1:178:THR:H	2.22	0.43
1:1:55:HIS:O	1:1:194:SER:HB2	2.18	0.43
1:1:56:VAL:HG13	1:1:193:GLY:O	2.17	0.43
1:1:181:LYS:O	1:1:182:ALA:CB	2.66	0.43
3:3:217:ARG:HD3	3:3:218:HIS:CD2	2.54	0.43
2:2:23:ILE:N	2:2:23:ILE:CD1	2.81	0.43
2:2:129:VAL:HA	2:2:130:PRO:HD3	1.78	0.43
1:1:79:PHE:C	1:1:79:PHE:CD1	2.92	0.43
1:1:52:PRO:HD3	1:1:115:THR:O	2.17	0.43
3:3:119:LYS:O	3:3:120:PHE:CB	2.67	0.43
2:2:140:LEU:HD22	2:2:190:ASN:CG	2.38	0.43
1:1:106:TRP:CZ2	1:1:158:VAL:HG13	2.54	0.43
2:2:22:THR:HG23	2:2:22:THR:O	2.18	0.43
1:1:26:VAL:HG12	1:1:27:HIS:N	2.32	0.43
2:2:152:TYR:CE1	3:3:60:PRO:CG	3.01	0.43
2:2:57:THR:O	2:2:59:SER:N	2.52	0.43
2:2:153:GLN:CD	3:3:55:SER:HB2	2.39	0.43
4:4:18:SER:O	4:4:23:GLN:NE2	2.52	0.43
1:1:184:TYR:HE1	2:2:139:ALA:HB3	1.84	0.43
3:3:84:GLU:CD	3:3:84:GLU:H	2.21	0.43
2:2:95:HIS:C	2:2:95:HIS:CD2	2.93	0.43
2:2:42:ARG:HA	2:2:43:PRO:HD2	1.64	0.43
2:2:83:LEU:HA	2:2:84:PRO:HA	1.60	0.42
1:1:101:PHE:CD1	1:1:143:VAL:CG1	2.91	0.42
2:2:139:ALA:C	2:2:141:LYS:H	2.21	0.42
2:2:216:ALA:HA	2:2:217:PRO:HD3	1.78	0.42
2:2:61:HIS:CG	2:2:216:ALA:HB2	2.54	0.42
1:1:22:VAL:HG12	1:1:23:ASP:N	2.33	0.42
2:2:121:SER:O	2:2:202:LEU:HA	2.19	0.42
2:2:69:TRP:HZ2	2:2:198:ILE:HG23	1.85	0.42
2:2:25:ASN:O	2:2:26:SER:HB3	2.18	0.42
2:2:135:THR:O	2:2:137:GLU:N	2.53	0.42
3:3:98:ALA:HB2	3:3:220:VAL:HG21	2.01	0.42
4:4:31:GLN:HE21	4:4:31:GLN:HA	1.85	0.42
2:2:152:TYR:HB3	2:2:197:LEU:HD22	2.00	0.42
1:1:128:VAL:HG13	1:1:128:VAL:O	2.19	0.42
2:2:77:HIS:HE1	2:2:144:GLU:HG2	1.84	0.42
1:1:172:ASN:HB2	2:2:132:TYR:O	2.19	0.42
2:2:135:THR:HB	2:2:139:ALA:CB	2.50	0.42
1:1:79:PHE:CE2	1:1:160:TYR:CD2	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:31:GLY:O	2:2:172:HIS:HB3	2.20	0.42
1:1:74:THR:HG22	1:1:74:THR:O	2.19	0.42
1:1:144:PHE:CD1	1:1:154:CYS:HB3	2.54	0.42
3:3:103:SER:HB3	3:3:159:PRO:C	2.40	0.42
4:4:29:GLN:HB2	4:4:30:TYR:HD1	1.84	0.42
2:2:160:HIS:HB2	2:2:161:GLN:H	1.70	0.42
2:2:74:SER:O	2:2:75:HIS:C	2.58	0.42
1:1:48:LEU:HA	1:1:198:THR:OG1	2.20	0.42
1:1:49:THR:CG2	1:1:50:GLY:N	2.83	0.42
1:1:219:TYR:CE1	3:3:39:ARG:HD2	2.55	0.42
2:2:57:THR:O	2:2:58:LEU:CB	2.66	0.41
2:2:153:GLN:HE22	3:3:55:SER:CB	2.33	0.41
2:2:211:VAL:HG12	2:2:212:THR:H	1.85	0.41
1:1:219:TYR:HA	3:3:39:ARG:HA	2.02	0.41
2:2:166:ARG:HD3	3:3:110:PHE:O	2.20	0.41
1:1:224:ILE:HD11	3:3:89:TYR:CE2	2.55	0.41
3:3:79:SER:O	3:3:81:SER:N	2.51	0.41
2:2:33:THR:HG21	2:2:160:HIS:O	2.20	0.41
