



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:07 PM GMT

PDB ID : 2R4R  
Title : Crystal structure of the human beta2 adrenoceptor  
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R.F.; Schertler, G.F.; Weis, W.I.; Kobilka, B.K.  
Deposited on : 2007-08-31  
Resolution : 3.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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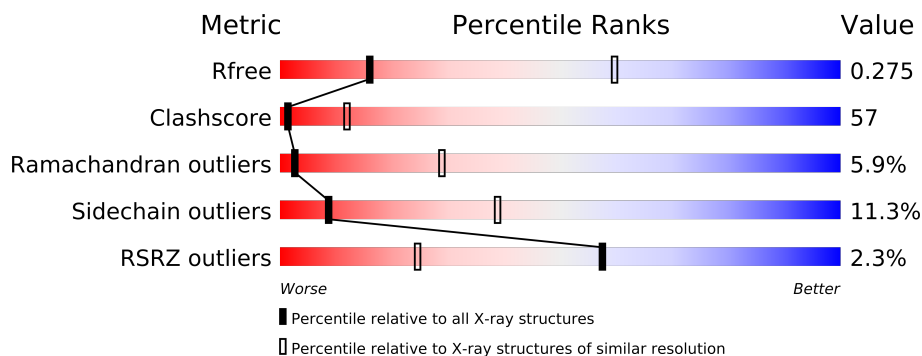
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.40 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))
$R_{free}$	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	365	
2	L	214	
3	H	217	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4925 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Beta-2 adrenergic receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1612	1052	271	279	10			

- Molecule 2 is a protein called antibody for beta2 adrenoceptor, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1678	1050	278	341	9			

- Molecule 3 is a protein called antibody for beta2 adrenoceptor, heavy chain.

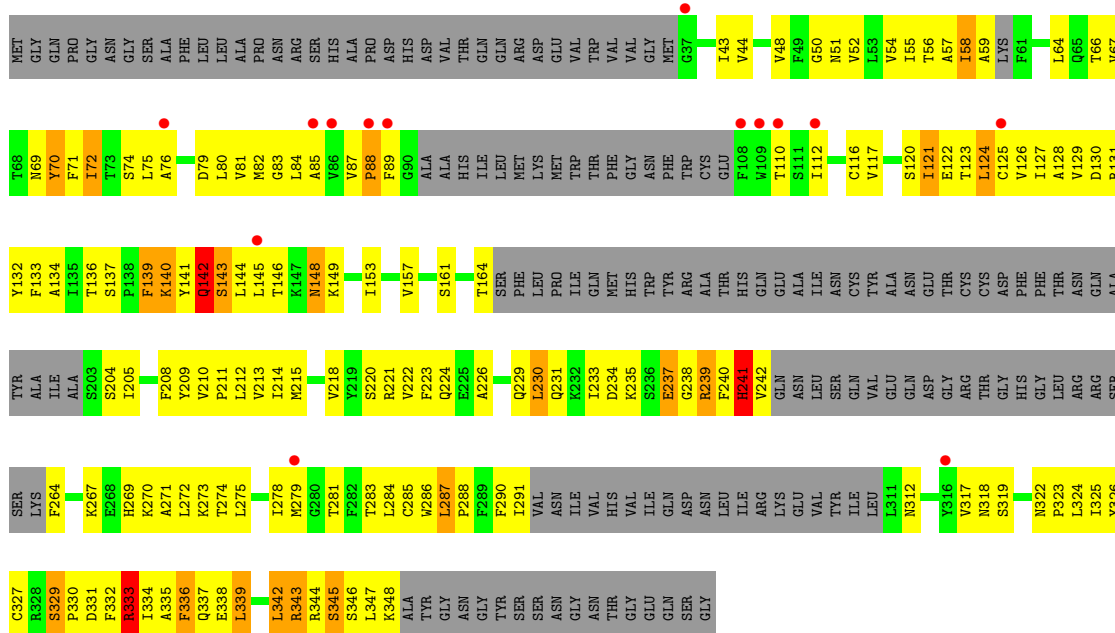
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	217	Total	C	N	O	S	0	0	0
			1635	1031	269	328	7			

### 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.

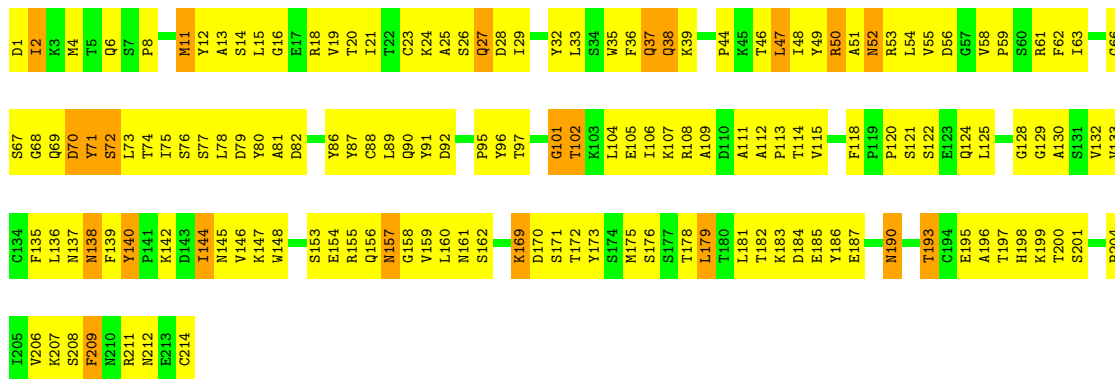
- Molecule 1: Beta-2 adrenergic receptor

Chain A: 



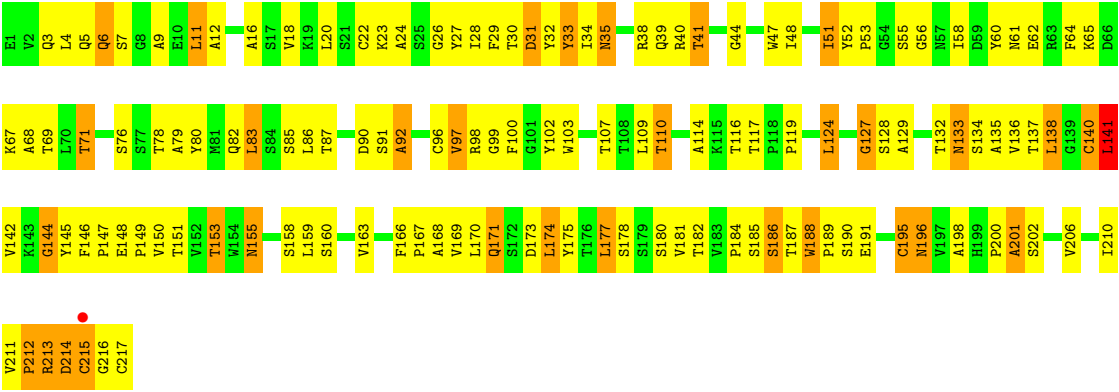
- Molecule 2: antibody for beta2 adrenoceptor, light chain

Chain L: 



- Molecule 3: antibody for beta2 adrenoceptor, heavy chain

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	338.38Å 48.48Å 89.35Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	19.99 – 3.40 85.92 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.99-3.40) 98.8 (85.92-3.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 3.41Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.217 , 0.270 0.226 , 0.275	Depositor DCC
$R_{free}$ test set	1902 reflections (9.72%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.1	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 103.0	EDS
Estimated twinning fraction	0.039 for -h-2*1,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 19671 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	4925	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.34	0/1636	0.57	0/2216
2	L	0.40	0/1716	0.73	0/2324
3	H	0.40	0/1677	0.74	1/2290 (0.0%)
All	All	0.38	0/5029	0.68	1/6830 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	141	LEU	CA-CB-CG	5.34	127.57	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1612	0	1610	195	0
2	L	1678	0	1610	208	0
3	H	1635	0	1578	177	0
All	All	4925	0	4798	556	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 57.

