



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:59 AM UTC

PDB ID : 2R4S / pdb_00002r4s
Title : Crystal structure of the human beta2 adrenoceptor
Authors : Rasmussen, S.G.F.; Choi, H.J.; Rosenbaum, D.M.; Kobilka, T.S.; Thian, F.S.;
Edwards, P.C.; Burghammer, M.; Ratnala, V.R.; Sanishvili, R.; Fischetti,
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

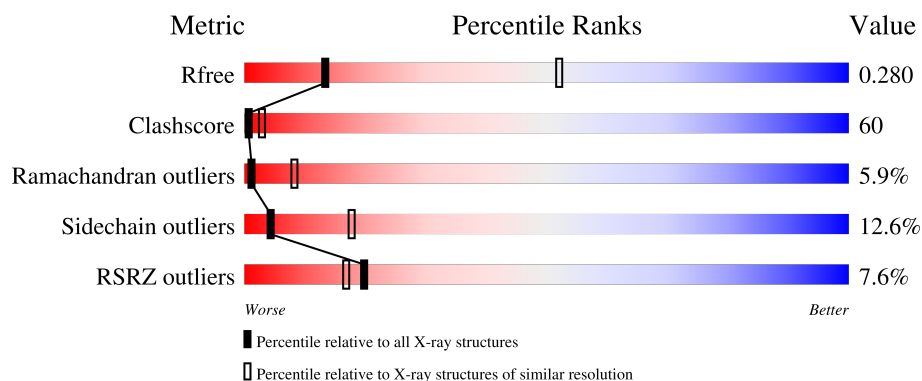
1 Overall quality at a glance

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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	342	
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 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.

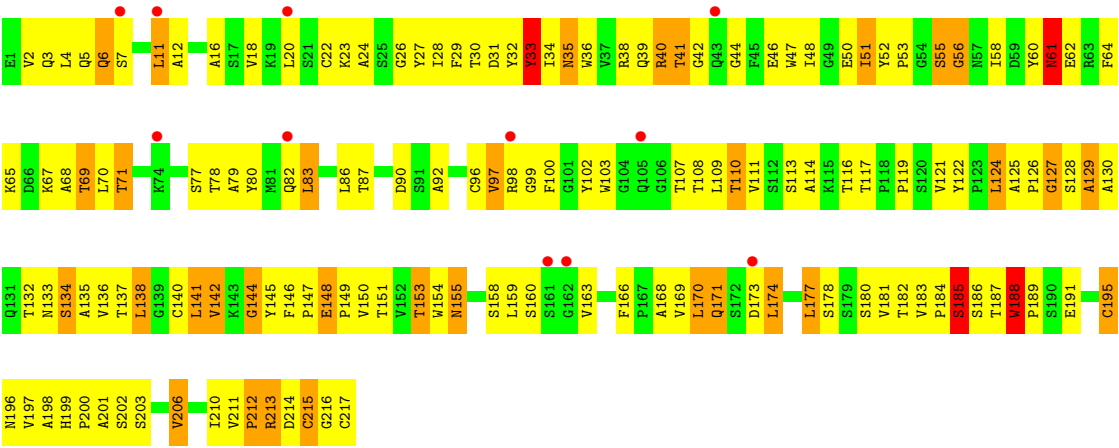
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1678	1050	278	341	9			

- 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 19.99 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.99-3.40) 97.2 (19.99-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.226 , 0.280 0.230 , 0.280	Depositor DCC
R_{free} test set	1904 reflections (9.77%)	wwPDB-VP
Wilson B-factor (Å ²)	97.9	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 97.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.018 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4925	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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, 0.333 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	0.39	0/1636	1.01	9/2216 (0.4%)
2	L	0.53	0/1716	1.06	9/2324 (0.4%)
3	H	0.56	0/1677	1.10	11/2290 (0.5%)
All	All	0.50	0/5029	1.06	29/6830 (0.4%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	LYS	N-CA-C	-12.24	98.39	113.20
2	L	183	LYS	N-CA-C	-10.97	99.34	111.07
3	H	33	TYR	N-CA-C	-8.75	99.24	110.53
3	H	134	SER	N-CA-C	-7.36	103.77	112.89
2	L	136	LEU	N-CA-C	-6.99	97.85	108.96
3	H	206	VAL	N-CA-C	6.80	117.33	108.35
2	L	102	THR	N-CA-C	-6.46	99.19	109.59
3	H	203	SER	N-CA-C	-6.26	103.20	111.02
1	A	161	SER	N-CA-C	-6.19	105.55	113.23
3	H	183	VAL	CA-C-N	-6.11	113.40	119.99
3	H	183	VAL	C-N-CA	-6.11	113.40	119.99
1	A	226	ALA	N-CA-C	-5.97	105.99	113.28
3	H	122	TYR	N-CA-C	-5.94	101.16	110.14
2	L	9	SER	N-CA-C	-5.90	104.22	112.12
2	L	205	ILE	N-CA-C	-5.87	101.23	109.21
1	A	150	ALA	N-CA-C	-5.72	104.50	112.45
3	H	185	SER	N-CA-C	-5.71	105.41	112.38
2	L	55	VAL	N-CA-C	-5.53	104.02	110.05
2	L	76	SER	N-CA-C	-5.43	101.69	110.32
1	A	272	LEU	N-CA-C	-5.39	106.37	113.17
1	A	279	MET	N-CA-C	-5.37	106.57	113.23
3	H	113	SER	N-CA-C	-5.33	106.28	112.89
1	A	273	LYS	N-CA-C	-5.28	105.12	112.45
2	L	137	ASN	N-CA-C	5.27	117.87	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	TYR	N-CA-C	-5.22	107.28	113.97
3	H	188	TRP	N-CA-C	5.18	121.25	109.81
2	L	202	THR	N-CA-C	-5.16	107.37	113.97
1	A	218	VAL	N-CA-C	-5.15	104.65	111.09
3	H	61	ASN	N-CA-C	-5.02	101.52	109.96

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	1612	0	1610	199	0
2	L	1678	0	1610	211	0
3	H	1635	0	1578	196	0
All	All	4925	0	4798	588	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 60.