1:1:65:GLN:HG2	1:1:70:ARG:HD2	2.01	0.41
1:1:30:VAL:HG13	1:1:218:MET:CE	2.49	0.41
1:1:239:PHE:CD2	3:3:226:GLN:NE2	2.87	0.41
2:2:111:VAL:HG22	2:2:172:HIS:HD2	1.85	0.41
1:1:115:THR:HG23	1:1:133:LEU:N	2.25	0.41
3:3:54:CYS:SG	3:3:208:VAL:HG21	2.61	0.41
2:2:22:THR:OG1	2:2:61:HIS:HB2	2.20	0.41
4:4:21:ILE:HG22	4:4:21:ILE:O	2.20	0.41
2:2:24:ILE:HD11	2:2:61:HIS:ND1	2.35	0.41
2:2:88:LEU:C	2:2:90:LYS:H	2.23	0.41
3:3:53:PHE:N	3:3:53:PHE:CD2	2.88	0.41
2:2:190:ASN:HA	2:2:191:PRO:HD3	1.87	0.41
2:2:69:TRP:CZ3	2:2:124:LEU:HD21	2.56	0.41
1:1:48:LEU:O	1:1:131:GLN:HG2	2.20	0.41
2:2:139:ALA:C	2:2:141:LYS:N	2.74	0.41
1:1:140:PRO:HB3	3:3:25:LEU:HB3	2.03	0.41
1:1:24:MET:O	1:1:25:HIS:HB2	2.21	0.41
1:1:38:PHE:CD1	1:1:68:TRP:HB2	2.56	0.41
2:2:28:GLY:O	2:2:168:ASN:HB2	2.21	0.41
3:3:152:SER:O	3:3:153:ALA:HB2	2.21	0.41
2:2:178:ILE:HG22	2:2:191:PRO:HB3	2.02	0.41
1:1:160:TYR:OH	1:1:167:VAL:HG23	2.21	0.41
1:1:7:ASP:O	1:1:8:GLY:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:175:GLY:N	1:1:183:THR:O	2.53	0.40
1:1:41:GLU:O	1:1:42:THR:HB	2.19	0.40
1:1:220:CYS:HA	1:1:221:PRO:HD2	1.82	0.40
2:2:153:GLN:HE22	3:3:55:SER:N	2.19	0.40
3:3:31:VAL:CB	4:4:34:ILE:O	2.69	0.40
3:3:47:ALA:HB2	3:3:89:TYR:CD1	2.56	0.40
3:3:120:PHE:HD1	3:3:146:TRP:CZ2	2.38	0.40
2:2:160:HIS:ND1	2:2:160:HIS:N	2.69	0.40
1:1:38:PHE:CE1	1:1:68:TRP:HB2	2.56	0.40
2:2:152:TYR:HB3	2:2:197:LEU:CD2	2.51	0.40
2:2:20:GLY:CA	2:2:56:PRO:O	2.67	0.40
2:2:166:ARG:HG3	2:2:166:ARG:O	2.22	0.40
1:1:55:HIS:O	1:1:194:SER:HA	2.21	0.40
4:4:32:ASN:HB3	4:4:33:SER:H	1.58	0.40
1:1:224:ILE:CD1	3:3:89:TYR:CE2	3.04	0.40
3:3:64:VAL:HG13	3:3:120:PHE:HE2	1.86	0.40
2:2:15:GLU:CB	2:2:29:SER:HB2	2.52	0.40
2:2:149:ALA:O	2:2:152:TYR:CD2	2.74	0.40
1:1:184:TYR:HE1	2:2:139:ALA:HB2	1.86	0.40
1:1:168:PRO:HB3	2:2:180:PRO:HB3	2.03	0.40
2:2:103:LEU:HD12	2:2:223:ASN:HB2	2.02	0.40
1:1:87:GLN:HA	1:1:153:ALA:HB2	2.02	0.40
1:1:87:GLN:O	1:1:88:PHE:CB	2.62	0.40
1:1:82:LEU:HG	1:1:83:GLU:H	1.86	0.40
1:1:174:TRP:CD1	1:1:184:TYR:HA	2.56	0.40
2:2:139:ALA:O	2:2:140:LEU:HB2	2.21	0.40
2:2:64:PHE:CD1	2:2:64:PHE:N	2.90	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	1	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
2	2	217/230 (94%)	145 (67%)	49 (23%)	23 (11%)	0	11
3	3	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
4	4	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	2
All	All	705/782 (90%)	455 (64%)	160 (23%)	90 (13%)	0	7