All (556) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:193:THR:HG23	2:L:208:SER:HB2	1.27	1.14
2:L:169:LYS:HD2	2:L:169:LYS:H	1.29	0.94
3:H:38:ARG:HB2	3:H:48:ILE:HD11	1.53	0.91
3:H:155:ASN:HB3	3:H:158:SER:HB2	1.53	0.90
2:L:38:GLN:HE21	3:H:39:GLN:HE22	1.16	0.89
2:L:89:LEU:HD12	2:L:90:GLN:N	1.87	0.89
2:L:38:GLN:NE2	3:H:39:GLN:HE22	1.69	0.89
2:L:44:PRO:HG2	3:H:103:TRP:CD2	2.07	0.89
3:H:35:ASN:HD22	3:H:35:ASN:H	1.22	0.85
1:A:71:PHE:HB3	1:A:127:ILE:HD11	1.57	0.85
1:A:231:GLN:HE21	1:A:235:LYS:HD2	1.42	0.85
2:L:66:GLY:HA3	2:L:71:TYR:HA	1.59	0.84
2:L:89:LEU:HD12	2:L:90:GLN:H	1.41	0.84
2:L:6:GLN:NE2	2:L:101:GLY:HA2	1.93	0.84
2:L:108:ARG:HG2	2:L:109:ALA:H	1.42	0.83
3:H:40:ARG:HH11	3:H:40:ARG:HB2	1.45	0.81
1:A:69:ASN:HA	1:A:72:ILE:HG22	1.60	0.81
2:L:132:VAL:HB	2:L:179:LEU:HD21	1.62	0.81
2:L:6:GLN:HE22	2:L:101:GLY:HA2	1.46	0.81
2:L:38:GLN:HE21	3:H:39:GLN:NE2	1.79	0.80
1:A:48:VAL:HG13	1:A:84:LEU:HD11	1.62	0.80
1:A:132:TYR:HE1	1:A:221:ARG:HG2	1.46	0.80
2:L:21:ILE:HB	2:L:102:THR:HG21	1.66	0.78
1:A:148:ASN:HD22	1:A:149:LYS:H	1.29	0.78
2:L:14:SER:HB3	2:L:107:LYS:HG3	1.65	0.78
2:L:16:GLY:O	2:L:77:SER:HA	1.84	0.77
3:H:68:ALA:HA	3:H:82:GLN:O	1.85	0.77
3:H:71:THR:HG23	3:H:80:TYR:HB2	1.68	0.76
2:L:112:ALA:HB2	2:L:200:THR:OG1	1.85	0.76
1:A:64:LEU:HD11	1:A:335:ALA:HB1	1.65	0.76
3:H:109:LEU:HD12	3:H:110:THR:N	2.01	0.76
3:H:11:LEU:HD13	3:H:12:ALA:N	2.01	0.75
2:L:182:THR:H	2:L:185:GLU:HB2	1.50	0.75
1:A:124:LEU:HD13	1:A:279:MET:HG2	1.68	0.75
3:H:18:VAL:HG22	3:H:86:LEU:HD11	1.69	0.74
2:L:120:PRO:CG	2:L:130:ALA:HB1	2.17	0.74
2:L:179:LEU:H	2:L:179:LEU:HD23	1.53	0.73
1:A:337:GLN:HE21	1:A:343:ARG:HG2	1.53	0.73
1:A:127:ILE:H	1:A:127:ILE:HD12	1.53	0.72
1:A:233:ILE:HG22	1:A:234:ASP:N	2.05	0.72
1:A:235:LYS:HB2	2:L:32:TYR:CZ	2.24	0.72
3:H:35:ASN:HD22	3:H:35:ASN:N	1.85	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:87:THR:HG22	3:H:90:ASP:OD2	1.89	0.72
2:L:108:ARG:HG2	2:L:109:ALA:N	2.05	0.71
2:L:24:LYS:HG2	2:L:70:ASP:HB3	1.72	0.71
2:L:59:PRO:HG2	2:L:62:PHE:CE1	2.26	0.71
3:H:110:THR:HG21	3:H:147:PRO:HB2	1.73	0.71
2:L:54:LEU:HD22	2:L:58:VAL:HB	1.73	0.70
1:A:336:PHE:HA	1:A:339:LEU:HD23	1.71	0.70
1:A:231:GLN:C	1:A:233:ILE:H	1.92	0.70
3:H:137:THR:HA	3:H:181:VAL:O	1.91	0.70
2:L:135:PHE:CZ	3:H:180:SER:HB3	2.27	0.70
2:L:46:THR:HG22	2:L:55:VAL:HG21	1.72	0.70
1:A:267:LYS:C	1:A:267:LYS:HD3	2.12	0.70
1:A:52:VAL:HG13	1:A:55:ILE:HD11	1.74	0.70
2:L:206:VAL:O	2:L:207:LYS:HD3	1.91	0.70
3:H:141:LEU:O	3:H:141:LEU:HD13	1.92	0.70
2:L:132:VAL:HB	2:L:179:LEU:CD2	2.22	0.69
3:H:68:ALA:HB2	3:H:83:LEU:HD13	1.74	0.69
2:L:79:ASP:HB3	2:L:82:ASP:OD2	1.93	0.68
3:H:97:VAL:HG12	3:H:103:TRP:HA	1.75	0.68
3:H:116:THR:HG23	3:H:146:PHE:O	1.92	0.68
3:H:7:SER:HB2	3:H:107:THR:HG23	1.75	0.68
3:H:40:ARG:HA	3:H:92:ALA:HB1	1.75	0.68
1:A:278:ILE:HG13	1:A:322:ASN:OD1	1.94	0.68
1:A:283:THR:O	1:A:287:LEU:HB2	1.94	0.68
1:A:87:VAL:N	1:A:88:PRO:HD2	2.09	0.68
1:A:148:ASN:ND2	1:A:149:LYS:H	1.92	0.67
2:L:211:ARG:HH11	2:L:211:ARG:HB3	1.58	0.67
1:A:343:ARG:HG3	1:A:344:ARG:N	2.09	0.67
1:A:52:VAL:HA	1:A:55:ILE:HG12	1.76	0.67
1:A:132:TYR:CE1	1:A:221:ARG:HG2	2.30	0.67
3:H:33:TYR:HA	3:H:53:PRO:HD2	1.75	0.67
2:L:125:LEU:CD2	2:L:130:ALA:HB2	2.25	0.67
1:A:58:ILE:HG23	1:A:59:ALA:H	1.59	0.67
2:L:125:LEU:HD23	2:L:130:ALA:HB2	1.76	0.66
1:A:58:ILE:HD13	1:A:59:ALA:N	2.10	0.66
3:H:144:GLY:HA2	3:H:174:LEU:HD12	1.76	0.66
2:L:148:TRP:CZ2	2:L:179:LEU:HD22	2.31	0.66
3:H:27:TYR:CE2	3:H:98:ARG:HD2	2.30	0.66
1:A:209:TYR:O	1:A:213:VAL:HG23	1.95	0.66
1:A:238:GLY:O	3:H:32:TYR:HA	1.96	0.66
2:L:157:ASN:C	2:L:157:ASN:HD22	1.97	0.66
3:H:153:THR:HG23	3:H:196:ASN:HB2	1.77	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:235:LYS:HB2	2:L:32:TYR:CE1	2.31	0.65
1:A:336:PHE:O	1:A:339:LEU:HG	1.97	0.65
3:H:35:ASN:N	3:H:35:ASN:ND2	2.43	0.65
1:A:71:PHE:CB	1:A:127:ILE:HD11	2.26	0.65
1:A:153:ILE:O	1:A:157:VAL:HG23	1.96	0.65
1:A:51:ASN:O	1:A:55:ILE:HG23	1.96	0.64
3:H:69:THR:OG1	3:H:82:GLN:HB3	1.98	0.63
2:L:136:LEU:CD1	2:L:196:ALA:HB2	2.27	0.63
3:H:67:LYS:HG3	3:H:83:LEU:CD1	2.28	0.63
2:L:193:THR:HG23	2:L:208:SER:CB	2.18	0.63
3:H:142:VAL:O	3:H:142:VAL:HG22	1.98	0.63
1:A:231:GLN:C	1:A:233:ILE:N	2.50	0.63
1:A:220:SER:O	1:A:224:GLN:HG2	1.99	0.63
3:H:109:LEU:HD12	3:H:110:THR:H	1.63	0.63
3:H:144:GLY:CA	3:H:174:LEU:HD12	2.29	0.63
2:L:160:LEU:HD23	2:L:160:LEU:C	2.18	0.63
1:A:332:PHE:HA	1:A:335:ALA:HB3	1.81	0.62
2:L:108:ARG:HH11	2:L:108:ARG:HG2	1.64	0.62
3:H:4:LEU:HB3	3:H:22:CYS:SG	2.39	0.62
2:L:53:ARG:HH11	2:L:53:ARG:HG3	1.63	0.62
2:L:27:GLN:O	2:L:69:GLN:HG3	1.99	0.62
1:A:234:ASP:O	1:A:237:GLU:HB2	2.00	0.62
2:L:2:ILE:HG13	2:L:26:SER:OG	2.00	0.62
1:A:44:VAL:HG22	1:A:87:VAL:HG11	1.82	0.61
1:A:329:SER:HB2	1:A:330:PRO:HD3	1.80	0.61
1:A:148:ASN:HD22	1:A:149:LYS:N	1.98	0.61
2:L:120:PRO:HG2	2:L:130:ALA:HB1	1.81	0.61
