



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 07:57 PM EDT

PDB ID : 2A6J  
Title : Crystal structure analysis of the anti-arsonate germline antibody 36-65  
Authors : Sethi, D.K.; Agarwal, A.; Manivel, V.; Rao, K.V.; Salunke, D.M.  
Deposited on : 2005-07-02  
Resolution : 2.70 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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030736

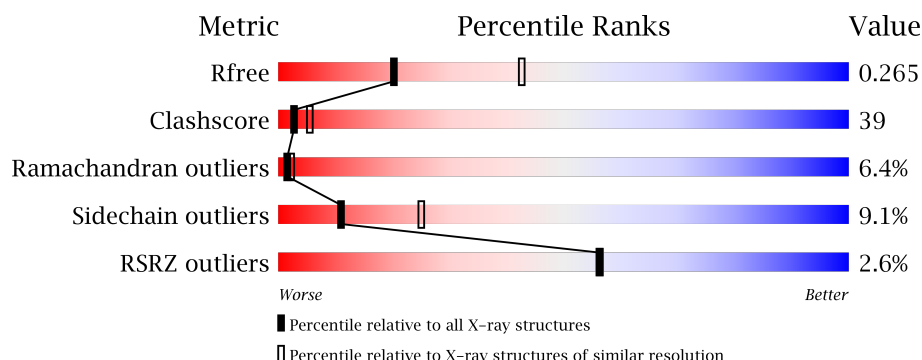
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	A	214	<div> <div>43%</div> <div>49%</div> <div>7%</div> </div>
1	L	214	<div>2%</div> <div>46%</div> <div>45%</div> <div>7%</div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6781 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 Germline antibody 36-65 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1649	1017	280	345	7			
1	A	214	Total	C	N	O	S	0	0	0
			1644	1017	283	337	7			

- Molecule 2 is a protein called Germline antibody 36-65 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	5	0	0
			1681	1064	276	334	7			
2	B	222	Total	C	N	O	S	8	0	0
			1670	1058	274	331	7			

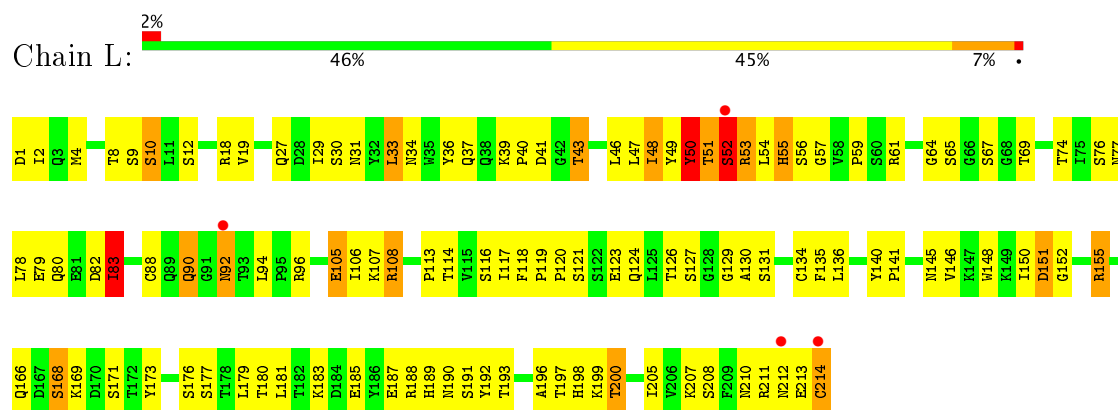
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	36	Total	O	0	0
			36	36		
3	H	39	Total	O	0	0
			39	39		
3	A	30	Total	O	0	0
			30	30		
3	B	32	Total	O	0	0
			32	32		

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

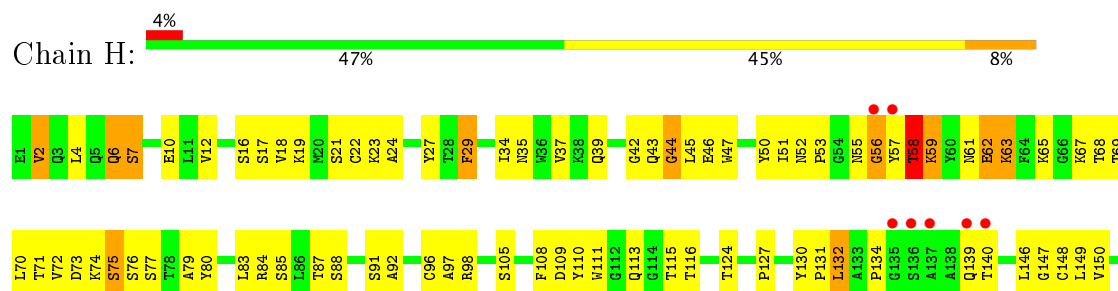
- Molecule 1: Germline antibody 36-65 Fab light chain



- Molecule 1: Germline antibody 36-65 Fab light chain

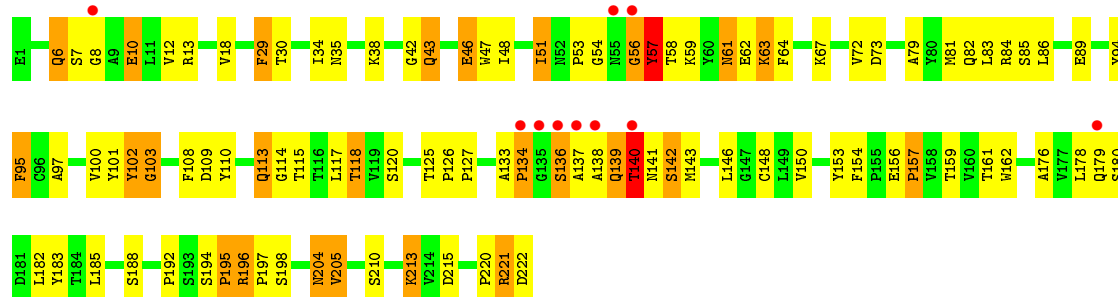


- Molecule 2: Germline antibody 36-65 Fab heavy chain





• Molecule 2: Germline antibody 36-65 Fab heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.14Å 73.95Å 85.92Å 90.00° 113.92° 90.00°	Depositor
Resolution (Å)	100.00 – 2.70 53.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (100.00-2.70) 79.2 (53.84-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.53 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.225 , 0.265 0.222 , 0.265	Depositor DCC
$R_{free}$ test set	1881 reflections (9.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6781	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.59	0/1677	0.83	1/2276 (0.0%)
1	L	0.62	0/1682	0.84	0/2283
2	B	0.62	0/1714	0.85	1/2339 (0.0%)
2	H	0.65	0/1725	0.87	2/2352 (0.1%)
All	All	0.62	0/6798	0.85	4/9250 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	58	THR	N-CA-C	5.70	126.39	111.00
2	H	6	GLN	N-CA-C	5.69	126.36	111.00
1	A	107	LYS	N-CA-C	5.24	125.16	111.00
2	B	140	THR	N-CA-C	-5.07	97.32	111.00

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	1644	0	1558	128	0
1	L	1649	0	1556	138	0
2	B	1670	0	1618	126	0
2	H	1681	0	1637	141	0
3	A	30	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	32	0	0	4	0
3	H	39	0	0	9	0
3	L	36	0	0	6	0
All	All	6781	0	6369	506	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 39.