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	10	PRO
1	1	18	ALA
1	1	22	VAL
1	1	26	VAL
1	1	63	THR
1	1	67	ALA
1	1	127	SER
1	1	135	VAL
1	1	162	SER
1	1	179	LYS
1	1	182	ALA
1	1	226	PRO
1	1	243	ILE
2	2	27	GLN
2	2	92	GLY
2	2	136	HIS
2	2	201	GLU
2	2	208	THR
2	2	209	VAL
2	2	224	GLY
3	3	20	ASP
3	3	21	ASN
3	3	27	PRO
3	3	78	VAL
3	3	80	LEU
3	3	120	PHE
3	3	153	ALA
3	3	191	LEU
4	4	17	ASN
1	1	21	PRO
1	1	42	THR
1	1	71	LEU
1	1	88	PHE

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Mol	Chain	Res	Type
1	1	99	GLU
1	1	100	GLY
1	1	114	LYS
1	1	118	ALA
1	1	140	PRO
1	1	150	ARG
1	1	151	SER
1	1	207	CYS
2	2	28	GLY
2	2	43	PRO
2	2	70	PRO
2	2	134	HIS
2	2	135	THR
3	3	14	PHE
3	3	15	MET
3	3	113	ALA
3	3	128	HIS
3	3	129	SER
3	3	150	LEU
3	3	152	SER
4	4	31	GLN
1	1	94	PRO
1	1	152	GLN
1	1	184	TYR
1	1	187	LEU
1	1	213	PHE
1	1	231	PRO
2	2	26	SER
2	2	89	LYS
2	2	102	HIS
2	2	159	PRO
3	3	60	PRO
3	3	174	ALA
3	3	223	PRO
4	4	29	GLN
1	1	9	GLU
1	1	65	GLN
2	2	58	LEU
2	2	86	ASP
2	2	149	ALA
3	3	11	SER
3	3	200	SER

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Mol	Chain	Res	Type
3	3	218	HIS
1	1	8	GLY
1	1	14	GLU
1	1	19	LEU
1	1	112	PRO
2	2	82	PRO
2	2	182	PRO
3	3	61	TYR
3	3	131	ALA
1	1	188	PRO
1	1	221	PRO
2	2	196	ILE
4	4	21	ILE
1	1	30	VAL
2	2	84	PRO

### 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	1	208/208 (100%)	173 (83%)	35 (17%)	2	20
2	2	193/204 (95%)	150 (78%)	43 (22%)	1	10
3	3	190/190 (100%)	146 (77%)	44 (23%)	1	8
4	4	18/65 (28%)	13 (72%)	5 (28%)	0	4
All	All	609/667 (91%)	482 (79%)	127 (21%)	1	11

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	10	PRO
1	1	14	GLU
1	1	19	LEU
1	1	20	SER
1	1	21	PRO
1	1	23	ASP