1:A:44:VAL:O	1:A:48:VAL:HG23	2.00	0.61
3:H:169:VAL:HG12	3:H:170:LEU:O	1.99	0.61
2:L:24:LYS:HG2	2:L:70:ASP:CB	2.29	0.61
3:H:33:TYR:HD2	3:H:52:TYR:HB2	1.65	0.61
1:A:71:PHE:O	1:A:74:SER:HB3	2.01	0.61
2:L:35:TRP:CD2	2:L:73:LEU:HB2	2.35	0.61
3:H:214:ASP:C	3:H:216:GLY:H	2.03	0.61
3:H:38:ARG:NH2	3:H:64:PHE:HE2	1.98	0.61
1:A:231:GLN:NE2	1:A:235:LYS:HD2	2.13	0.61
3:H:34:ILE:O	3:H:34:ILE:HG13	2.01	0.60
2:L:108:ARG:CG	2:L:109:ALA:H	2.14	0.60
3:H:136:VAL:HG12	3:H:138:LEU:HD23	1.83	0.60
1:A:229:GLN:NE2	1:A:264:PHE:HB3	2.16	0.60
1:A:333:ARG:HG2	1:A:333:ARG:HH11	1.67	0.59
1:A:339:LEU:C	1:A:339:LEU:HD12	2.22	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:283:THR:HG23	1:A:284:LEU:CD1	2.32	0.59
3:H:4:LEU:HA	3:H:24:ALA:HA	1.84	0.59
1:A:337:GLN:O	1:A:343:ARG:HB2	2.02	0.59
1:A:326:TYR:HA	1:A:330:PRO:CD	2.31	0.59
2:L:190:ASN:HD22	2:L:190:ASN:N	2.01	0.59
1:A:205:ILE:O	1:A:210:VAL:HG23	2.03	0.59
1:A:270:LYS:O	1:A:273:LYS:HB3	2.02	0.59
3:H:138:LEU:HD12	3:H:210:ILE:HD12	1.85	0.59
1:A:50:GLY:O	1:A:54:VAL:HG23	2.03	0.59
1:A:233:ILE:CG2	1:A:234:ASP:N	2.65	0.59
1:A:327:CYS:O	1:A:333:ARG:HG2	2.03	0.58
3:H:48:ILE:HG23	3:H:64:PHE:CG	2.38	0.58
3:H:67:LYS:HG3	3:H:83:LEU:HD12	1.85	0.58
2:L:135:PHE:CE2	3:H:180:SER:HB3	2.38	0.58
2:L:144:ILE:CD1	2:L:145:ASN:H	2.16	0.58
1:A:83:GLY:HA2	1:A:87:VAL:CG2	2.34	0.58
1:A:287:LEU:HD22	1:A:291:ILE:HG13	1.84	0.58
2:L:71:TYR:N	2:L:71:TYR:CD1	2.72	0.58
2:L:91:TYR:HA	2:L:96:TYR:CD2	2.38	0.58
3:H:136:VAL:O	3:H:182:THR:HA	2.04	0.58
2:L:63:ILE:N	2:L:74:THR:O	2.36	0.58
3:H:155:ASN:ND2	3:H:159:LEU:HD13	2.19	0.58
3:H:91:SER:O	3:H:92:ALA:HB2	2.03	0.58
1:A:337:GLN:NE2	1:A:343:ARG:HG2	2.18	0.58
1:A:52:VAL:O	1:A:55:ILE:HG12	2.04	0.58
2:L:136:LEU:N	2:L:136:LEU:HD22	2.19	0.58
2:L:2:ILE:O	2:L:2:ILE:HG12	2.03	0.58
1:A:336:PHE:HD2	1:A:337:GLN:N	2.00	0.58
2:L:59:PRO:HG2	2:L:62:PHE:HE1	1.66	0.58
1:A:121:ILE:HD13	1:A:121:ILE:O	2.04	0.58
2:L:159:VAL:HG12	2:L:161:ASN:ND2	2.19	0.57
1:A:235:LYS:HE3	2:L:92:ASP:O	2.04	0.57
2:L:144:ILE:HD13	2:L:145:ASN:H	1.69	0.57
2:L:80:TYR:CD1	2:L:81:ALA:N	2.72	0.57
3:H:40:ARG:HB2	3:H:40:ARG:NH1	2.16	0.57
3:H:40:ARG:HG2	3:H:41:THR:N	2.20	0.57
3:H:137:THR:HG22	3:H:182:THR:OG1	2.05	0.57
3:H:166:PHE:CD1	3:H:166:PHE:N	2.72	0.57
2:L:52:ASN:HD22	2:L:52:ASN:H	1.51	0.57
1:A:148:ASN:N	1:A:148:ASN:HD22	2.02	0.57
1:A:81:VAL:O	1:A:85:ALA:HB3	2.05	0.57
2:L:159:VAL:HG12	2:L:161:ASN:HD21	1.69	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:44:PRO:HG2	3:H:103:TRP:CG	2.40	0.57
3:H:117:THR:O	3:H:145:TYR:HA	2.05	0.57
2:L:157:ASN:HD22	2:L:158:GLY:N	2.03	0.57
1:A:83:GLY:HA2	1:A:87:VAL:HG23	1.86	0.56
2:L:1:ASP:HB3	2:L:95:PRO:HD2	1.85	0.56
1:A:240:PHE:O	1:A:242:VAL:N	2.37	0.56
1:A:124:LEU:CD1	1:A:279:MET:HG2	2.34	0.56
3:H:40:ARG:HA	3:H:92:ALA:CB	2.34	0.56
1:A:82:MET:O	1:A:87:VAL:HG23	2.06	0.56
3:H:177:LEU:C	3:H:177:LEU:HD12	2.26	0.56
2:L:183:LYS:O	2:L:187:GLU:HG2	2.03	0.56
3:H:6:GLN:HE22	3:H:96:CYS:CB	2.18	0.56
2:L:136:LEU:HD11	2:L:196:ALA:HB2	1.85	0.56
2:L:11:MET:SD	2:L:19:VAL:HG23	2.46	0.56
2:L:36:PHE:HA	2:L:47:LEU:HD22	1.88	0.56
3:H:188:TRP:CH2	3:H:212:PRO:HA	2.41	0.56
3:H:150:VAL:HG23	3:H:150:VAL:O	2.06	0.55
2:L:142:LYS:HA	2:L:173:TYR:CD2	2.41	0.55
2:L:13:ALA:O	2:L:106:ILE:HA	2.06	0.55
1:A:214:ILE:HG13	1:A:215:MET:N	2.21	0.55
3:H:5:GLN:O	3:H:22:CYS:HA	2.06	0.55
2:L:209:PHE:CD1	2:L:209:PHE:C	2.78	0.55
3:H:142:VAL:O	3:H:142:VAL:CG2	2.54	0.55
2:L:108:ARG:HB3	2:L:140:TYR:CD2	2.41	0.55
2:L:52:ASN:HD22	2:L:52:ASN:N	2.03	0.55
1:A:66:THR:O	1:A:70:TYR:HB2	2.07	0.55
1:A:83:GLY:O	1:A:88:PRO:HD3	2.05	0.55
3:H:40:ARG:HG2	3:H:41:THR:H	1.72	0.55
2:L:144:ILE:HG23	2:L:145:ASN:N	2.22	0.55
2:L:29:ILE:HG13	2:L:71:TYR:OH	2.07	0.54
3:H:60:TYR:CE2	3:H:69:THR:HA	2.42	0.54
1:A:209:TYR:C	1:A:213:VAL:HG23	2.28	0.54
2:L:18:ARG:HB3	2:L:76:SER:HA	1.90	0.54
1:A:275:LEU:HA	1:A:278:ILE:HG22	1.90	0.54
3:H:147:PRO:HD2	3:H:201:ALA:HB1	1.89	0.54
2:L:169:LYS:CD	2:L:169:LYS:H	2.11	0.54
3:H:38:ARG:CZ	3:H:64:PHE:HE2	2.21	0.54
2:L:108:ARG:NH1	2:L:108:ARG:HG2	2.22	0.54
1:A:235:LYS:O	1:A:239:ARG:HD3	2.07	0.54
2:L:120:PRO:CB	2:L:130:ALA:HB1	2.38	0.53
2:L:47:LEU:O	2:L:55:VAL:HG23	2.09	0.53
2:L:89:LEU:HD21	3:H:100:PHE:CE2	2.43	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:115:VAL:HA	2:L:135:PHE:O	2.07	0.53
3:H:11:LEU:HD23	3:H:147:PRO:HG3	1.90	0.53
1:A:139:PHE:CZ	1:A:140:LYS:HE2	2.43	0.53
3:H:110:THR:HG21	3:H:147:PRO:CB	2.38	0.53
3:H:188:TRP:CE3	3:H:189:PRO:HD3	2.43	0.53
2:L:170:ASP:OD2	2:L:172:THR:HB	2.09	0.53
1:A:124:LEU:HD12	1:A:215:MET:HE2	1.91	0.53
1:A:54:VAL:O	1:A:58:ILE:HG22	2.09	0.53
2:L:19:VAL:HG21	2:L:104:LEU:HD11	1.91	0.53
2:L:47:LEU:HA	2:L:58:VAL:HG21	1.89	0.53
3:H:23:LYS:HG3	3:H:78:THR:HG22	1.90	0.53
3:H:76:SER:HB3	3:H:78:THR:HG23	1.89	0.53
2:L:146:VAL:HG13	2:L:175:MET:HE1	1.90	0.53