All (506) 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:L:94:LEU:HD13	2:H:59:LYS:CE	1.23	1.65
1:L:94:LEU:CD1	2:H:59:LYS:HE3	1.29	1.62
2:B:82:GLN:HE21	2:B:84:ARG:NH1	1.38	1.22
2:H:51:ILE:HG13	2:H:57:TYR:HB2	1.19	1.09
1:L:46:LEU:HD12	1:L:56:SER:HB2	1.33	1.09
1:L:94:LEU:HD13	2:H:59:LYS:NZ	1.68	1.08
1:L:124:GLN:HE22	1:L:131:SER:HB2	1.18	1.03
1:L:94:LEU:HB3	2:H:59:LYS:NZ	1.76	1.00
2:B:142:SER:HB2	3:B:229:HOH:O	1.59	1.00
2:B:82:GLN:NE2	2:B:84:ARG:HH11	1.61	0.98
2:B:221:ARG:HG3	2:B:222:ASP:H	1.26	0.98
2:H:161:THR:HG22	2:H:204:ASN:HB2	1.44	0.95
1:L:52:SER:HB2	1:L:64:GLY:HA3	1.48	0.95
2:B:6:GLN:H	2:B:113:GLN:HE22	1.07	0.95
2:B:82:GLN:NE2	2:B:84:ARG:NH1	2.14	0.93
2:B:192:PRO:O	2:B:195:PRO:HD2	1.68	0.93
1:A:52:SER:HB3	1:A:64:GLY:HA3	1.53	0.90
1:A:117:ILE:HD12	1:A:117:ILE:H	1.34	0.88
1:L:94:LEU:CD1	2:H:59:LYS:CE	2.11	0.87
2:B:82:GLN:HE21	2:B:84:ARG:HH11	0.88	0.87
1:A:2:ILE:HD11	1:A:27:GLN:HE21	1.41	0.85
2:H:159:THR:HG22	2:H:206:ALA:HB3	1.57	0.85
2:B:48:ILE:HD13	2:B:81:MET:CE	2.06	0.84
2:H:51:ILE:CG1	2:H:57:TYR:HB2	2.07	0.83
1:L:48:ILE:HG21	1:L:52:SER:HA	1.59	0.83
2:B:195:PRO:O	2:B:198:SER:HB3	1.79	0.82
1:L:46:LEU:CD1	1:L:56:SER:HB2	2.10	0.81
1:L:94:LEU:HD11	2:H:59:LYS:HE3	1.59	0.81
2:B:51:ILE:HG12	2:B:58:THR:HG22	1.63	0.81
1:L:18:ARG:HG3	1:L:76:SER:HA	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:94:LEU:HB3	2:H:59:LYS:HZ2	1.47	0.79
1:L:94:LEU:HB3	2:H:59:LYS:HZ1	1.43	0.78
1:A:52:SER:HB3	1:A:64:GLY:CA	2.12	0.78
1:L:48:ILE:CG2	1:L:52:SER:HA	2.14	0.78
2:H:51:ILE:HG13	2:H:57:TYR:CB	2.09	0.77
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.66	0.77
1:L:114:THR:HG23	2:H:140:THR:OG1	1.85	0.77
1:A:199:LYS:H	1:A:199:LYS:HE2	1.50	0.77
2:B:35:ASN:HD22	2:B:47:TRP:HE1	1.33	0.77
2:B:83:LEU:HB2	2:B:86:LEU:HD21	1.67	0.77
2:B:48:ILE:HD13	2:B:81:MET:HE1	1.67	0.76
1:A:106:ILE:HG22	1:A:107:LYS:HD2	1.64	0.76
1:A:163:TRP:HE1	1:A:175:MET:HE3	1.49	0.76
1:A:183:LYS:O	1:A:187:GLU:HG3	1.86	0.76
2:B:6:GLN:H	2:B:113:GLN:NE2	1.83	0.76
2:B:102:TYR:O	2:B:103:GLY:O	2.04	0.75
1:L:50:TYR:O	1:L:51:THR:O	2.04	0.75
1:L:55:HIS:ND1	1:L:55:HIS:N	2.35	0.75
1:L:124:GLN:HE22	1:L:131:SER:CB	1.99	0.75
2:H:134:PRO:HD3	2:H:146:LEU:CD2	2.16	0.75
2:B:56:GLY:O	2:B:57:TYR:HB3	1.84	0.75
1:L:52:SER:HB2	1:L:64:GLY:CA	2.17	0.74
1:L:50:TYR:HB3	1:L:54:LEU:HD12	1.67	0.74
1:A:33:LEU:HD12	1:A:35:TRP:CZ3	2.23	0.74
2:B:125:THR:HG21	2:B:182:LEU:HD22	1.68	0.74
1:A:55:HIS:NE2	1:A:60:SER:HA	2.03	0.74
1:L:94:LEU:CB	2:H:59:LYS:NZ	2.50	0.74
1:L:94:LEU:CB	2:H:59:LYS:HZ1	2.00	0.73
2:B:221:ARG:HH12	2:B:222:ASP:HB2	1.53	0.73
2:H:6:GLN:O	2:H:7:SER:CB	2.36	0.73
2:B:38:LYS:HZ3	2:B:64:PHE:HE1	1.35	0.72
2:B:134:PRO:HD3	2:B:146:LEU:HD23	1.71	0.72
1:L:31:ASN:HB3	1:L:51:THR:HB	1.71	0.72
2:H:139:GLN:CB	3:H:225:HOH:O	2.38	0.71
2:H:51:ILE:O	2:H:53:PRO:HD3	1.89	0.71
1:A:136:LEU:HD21	1:A:196:ALA:HB2	1.73	0.70
2:B:142:SER:CB	3:B:229:HOH:O	2.28	0.70
1:A:31:ASN:CA	1:A:51:THR:HB	2.22	0.70
2:H:7:SER:O	2:H:115:THR:HG22	1.91	0.70
2:B:48:ILE:HD13	2:B:81:MET:HE3	1.73	0.70
2:B:48:ILE:CD1	2:B:81:MET:HE3	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:GLY:HA2	3:B:233:HOH:O	1.92	0.69
2:H:52:ASN:OD1	2:H:55:ASN:HB2	1.91	0.69
2:H:194:SER:HB2	2:H:195:PRO:HD3	1.75	0.69
1:A:149:LYS:HA	1:A:153:SER:O	1.93	0.69
1:L:207:LYS:HD2	2:H:139:GLN:CB	2.22	0.69
2:H:6:GLN:HB3	2:H:115:THR:HG23	1.75	0.69
1:A:185:GLU:HA	1:A:188:ARG:HE	1.58	0.69
1:L:124:GLN:NE2	1:L:131:SER:HB2	2.02	0.68
1:L:90:GLN:NE2	1:L:92:ASN:HB3	2.08	0.68
2:B:192:PRO:C	2:B:195:PRO:HD2	2.14	0.68
1:A:106:ILE:HG22	1:A:107:LYS:CD	2.24	0.68
2:H:35:ASN:ND2	2:H:50:TYR:HB2	2.08	0.68
1:L:46:LEU:HD13	1:L:46:LEU:C	2.14	0.68
1:A:79:GLU:HB2	1:A:82:ASP:OD2	1.94	0.68
1:A:199:LYS:H	1:A:199:LYS:CE	2.06	0.68
1:L:51:THR:O	1:L:53:ARG:N	2.26	0.68
1:A:189:HIS:O	1:A:211:ARG:HD3	1.94	0.68
2:H:7:SER:O	2:H:115:THR:CG2	2.41	0.68
2:H:12:VAL:HG21	2:H:18:VAL:CG2	2.23	0.68
2:B:38:LYS:HB3	2:B:46:GLU:HB3	1.76	0.68
2:H:207:HIS:CE1	2:H:210:SER:HG	2.12	0.68
2:H:62:GLU:O	2:H:63:LYS:HB2	1.93	0.67
1:L:39:LYS:HB2	1:L:43:THR:HG23	1.76	0.67
2:B:72:VAL:HG23	2:B:79:ALA:HA	1.75	0.67
1:L:108:ARG:HD3	1:L:171:SER:O	1.95	0.67
1:L:94:LEU:CD1	2:H:59:LYS:NZ	2.46	0.67
1:L:198:HIS:ND1	1:L:200:THR:HG21	2.10	0.67
1:L:4:MET:CE	1:L:33:LEU:HD21	2.24	0.67
2:B:161:THR:HG22	2:B:204:ASN:HB2	1.76	0.66
2:B:29:PHE:CE2	2:B:72:VAL:HG21	2.29	0.66
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.77	0.66
2:H:130:TYR:HD2	2:H:149:LEU:HD23	1.61	0.66
1:L:145:ASN:HB3	1:L:197:THR:CG2	2.25	0.66
2:B:221:ARG:HG3	2:B:222:ASP:N	2.08	0.65
2:B:38:LYS:HD2	2:B:64:PHE:CZ	2.32	0.65
2:B:221:ARG:NH1	2:B:222:ASP:HB2	2.12	0.65
1:L:145:ASN:HB3	1:L:197:THR:HG22	1.77	0.65
1:A:2:ILE:CD1	1:A:27:GLN:HE21	2.09	0.65
1:A:163:TRP:NE1	1:A:175:MET:HE3	2.12	0.65
1:L:116:SER:O	1:L:134:CYS:HA	1.98	0.65
2:B:178:LEU:HD21	2:B:183:TYR:CZ	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:GLN:HG2	1:L:129:GLY:O	1.98	0.64
2:B:196:ARG:HG2	2:B:197:PRO:HA	1.79	0.64
2:H:69:THR:OG1	2:H:84:ARG:NH1	2.31	0.64
1:L:46:LEU:HD12	1:L:56:SER:CB	2.21	0.64
2:B:29:PHE:HE2	2:B:72:VAL:HG21	1.62	0.64
1:L:61:ARG:CZ	1:L:79:GLU:HG3	2.28	0.64
2:B:62:GLU:O	2:B:63:LYS:CB	2.46	0.64
1:L:1:ASP:HB2	3:L:233:HOH:O	1.97	0.64
1:A:108:ARG:HD2	1:A:172:THR:HG22	1.80	0.63
1:A:29:ILE:HD11	1:A:90:GLN:HE21	1.62	0.63
1:L:198:HIS:ND1	1:L:200:THR:CG2	2.61	0.63
1:A:31:ASN:C	1:A:51:THR:HB	2.19	0.63
1:L:31:ASN:O	1:L:51:THR:HB	1.98	0.63
2:B:148:CYS:HB2	2:B:162:TRP:CH2	2.34	0.63