All (588) 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	1.29	1.10
2:L:169:LYS:H	2:L:169:LYS:HD2	1.20	1.03
2:L:108:ARG:HG2	2:L:109:ALA:H	1.25	0.99
2:L:38:GLN:NE2	3:H:39:GLN:HE22	1.60	0.98
2:L:38:GLN:HE21	3:H:39:GLN:HE22	0.98	0.94
3:H:155:ASN:HB3	3:H:158:SER:HB2	1.52	0.90
2:L:38:GLN:HE21	3:H:39:GLN:NE2	1.70	0.88
2:L:66:GLY:HA3	2:L:71:TYR:HA	1.55	0.87
2:L:44:PRO:HG2	3:H:103:TRP:CD2	2.09	0.86
1:A:69:ASN:HA	1:A:72:ILE:HG22	1.57	0.85
2:L:211:ARG:HH11	2:L:211:ARG:HB3	1.42	0.83
1:A:64:LEU:HD11	1:A:335:ALA:HB1	1.58	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:TYR:HE1	1:A:221:ARG:HG2	1.45	0.82
2:L:206:VAL:O	2:L:207:LYS:HD3	1.79	0.82
3:H:153:THR:HG23	3:H:196:ASN:HB2	1.62	0.81
1:A:71:PHE:HB3	1:A:127:ILE:HD11	1.60	0.81
3:H:147:PRO:HD2	3:H:201:ALA:HB1	1.62	0.81
2:L:190:ASN:N	2:L:190:ASN:HD22	1.79	0.80
2:L:52:ASN:HD22	2:L:53:ARG:N	1.80	0.80
2:L:182:THR:H	2:L:185:GLU:HB2	1.47	0.79
3:H:40:ARG:HB2	3:H:40:ARG:HH11	1.47	0.78
2:L:27:GLN:O	2:L:69:GLN:HG3	1.83	0.78
1:A:48:VAL:HG13	1:A:84:LEU:HD11	1.64	0.77
3:H:87:THR:HG22	3:H:90:ASP:OD2	1.85	0.77
3:H:141:LEU:HD13	3:H:141:LEU:O	1.84	0.77
1:A:337:GLN:HE21	1:A:343:ARG:HG2	1.47	0.77
3:H:109:LEU:HD12	3:H:110:THR:N	2.00	0.77
3:H:35:ASN:HD22	3:H:35:ASN:H	1.33	0.76
3:H:83:LEU:HB3	3:H:86:LEU:HD21	1.66	0.76
2:L:47:LEU:HA	2:L:58:VAL:HG21	1.69	0.75
3:H:137:THR:HA	3:H:181:VAL:O	1.87	0.75
3:H:169:VAL:HG12	3:H:170:LEU:O	1.86	0.75
3:H:40:ARG:HA	3:H:92:ALA:HB1	1.66	0.75
3:H:38:ARG:HB2	3:H:48:ILE:HD11	1.69	0.75
2:L:89:LEU:HD12	2:L:90:GLN:N	2.02	0.74
2:L:112:ALA:HB2	2:L:200:THR:OG1	1.86	0.74
2:L:14:SER:HB3	2:L:107:LYS:HG3	1.68	0.74
2:L:16:GLY:O	2:L:77:SER:HA	1.86	0.74
2:L:157:ASN:C	2:L:157:ASN:HD22	1.94	0.73
3:H:177:LEU:HD12	3:H:178:SER:N	2.03	0.73
3:H:109:LEU:HD12	3:H:110:THR:H	1.54	0.73
1:A:336:PHE:HA	1:A:339:LEU:HD23	1.68	0.73
3:H:116:THR:HG23	3:H:146:PHE:O	1.89	0.73
2:L:108:ARG:HG2	2:L:109:ALA:N	1.99	0.73
2:L:179:LEU:HD23	2:L:179:LEU:H	1.54	0.72
3:H:127:GLY:HA2	3:H:213:ARG:HH12	1.53	0.72
2:L:89:LEU:HD12	2:L:90:GLN:H	1.54	0.72
3:H:199:HIS:NE2	3:H:201:ALA:HB3	2.04	0.72
3:H:11:LEU:HD13	3:H:12:ALA:N	2.03	0.72
2:L:53:ARG:HG3	2:L:53:ARG:HH11	1.54	0.71
1:A:51:ASN:O	1:A:55:ILE:HG23	1.89	0.71
1:A:148:ASN:HD22	1:A:149:LYS:H	1.34	0.71
1:A:235:LYS:HB2	2:L:32:TYR:CZ	2.26	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:THR:O	1:A:287:LEU:HB2	1.91	0.70
1:A:267:LYS:C	1:A:267:LYS:HD3	2.17	0.70
1:A:231:GLN:C	1:A:233:ILE:H	1.97	0.70
3:H:214:ASP:C	3:H:216:GLY:H	2.00	0.69
1:A:124:LEU:HD13	1:A:279:MET:HG2	1.74	0.69
2:L:24:LYS:HG2	2:L:70:ASP:HB3	1.73	0.69
1:A:87:VAL:N	1:A:88:PRO:HD2	2.07	0.69
3:H:69:THR:OG1	3:H:82:GLN:HB3	1.91	0.69
2:L:11:MET:SD	2:L:19:VAL:HG23	2.32	0.69
1:A:52:VAL:HG13	1:A:55:ILE:HD11	1.75	0.69
1:A:52:VAL:HA	1:A:55:ILE:HG12	1.74	0.69
3:H:4:LEU:HB3	3:H:22:CYS:SG	2.33	0.69
3:H:18:VAL:HG22	3:H:86:LEU:HD11	1.74	0.69
2:L:144:ILE:HD13	2:L:145:ASN:H	1.57	0.68
1:A:127:ILE:HD12	1:A:127:ILE:H	1.56	0.68
2:L:6:GLN:HE22	2:L:101:GLY:HA2	1.57	0.68
3:H:127:GLY:HA2	3:H:213:ARG:NH1	2.08	0.68
3:H:27:TYR:CE2	3:H:98:ARG:HD2	2.28	0.68
1:A:209:TYR:O	1:A:213:VAL:HG23	1.93	0.68
2:L:136:LEU:HD21	2:L:146:VAL:HG11	1.76	0.68
3:H:97:VAL:HG12	3:H:103:TRP:HA	1.75	0.68
1:A:148:ASN:ND2	1:A:149:LYS:H	1.92	0.68
2:L:35:TRP:CD2	2:L:73:LEU:HB2	2.28	0.68
2:L:21:ILE:HB	2:L:102:THR:HG21	1.74	0.67
2:L:18:ARG:HB3	2:L:76:SER:HA	1.76	0.67
1:A:132:TYR:CE1	1:A:221:ARG:HG2	2.30	0.67
3:H:35:ASN:HD21	3:H:99:GLY:HA2	1.59	0.67
3:H:40:ARG:HB2	3:H:40:ARG:NH1	2.11	0.66
1:A:231:GLN:HE21	1:A:235:LYS:HD2	1.60	0.66
1:A:278:ILE:HG13	1:A:322:ASN:OD1	1.96	0.66
2:L:136:LEU:HD11	2:L:196:ALA:HB2	1.77	0.66
2:L:142:LYS:HA	2:L:173:TYR:CD2	2.31	0.66
2:L:108:ARG:CG	2:L:109:ALA:H	2.03	0.65
3:H:6:GLN:HE22	3:H:96:CYS:CB	2.08	0.65
2:L:54:LEU:HD22	2:L:58:VAL:HB	1.79	0.65