1:A:69:ASN:HA	1:A:72:ILE:CG2	2.34	0.53
3:H:114:ALA:HB3	3:H:146:PHE:CZ	2.44	0.53
1:A:80:LEU:C	1:A:80:LEU:HD23	2.29	0.53
2:L:20:THR:HG23	2:L:74:THR:OG1	2.09	0.53
2:L:108:ARG:NH1	2:L:109:ALA:O	2.42	0.52
3:H:6:GLN:NE2	3:H:96:CYS:CB	2.72	0.52
1:A:283:THR:HG23	1:A:284:LEU:HD12	1.89	0.52
1:A:329:SER:HB2	1:A:330:PRO:CD	2.39	0.52
3:H:163:VAL:O	3:H:163:VAL:HG13	2.10	0.52
3:H:187:THR:O	3:H:190:SER:HB2	2.09	0.52
1:A:326:TYR:C	1:A:330:PRO:HD2	2.30	0.52
2:L:11:MET:CE	2:L:19:VAL:HG23	2.39	0.52
3:H:56:GLY:O	3:H:58:ILE:HG13	2.09	0.52
1:A:148:ASN:H	1:A:148:ASN:ND2	2.08	0.52
3:H:40:ARG:HH11	3:H:40:ARG:CB	2.20	0.52
2:L:148:TRP:CE2	2:L:179:LEU:HD22	2.45	0.52
3:H:6:GLN:NE2	3:H:96:CYS:HB3	2.25	0.52
2:L:59:PRO:HG2	2:L:62:PHE:CD1	2.44	0.52
2:L:118:PHE:O	2:L:132:VAL:HG13	2.09	0.52
1:A:336:PHE:CD2	1:A:337:GLN:N	2.78	0.52
2:L:175:MET:HG2	2:L:176:SER:N	2.25	0.52
1:A:230:LEU:HD22	1:A:269:HIS:CE1	2.44	0.51
2:L:6:GLN:HE22	2:L:87:TYR:HA	1.74	0.51
2:L:195:GLU:HG2	2:L:206:VAL:HG13	1.92	0.51
3:H:214:ASP:O	3:H:216:GLY:N	2.42	0.51
3:H:127:GLY:HA2	3:H:213:ARG:NH1	2.26	0.51
3:H:128:SER:HA	3:H:217:CYS:O	2.10	0.51
3:H:132:THR:O	3:H:133:ASN:HB2	2.10	0.51
3:H:52:TYR:HD2	3:H:55:SER:HB3	1.76	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:128:ALA:O	1:A:218:VAL:HG12	2.11	0.51
1:A:212:LEU:HD23	1:A:212:LEU:O	2.10	0.51
2:L:8:PRO:O	2:L:102:THR:HB	2.10	0.51
3:H:124:LEU:HD21	3:H:141:LEU:H	1.76	0.51
3:H:170:LEU:HD12	3:H:174:LEU:O	2.11	0.51
1:A:332:PHE:O	1:A:333:ARG:C	2.49	0.51
3:H:133:ASN:HB3	3:H:135:ALA:O	2.11	0.51
1:A:48:VAL:HG22	1:A:84:LEU:HG	1.93	0.51
2:L:200:THR:HG23	2:L:201:SER:N	2.26	0.51
2:L:187:GLU:CD	2:L:211:ARG:HE	2.14	0.51
1:A:239:ARG:HG2	1:A:240:PHE:CD2	2.46	0.51
2:L:29:ILE:HG22	2:L:92:ASP:CB	2.40	0.51
3:H:9:ALA:HB2	3:H:149:PRO:HD2	1.92	0.51
1:A:127:ILE:HD12	1:A:127:ILE:N	2.24	0.50
2:L:136:LEU:HD12	2:L:196:ALA:HB2	1.92	0.50
1:A:71:PHE:O	1:A:75:LEU:HD13	2.11	0.50
2:L:184:ASP:O	2:L:185:GLU:C	2.49	0.50
2:L:142:LYS:HB2	2:L:173:TYR:CE2	2.46	0.50
3:H:11:LEU:HD23	3:H:147:PRO:CG	2.41	0.50
1:A:242:VAL:HG23	3:H:32:TYR:OH	2.10	0.50
1:A:148:ASN:ND2	1:A:149:LYS:N	2.56	0.50
2:L:182:THR:HG22	2:L:183:LYS:H	1.77	0.50
1:A:326:TYR:HA	1:A:330:PRO:HD2	1.93	0.50
3:H:34:ILE:HD11	3:H:79:ALA:CB	2.41	0.50
3:H:35:ASN:HD21	3:H:99:GLY:HA2	1.77	0.50
1:A:148:ASN:N	1:A:148:ASN:ND2	2.60	0.50
1:A:161:SER:C	1:A:164:THR:HG22	2.31	0.50
2:L:162:SER:OG	3:H:167:PRO:HG2	2.12	0.50
1:A:122:GLU:O	1:A:126:VAL:HG23	2.10	0.50
2:L:113:PRO:HA	2:L:137:ASN:O	2.12	0.50
2:L:50:ARG:HH21	2:L:53:ARG:HH12	1.59	0.50
3:H:195:CYS:SG	3:H:195:CYS:O	2.70	0.50
1:A:110:THR:O	1:A:110:THR:HG22	2.11	0.50
3:H:150:VAL:CG2	3:H:177:LEU:HD21	2.42	0.50
2:L:182:THR:HG22	2:L:183:LYS:N	2.26	0.50
1:A:267:LYS:C	1:A:269:HIS:H	2.15	0.50
2:L:53:ARG:NH1	2:L:53:ARG:HG3	2.27	0.50
1:A:344:ARG:C	1:A:346:SER:H	2.16	0.50
2:L:19:VAL:HG13	2:L:75:ILE:HG23	1.93	0.50
1:A:52:VAL:HG22	1:A:80:LEU:HD12	1.94	0.49
1:A:325:ILE:O	1:A:329:SER:HB2	2.11	0.49
3:H:211:VAL:HG13	3:H:212:PRO:HD2	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:168:ALA:HB2	3:H:177:LEU:HD23	1.94	0.49
3:H:11:LEU:HD13	3:H:12:ALA:H	1.75	0.49
3:H:7:SER:HB2	3:H:107:THR:CG2	2.40	0.49
2:L:170:ASP:OD2	2:L:172:THR:CG2	2.60	0.49
1:A:67:VAL:HG11	1:A:130:ASP:OD2	2.12	0.49
1:A:271:ALA:O	1:A:274:THR:HG22	2.13	0.49
2:L:52:ASN:HD22	2:L:53:ARG:N	2.09	0.49
1:A:124:LEU:HB3	1:A:215:MET:CE	2.43	0.49
2:L:4:MET:CE	2:L:25:ALA:HB2	2.42	0.49
2:L:157:ASN:C	2:L:157:ASN:ND2	2.65	0.49
1:A:329:SER:CB	1:A:330:PRO:HD3	2.42	0.49
3:H:128:SER:HA	3:H:217:CYS:C	2.33	0.49
1:A:131:ARG:NH1	1:A:141:TYR:HE1	2.10	0.49
3:H:51:ILE:HD13	3:H:51:ILE:C	2.33	0.49
2:L:48:ILE:HG22	2:L:49:TYR:N	2.27	0.49
2:L:4:MET:SD	2:L:90:GLN:HB3	2.53	0.48
3:H:144:GLY:C	3:H:174:LEU:HD12	2.33	0.48
1:A:146:THR:HG1	1:A:149:LYS:HB2	1.77	0.48
1:A:208:PHE:O	1:A:211:PRO:HG2	2.12	0.48
2:L:86:TYR:N	2:L:86:TYR:CD1	2.81	0.48
2:L:147:LYS:CE	2:L:195:GLU:OE2	2.61	0.48
3:H:40:ARG:O	3:H:41:THR:O	2.32	0.48
3:H:83:LEU:O	3:H:86:LEU:HD21	2.13	0.48
1:A:336:PHE:HD2	1:A:337:GLN:H	1.60	0.48
1:A:287:LEU:HD22	1:A:291:ILE:CG1	2.43	0.48
1:A:75:LEU:HD21	1:A:124:LEU:HD21	1.95	0.48
2:L:211:ARG:O	2:L:211:ARG:HG2	2.14	0.48
2:L:95:PRO:O	2:L:97:THR:HG23	2.13	0.48
2:L:155:ARG:HG2	2:L:156:GLN:N	2.28	0.48
1:A:75:LEU:HD21	1:A:124:LEU:CD2	2.43	0.48
1:A:88:PRO:HG2	1:A:89:PHE:H	1.79	0.47
3:H:146:PHE:CD1	3:H:146:PHE:C	2.87	0.47
3:H:34:ILE:HD11	3:H:79:ALA:HB3	1.96	0.47
3:H:188:TRP:CG	3:H:189:PRO:N	2.82	0.47
3:H:188:TRP:CZ2	3:H:212:PRO:HA	2.49	0.47
3:H:184:PRO:HD2	3:H:187:THR:OG1	2.13	0.47
1:A:79:ASP:OD1	1:A:319:SER:HA	2.14	0.47
1:A:58:ILE:HG23	1:A:59:ALA:N	2.28	0.47
1:A:117:VAL:HG21	1:A:286:TRP:CH2	2.49	0.47
1:A:146:THR:OG1	1:A:148:ASN:ND2	2.47	0.47
3:H:40:ARG:C	3:H:41:THR:O	2.51	0.47