1:L:207:LYS:HZ2	2:H:139:GLN:HA	1.64	0.62
1:A:52:SER:HB3	1:A:64:GLY:C	2.18	0.62
2:H:18:VAL:HG12	2:H:19:LYS:N	2.14	0.62
2:B:125:THR:HG21	2:B:182:LEU:CD2	2.29	0.62
2:B:57:TYR:C	2:B:57:TYR:CD2	2.73	0.62
1:A:167:ASP:HB3	1:A:170:ASP:O	1.99	0.62
2:B:192:PRO:HB2	2:B:195:PRO:HD3	1.81	0.62
2:H:68:THR:HG22	2:H:69:THR:N	2.15	0.62
1:A:31:ASN:HA	1:A:51:THR:HB	1.80	0.61
2:H:55:ASN:C	2:H:57:TYR:H	2.03	0.61
1:A:66:GLY:O	1:A:67:SER:HB3	2.01	0.61
2:B:94:TYR:O	2:B:114:GLY:HA2	2.01	0.61
1:L:19:VAL:HG21	1:L:78:LEU:HD22	1.82	0.61
2:H:12:VAL:HG21	2:H:18:VAL:HG21	1.81	0.61
2:H:204:ASN:ND2	2:H:215:ASP:OD1	2.30	0.61
1:L:155:ARG:HD2	1:L:179:LEU:HD11	1.83	0.61
1:A:198:HIS:ND1	1:A:200:THR:HB	2.16	0.61
2:B:176:ALA:HA	2:B:185:LEU:HB3	1.83	0.61
2:H:37:VAL:HG13	2:H:46:GLU:O	2.00	0.60
1:L:106:ILE:N	1:L:166:GLN:HE22	1.99	0.60
1:L:136:LEU:N	1:L:136:LEU:HD12	2.15	0.60
2:B:46:GLU:HG2	2:B:64:PHE:CE2	2.37	0.60
1:L:210:ASN:O	1:L:213:GLU:HG2	2.01	0.60
1:L:183:LYS:NZ	1:L:187:GLU:OE2	2.33	0.60
2:B:102:TYR:O	2:B:103:GLY:C	2.39	0.60
2:H:42:GLY:O	2:H:44:GLY:N	2.34	0.60
2:H:68:THR:HG22	2:H:69:THR:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TRP:CG	1:A:73:LEU:HD13	2.37	0.60
1:L:4:MET:HE2	1:L:33:LEU:HD21	1.84	0.60
2:B:185:LEU:HD12	2:B:185:LEU:C	2.21	0.60
2:B:125:THR:CG2	2:B:182:LEU:HD22	2.32	0.60
1:L:207:LYS:NZ	2:H:139:GLN:HA	2.16	0.60
2:B:38:LYS:HD2	2:B:64:PHE:HZ	1.65	0.59
1:L:52:SER:O	1:L:64:GLY:C	2.40	0.59
2:B:8:GLY:O	2:B:10:GLU:HG2	2.01	0.59
1:A:31:ASN:HB3	1:A:51:THR:HG21	1.85	0.59
2:B:48:ILE:HG21	2:B:81:MET:CE	2.31	0.59
2:H:35:ASN:HD22	2:H:47:TRP:HE1	1.49	0.59
2:H:132:LEU:HB2	2:H:147:GLY:O	2.03	0.59
1:A:115:VAL:HA	1:A:135:PHE:O	2.03	0.59
1:A:18:ARG:HA	1:A:75:ILE:O	2.03	0.59
2:B:161:THR:CG2	2:B:204:ASN:HB2	2.33	0.58
1:L:29:ILE:O	1:L:29:ILE:HG22	2.02	0.58
1:A:106:ILE:CG2	1:A:107:LYS:HD2	2.33	0.58
1:L:108:ARG:HG2	1:L:140:TYR:CD2	2.38	0.58
2:H:200:THR:HG22	2:H:201:VAL:N	2.18	0.58
1:A:52:SER:O	1:A:53:ARG:HB3	2.04	0.58
1:L:61:ARG:HD2	3:L:223:HOH:O	2.02	0.58
1:A:46:LEU:HD22	1:A:47:LEU:N	2.19	0.57
2:H:98:ARG:NH2	2:H:109:ASP:OD2	2.31	0.57
1:L:140:TYR:CD1	1:L:141:PRO:HA	2.39	0.57
2:B:221:ARG:HG3	2:B:221:ARG:HH11	1.68	0.57
2:H:132:LEU:HB2	2:H:147:GLY:C	2.24	0.57
1:A:14:SER:OG	1:A:107:LYS:HB3	2.05	0.57
2:H:179:GLN:HG2	2:H:180:SER:H	1.70	0.57
1:L:113:PRO:HG2	1:L:205:ILE:HD12	1.86	0.57
1:L:33:LEU:HD11	1:L:88:CYS:HB2	1.86	0.57
1:L:90:GLN:HE21	1:L:92:ASN:H	1.52	0.57
2:H:192:PRO:O	2:H:195:PRO:HD2	2.05	0.57
1:L:94:LEU:HD13	2:H:59:LYS:HE3	0.71	0.57
2:B:101:TYR:O	2:B:102:TYR:O	2.22	0.56
1:L:155:ARG:NH1	1:L:181:LEU:CD2	2.68	0.56
2:B:100:VAL:HG12	2:B:101:TYR:N	2.19	0.56
2:B:161:THR:HG23	2:B:204:ASN:OD1	2.05	0.56
1:L:119:PRO:HD2	3:H:224:HOH:O	2.05	0.56
2:B:12:VAL:HG21	2:B:86:LEU:CD1	2.35	0.56
1:L:90:GLN:NE2	1:L:92:ASN:H	2.04	0.56
2:B:180:SER:C	2:B:182:LEU:H	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ASP:OD1	1:A:172:THR:HG23	2.05	0.56
2:B:57:TYR:CD2	2:B:58:THR:N	2.73	0.56
1:L:77:ASN:N	3:L:223:HOH:O	2.38	0.56
1:L:126:THR:HB	3:L:243:HOH:O	2.05	0.55
1:L:150:ILE:O	1:L:151:ASP:C	2.44	0.55
2:B:95:PHE:CD1	2:B:95:PHE:N	2.73	0.55
2:B:221:ARG:NH1	2:B:221:ARG:HG3	2.21	0.55
2:H:6:GLN:O	2:H:7:SER:HB3	2.06	0.55
2:B:6:GLN:N	2:B:113:GLN:HE22	1.90	0.55
1:A:47:LEU:HD23	1:A:58:VAL:HG11	1.87	0.55
2:B:159:THR:O	2:B:205:VAL:HA	2.07	0.55
1:A:117:ILE:CD1	1:A:117:ILE:H	2.06	0.55
1:A:124:GLN:HG2	1:A:129:GLY:O	2.07	0.55
2:B:42:GLY:O	2:B:43:GLN:O	2.25	0.54
1:L:30:SER:O	1:L:31:ASN:HB2	2.08	0.54
1:L:52:SER:HB2	1:L:64:GLY:C	2.28	0.54
1:A:89:GLN:HG2	1:A:90:GLN:N	2.21	0.54
1:A:19:VAL:CG2	1:A:78:LEU:HD22	2.38	0.54
1:L:198:HIS:O	1:L:200:THR:N	2.40	0.54
1:L:47:LEU:O	1:L:48:ILE:HD12	2.08	0.54
2:H:35:ASN:ND2	2:H:47:TRP:HE1	2.05	0.54
1:L:148:TRP:HE1	1:L:177:SER:HG	1.54	0.54
1:A:108:ARG:NE	1:A:109:ALA:O	2.35	0.54
1:L:4:MET:HE1	1:L:33:LEU:HD21	1.88	0.54
2:B:18:VAL:O	2:B:82:GLN:HA	2.08	0.54
2:H:58:THR:O	2:H:59:LYS:HB2	2.07	0.54
1:L:150:ILE:C	1:L:152:GLY:N	2.59	0.54
1:L:9:SER:O	1:L:10:SER:HB3	2.08	0.54
2:B:156:GLU:HB3	2:B:157:PRO:HA	1.90	0.54
2:B:48:ILE:CD1	2:B:81:MET:CE	2.81	0.54
2:B:192:PRO:HD2	2:B:195:PRO:HG2	1.90	0.54
1:L:90:GLN:NE2	1:L:92:ASN:N	2.56	0.54
1:A:210:ASN:O	1:A:212:ASN:N	2.41	0.53
2:B:213:LYS:NZ	2:B:215:ASP:OD2	2.41	0.53
1:A:111:ALA:O	1:A:112:ALA:HB3	2.09	0.53
1:A:112:ALA:HA	1:A:200:THR:HG21	1.90	0.53
1:A:89:GLN:HB2	1:A:98:PHE:CD1	2.43	0.53
1:L:150:ILE:HD11	1:L:155:ARG:HG2	1.89	0.53
1:L:189:HIS:O	1:L:211:ARG:HD3	2.08	0.53
1:A:18:ARG:O	1:A:18:ARG:HG2	2.08	0.53
2:H:58:THR:CG2	2:H:59:LYS:N	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:SER:O	2:B:86:LEU:C	2.45	0.53
2:H:202:THR:HG23	2:H:216:LYS:C	2.29	0.53
2:H:37:VAL:HG11	2:H:45:LEU:HG	1.91	0.53
1:L:79:GLU:N	1:L:82:ASP:OD2	2.35	0.53
1:A:19:VAL:HG21	1:A:78:LEU:HD22	1.89	0.53
2:B:56:GLY:O	2:B:57:TYR:CB	2.55	0.53
2:H:134:PRO:HD3	2:H:146:LEU:HD22	1.88	0.53
2:B:47:TRP:CE3	2:B:61:ASN:HB2	2.44	0.53
1:L:105:GLU:O	1:L:105:GLU:HG3	2.08	0.53
1:A:25:ALA:O	1:A:27:GLN:N	2.42	0.53
2:H:37:VAL:HA	2:H:46:GLU:O	2.09	0.53
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.91	0.53
1:L:124:GLN:O	1:L:127:SER:HB2	2.08	0.53
1:L:50:TYR:CB	1:L:54:LEU:HD12	2.38	0.53
1:L:207:LYS:NZ	2:H:139:GLN:O	2.35	0.52
2:H:18:VAL:CG1	2:H:19:LYS:N	2.72	0.52
2:H:65:LYS:HD3	3:H:226:HOH:O	2.10	0.52
2:H:22:CYS:HB3	2:H:79:ALA:HB3	1.89	0.52
1:L:150:ILE:O	1:L:152:GLY:N	2.43	0.52
2:H:192:PRO:HD2	2:H:195:PRO:HG2	1.92	0.52