1:A:343:ARG:HG3	1:A:344:ARG:N	2.11	0.65
1:A:231:GLN:C	1:A:233:ILE:N	2.54	0.65
2:L:95:PRO:O	2:L:97:THR:HG23	1.97	0.65
1:A:124:LEU:HB3	1:A:215:MET:HE2	1.80	0.64
2:L:148:TRP:CE2	2:L:179:LEU:HD22	2.32	0.64
1:A:336:PHE:O	1:A:339:LEU:HG	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:11:LEU:HD23	3:H:147:PRO:HG3	1.80	0.64
3:H:23:LYS:HG3	3:H:78:THR:HG22	1.78	0.64
2:L:159:VAL:HG12	2:L:161:ASN:HD21	1.61	0.64
3:H:5:GLN:O	3:H:22:CYS:HA	1.97	0.64
2:L:20:THR:HG23	2:L:74:THR:OG1	1.98	0.64
2:L:24:LYS:HG2	2:L:70:ASP:CB	2.28	0.64
3:H:40:ARG:HG2	3:H:41:THR:H	1.63	0.64
1:A:71:PHE:CB	1:A:127:ILE:HD11	2.27	0.63
2:L:157:ASN:HD22	2:L:158:GLY:N	1.95	0.63
2:L:159:VAL:HG12	2:L:161:ASN:ND2	2.12	0.63
2:L:120:PRO:CG	2:L:130:ALA:HB1	2.27	0.63
1:A:235:LYS:HE3	2:L:92:ASP:O	1.99	0.63
1:A:44:VAL:O	1:A:48:VAL:HG23	1.98	0.62
1:A:153:ILE:O	1:A:157:VAL:HG23	1.98	0.62
2:L:79:ASP:HB3	2:L:82:ASP:OD2	1.98	0.62
1:A:148:ASN:HD22	1:A:148:ASN:N	1.97	0.62
2:L:2:ILE:HG12	2:L:2:ILE:O	1.97	0.62
1:A:270:LYS:O	1:A:273:LYS:HB3	2.00	0.62
1:A:69:ASN:HA	1:A:72:ILE:CG2	2.28	0.62
1:A:339:LEU:HD12	1:A:339:LEU:C	2.25	0.62
2:L:4:MET:HE3	2:L:25:ALA:HB2	1.80	0.62
2:L:6:GLN:NE2	2:L:101:GLY:HA2	2.14	0.62
2:L:148:TRP:CZ2	2:L:179:LEU:HD22	2.35	0.62
3:H:35:ASN:HD22	3:H:35:ASN:N	1.96	0.62
1:A:134:ALA:O	1:A:137:SER:HB3	2.00	0.61
2:L:132:VAL:HB	2:L:179:LEU:HD21	1.81	0.61
2:L:160:LEU:HD23	2:L:160:LEU:C	2.25	0.61
3:H:188:TRP:CE3	3:H:189:PRO:HD3	2.35	0.61
2:L:49:TYR:CD1	2:L:50:ARG:HB2	2.34	0.61
1:A:205:ILE:O	1:A:210:VAL:HG23	1.99	0.61
3:H:133:ASN:ND2	3:H:134:SER:H	1.99	0.61
3:H:136:VAL:O	3:H:182:THR:HA	2.01	0.61
2:L:144:ILE:CD1	2:L:145:ASN:H	2.12	0.61
2:L:10:SER:O	2:L:11:MET:HB2	2.01	0.61
3:H:6:GLN:HE22	3:H:96:CYS:HB3	1.66	0.61
1:A:58:ILE:HD13	1:A:58:ILE:C	2.26	0.61
1:A:337:GLN:NE2	1:A:343:ARG:HG2	2.16	0.61
3:H:56:GLY:O	3:H:58:ILE:HG13	2.00	0.61
1:A:242:VAL:HG23	3:H:32:TYR:OH	2.00	0.60
3:H:33:TYR:HA	3:H:53:PRO:HD2	1.83	0.60
2:L:59:PRO:HG2	2:L:62:PHE:CE1	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:34:ILE:HD11	3:H:79:ALA:HB3	1.82	0.60
3:H:6:GLN:NE2	3:H:96:CYS:HB3	2.16	0.60
3:H:40:ARG:HA	3:H:92:ALA:CB	2.30	0.60
3:H:142:VAL:O	3:H:142:VAL:HG22	2.00	0.60
1:A:333:ARG:HG2	1:A:333:ARG:HH11	1.67	0.60
2:L:44:PRO:HG2	3:H:103:TRP:CG	2.37	0.60
2:L:108:ARG:HG2	2:L:108:ARG:HH11	1.67	0.60
1:A:275:LEU:HA	1:A:278:ILE:HG22	1.84	0.59
1:A:124:LEU:CD1	1:A:279:MET:HG2	2.31	0.59
3:H:40:ARG:HG2	3:H:41:THR:N	2.17	0.59
2:L:47:LEU:O	2:L:55:VAL:HG23	2.01	0.59
2:L:132:VAL:HB	2:L:179:LEU:CD2	2.33	0.59
2:L:113:PRO:HA	2:L:137:ASN:O	2.03	0.59
1:A:235:LYS:O	1:A:239:ARG:HD3	2.02	0.59
1:A:283:THR:HG23	1:A:284:LEU:HD12	1.84	0.59
2:L:135:PHE:CZ	3:H:180:SER:HB3	2.38	0.59
3:H:68:ALA:HA	3:H:82:GLN:O	2.02	0.59
3:H:35:ASN:N	3:H:35:ASN:ND2	2.50	0.59
2:L:71:TYR:CD1	2:L:71:TYR:N	2.70	0.58
3:H:2:VAL:O	3:H:3:GLN:HB3	2.02	0.58
1:A:209:TYR:C	1:A:213:VAL:HG23	2.29	0.58
2:L:190:ASN:N	2:L:190:ASN:ND2	2.51	0.58
3:H:38:ARG:HD2	3:H:46:GLU:CD	2.29	0.58
2:L:1:ASP:HB3	2:L:95:PRO:HD2	1.85	0.58
2:L:47:LEU:C	2:L:55:VAL:HG23	2.28	0.58
3:H:7:SER:HB2	3:H:107:THR:HG23	1.85	0.58
1:A:44:VAL:HG22	1:A:87:VAL:HG11	1.85	0.58
1:A:83:GLY:HA2	1:A:87:VAL:CG2	2.34	0.58
2:L:111:ALA:O	2:L:139:PHE:HA	2.04	0.58
2:L:184:ASP:O	2:L:185:GLU:C	2.47	0.58
2:L:80:TYR:CD1	2:L:81:ALA:N	2.72	0.58
2:L:6:GLN:HE21	2:L:102:THR:HG22	1.69	0.58
3:H:6:GLN:NE2	3:H:96:CYS:CB	2.67	0.58
3:H:124:LEU:HD21	3:H:141:LEU:H	1.69	0.58
1:A:71:PHE:O	1:A:74:SER:HB3	2.05	0.57
1:A:239:ARG:HB2	3:H:99:GLY:O	2.04	0.57
1:A:332:PHE:HA	1:A:335:ALA:HB3	1.86	0.57
2:L:53:ARG:HG3	2:L:53:ARG:NH1	2.19	0.57
2:L:8:PRO:O	2:L:102:THR:HB	2.04	0.57
2:L:160:LEU:HD23	2:L:160:LEU:O	2.05	0.57
3:H:138:LEU:HD12	3:H:210:ILE:HD12	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:166:PHE:N	3:H:166:PHE:CD1	2.71	0.57