1:A:87:VAL:N	1:A:88:PRO:CD	2.76	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:12:TYR:HA	2:L:105:GLU:O	2.15	0.47
3:H:173:ASP:O	3:H:174:LEU:CD2	2.63	0.47
2:L:19:VAL:HG13	2:L:75:ILE:CG2	2.44	0.47
2:L:179:LEU:H	2:L:179:LEU:CD2	2.26	0.47
3:H:138:LEU:O	3:H:181:VAL:N	2.45	0.47
2:L:61:ARG:O	2:L:75:ILE:HA	2.14	0.47
1:A:240:PHE:O	1:A:241:HIS:C	2.52	0.47
3:H:39:GLN:HG3	3:H:44:GLY:O	2.14	0.47
2:L:24:LYS:CG	2:L:70:ASP:HB3	2.41	0.47
1:A:324:LEU:HD23	1:A:324:LEU:C	2.35	0.47
1:A:212:LEU:HD23	1:A:212:LEU:C	2.35	0.47
3:H:133:ASN:ND2	3:H:134:SER:H	2.12	0.47
1:A:131:ARG:O	1:A:134:ALA:HB3	2.15	0.47
3:H:141:LEU:HB2	3:H:178:SER:HB3	1.97	0.47
2:L:118:PHE:CG	3:H:124:LEU:HB3	2.50	0.47
1:A:204:SER:O	1:A:208:PHE:HB3	2.15	0.47
3:H:151:THR:HB	3:H:198:ALA:HB3	1.97	0.47
3:H:62:GLU:O	3:H:65:LYS:CB	2.63	0.47
1:A:133:PHE:HA	1:A:136:THR:CG2	2.45	0.47
2:L:120:PRO:HG2	2:L:186:TYR:CE2	2.50	0.47
2:L:111:ALA:O	2:L:139:PHE:HA	2.15	0.46
3:H:61:ASN:O	3:H:62:GLU:C	2.53	0.46
2:L:139:PHE:CE1	2:L:144:ILE:HB	2.51	0.46
1:A:157:VAL:O	1:A:161:SER:HB2	2.16	0.46
2:L:170:ASP:OD2	2:L:172:THR:HG21	2.15	0.46
1:A:267:LYS:O	1:A:267:LYS:HD3	2.14	0.46
2:L:198:HIS:CD2	2:L:200:THR:HB	2.50	0.46
3:H:213:ARG:C	3:H:215:CYS:H	2.18	0.46
1:A:317:VAL:C	1:A:319:SER:H	2.19	0.46
2:L:78:LEU:CD1	2:L:82:ASP:HB2	2.45	0.46
3:H:184:PRO:C	3:H:186:SER:N	2.68	0.46
1:A:123:THR:HG22	1:A:127:ILE:CD1	2.46	0.46
1:A:224:GLN:C	1:A:226:ALA:H	2.19	0.46
3:H:145:TYR:N	3:H:174:LEU:CD1	2.79	0.46
1:A:52:VAL:CA	1:A:55:ILE:HG12	2.44	0.46
2:L:169:LYS:HD2	2:L:169:LYS:N	2.13	0.46
1:A:239:ARG:CZ	3:H:33:TYR:CE1	2.99	0.46
2:L:6:GLN:HG2	2:L:102:THR:HG22	1.97	0.46
3:H:145:TYR:O	3:H:146:PHE:HB2	2.16	0.46
3:H:170:LEU:O	3:H:171:GLN:HB2	2.16	0.46
2:L:79:ASP:N	2:L:82:ASP:OD2	2.48	0.45
2:L:19:VAL:HG21	2:L:104:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:124:GLN:HG2	2:L:129:GLY:O	2.17	0.45
2:L:125:LEU:HD21	2:L:130:ALA:HB2	1.98	0.45
1:A:58:ILE:HD13	1:A:58:ILE:C	2.36	0.45
2:L:190:ASN:OD1	2:L:212:ASN:ND2	2.34	0.45
1:A:43:ILE:HG22	1:A:43:ILE:O	2.14	0.45
2:L:50:ARG:O	2:L:52:ASN:ND2	2.50	0.45
1:A:283:THR:HG23	1:A:284:LEU:HD13	1.97	0.45
2:L:67:SER:O	2:L:69:GLN:N	2.50	0.45
2:L:27:GLN:HB3	2:L:28:ASP:H	1.44	0.45
1:A:286:TRP:O	1:A:290:PHE:HD1	1.99	0.45
3:H:62:GLU:O	3:H:65:LYS:HB2	2.16	0.45
2:L:49:TYR:CD1	2:L:50:ARG:HB2	2.52	0.45
1:A:275:LEU:HA	1:A:278:ILE:CG2	2.46	0.45
1:A:322:ASN:C	1:A:324:LEU:H	2.20	0.45
3:H:177:LEU:HD12	3:H:178:SER:N	2.31	0.45
2:L:160:LEU:C	2:L:161:ASN:HD22	2.20	0.45
1:A:344:ARG:O	1:A:348:LYS:HB2	2.17	0.45
2:L:29:ILE:HG22	2:L:92:ASP:HB3	1.98	0.45
1:A:52:VAL:O	1:A:56:THR:HG22	2.16	0.45
2:L:71:TYR:O	2:L:72:SER:HB3	2.17	0.45
3:H:136:VAL:HG12	3:H:137:THR:N	2.31	0.45
1:A:334:ILE:HG23	1:A:338:GLU:CD	2.37	0.45
3:H:155:ASN:HB2	3:H:159:LEU:HB2	1.99	0.44
2:L:161:ASN:O	3:H:169:VAL:HG21	2.17	0.44
2:L:198:HIS:HD2	2:L:200:THR:HB	1.82	0.44
3:H:38:ARG:CB	3:H:48:ILE:HD11	2.34	0.44
3:H:127:GLY:HA2	3:H:213:ARG:HH12	1.83	0.44
2:L:66:GLY:HA3	2:L:71:TYR:CA	2.40	0.44
2:L:38:GLN:HB2	2:L:87:TYR:HE1	1.82	0.44
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.52	0.44
3:H:4:LEU:CD1	3:H:102:TYR:HD2	2.30	0.44
3:H:28:ILE:O	3:H:29:PHE:C	2.55	0.44
2:L:19:VAL:HG11	2:L:104:LEU:HD11	1.98	0.44
2:L:33:LEU:C	2:L:33:LEU:HD23	2.37	0.44
2:L:52:ASN:ND2	2:L:52:ASN:N	2.66	0.44
1:A:127:ILE:H	1:A:127:ILE:CD1	2.25	0.44
1:A:283:THR:HG23	1:A:284:LEU:N	2.32	0.44
3:H:51:ILE:HG12	3:H:58:ILE:HG12	1.99	0.44
3:H:148:GLU:OE1	3:H:149:PRO:HA	2.17	0.44
1:A:239:ARG:HG3	1:A:240:PHE:CE2	2.52	0.44
2:L:50:ARG:O	2:L:52:ASN:N	2.48	0.44
2:L:52:ASN:HD22	2:L:53:ARG:H	1.65	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:198:HIS:HB3	2:L:200:THR:HG22	2.00	0.44
1:A:342:LEU:HB3	1:A:346:SER:CB	2.47	0.44
3:H:214:ASP:C	3:H:216:GLY:N	2.69	0.44
1:A:233:ILE:CG2	1:A:234:ASP:H	2.30	0.44
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.53	0.44
2:L:66:GLY:CA	2:L:71:TYR:HA	2.41	0.44
1:A:48:VAL:O	1:A:48:VAL:HG12	2.16	0.44
1:A:82:MET:HG2	1:A:82:MET:O	2.18	0.44
1:A:333:ARG:NH1	1:A:333:ARG:HG2	2.32	0.44
1:A:55:ILE:HG13	1:A:56:THR:N	2.33	0.44
3:H:4:LEU:N	3:H:4:LEU:HD12	2.33	0.44
2:L:133:VAL:HG22	2:L:178:THR:OG1	2.18	0.44
2:L:148:TRP:CD2	2:L:179:LEU:HD13	2.53	0.44
2:L:206:VAL:HG12	2:L:207:LYS:N	2.33	0.44
1:A:347:LEU:N	1:A:347:LEU:HD22	2.33	0.44
2:L:198:HIS:O	2:L:199:LYS:C	2.57	0.44
1:A:205:ILE:HA	1:A:209:TYR:CB	2.47	0.44
1:A:329:SER:CB	1:A:330:PRO:CD	2.96	0.44
1:A:120:SER:C	1:A:122:GLU:H	2.21	0.44
3:H:146:PHE:CD1	3:H:147:PRO:N	2.86	0.43
2:L:35:TRP:HB3	2:L:73:LEU:HD22	2.01	0.43
1:A:230:LEU:O	1:A:233:ILE:HD12	2.18	0.43
3:H:33:TYR:CD2	3:H:52:TYR:HB2	2.49	0.43
2:L:48:ILE:HG12	2:L:54:LEU:HA	2.01	0.43
2:L:6:GLN:O	2:L:8:PRO:O	2.37	0.43
1:A:222:VAL:O	1:A:224:GLN:N	2.51	0.43
3:H:67:LYS:HG3	3:H:83:LEU:HD11	1.98	0.43
2:L:170:ASP:O	2:L:171:SER:C	2.56	0.43
1:A:286:TRP:O	1:A:290:PHE:CD1	2.71	0.43