2:H:200:THR:CG2	2:H:201:VAL:N	2.72	0.52
2:B:72:VAL:HG23	2:B:79:ALA:CA	2.40	0.52
2:H:29:PHE:HZ	2:H:72:VAL:CG2	2.23	0.52
1:A:36:TYR:CE2	1:A:46:LEU:HD23	2.45	0.52
2:B:142:SER:OG	2:B:143:MET:N	2.43	0.52
1:L:12:SER:HB3	1:L:107:LYS:CG	2.39	0.52
1:A:180:THR:O	1:A:180:THR:HG23	2.09	0.52
1:A:33:LEU:HD13	1:A:34:ASN:N	2.25	0.52
2:H:24:ALA:HB1	2:H:27:TYR:CE2	2.45	0.51
2:H:6:GLN:H	2:H:113:GLN:HE22	1.57	0.51
1:L:106:ILE:H	1:L:166:GLN:HE22	1.59	0.51
1:L:53:ARG:HD2	1:L:54:LEU:HG	1.92	0.51
1:A:112:ALA:HB2	1:A:200:THR:OG1	2.10	0.51
1:A:49:TYR:O	1:A:54:LEU:HB2	2.10	0.51
2:B:54:GLY:C	2:B:56:GLY:H	2.14	0.51
1:A:161:ASN:ND2	1:A:177:SER:HB2	2.25	0.51
2:H:29:PHE:CZ	2:H:72:VAL:CG2	2.93	0.51
2:B:18:VAL:HG13	2:B:86:LEU:HD11	1.92	0.51
2:B:29:PHE:CE2	2:B:72:VAL:CG2	2.93	0.51
2:H:192:PRO:HB2	2:H:195:PRO:HD2	1.91	0.51
1:A:52:SER:CB	1:A:64:GLY:C	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:PRO:HB2	2:B:150:VAL:HG12	1.92	0.51
2:H:39:GLN:HA	3:H:254:HOH:O	2.11	0.51
2:H:62:GLU:O	2:H:63:LYS:CB	2.59	0.51
1:L:52:SER:O	1:L:64:GLY:O	2.29	0.51
1:A:48:ILE:CG2	1:A:52:SER:HA	2.42	0.50
2:H:74:LYS:C	2:H:76:SER:H	2.15	0.50
1:L:168:SER:HA	3:L:230:HOH:O	2.09	0.50
2:H:29:PHE:CD2	2:H:77:SER:HA	2.45	0.50
1:L:120:PRO:HG2	1:L:130:ALA:HB1	1.93	0.50
1:L:51:THR:O	1:L:52:SER:C	2.50	0.50
2:B:133:ALA:HB1	2:B:134:PRO:HD2	1.92	0.50
2:H:172:HIS:HA	3:H:240:HOH:O	2.11	0.50
1:L:59:PRO:HB2	1:L:61:ARG:HG2	1.94	0.50
1:A:163:TRP:NE1	1:A:175:MET:CE	2.74	0.50
1:A:135:PHE:CE2	2:B:188:SER:HB3	2.46	0.50
2:B:29:PHE:HE2	2:B:72:VAL:CG2	2.25	0.50
1:L:121:SER:CB	2:H:131:PRO:HD2	2.42	0.50
1:L:37:GLN:HB2	1:L:47:LEU:HD22	1.94	0.50
1:A:106:ILE:HG22	1:A:107:LYS:N	2.27	0.50
2:B:192:PRO:HB2	2:B:195:PRO:CD	2.40	0.50
2:H:153:TYR:CE2	2:H:158:VAL:HG23	2.46	0.50
1:A:146:VAL:HG11	1:A:161:ASN:HD21	1.77	0.49
2:B:38:LYS:NZ	2:B:64:PHE:HE1	2.06	0.49
2:H:6:GLN:H	2:H:113:GLN:NE2	2.09	0.49
1:A:117:ILE:HG13	1:A:207:LYS:HB3	1.94	0.49
2:H:19:LYS:O	2:H:19:LYS:HE2	2.12	0.49
1:A:209:PHE:HB2	2:B:136:SER:OG	2.12	0.49
1:L:51:THR:O	1:L:51:THR:HG23	2.12	0.49
1:A:108:ARG:HB3	1:A:140:TYR:CD2	2.48	0.49
1:A:35:TRP:CH2	1:A:71:TYR:HB3	2.48	0.49
2:H:192:PRO:HB2	2:H:195:PRO:CD	2.43	0.49
2:H:52:ASN:OD1	2:H:55:ASN:OD1	2.30	0.49
1:A:199:LYS:N	1:A:199:LYS:HZ3	2.11	0.49
2:H:4:LEU:HA	2:H:23:LYS:O	2.12	0.49
1:L:192:TYR:O	1:L:208:SER:HB2	2.12	0.49
1:A:46:LEU:HD22	1:A:47:LEU:H	1.77	0.49
2:B:57:TYR:CG	2:B:58:THR:N	2.80	0.49
2:H:171:VAL:HG13	2:H:171:VAL:O	2.13	0.49
2:B:34:ILE:CG2	2:B:35:ASN:N	2.75	0.49
1:A:31:ASN:ND2	1:A:51:THR:HG21	2.28	0.48
1:A:55:HIS:CE1	1:A:58:VAL:HG23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:67:LYS:NZ	2:H:85:SER:O	2.46	0.48
1:A:209:PHE:C	1:A:209:PHE:CD1	2.87	0.48
2:H:6:GLN:CB	2:H:115:THR:HG23	2.41	0.48
1:A:155:ARG:HD3	3:A:227:HOH:O	2.13	0.48
1:L:49:TYR:CE2	1:L:54:LEU:HD13	2.48	0.48
1:L:27:GLN:O	1:L:69:THR:HG22	2.14	0.48
1:L:51:THR:O	1:L:51:THR:CG2	2.62	0.48
2:H:153:TYR:CZ	2:H:158:VAL:HG21	2.48	0.48
1:A:90:GLN:HE22	1:A:93:THR:H	1.61	0.47
1:A:214:CYS:OXT	2:B:221:ARG:NH2	2.47	0.47
2:B:67:LYS:HB2	3:B:242:HOH:O	2.14	0.47
1:A:148:TRP:O	1:A:154:GLU:O	2.32	0.47
2:B:134:PRO:HD3	2:B:146:LEU:CD2	2.42	0.47
2:H:185:LEU:C	2:H:185:LEU:HD12	2.34	0.47
2:H:61:ASN:O	2:H:63:LYS:N	2.47	0.47
1:L:53:ARG:HH11	1:L:54:LEU:CG	2.28	0.47
1:A:61:ARG:CZ	1:A:79:GLU:HG3	2.45	0.47
1:A:164:THR:HG21	1:A:174:SER:HB2	1.97	0.47
1:L:119:PRO:HB2	2:H:222:ASP:OD2	2.15	0.47
1:L:94:LEU:HD12	2:H:59:LYS:HE3	1.68	0.47
2:H:6:GLN:OE1	2:H:96:CYS:N	2.47	0.47
1:L:185:GLU:HG2	1:L:188:ARG:NH2	2.29	0.47
2:H:17:SER:HB2	2:H:83:LEU:O	2.14	0.47
2:B:83:LEU:CB	2:B:86:LEU:HD21	2.40	0.47
2:H:196:ARG:HB3	2:H:196:ARG:HE	1.36	0.47
1:L:52:SER:HB2	1:L:65:SER:N	2.29	0.47
2:H:221:ARG:HD3	3:H:257:HOH:O	2.13	0.47
2:B:61:ASN:HD22	2:B:62:GLU:N	2.13	0.47
1:L:214:CYS:O	2:H:221:ARG:NH2	2.48	0.47
2:B:125:THR:HG22	2:B:154:PHE:HB3	1.97	0.46
2:B:127:PRO:HB2	2:B:150:VAL:CG1	2.45	0.46
2:B:72:VAL:HG22	2:B:73:ASP:N	2.29	0.46
2:H:19:LYS:HZ2	2:H:80:TYR:HE2	1.62	0.46
2:H:6:GLN:O	2:H:7:SER:OG	2.32	0.46
2:H:74:LYS:O	2:H:76:SER:N	2.47	0.46
2:H:19:LYS:HD2	2:H:80:TYR:CD2	2.49	0.46
1:A:90:GLN:NE2	1:A:92:ASN:H	2.13	0.46
2:B:178:LEU:HD21	2:B:183:TYR:CE1	2.51	0.46
2:H:97:ALA:HB1	2:H:108:PHE:HB3	1.97	0.46
1:L:12:SER:HB3	1:L:107:LYS:HG3	1.96	0.46
1:A:161:ASN:HD21	1:A:177:SER:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:N	1:A:117:ILE:HD12	2.12	0.46
1:L:135:PHE:CE2	2:H:188:SER:HB3	2.50	0.46
1:L:83:ILE:HG22	1:L:83:ILE:O	2.15	0.46
1:A:25:ALA:O	1:A:69:THR:HG23	2.16	0.46
1:A:167:ASP:O	1:A:170:ASP:O	2.33	0.46
2:B:97:ALA:HA	2:B:110:TYR:O	2.16	0.46
1:L:53:ARG:HH11	1:L:54:LEU:HG	1.80	0.46
2:H:29:PHE:HZ	2:H:72:VAL:HG23	1.81	0.46
1:A:52:SER:O	1:A:53:ARG:CB	2.64	0.45
1:A:119:PRO:HG3	1:A:209:PHE:CD2	2.51	0.45
2:B:194:SER:N	2:B:195:PRO:CD	2.78	0.45
2:B:126:PRO:HG3	2:B:210:SER:HB2	1.98	0.45
2:B:7:SER:HA	2:B:115:THR:OG1	2.15	0.45
2:H:194:SER:CB	2:H:195:PRO:HD3	2.45	0.45
2:H:146:LEU:HD13	2:H:218:ILE:HG21	1.98	0.45
1:A:156:GLN:O	1:A:159:VAL:HG23	2.16	0.45
2:H:56:GLY:C	2:H:57:TYR:CD1	2.90	0.45
2:B:196:ARG:HE	2:B:196:ARG:HB3	1.41	0.45
2:H:159:THR:HG23	2:H:159:THR:O	2.16	0.45
1:L:140:TYR:HA	1:L:141:PRO:O	2.17	0.45
2:B:213:LYS:NZ	2:B:215:ASP:CG	2.70	0.45
1:A:37:GLN:O	1:A:44:VAL:HA	2.17	0.45
2:H:213:LYS:HA	2:H:213:LYS:HD2	1.79	0.45
2:H:6:GLN:O	2:H:21:SER:O	2.35	0.45
1:A:107:LYS:O	1:A:108:ARG:O	2.35	0.45
1:A:179:LEU:CD1	1:A:181:LEU:HG	2.47	0.45
1:A:35:TRP:HH2	1:A:71:TYR:HB3	1.82	0.45