2:L:15:LEU:CD1	2:L:106:ILE:HG21	2.34	0.57
2:L:4:MET:SD	2:L:90:GLN:HB3	2.44	0.57
3:H:71:THR:HG23	3:H:80:TYR:HB2	1.86	0.57
1:A:235:LYS:HB2	2:L:32:TYR:CE1	2.40	0.57
2:L:136:LEU:CD1	2:L:196:ALA:HB2	2.34	0.57
1:A:230:LEU:O	1:A:233:ILE:HD12	2.05	0.57
2:L:182:THR:HG22	2:L:183:LYS:H	1.69	0.57
1:A:52:VAL:O	1:A:55:ILE:HG12	2.05	0.57
1:A:327:CYS:O	1:A:333:ARG:HG2	2.05	0.57
2:L:52:ASN:HD22	2:L:53:ARG:H	1.49	0.57
2:L:63:ILE:N	2:L:74:THR:O	2.37	0.57
1:A:128:ALA:O	1:A:218:VAL:HG12	2.05	0.56
1:A:148:ASN:HD22	1:A:149:LYS:N	2.03	0.56
2:L:209:PHE:CD1	2:L:209:PHE:C	2.82	0.56
1:A:83:GLY:HA2	1:A:87:VAL:HG23	1.86	0.56
1:A:283:THR:HG23	1:A:284:LEU:CD1	2.35	0.56
1:A:337:GLN:O	1:A:343:ARG:HB2	2.05	0.56
2:L:170:ASP:OD2	2:L:172:THR:HG21	2.05	0.56
2:L:59:PRO:HG2	2:L:62:PHE:HE1	1.70	0.56
3:H:214:ASP:O	3:H:216:GLY:N	2.38	0.56
3:H:121:VAL:CG2	3:H:197:VAL:HG21	2.36	0.56
2:L:29:ILE:HG22	2:L:92:ASP:HB3	1.87	0.56
3:H:144:GLY:C	3:H:174:LEU:HD12	2.31	0.56
1:A:83:GLY:O	1:A:88:PRO:HD3	2.04	0.56
3:H:136:VAL:HG12	3:H:138:LEU:HD23	1.87	0.56
3:H:188:TRP:CH2	3:H:212:PRO:HA	2.41	0.56
1:A:81:VAL:O	1:A:85:ALA:HB3	2.06	0.56
2:L:13:ALA:O	2:L:106:ILE:HA	2.06	0.56
3:H:40:ARG:HH11	3:H:40:ARG:CB	2.18	0.56
1:A:148:ASN:ND2	1:A:148:ASN:H	2.04	0.55
1:A:344:ARG:C	1:A:346:SER:H	2.14	0.55
2:L:120:PRO:HG2	2:L:130:ALA:HB1	1.88	0.55
2:L:142:LYS:HB2	2:L:173:TYR:CE2	2.41	0.55
3:H:116:THR:HG22	3:H:117:THR:N	2.21	0.55
1:A:58:ILE:HG23	1:A:59:ALA:H	1.70	0.55
1:A:233:ILE:HG22	1:A:234:ASP:N	2.21	0.55
1:A:141:TYR:OH	1:A:272:LEU:HD21	2.07	0.55
2:L:139:PHE:CE1	2:L:144:ILE:HB	2.41	0.55
2:L:199:LYS:O	2:L:200:THR:C	2.49	0.55
3:H:67:LYS:HG3	3:H:83:LEU:CD1	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ILE:HD13	1:A:121:ILE:O	2.06	0.55
1:A:220:SER:O	1:A:224:GLN:HG2	2.07	0.55
2:L:200:THR:HG23	2:L:201:SER:N	2.22	0.55
3:H:51:ILE:HG12	3:H:58:ILE:HG12	1.87	0.55
1:A:267:LYS:C	1:A:269:HIS:H	2.15	0.55
1:A:326:TYR:HA	1:A:330:PRO:CD	2.36	0.55
2:L:198:HIS:HD2	2:L:200:THR:HB	1.72	0.55
2:L:50:ARG:HH21	2:L:53:ARG:HH12	1.55	0.54
3:H:40:ARG:C	3:H:41:THR:O	2.49	0.54
3:H:51:ILE:CG1	3:H:58:ILE:HG12	2.36	0.54
2:L:52:ASN:ND2	2:L:53:ARG:N	2.55	0.54
3:H:35:ASN:ND2	3:H:99:GLY:HA2	2.21	0.54
1:A:110:THR:O	1:A:110:THR:HG22	2.07	0.54
3:H:6:GLN:HG2	3:H:107:THR:OG1	2.08	0.54
1:A:240:PHE:O	1:A:242:VAL:N	2.39	0.54
2:L:33:LEU:C	2:L:33:LEU:HD23	2.32	0.54
3:H:138:LEU:HD23	3:H:138:LEU:N	2.23	0.54
3:H:151:THR:HB	3:H:198:ALA:HB3	1.90	0.54
1:A:80:LEU:C	1:A:80:LEU:HD23	2.33	0.54
2:L:38:GLN:NE2	3:H:39:GLN:NE2	2.38	0.54
3:H:110:THR:HG21	3:H:147:PRO:HB2	1.89	0.54
1:A:58:ILE:HD13	1:A:59:ALA:N	2.23	0.54
1:A:229:GLN:NE2	1:A:264:PHE:HB3	2.22	0.54
3:H:146:PHE:CD1	3:H:146:PHE:C	2.86	0.54
2:L:11:MET:CE	2:L:13:ALA:HB2	2.38	0.53
1:A:135:ILE:HD12	1:A:222:VAL:HG13	1.89	0.53
1:A:324:LEU:C	1:A:324:LEU:HD23	2.33	0.53
1:A:332:PHE:O	1:A:333:ARG:C	2.51	0.53
3:H:47:TRP:CE3	3:H:61:ASN:HB2	2.44	0.53
3:H:48:ILE:O	3:H:48:ILE:HG22	2.07	0.53
3:H:145:TYR:O	3:H:146:PHE:HB2	2.08	0.53
1:A:50:GLY:O	1:A:54:VAL:HG23	2.08	0.53
1:A:229:GLN:O	1:A:231:GLN:N	2.41	0.53
3:H:60:TYR:CE2	3:H:69:THR:HA	2.43	0.53
1:A:336:PHE:HD2	1:A:337:GLN:N	2.05	0.53
2:L:125:LEU:CD2	2:L:130:ALA:HB2	2.38	0.53
1:A:287:LEU:HD22	1:A:291:ILE:HG13	1.89	0.53
2:L:29:ILE:HG22	2:L:92:ASP:CB	2.38	0.53
2:L:103:LYS:HZ3	2:L:105:GLU:HG3	1.74	0.53
3:H:36:TRP:O	3:H:48:ILE:HB	2.09	0.53
1:A:54:VAL:O	1:A:58:ILE:HG22	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:52:ASN:HD21	2:L:53:ARG:HH11	1.57	0.53
3:H:132:THR:O	3:H:133:ASN:HB2	2.09	0.53
3:H:137:THR:HG22	3:H:182:THR:OG1	2.09	0.53
3:H:148:GLU:OE1	3:H:149:PRO:HA	2.07	0.53
1:A:66:THR:O	1:A:70:TYR:HB2	2.09	0.53
2:L:115:VAL:HA	2:L:135:PHE:O	2.09	0.53
1:A:275:LEU:HA	1:A:278:ILE:CG2	2.38	0.52
2:L:137:ASN:HD22	2:L:174:SER:HB3	1.74	0.52