1:A:239:ARG:HG2	1:A:240:PHE:HD2	1.83	0.43
2:L:44:PRO:O	3:H:103:TRP:CD1	2.72	0.43
3:H:124:LEU:HD22	3:H:124:LEU:N	2.33	0.43
3:H:168:ALA:HA	3:H:177:LEU:HB3	1.98	0.43
1:A:218:VAL:O	1:A:222:VAL:HG23	2.18	0.43
3:H:30:THR:O	3:H:31:ASP:OD1	2.36	0.43
2:L:44:PRO:HG2	3:H:103:TRP:CE2	2.53	0.43
2:L:61:ARG:HH11	2:L:61:ARG:HG2	1.83	0.43
3:H:76:SER:CB	3:H:78:THR:HG23	2.48	0.43
3:H:47:TRP:CE3	3:H:61:ASN:HB2	2.54	0.43
1:A:129:VAL:O	1:A:132:TYR:HB3	2.18	0.43
2:L:140:TYR:CD1	2:L:140:TYR:C	2.92	0.43
3:H:6:GLN:NE2	3:H:96:CYS:HB2	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:74:SER:C	1:A:76:ALA:H	2.22	0.42
1:A:132:TYR:O	1:A:136:THR:HG22	2.18	0.42
2:L:160:LEU:HD21	3:H:169:VAL:HB	2.00	0.42
1:A:56:THR:HG23	1:A:57:ALA:N	2.34	0.42
2:L:190:ASN:ND2	2:L:190:ASN:N	2.67	0.42
3:H:188:TRP:O	3:H:191:GLU:O	2.37	0.42
3:H:210:ILE:HG22	3:H:210:ILE:O	2.19	0.42
2:L:91:TYR:HA	2:L:96:TYR:HD2	1.81	0.42
3:H:160:SER:O	3:H:163:VAL:HG12	2.18	0.42
1:A:124:LEU:HB3	1:A:215:MET:HE2	2.01	0.42
3:H:124:LEU:HD22	3:H:140:CYS:HA	2.00	0.42
1:A:44:VAL:HG22	1:A:87:VAL:CG1	2.49	0.42
2:L:19:VAL:CG1	2:L:75:ILE:HG23	2.49	0.42
3:H:155:ASN:O	3:H:158:SER:HB2	2.18	0.42
1:A:337:GLN:HG2	1:A:343:ARG:CB	2.50	0.42
2:L:147:LYS:HE3	2:L:195:GLU:OE2	2.20	0.42
3:H:3:GLN:O	3:H:24:ALA:HA	2.19	0.42
1:A:112:ILE:O	1:A:116:CYS:SG	2.76	0.42
1:A:229:GLN:O	1:A:230:LEU:C	2.57	0.42
2:L:21:ILE:HD11	2:L:35:TRP:CZ3	2.55	0.42
2:L:29:ILE:HD12	2:L:33:LEU:HB2	2.01	0.42
1:A:131:ARG:NH1	1:A:141:TYR:CE1	2.87	0.42
2:L:197:THR:HG22	2:L:204:PRO:HG3	2.01	0.42
2:L:182:THR:OG1	2:L:185:GLU:HG3	2.20	0.42
3:H:34:ILE:O	3:H:34:ILE:CG1	2.66	0.42
2:L:212:ASN:C	2:L:214:CYS:N	2.73	0.42
2:L:138:ASN:HA	2:L:172:THR:CG2	2.49	0.42
1:A:134:ALA:O	1:A:137:SER:HB3	2.20	0.42
1:A:117:VAL:HG12	1:A:117:VAL:O	2.19	0.42
1:A:142:GLN:O	1:A:143:SER:O	2.38	0.42
1:A:241:HIS:HB2	3:H:32:TYR:CE1	2.54	0.42
2:L:161:ASN:N	2:L:161:ASN:HD22	2.17	0.42
2:L:35:TRP:O	2:L:47:LEU:HD22	2.19	0.42
3:H:169:VAL:HG12	3:H:170:LEU:N	2.35	0.42
3:H:29:PHE:HZ	3:H:79:ALA:HB2	1.85	0.42
1:A:141:TYR:OH	1:A:272:LEU:HD21	2.19	0.42
2:L:52:ASN:ND2	2:L:53:ARG:N	2.68	0.42
1:A:239:ARG:HB2	3:H:99:GLY:O	2.20	0.42
2:L:199:LYS:O	2:L:200:THR:C	2.57	0.42
2:L:170:ASP:OD2	2:L:172:THR:CB	2.68	0.42
3:H:173:ASP:O	3:H:174:LEU:HD22	2.20	0.41
2:L:4:MET:HG2	2:L:25:ALA:CB	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:331:ASP:O	1:A:332:PHE:C	2.58	0.41
1:A:287:LEU:HB3	1:A:288:PRO:HD3	2.02	0.41
1:A:231:GLN:HE21	1:A:235:LYS:CD	2.21	0.41
1:A:129:VAL:HA	1:A:218:VAL:HG11	2.02	0.41
1:A:222:VAL:C	1:A:224:GLN:N	2.74	0.41
3:H:146:PHE:CG	3:H:147:PRO:HA	2.55	0.41
1:A:52:VAL:CG2	1:A:80:LEU:HD12	2.50	0.41
3:H:48:ILE:O	3:H:48:ILE:HG22	2.19	0.41
2:L:36:PHE:O	2:L:86:TYR:HA	2.20	0.41
1:A:146:THR:OG1	1:A:149:LYS:HB2	2.20	0.41
3:H:60:TYR:CZ	3:H:69:THR:HA	2.56	0.41
3:H:67:LYS:NZ	3:H:85:SER:O	2.53	0.41
2:L:15:LEU:CD1	2:L:106:ILE:HG21	2.51	0.41
2:L:49:TYR:O	2:L:50:ARG:C	2.59	0.41
3:H:60:TYR:OH	3:H:69:THR:HA	2.21	0.41
1:A:322:ASN:N	1:A:323:PRO:HD2	2.36	0.41
1:A:121:ILE:HD11	1:A:212:LEU:HB2	2.01	0.41
2:L:209:PHE:HD1	2:L:209:PHE:C	2.22	0.41
3:H:200:PRO:C	3:H:202:SER:N	2.74	0.41
2:L:37:GLN:NE2	2:L:39:LYS:HE2	2.36	0.41
2:L:121:SER:O	2:L:122:SER:C	2.59	0.41
2:L:4:MET:HE2	2:L:25:ALA:HB2	2.03	0.41
2:L:4:MET:HE1	2:L:23:CYS:SG	2.60	0.41
2:L:55:VAL:HG12	2:L:56:ASP:N	2.36	0.41
1:A:125:CYS:SG	1:A:214:ILE:HD11	2.61	0.41
2:L:112:ALA:CB	2:L:200:THR:HG21	2.51	0.41
1:A:326:TYR:CA	1:A:330:PRO:HD2	2.51	0.41
1:A:345:SER:O	1:A:347:LEU:N	2.46	0.41
1:A:240:PHE:CZ	3:H:100:PHE:HB2	2.55	0.41
1:A:267:LYS:C	1:A:269:HIS:N	2.74	0.41
3:H:170:LEU:HD13	3:H:175:TYR:CE1	2.55	0.41
2:L:129:GLY:HA2	2:L:183:LYS:N	2.35	0.41
1:A:287:LEU:CB	1:A:288:PRO:HD3	2.51	0.41
2:L:136:LEU:HD23	2:L:175:MET:HE3	2.03	0.41
2:L:179:LEU:N	2:L:179:LEU:CD2	2.84	0.41
1:A:133:PHE:HA	1:A:136:THR:HG22	2.03	0.41
3:H:211:VAL:CG1	3:H:212:PRO:HD2	2.50	0.41
1:A:239:ARG:HB2	3:H:99:GLY:HA3	2.03	0.40
2:L:52:ASN:HD21	2:L:53:ARG:HH11	1.66	0.40
3:H:18:VAL:HG21	3:H:109:LEU:HD22	2.02	0.40
3:H:137:THR:HG22	3:H:182:THR:HG23	2.03	0.40
2:L:136:LEU:HD12	2:L:196:ALA:CB	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:181:LEU:HA	2:L:181:LEU:HD23	1.83	0.40
2:L:29:ILE:HG21	2:L:90:GLN:HB2	2.02	0.40
2:L:108:ARG:CG	2:L:109:ALA:N	2.72	0.40
1:A:144:LEU:N	1:A:144:LEU:HD23	2.36	0.40
1:A:69:ASN:CA	1:A:72:ILE:HG22	2.42	0.40
2:L:179:LEU:N	2:L:179:LEU:HD23	2.24	0.40
3:H:6:GLN:HG2	3:H:107:THR:OG1	2.20	0.40
1:A:281:THR:O	1:A:285:CYS:SG	2.78	0.40
3:H:200:PRO:O	3:H:202:SER:N	2.53	0.40
1:A:235:LYS:O	1:A:239:ARG:CD	2.69	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	204/365 (56%)	151 (74%)	39 (19%)	14 (7%)	2	24
2	L	212/214 (99%)	172 (81%)	31 (15%)	9 (4%)	4	41
3	H	215/217 (99%)	159 (74%)	42 (20%)	14 (6%)	2	25
All	All	631/796 (79%)	482 (76%)	112 (18%)	37 (6%)	2	29