1:A:29:ILE:HG22	1:A:71:TYR:OH	2.17	0.45
2:B:30:THR:HA	2:B:53:PRO:O	2.16	0.45
1:A:179:LEU:HD13	1:A:181:LEU:HG	1.99	0.44
1:L:180:THR:HG21	2:H:179:GLN:HE22	1.82	0.44
1:L:36:TYR:CD2	1:L:46:LEU:HA	2.52	0.44
1:A:142:LYS:HB3	1:A:173:TYR:CZ	2.52	0.44
1:A:46:LEU:CD1	1:A:56:SER:HB2	2.47	0.44
2:H:12:VAL:CG1	2:H:16:SER:OG	2.65	0.44
1:L:46:LEU:CD1	1:L:46:LEU:C	2.85	0.44
2:B:125:THR:O	2:B:153:TYR:HA	2.17	0.44
2:B:180:SER:C	2:B:182:LEU:N	2.71	0.44
2:H:153:TYR:CE2	2:H:158:VAL:CG2	3.00	0.44
1:A:164:THR:CG2	1:A:174:SER:HB2	2.47	0.44
1:A:15:LEU:HD21	1:A:80:GLN:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:ASN:O	2:B:62:GLU:C	2.56	0.44
2:H:34:ILE:HB	2:H:51:ILE:HG23	2.00	0.44
1:L:46:LEU:HD22	1:L:47:LEU:N	2.32	0.44
2:B:117:LEU:HD12	2:B:118:THR:H	1.83	0.44
1:L:198:HIS:HB3	1:L:200:THR:HG22	1.99	0.44
1:A:86:TYR:O	1:A:101:GLY:HA2	2.17	0.44
2:B:34:ILE:HG23	2:B:35:ASN:N	2.32	0.44
2:B:57:TYR:HD2	2:B:57:TYR:C	2.18	0.44
2:H:42:GLY:HA3	3:H:227:HOH:O	2.16	0.44
1:L:19:VAL:O	1:L:74:THR:HA	2.17	0.44
1:A:185:GLU:O	1:A:188:ARG:HB2	2.18	0.44
2:B:213:LYS:NZ	2:B:215:ASP:OD1	2.46	0.44
2:B:220:PRO:O	2:B:221:ARG:HB3	2.18	0.44
2:H:57:TYR:CE2	2:H:70:LEU:O	2.71	0.44
1:L:193:THR:HA	1:L:208:SER:HB3	1.99	0.44
1:L:145:ASN:ND2	1:L:146:VAL:H	2.16	0.43
1:L:29:ILE:O	1:L:29:ILE:CG2	2.65	0.43
1:L:34:ASN:HD22	1:L:49:TYR:HA	1.83	0.43
1:A:116:SER:O	1:A:134:CYS:HA	2.18	0.43
2:H:12:VAL:HG12	2:H:16:SER:OG	2.19	0.43
1:L:12:SER:HB3	1:L:107:LYS:HG2	2.00	0.43
1:L:190:ASN:ND2	1:L:212:ASN:ND2	2.66	0.43
1:A:199:LYS:N	1:A:199:LYS:HE2	2.26	0.43
1:A:186:TYR:O	1:A:192:TYR:OH	2.37	0.43
2:H:37:VAL:HG21	2:H:111:TRP:CH2	2.54	0.43
2:H:12:VAL:HG21	2:H:18:VAL:HG22	1.98	0.43
2:H:154:PHE:HA	2:H:155:PRO:HA	1.83	0.43
1:A:37:GLN:O	1:A:44:VAL:HG13	2.19	0.43
2:B:109:ASP:CG	2:B:110:TYR:HD1	2.22	0.43
2:H:140:THR:N	3:H:225:HOH:O	2.51	0.43
1:A:12:SER:HB3	1:A:105:GLU:OE1	2.18	0.43
2:H:7:SER:O	2:H:115:THR:HG21	2.18	0.43
1:A:25:ALA:C	1:A:27:GLN:H	2.23	0.42
2:B:221:ARG:HH11	2:B:222:ASP:N	2.17	0.42
1:A:33:LEU:HD12	1:A:35:TRP:CE3	2.53	0.42
2:B:221:ARG:HH11	2:B:222:ASP:H	1.67	0.42
2:B:48:ILE:HD12	2:B:81:MET:HE3	2.00	0.42
1:A:142:LYS:HB3	1:A:173:TYR:CE2	2.54	0.42
1:A:31:ASN:HB3	1:A:51:THR:CG2	2.48	0.42
2:B:46:GLU:HG2	2:B:64:PHE:HE2	1.80	0.42
2:H:221:ARG:CG	2:H:222:ASP:H	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:GLN:C	2:H:92:ALA:HB1	2.40	0.42
1:A:107:LYS:O	1:A:108:ARG:C	2.57	0.42
1:A:198:HIS:HB3	1:A:200:THR:HG22	2.01	0.42
2:B:13:ARG:HA	2:B:120:SER:O	2.20	0.42
2:H:159:THR:O	2:H:159:THR:CG2	2.66	0.42
2:B:117:LEU:HD12	2:B:118:THR:N	2.34	0.42
2:B:100:VAL:CG1	2:B:101:TYR:N	2.83	0.42
1:L:176:SER:HB2	2:H:174:PHE:CE2	2.55	0.42
1:L:50:TYR:O	1:L:51:THR:C	2.57	0.42
1:A:29:ILE:HD12	1:A:29:ILE:HA	1.59	0.42
2:H:130:TYR:HA	2:H:131:PRO:HD3	1.82	0.42
2:H:87:THR:O	2:H:88:SER:C	2.57	0.42
1:L:39:LYS:O	1:L:41:ASP:N	2.52	0.42
1:A:190:ASN:ND2	1:A:210:ASN:ND2	2.66	0.41
1:A:31:ASN:CB	1:A:51:THR:HG21	2.48	0.41
2:B:48:ILE:O	2:B:61:ASN:HB2	2.20	0.41
2:H:58:THR:HG23	2:H:59:LYS:N	2.35	0.41
1:A:48:ILE:HG22	1:A:52:SER:HA	2.01	0.41
1:A:31:ASN:O	1:A:51:THR:HB	2.19	0.41
2:B:82:GLN:NE2	2:B:84:ARG:HH12	2.12	0.41
1:L:121:SER:HB2	1:L:123:GLU:OE2	2.21	0.41
1:L:80:GLN:NE2	3:L:238:HOH:O	2.53	0.41
1:A:199:LYS:N	1:A:199:LYS:CE	2.77	0.41
2:H:127:PRO:HB2	2:H:150:VAL:HG13	2.01	0.41
2:H:55:ASN:C	2:H:57:TYR:N	2.71	0.41
2:H:71:THR:OG1	2:H:80:TYR:HB2	2.20	0.41
1:L:166:GLN:HB2	1:L:173:TYR:CZ	2.55	0.41
1:A:159:VAL:HA	1:A:178:THR:O	2.21	0.41
2:B:108:PHE:CD1	2:B:108:PHE:N	2.87	0.41
2:H:221:ARG:HG3	2:H:222:ASP:H	1.85	0.41
2:H:72:VAL:HG22	2:H:73:ASP:H	1.85	0.41
1:L:2:ILE:HG21	1:L:29:ILE:HD11	2.02	0.41
1:A:182:THR:HG23	3:A:229:HOH:O	2.20	0.41
2:B:46:GLU:HG2	2:B:64:PHE:CZ	2.55	0.41
2:H:68:THR:CG2	2:H:69:THR:H	2.33	0.41
1:L:145:ASN:ND2	1:L:146:VAL:N	2.68	0.41
1:A:10:SER:HA	1:A:103:LYS:O	2.21	0.41
1:A:119:PRO:HG3	1:A:209:PHE:CE2	2.56	0.41
1:A:195:GLU:HG2	1:A:206:VAL:HG22	2.02	0.41
1:A:38:GLN:O	1:A:84:ALA:HB1	2.21	0.41
1:A:48:ILE:CD1	1:A:63:SER:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:140:TYR:CD1	1:L:141:PRO:CA	3.03	0.41
1:A:155:ARG:HA	1:A:155:ARG:HD2	1.66	0.41
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.79	0.41
1:L:41:ASP:CG	1:L:43:THR:HG22	2.41	0.41
2:B:195:PRO:HB2	2:B:196:ARG:H	1.75	0.41
2:H:194:SER:HB2	2:H:195:PRO:CD	2.49	0.41
1:L:108:ARG:HD3	1:L:171:SER:C	2.42	0.41
1:A:161:ASN:ND2	1:A:175:MET:HE1	2.35	0.40
2:B:101:TYR:CD2	2:B:102:TYR:N	2.89	0.40
2:H:62:GLU:HG2	3:H:226:HOH:O	2.20	0.40
2:H:84:ARG:O	2:H:85:SER:C	2.59	0.40
2:B:48:ILE:HG21	2:B:81:MET:HE3	2.03	0.40
1:L:150:ILE:HD11	1:L:155:ARG:CG	2.51	0.40
1:L:31:ASN:CB	1:L:51:THR:HB	2.48	0.40
2:H:2:VAL:HG21	2:H:110:TYR:CD1	2.57	0.40
2:H:65:LYS:C	2:H:67:LYS:H	2.25	0.40
2:H:91:SER:O	2:H:92:ALA:HB2	2.21	0.40
1:L:136:LEU:HD21	1:L:196:ALA:HB2	2.03	0.40
1:L:145:ASN:HD22	1:L:146:VAL:H	1.70	0.40
1:A:108:ARG:HD3	1:A:140:TYR:HB2	2.04	0.40
1:A:163:TRP:HE1	1:A:175:MET:CE	2.26	0.40
1:A:35:TRP:CZ3	1:A:52:SER:OG	2.72	0.40
2:B:6:GLN:O	2:B:7:SER:HB2	2.22	0.40
2:H:181:ASP:O	2:H:182:LEU:HD23	2.21	0.40
1:A:58:VAL:HB	1:A:59:PRO:CD	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	212/214 (99%)	184 (87%)	18 (8%)	10 (5%)	<b>3</b> <b>5</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	212/214 (99%)	179 (84%)	20 (9%)	13 (6%)	2	2
2	B	220/222 (99%)	174 (79%)	27 (12%)	19 (9%)	1	1
2	H	220/222 (99%)	184 (84%)	23 (10%)	13 (6%)	2	3
All	All	864/872 (99%)	721 (83%)	88 (10%)	55 (6%)	1	2