3:H:177:LEU:HD12	3:H:177:LEU:C	2.33	0.52
2:L:85:ILE:HG12	2:L:103:LYS:HG3	1.92	0.52
2:L:140:TYR:CD1	2:L:140:TYR:C	2.88	0.52
1:A:326:TYR:C	1:A:330:PRO:HD2	2.35	0.52
3:H:99:GLY:O	3:H:100:PHE:HB2	2.10	0.52
1:A:329:SER:HB2	1:A:330:PRO:HD3	1.90	0.52
1:A:234:ASP:O	1:A:237:GLU:HB2	2.09	0.52
2:L:108:ARG:HG2	2:L:108:ARG:NH1	2.25	0.52
2:L:206:VAL:HG12	2:L:207:LYS:N	2.25	0.52
1:A:139:PHE:CZ	1:A:140:LYS:HE2	2.45	0.52
2:L:125:LEU:HD23	2:L:130:ALA:HB2	1.91	0.52
3:H:11:LEU:HD23	3:H:147:PRO:CG	2.40	0.52
2:L:19:VAL:HG13	2:L:75:ILE:HG23	1.92	0.52
2:L:70:ASP:C	2:L:71:TYR:CD1	2.88	0.51
3:H:147:PRO:HD2	3:H:201:ALA:CB	2.38	0.51
1:A:82:MET:O	1:A:87:VAL:HG23	2.11	0.51
1:A:71:PHE:O	1:A:75:LEU:HD13	2.11	0.51
3:H:34:ILE:HD11	3:H:79:ALA:CB	2.39	0.51
3:H:34:ILE:HB	3:H:97:VAL:O	2.10	0.51
3:H:133:ASN:HB3	3:H:135:ALA:O	2.10	0.51
1:A:240:PHE:O	1:A:241:HIS:C	2.52	0.51
3:H:150:VAL:HG23	3:H:150:VAL:O	2.10	0.51
1:A:161:SER:C	1:A:164:THR:HG22	2.35	0.51
2:L:182:THR:HG22	2:L:183:LYS:N	2.26	0.51
3:H:200:PRO:O	3:H:201:ALA:C	2.53	0.51
2:L:135:PHE:CE1	3:H:180:SER:HB3	2.45	0.51
3:H:128:SER:HA	3:H:217:CYS:C	2.36	0.51
2:L:11:MET:HE1	2:L:13:ALA:HB2	1.93	0.51
2:L:61:ARG:O	2:L:75:ILE:HA	2.10	0.51
3:H:144:GLY:CA	3:H:174:LEU:HD12	2.41	0.51
3:H:4:LEU:CD1	3:H:102:TYR:HD2	2.24	0.51
3:H:11:LEU:HD13	3:H:12:ALA:H	1.75	0.51
3:H:188:TRP:CZ2	3:H:212:PRO:HA	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:214:ASP:C	3:H:216:GLY:N	2.67	0.51
1:A:127:ILE:HD12	1:A:127:ILE:N	2.24	0.51
1:A:146:THR:HG1	1:A:149:LYS:HB2	1.75	0.51
2:L:198:HIS:CD2	2:L:200:THR:HB	2.46	0.51
2:L:35:TRP:HB3	2:L:73:LEU:HD22	1.93	0.50
1:A:212:LEU:HD23	1:A:212:LEU:O	2.11	0.50
2:L:170:ASP:O	2:L:171:SER:C	2.54	0.50
3:H:114:ALA:HB3	3:H:146:PHE:CZ	2.47	0.50
3:H:148:GLU:OE1	3:H:148:GLU:HA	2.11	0.50
1:A:325:ILE:O	1:A:329:SER:HB2	2.12	0.50
2:L:6:GLN:HE21	2:L:102:THR:CG2	2.25	0.50
2:L:157:ASN:C	2:L:157:ASN:ND2	2.65	0.50
2:L:189:HIS:C	2:L:190:ASN:HD22	2.19	0.50
2:L:197:THR:HG22	2:L:204:PRO:HG3	1.94	0.50
3:H:200:PRO:C	3:H:202:SER:N	2.66	0.50
1:A:88:PRO:HG2	1:A:89:PHE:H	1.77	0.50
1:A:233:ILE:CG2	1:A:234:ASP:N	2.74	0.50
1:A:322:ASN:C	1:A:324:LEU:H	2.20	0.50
2:L:19:VAL:HG22	2:L:20:THR:N	2.27	0.50
2:L:155:ARG:HG2	2:L:156:GLN:N	2.26	0.50
3:H:136:VAL:HG12	3:H:137:THR:N	2.26	0.50
3:H:145:TYR:N	3:H:174:LEU:CD1	2.75	0.50
1:A:157:VAL:O	1:A:161:SER:HB2	2.12	0.49
2:L:4:MET:HG2	2:L:25:ALA:CB	2.42	0.49
2:L:52:ASN:HD22	2:L:52:ASN:C	2.18	0.49
2:L:170:ASP:OD2	2:L:172:THR:CG2	2.60	0.49
3:H:12:ALA:O	3:H:111:VAL:HA	2.12	0.49
1:A:117:VAL:HG21	1:A:286:TRP:CH2	2.46	0.49
1:A:148:ASN:ND2	1:A:149:LYS:N	2.58	0.49
2:L:49:TYR:HD1	2:L:50:ARG:HB2	1.74	0.49
1:A:317:VAL:C	1:A:319:SER:H	2.21	0.49
3:H:168:ALA:HB2	3:H:177:LEU:HD23	1.94	0.49
3:H:48:ILE:HG23	3:H:64:PHE:CG	2.47	0.49
1:A:224:GLN:O	1:A:227:LYS:HB2	2.12	0.49
1:A:212:LEU:HD23	1:A:212:LEU:C	2.37	0.49
2:L:2:ILE:HG13	2:L:26:SER:OG	2.13	0.49
1:A:146:THR:OG1	1:A:148:ASN:ND2	2.46	0.49
2:L:18:ARG:CB	2:L:76:SER:HA	2.41	0.49
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.47	0.49
2:L:121:SER:O	2:L:122:SER:C	2.54	0.49
1:A:229:GLN:O	1:A:230:LEU:C	2.56	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:52:TYR:HD2	3:H:55:SER:HB3	1.77	0.49
3:H:136:VAL:HG23	3:H:185:SER:HB3	1.95	0.49
2:L:47:LEU:HA	2:L:58:VAL:CG2	2.41	0.49
2:L:139:PHE:CD2	2:L:173:TYR:O	2.66	0.49
1:A:52:VAL:CA	1:A:55:ILE:HG12	2.42	0.48
3:H:11:LEU:HD21	3:H:146:PHE:HE1	1.78	0.48
3:H:163:VAL:HG13	3:H:163:VAL:O	2.13	0.48
3:H:188:TRP:CG	3:H:189:PRO:N	2.81	0.48
2:L:108:ARG:HB3	2:L:140:TYR:CD2	2.48	0.48
3:H:138:LEU:HD12	3:H:210:ILE:CD1	2.42	0.48
1:A:87:VAL:N	1:A:88:PRO:CD	2.75	0.48
1:A:344:ARG:O	1:A:348:LYS:HB2	2.13	0.48
2:L:29:ILE:HD12	2:L:33:LEU:HB2	1.95	0.48
2:L:78:LEU:HD12	2:L:82:ASP:HB2	1.93	0.48
3:H:116:THR:CG2	3:H:117:THR:N	2.77	0.48