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	LYS
1	A	142	GLN
1	A	143	SER
1	A	241	HIS
1	A	343	ARG
2	L	2	ILE
2	L	68	GLY
2	L	153	SER
3	H	41	THR

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Mol	Chain	Res	Type
3	H	188	TRP
3	H	212	PRO
1	A	342	LEU
1	A	345	SER
2	L	51	ALA
2	L	101	GLY
2	L	138	ASN
3	H	92	ALA
3	H	127	GLY
3	H	129	ALA
3	H	144	GLY
1	A	145	LEU
1	A	329	SER
1	A	333	ARG
2	L	169	LYS
3	H	119	PRO
3	H	171	GLN
1	A	230	LEU
2	L	72	SER
3	H	26	GLY
1	A	223	PHE
3	H	16	ALA
3	H	201	ALA
3	H	214	ASP
1	A	318	ASN
3	H	215	CYS
1	A	88	PRO
2	L	128	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	167/317 (53%)	151 (90%)	16 (10%)	12	49
2	L	191/191 (100%)	172 (90%)	19 (10%)	11	47
3	H	183/183 (100%)	157 (86%)	26 (14%)	5	27
All	All	541/691 (78%)	480 (89%)	61 (11%)	9	39

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ILE
1	A	70	TYR
1	A	72	ILE
1	A	121	ILE
1	A	124	LEU
1	A	139	PHE
1	A	142	GLN
1	A	148	ASN
1	A	237	GLU
1	A	239	ARG
1	A	241	HIS
1	A	287	LEU
1	A	312	ASN
1	A	333	ARG
1	A	336	PHE
1	A	339	LEU
2	L	11	MET
2	L	27	GLN
2	L	37	GLN
2	L	38	GLN
2	L	47	LEU
2	L	50	ARG
2	L	52	ASN
2	L	70	ASP
2	L	71	TYR
2	L	102	THR
2	L	114	THR
2	L	140	TYR
2	L	144	ILE
2	L	154	GLU
2	L	157	ASN
2	L	179	LEU
2	L	190	ASN
2	L	193	THR
2	L	209	PHE
3	H	6	GLN
3	H	11	LEU
3	H	20	LEU
3	H	31	ASP
3	H	33	TYR
3	H	35	ASN
3	H	51	ILE