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	51	THR
1	L	52	SER
2	H	43	GLN
2	H	58	THR
2	H	59	LYS
2	H	63	LYS
1	A	26	SER
1	A	107	LYS
1	A	108	ARG
1	A	154	GLU
1	A	211	ARG
2	B	43	GLN
2	B	56	GLY
2	B	57	TYR
2	B	102	TYR
2	B	103	GLY
2	B	139	GLN
2	B	140	THR
2	B	142	SER
2	B	195	PRO
1	L	169	LYS
2	H	7	SER
2	H	44	GLY
2	H	62	GLU
2	H	75	SER
1	A	17	ASP
1	A	67	SER
2	B	59	LYS
2	B	63	LYS
2	B	136	SER
2	B	138	ALA
2	B	141	ASN
1	L	57	GLY

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Mol	Chain	Res	Type
1	L	92	ASN
1	L	199	LYS
1	L	200	THR
2	H	179	GLN
2	H	180	SER
2	H	220	PRO
2	B	137	ALA
2	B	179	GLN
1	L	10	SER
1	L	50	TYR
2	H	29	PHE
1	A	112	ALA
2	B	134	PRO
1	L	67	SER
1	L	151	ASP
1	A	50	TYR
2	B	29	PHE
2	B	221	ARG
1	L	40	PRO
1	A	8	THR
1	L	83	ILE
2	H	56	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/192 (96%)	167 (90%)	18 (10%)	9	22
1	L	188/192 (98%)	170 (90%)	18 (10%)	10	22
2	B	186/190 (98%)	169 (91%)	17 (9%)	11	25
2	H	189/190 (100%)	174 (92%)	15 (8%)	14	33
All	All	748/764 (98%)	680 (91%)	68 (9%)	11	25