3:H:30:THR:O	3:H:31:ASP:OD1	2.31	0.48
3:H:146:PHE:CD1	3:H:147:PRO:N	2.81	0.48
1:A:329:SER:CB	1:A:330:PRO:HD3	2.44	0.48
1:A:336:PHE:CD2	1:A:337:GLN:N	2.81	0.48
1:A:58:ILE:HG23	1:A:59:ALA:N	2.29	0.48
2:L:144:ILE:HG23	2:L:145:ASN:N	2.29	0.48
2:L:151:ASP:C	2:L:153:SER:H	2.22	0.48
3:H:47:TRP:CZ3	3:H:61:ASN:HB2	2.49	0.48
1:A:133:PHE:O	1:A:137:SER:HB2	2.14	0.47
2:L:198:HIS:O	2:L:199:LYS:C	2.57	0.47
3:H:121:VAL:HG21	3:H:197:VAL:HG21	1.96	0.47
1:A:132:TYR:O	1:A:136:THR:HG22	2.14	0.47
1:A:52:VAL:O	1:A:56:THR:HG22	2.13	0.47
1:A:112:ILE:O	1:A:116:CYS:SG	2.71	0.47
1:A:117:VAL:HG11	1:A:286:TRP:CZ3	2.49	0.47
3:H:188:TRP:O	3:H:191:GLU:O	2.33	0.47
2:L:136:LEU:HD23	2:L:175:MET:HE3	1.96	0.47
3:H:4:LEU:N	3:H:4:LEU:HD12	2.30	0.47
3:H:124:LEU:HD22	3:H:140:CYS:HA	1.96	0.47
3:H:142:VAL:O	3:H:142:VAL:CG2	2.62	0.47
3:H:153:THR:OG1	3:H:154:TRP:N	2.48	0.47
1:A:238:GLY:O	3:H:32:TYR:HA	2.15	0.47
1:A:334:ILE:HG23	1:A:338:GLU:CD	2.40	0.47
1:A:342:LEU:HB3	1:A:346:SER:CB	2.44	0.47
1:A:345:SER:C	1:A:347:LEU:H	2.22	0.47
3:H:128:SER:HA	3:H:217:CYS:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:145:TYR:CE1	3:H:150:VAL:HG13	2.49	0.47
2:L:49:TYR:CD1	2:L:49:TYR:C	2.92	0.47
2:L:161:ASN:N	2:L:161:ASN:HD22	2.11	0.47
2:L:211:ARG:HH11	2:L:211:ARG:CB	2.21	0.47
3:H:67:LYS:HG3	3:H:83:LEU:HD11	1.96	0.47
3:H:213:ARG:C	3:H:215:CYS:H	2.21	0.47
2:L:19:VAL:CG1	2:L:75:ILE:HG23	2.45	0.47
2:L:195:GLU:HG2	2:L:206:VAL:HG22	1.96	0.47
3:H:146:PHE:CG	3:H:147:PRO:HA	2.50	0.47
3:H:199:HIS:HE2	3:H:201:ALA:HB3	1.77	0.47
2:L:19:VAL:CG2	2:L:20:THR:N	2.78	0.47
1:A:52:VAL:HG22	1:A:80:LEU:HD12	1.97	0.47
1:A:230:LEU:HD22	1:A:269:HIS:CE1	2.49	0.47
1:A:331:ASP:O	1:A:332:PHE:C	2.58	0.47
3:H:200:PRO:O	3:H:202:SER:N	2.48	0.47
1:A:43:ILE:HG22	1:A:43:ILE:O	2.14	0.46
3:H:154:TRP:CZ3	3:H:181:VAL:HG11	2.50	0.46
3:H:155:ASN:ND2	3:H:159:LEU:HD13	2.31	0.46
2:L:136:LEU:CD2	2:L:146:VAL:HG11	2.43	0.46
3:H:160:SER:O	3:H:163:VAL:HG12	2.16	0.46
2:L:27:GLN:HB3	2:L:28:ASP:H	1.34	0.46
2:L:179:LEU:HD23	2:L:179:LEU:N	2.25	0.46
3:H:24:ALA:HB1	3:H:27:TYR:HE1	1.80	0.46
1:A:204:SER:O	1:A:208:PHE:HB3	2.16	0.46
1:A:218:VAL:O	1:A:222:VAL:HG23	2.15	0.46
2:L:59:PRO:HB2	2:L:61:ARG:NH1	2.31	0.46
3:H:39:GLN:HG3	3:H:44:GLY:O	2.15	0.46
1:A:75:LEU:HD21	1:A:124:LEU:HD21	1.97	0.46
2:L:30:ASN:N	2:L:30:ASN:HD22	2.12	0.46
3:H:41:THR:O	3:H:42:GLY:C	2.56	0.46
1:A:82:MET:O	1:A:82:MET:HG2	2.16	0.46
1:A:120:SER:O	1:A:124:LEU:HD23	2.16	0.46
2:L:212:ASN:C	2:L:214:CYS:N	2.72	0.46
3:H:40:ARG:HG2	3:H:41:THR:HG22	1.97	0.46
1:A:267:LYS:C	1:A:269:HIS:N	2.74	0.46
3:H:199:HIS:CD2	3:H:201:ALA:HB3	2.51	0.46
3:H:211:VAL:HG13	3:H:212:PRO:HD2	1.98	0.46
1:A:287:LEU:HB3	1:A:288:PRO:HD3	1.97	0.45
1:A:347:LEU:N	1:A:347:LEU:HD22	2.31	0.45
2:L:4:MET:HE2	2:L:23:CYS:SG	2.56	0.45
1:A:74:SER:C	1:A:76:ALA:H	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LYS:O	1:A:239:ARG:CD	2.63	0.45
2:L:86:TYR:N	2:L:86:TYR:CD1	2.84	0.45
1:A:48:VAL:HG22	1:A:84:LEU:HG	1.99	0.45
2:L:142:LYS:CA	2:L:173:TYR:CD2	2.99	0.45
1:A:283:THR:HG23	1:A:284:LEU:N	2.31	0.45
2:L:52:ASN:HD21	2:L:53:ARG:NH1	2.14	0.45
1:A:48:VAL:HG12	1:A:48:VAL:O	2.17	0.45
2:L:28:ASP:OD2	2:L:28:ASP:C	2.58	0.45
2:L:44:PRO:CG	3:H:103:TRP:CD2	2.93	0.45
2:L:91:TYR:HA	2:L:96:TYR:CD2	2.52	0.45
3:H:3:GLN:HA	3:H:102:TYR:CE2	2.51	0.45
1:A:326:TYR:HA	1:A:330:PRO:HD2	1.98	0.45
1:A:75:LEU:HD21	1:A:124:LEU:CD2	2.47	0.45
1:A:333:ARG:HG2	1:A:333:ARG:NH1	2.31	0.45
2:L:136:LEU:N	2:L:136:LEU:HD22	2.32	0.45
3:H:184:PRO:C	3:H:186:SER:N	2.73	0.45
1:A:79:ASP:OD1	1:A:319:SER:HA	2.17	0.45
2:L:19:VAL:HG11	2:L:104:LEU:HD11	1.99	0.45
1:A:121:ILE:HD11	1:A:212:LEU:HB2	1.98	0.44
3:H:64:PHE:O	3:H:65:LYS:C	2.60	0.44
3:H:67:LYS:HE2	3:H:90:ASP:OD1	2.17	0.44
1:A:117:VAL:HG12	1:A:117:VAL:O	2.16	0.44
1:A:208:PHE:O	1:A:211:PRO:HG2	2.16	0.44