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Mol	Chain	Res	Type
3	H	71	THR
3	H	83	LEU
3	H	97	VAL
3	H	110	THR
3	H	124	LEU
3	H	133	ASN
3	H	138	LEU
3	H	140	CYS
3	H	141	LEU
3	H	153	THR
3	H	155	ASN
3	H	174	LEU
3	H	177	LEU
3	H	185	SER
3	H	186	SER
3	H	195	CYS
3	H	196	ASN
3	H	206	VAL
3	H	213	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	231	GLN
2	L	6	GLN
2	L	30	ASN
2	L	38	GLN
2	L	52	ASN
2	L	137	ASN
2	L	161	ASN
2	L	198	HIS
3	H	6	GLN
3	H	35	ASN
3	H	133	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	216/365 (59%)	0.51	14 (6%) 18 7	26, 154, 221, 266	0
2	L	214/214 (100%)	-0.06	0 100 100	13, 58, 108, 171	0
3	H	217/217 (100%)	-0.01	1 (0%) 88 61	12, 57, 137, 198	0
All	All	647/796 (81%)	0.15	15 (2%) 57 24	12, 74, 197, 266	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	TRP	4.1
1	A	76	ALA	4.0
1	A	85	ALA	2.8
1	A	108	PHE	2.8
1	A	88	PRO	2.8
1	A	110	THR	2.7
1	A	316	TYR	2.6
1	A	145	LEU	2.4
1	A	125	CYS	2.4
3	H	215	CYS	2.4
1	A	89	PHE	2.3
1	A	112	ILE	2.3
1	A	279	MET	2.3
1	A	37	GLY	2.3
1	A	86	VAL	2.2

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.