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	8	THR
1	L	33	LEU
1	L	43	THR
1	L	48	ILE
1	L	50	TYR
1	L	52	SER
1	L	53	ARG
1	L	55	HIS
1	L	83	ILE
1	L	90	GLN
1	L	96	ARG
1	L	105	GLU
1	L	108	ARG
1	L	117	ILE
1	L	155	ARG
1	L	168	SER
1	L	191	SER
1	L	214	CYS
2	H	2	VAL
2	H	10	GLU
2	H	75	SER
2	H	105	SER
2	H	116	THR
2	H	124	THR
2	H	132	LEU
2	H	148	CYS
2	H	157	PRO
2	H	161	THR
2	H	194	SER
2	H	195	PRO
2	H	196	ARG
2	H	203	CYS
2	H	222	ASP
1	A	1	ASP
1	A	10	SER
1	A	12	SER
1	A	17	ASP
1	A	29	ILE
1	A	46	LEU
1	A	52	SER
1	A	55	HIS
1	A	83	ILE
1	A	90	GLN

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Mol	Chain	Res	Type
1	A	107	LYS
1	A	108	ARG
1	A	117	ILE
1	A	151	ASP
1	A	164	THR
1	A	171	SER
1	A	199	LYS
1	A	210	ASN
2	B	6	GLN
2	B	10	GLU
2	B	46	GLU
2	B	51	ILE
2	B	57	TYR
2	B	61	ASN
2	B	89	GLU
2	B	95	PHE
2	B	113	GLN
2	B	118	THR
2	B	139	GLN
2	B	140	THR
2	B	157	PRO
2	B	196	ARG
2	B	204	ASN
2	B	205	VAL
2	B	213	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	34	ASN
1	L	80	GLN
1	L	90	GLN
1	L	92	ASN
1	L	124	GLN
1	L	137	ASN
1	L	145	ASN
1	L	161	ASN
1	L	166	GLN
1	L	189	HIS
2	H	3	GLN
2	H	35	ASN
2	H	43	GLN