1:A:275:LEU:CA	1:A:278:ILE:HG22	2.48	0.44
1:A:281:THR:O	1:A:285:CYS:SG	2.76	0.44
2:L:85:ILE:HG23	2:L:103:LYS:HB2	1.99	0.44
2:L:195:GLU:HG2	2:L:206:VAL:HG13	1.99	0.44
3:H:145:TYR:O	3:H:174:LEU:HD13	2.17	0.44
1:A:131:ARG:O	1:A:134:ALA:HB3	2.18	0.44
1:A:122:GLU:O	1:A:126:VAL:HG23	2.17	0.44
1:A:135:ILE:C	1:A:137:SER:N	2.76	0.44
1:A:162:GLY:C	1:A:164:THR:H	2.24	0.44
1:A:271:ALA:O	1:A:274:THR:HG22	2.18	0.44
2:L:124:GLN:HG2	2:L:129:GLY:O	2.17	0.44
1:A:287:LEU:O	1:A:291:ILE:HG13	2.18	0.44
2:L:37:GLN:O	2:L:37:GLN:HG2	2.17	0.44
3:H:128:SER:O	3:H:130:ALA:N	2.51	0.44
3:H:144:GLY:HA2	3:H:174:LEU:HD12	1.98	0.44
3:H:211:VAL:O	3:H:212:PRO:C	2.60	0.44
1:A:67:VAL:HG11	1:A:130:ASP:OD2	2.18	0.44
1:A:329:SER:HB2	1:A:330:PRO:CD	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:15:LEU:HD11	2:L:106:ILE:HG21	2.00	0.44
2:L:30:ASN:N	2:L:30:ASN:ND2	2.66	0.44
3:H:34:ILE:HG13	3:H:34:ILE:O	2.18	0.44
2:L:36:PHE:O	2:L:86:TYR:HA	2.18	0.44
2:L:78:LEU:CD1	2:L:82:ASP:HB2	2.47	0.44
3:H:173:ASP:O	3:H:174:LEU:CD2	2.66	0.44
1:A:287:LEU:HD22	1:A:291:ILE:CG1	2.47	0.43
2:L:91:TYR:N	2:L:91:TYR:CD1	2.86	0.43
1:A:217:PHE:HA	1:A:220:SER:HB3	1.99	0.43
1:A:231:GLN:NE2	1:A:235:LYS:HD2	2.29	0.43
3:H:125:ALA:HB1	3:H:126:PRO:HD2	2.00	0.43
1:A:120:SER:C	1:A:122:GLU:H	2.26	0.43
2:L:140:TYR:C	2:L:140:TYR:HD1	2.26	0.43
2:L:48:ILE:HG12	2:L:54:LEU:HA	2.01	0.43
2:L:49:TYR:O	2:L:50:ARG:C	2.61	0.43
2:L:52:ASN:ND2	2:L:52:ASN:C	2.76	0.43
3:H:170:LEU:O	3:H:171:GLN:HB2	2.17	0.43
2:L:198:HIS:O	2:L:200:THR:HG22	2.18	0.43
3:H:6:GLN:NE2	3:H:96:CYS:HB2	2.32	0.43
3:H:133:ASN:HD22	3:H:134:SER:H	1.66	0.43
2:L:4:MET:HA	2:L:25:ALA:HA	2.01	0.43
2:L:11:MET:HE1	2:L:19:VAL:HG23	2.00	0.43
2:L:212:ASN:O	2:L:213:GLU:C	2.61	0.43
3:H:145:TYR:CD1	3:H:145:TYR:C	2.96	0.43
1:A:69:ASN:CA	1:A:72:ILE:HG22	2.38	0.43
1:A:271:ALA:C	1:A:274:THR:HG22	2.43	0.43
2:L:19:VAL:HG13	2:L:75:ILE:CG2	2.49	0.43
2:L:21:ILE:HD11	2:L:35:TRP:CZ3	2.54	0.43
2:L:150:ILE:O	2:L:153:SER:HB3	2.19	0.43
2:L:169:LYS:HD2	2:L:169:LYS:N	2.04	0.43
3:H:7:SER:HB2	3:H:107:THR:CG2	2.46	0.43
3:H:40:ARG:O	3:H:41:THR:O	2.37	0.43
3:H:155:ASN:O	3:H:158:SER:HB2	2.18	0.43
3:H:195:CYS:O	3:H:195:CYS:SG	2.76	0.43
1:A:336:PHE:HD2	1:A:337:GLN:H	1.65	0.43
3:H:4:LEU:CD1	3:H:102:TYR:CD2	3.02	0.43
3:H:141:LEU:HD13	3:H:141:LEU:C	2.44	0.43
1:A:141:TYR:CD1	1:A:141:TYR:C	2.96	0.43
2:L:151:ASP:OD2	2:L:189:HIS:ND1	2.50	0.43
3:H:128:SER:O	3:H:129:ALA:C	2.62	0.42
1:A:224:GLN:C	1:A:226:ALA:H	2.26	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:PHE:CE2	1:A:312:ASN:OD1	2.72	0.42
2:L:152:GLY:O	2:L:153:SER:O	2.37	0.42
1:A:267:LYS:HD3	1:A:267:LYS:O	2.18	0.42
1:A:329:SER:CB	1:A:330:PRO:CD	2.97	0.42
2:L:161:ASN:O	3:H:169:VAL:HG21	2.18	0.42
3:H:61:ASN:O	3:H:62:GLU:C	2.59	0.42
2:L:200:THR:HG23	2:L:201:SER:H	1.84	0.42
3:H:97:VAL:CG1	3:H:103:TRP:CD2	3.03	0.42
1:A:120:SER:C	1:A:122:GLU:N	2.78	0.42
2:L:6:GLN:O	2:L:8:PRO:O	2.38	0.42
2:L:112:ALA:CB	2:L:200:THR:HG21	2.49	0.42
2:L:120:PRO:CB	2:L:130:ALA:HB1	2.49	0.42
3:H:11:LEU:HD21	3:H:146:PHE:CE1	2.54	0.42
3:H:184:PRO:O	3:H:187:THR:OG1	2.36	0.42
3:H:188:TRP:O	3:H:189:PRO:C	2.61	0.42
1:A:127:ILE:H	1:A:127:ILE:CD1	2.26	0.42
1:A:345:SER:C	1:A:347:LEU:N	2.78	0.42
1:A:345:SER:O	1:A:347:LEU:N	2.46	0.42
1:A:133:PHE:HA	1:A:136:THR:CG2	2.50	0.42
2:L:50:ARG:C	2:L:52:ASN:H	2.28	0.42
3:H:97:VAL:CG1	3:H:103:TRP:HA	2.48	0.42
3:H:99:GLY:O	3:H:100:PHE:CB	2.66	0.42
3:H:124:LEU:HD21	3:H:141:LEU:HB3	2.02	0.42
1:A:56:THR:HG23	1:A:57:ALA:N	2.34	0.42
1:A:275:LEU:O	1:A:279:MET:HG3	2.20	0.42
2:L:70:ASP:OD1	2:L:70:ASP:N	2.52	0.42
1:A:88:PRO:C	1:A:90:GLY:H	2.27	0.42
1:A:214:ILE:HG13	1:A:215:MET:N	2.35	0.42
1:A:222:VAL:O	1:A:224:GLN:N	2.53	0.42
1:A:88:PRO:C	1:A:90:GLY:N	2.78	0.41
1:A:216:VAL:O	1:A:216:VAL:HG12	2.20	0.41