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Mol	Chain	Res	Type
1	1	28	THR
1	1	36	ARG
1	1	39	ASP
1	1	40	VAL
1	1	43	LEU
1	1	45	LEU
1	1	46	SER
1	1	47	ASN
1	1	59	PRO
1	1	71	LEU
1	1	87	GLN
1	1	90	PHE
1	1	92	THR
1	1	119	TRP
1	1	130	ILE
1	1	132	GLN
1	1	138	MET
1	1	144	PHE
1	1	150	ARG
1	1	163	MET
1	1	177	PRO
1	1	178	THR
1	1	195	ILE
1	1	196	LEU
1	1	202	HIS
1	1	207	CYS
1	1	209	LEU
1	1	226	PRO
1	1	241	THR
2	2	13	ARG
2	2	18	VAL
2	2	22	THR
2	2	29	SER
2	2	45	SER
2	2	53	ARG
2	2	56	PRO
2	2	58	LEU
2	2	71	HIS
2	2	73	GLN
2	2	75	HIS
2	2	84	PRO
2	2	88	LEU

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Mol	Chain	Res	Type
2	2	93	SER
2	2	103	LEU
2	2	104	VAL
2	2	110	VAL
2	2	126	VAL
2	2	134	HIS
2	2	135	THR
2	2	150	TYR
2	2	152	TYR
2	2	159	PRO
2	2	160	HIS
2	2	162	LEU
2	2	166	ARG
2	2	167	THR
2	2	174	VAL
2	2	176	PRO
2	2	178	ILE
2	2	184	THR
2	2	186	LEU
2	2	188	LEU
2	2	193	THR
2	2	194	ILE
2	2	195	VAL
2	2	197	LEU
2	2	200	SER
2	2	202	LEU
2	2	203	THR
2	2	210	PRO
2	2	214	SER
2	2	223	ASN
3	3	15	MET
3	3	16	SER
3	3	18	VAL
3	3	26	TYR
3	3	31	VAL
3	3	35	GLN
3	3	36	VAL
3	3	41	THR
3	3	42	ASN
3	3	46	VAL
3	3	50	THR
3	3	51	TYR

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Mol	Chain	Res	Type
3	3	54	CYS
3	3	56	ILE
3	3	59	LYS
3	3	63	GLU
3	3	65	THR
3	3	67	THR
3	3	76	MET
3	3	84	GLU
3	3	86	HIS
3	3	90	VAL
3	3	93	LEU
3	3	103	SER
3	3	120	PHE
3	3	133	LYS
3	3	134	THR
3	3	139	MET
3	3	142	ILE
3	3	146	TRP
3	3	148	VAL
3	3	150	LEU
3	3	157	ASN
3	3	160	TYR
3	3	162	SER
3	3	165	ASP
3	3	178	ASN
3	3	188	LEU
3	3	189	THR
3	3	195	ASP
3	3	204	VAL
3	3	217	ARG
3	3	222	LEU
3	3	224	ASP
4	4	17	ASN
4	4	30	TYR
4	4	31	GLN
4	4	33	SER
4	4	35	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	27	HIS

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Mol	Chain	Res	Type
1	1	47	ASN
1	1	73	ASN
1	1	87	GLN
1	1	132	GLN
1	1	191	HIS
1	1	202	HIS
2	2	71	HIS
2	2	73	GLN
2	2	95	HIS
2	2	101	HIS
2	2	134	HIS
2	2	136	HIS
2	2	153	GLN
2	2	223	ASN
3	3	42	ASN
3	3	49	GLN
3	3	178	ASN
3	3	226	GLN
4	4	17	ASN
4	4	23	GLN
4	4	24	ASN
4	4	31	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1	246/246 (100%)	-0.66	0 100 100	2, 4, 42, 72	0
2	2	219/230 (95%)	-0.65	0 100 100	2, 4, 47, 93	0
3	3	226/226 (100%)	-0.76	0 100 100	2, 3, 23, 56	0
4	4	22/80 (27%)	-0.49	0 100 100	13, 36, 45, 55	0
All	All	713/782 (91%)	-0.68	0 100 100	2, 4, 41, 93	0

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.