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Mol	Chain	Res	Type
2	H	55	ASN
2	H	179	GLN
1	A	27	GLN
1	A	80	GLN
1	A	90	GLN
1	A	92	ASN
1	A	161	ASN
1	A	189	HIS
1	A	210	ASN
2	B	3	GLN
2	B	35	ASN
2	B	52	ASN
2	B	55	ASN
2	B	61	ASN
2	B	82	GLN
2	B	113	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	A	214/214 (100%)	-0.19	1 (0%) 90 92	3, 17, 38, 49	0
1	L	214/214 (100%)	-0.16	4 (1%) 67 68	1, 15, 38, 67	0
2	B	221/222 (99%)	-0.02	10 (4%) 34 32	1, 17, 45, 65	2 (0%)
2	H	221/222 (99%)	-0.11	8 (3%) 43 42	2, 15, 45, 61	0
All	All	870/872 (99%)	-0.12	23 (2%) 56 56	1, 16, 42, 67	2 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	140	THR	9.9
2	B	8	GLY	7.8
1	L	214	CYS	5.9
2	H	140	THR	5.0
2	B	134	PRO	4.9
2	B	137	ALA	4.5
2	H	139	GLN	4.1
2	B	55	ASN	3.8
2	H	57	TYR	3.7
2	B	135	GLY	3.2
2	H	135	GLY	3.1
2	H	56	GLY	3.0
2	B	138	ALA	2.8
2	H	137	ALA	2.7
2	H	222	ASP	2.7
2	H	136	SER	2.6
2	B	136	SER	2.6
2	B	56	GLY	2.4
1	L	52	SER	2.4
2	B	179	GLN	2.3
1	L	212	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	92	ASN	2.1
1	A	52	SER	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.