



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:32 AM 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

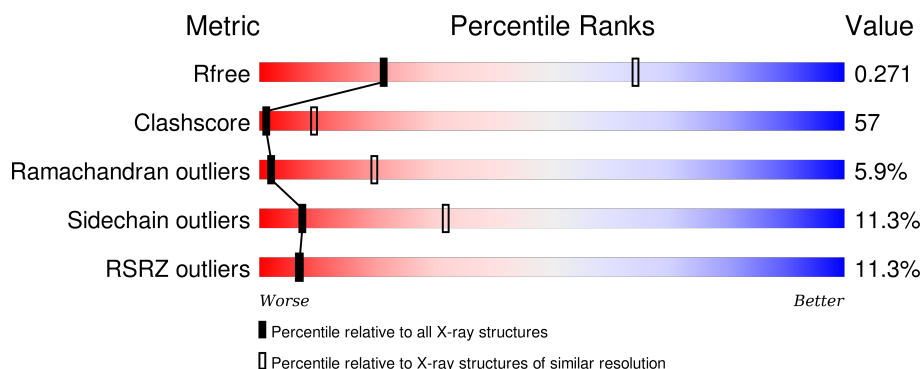
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	365	<div> <div>19%</div> <div>20% 33% 5% 41%</div> </div>
2	L	214	<div> <div>29% 61% 10%</div> </div>
3	H	217	<div> <div>% 37% 48% 15%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4925 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 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			

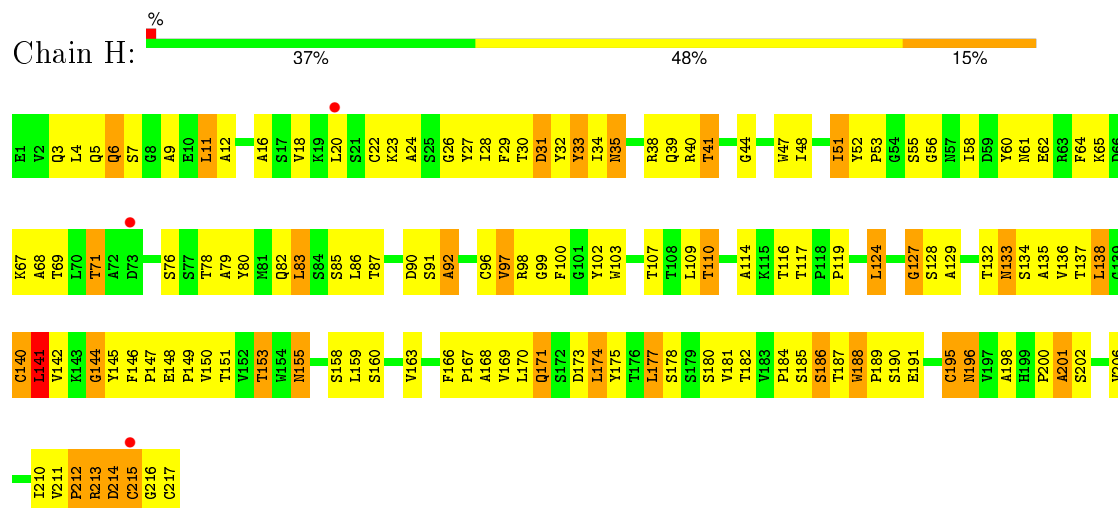
- Molecule 2 is a protein called antibody for beta2 adrenoceptor, light chain.

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			

- Molecule 3: antibody for beta2 adrenoceptor, heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.41Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.217 , 0.270 0.218 , 0.271	Depositor DCC
R_{free} test set	1902 reflections (9.72%)	DCC
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 146.3	EDS
Estimated twinning fraction	0.039 for -h-2*k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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($^{\circ}$)	Ideal($^{\circ}$)
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 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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 57.

All (556) 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)
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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:153:THR:HG23	3:H:196:ASN:HB2	1.77	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [i](#)

5.3.1 Protein backbone [i](#)

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%)	1	15
2	L	212/214 (99%)	172 (81%)	31 (15%)	9 (4%)	3	29
3	H	215/217 (99%)	159 (74%)	42 (20%)	14 (6%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	631/796 (79%)	482 (76%)	112 (18%)	37 (6%)	2	19

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
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%)	10	40
2	L	191/191 (100%)	172 (90%)	19 (10%)	10	39
3	H	183/183 (100%)	157 (86%)	26 (14%)	4	22
All	All	541/691 (78%)	480 (89%)	61 (11%)	7	32

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [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 [i](#)

There are no such residues in this entry.









5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	216/365 (59%)	1.57	70 (32%)  	26, 154, 221, 266	0
2	L	214/214 (100%)	0.10	0  	13, 58, 108, 171	0
3	H	217/217 (100%)	0.18	3 (1%)  	12, 57, 137, 198	0
All	All	647/796 (81%)	0.62	73 (11%)  	12, 74, 197, 266	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	ALA	7.3
1	A	109	TRP	6.8
1	A	112	ILE	5.4
1	A	145	LEU	5.3
1	A	281	THR	5.3
1	A	203	SER	5.2
1	A	279	MET	5.1
1	A	164	THR	5.1
1	A	37	GLY	5.0
1	A	285	CYS	5.0
1	A	146	THR	5.0
1	A	108	PHE	5.0
1	A	204	SER	4.9
1	A	85	ALA	4.8
1	A	88	PRO	4.7
1	A	51	ASN	4.6
1	A	50	GLY	4.6
1	A	125	CYS	4.2
1	A	110	THR	4.1
1	A	86	VAL	4.1
1	A	77	CYS	4.0
1	A	316	TYR	4.0
1	A	143	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	205	ILE	3.8
1	A	113	ASP	3.8
1	A	284	LEU	3.8
1	A	290	PHE	3.8
1	A	83	GLY	3.7
1	A	286	TRP	3.7
1	A	280	GLY	3.7
1	A	320	GLY	3.7
1	A	157	VAL	3.6
1	A	218	VAL	3.4
1	A	152	VAL	3.4
1	A	87	VAL	3.4
1	A	111	SER	3.3
1	A	114	VAL	3.2
1	A	158	TRP	3.1
1	A	317	VAL	3.0
1	A	116	CYS	3.0
3	H	215	CYS	3.0
1	A	150	ALA	3.0
1	A	315	GLY	3.0
1	A	230	LEU	2.9
1	A	289	PHE	2.9
1	A	211	PRO	2.8
1	A	207	SER	2.8
1	A	154	ILE	2.8
1	A	121	ILE	2.8
1	A	140	LYS	2.7
1	A	148	ASN	2.7
1	A	124	LEU	2.7
1	A	215	MET	2.7
1	A	288	PRO	2.6
1	A	89	PHE	2.6
3	H	73	ASP	2.5
1	A	144	LEU	2.5
1	A	156	MET	2.4
1	A	82	MET	2.4
1	A	162	GLY	2.4
1	A	73	THR	2.4
3	H	20	LEU	2.4
1	A	84	LEU	2.3
1	A	210	VAL	2.3
1	A	118	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	216	VAL	2.2
1	A	128	ALA	2.2
1	A	147	LYS	2.1
1	A	283	THR	2.1
1	A	282	PHE	2.1
1	A	44	VAL	2.1
1	A	208	PHE	2.0
1	A	311	LEU	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.