2:L:24:LYS:CG	2:L:70:ASP:HB3	2.46	0.41
2:L:79:ASP:N	2:L:82:ASP:OD2	2.48	0.41
1:A:123:THR:HG22	1:A:127:ILE:CD1	2.50	0.41
2:L:163:TRP:NE1	2:L:175:MET:SD	2.93	0.41
1:A:148:ASN:HD22	1:A:148:ASN:H	1.60	0.41
1:A:222:VAL:C	1:A:224:GLN:N	2.76	0.41
1:A:337:GLN:HG2	1:A:343:ARG:CB	2.51	0.41
2:L:4:MET:HE2	2:L:4:MET:HB3	1.80	0.41
2:L:211:ARG:O	2:L:211:ARG:HG2	2.21	0.41
1:A:336:PHE:CA	1:A:339:LEU:HD23	2.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:140:TYR:CD1	2:L:141:PRO:N	2.88	0.41
3:H:28:ILE:O	3:H:29:PHE:C	2.63	0.41
3:H:185:SER:C	3:H:187:THR:H	2.29	0.41
1:A:220:SER:O	1:A:221:ARG:C	2.64	0.41
2:L:14:SER:O	2:L:78:LEU:HD23	2.21	0.41
2:L:159:VAL:CG1	2:L:161:ASN:HD21	2.29	0.41
1:A:57:ALA:O	1:A:61:PHE:N	2.53	0.41
1:A:344:ARG:C	1:A:346:SER:N	2.79	0.41
3:H:4:LEU:HA	3:H:24:ALA:HA	2.02	0.41
3:H:121:VAL:HG22	3:H:197:VAL:HG21	2.01	0.41
3:H:196:ASN:C	3:H:197:VAL:HG23	2.46	0.41
1:A:146:THR:OG1	1:A:149:LYS:HB2	2.20	0.41
2:L:44:PRO:O	3:H:103:TRP:CD1	2.74	0.41
2:L:55:VAL:HG12	2:L:56:ASP:N	2.36	0.41
2:L:152:GLY:C	2:L:153:SER:O	2.63	0.41
3:H:136:VAL:HG23	3:H:185:SER:HA	2.03	0.41
1:A:37:GLY:C	1:A:39:VAL:H	2.29	0.41
1:A:234:ASP:O	1:A:235:LYS:C	2.63	0.41
2:L:149:LYS:HG2	2:L:154:GLU:HB2	2.02	0.41
3:H:58:ILE:HG21	3:H:70:LEU:HB2	2.02	0.41
1:A:239:ARG:HH21	3:H:50:GLU:CD	2.29	0.41
2:L:160:LEU:C	2:L:161:ASN:HD22	2.29	0.41
3:H:18:VAL:HG13	3:H:86:LEU:HD11	2.03	0.41
3:H:117:THR:O	3:H:145:TYR:HA	2.20	0.41
3:H:145:TYR:N	3:H:174:LEU:HD12	2.34	0.41
2:L:50:ARG:O	2:L:52:ASN:N	2.51	0.41
3:H:126:PRO:O	3:H:213:ARG:HG3	2.21	0.41
3:H:170:LEU:HD12	3:H:171:GLN:H	1.86	0.41
1:A:127:ILE:HG23	1:A:131:ARG:HG2	2.03	0.40
1:A:142:GLN:O	1:A:143:SER:O	2.38	0.40
2:L:29:ILE:HA	2:L:92:ASP:CG	2.46	0.40
2:L:67:SER:O	2:L:69:GLN:N	2.54	0.40
2:L:71:TYR:N	2:L:71:TYR:HD1	2.19	0.40
2:L:136:LEU:HD21	2:L:146:VAL:CG1	2.49	0.40
3:H:67:LYS:HG3	3:H:83:LEU:HD12	2.01	0.40
1:A:52:VAL:HG22	1:A:80:LEU:CD1	2.51	0.40
2:L:98:PHE:C	2:L:99:GLY:O	2.62	0.40
1:A:266:LEU:O	1:A:269:HIS:HB3	2.21	0.40
2:L:61:ARG:HG2	2:L:61:ARG:HH11	1.86	0.40
1:A:131:ARG:NH1	1:A:141:TYR:HE1	2.19	0.40
3:H:6:GLN:HE22	3:H:96:CYS:HB2	1.82	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:29:PHE:HZ	3:H:79:ALA:HB2	1.87	0.40
3:H:168:ALA:HA	3:H:177:LEU:HB3	2.02	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	204/342 (60%)	155 (76%)	36 (18%)	13 (6%)	1	7
2	L	212/214 (99%)	174 (82%)	27 (13%)	11 (5%)	1	10
3	H	215/217 (99%)	157 (73%)	45 (21%)	13 (6%)	1	7
All	All	631/773 (82%)	486 (77%)	108 (17%)	37 (6%)	1	8

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	129	ALA
3	H	188	TRP
3	H	212	PRO
1	A	145	LEU
1	A	230	LEU
1	A	342	LEU
1	A	345	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	138	ASN
3	H	41	THR
3	H	127	GLY
3	H	144	GLY
3	H	171	GLN
1	A	329	SER
1	A	333	ARG
2	L	11	MET
2	L	27	GLN
3	H	16	ALA
3	H	215	CYS
2	L	169	LYS
2	L	199	LYS
2	L	72	SER
3	H	55	SER
2	L	51	ALA
2	L	101	GLY
3	H	26	GLY
3	H	119	PRO
1	A	222	VAL
1	A	83	GLY
3	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	167/300 (56%)	153 (92%)	14 (8%)	10	34
2	L	191/191 (100%)	166 (87%)	25 (13%)	4	16
3	H	183/183 (100%)	154 (84%)	29 (16%)	2	10
All	All	541/674 (80%)	473 (87%)	68 (13%)	4	18

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

Mol	Chain	Res	Type
1	A	58	ILE
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	239	ARG
1	A	287	LEU
1	A	312	ASN
1	A	333	ARG
1	A	336	PHE
1	A	339	LEU
1	A	347	LEU
2	L	11	MET
2	L	19	VAL
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	75	ILE
2	L	85	ILE
2	L	87	TYR
2	L	102	THR
2	L	104	LEU
2	L	114	THR
2	L	140	TYR
2	L	144	ILE
2	L	146	VAL
2	L	154	GLU
2	L	157	ASN
2	L	179	LEU
2	L	190	ASN
2	L	193	THR
2	L	211	ARG
3	H	6	GLN
3	H	11	LEU
3	H	20	LEU
3	H	33	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	35	ASN
3	H	40	ARG
3	H	51	ILE
3	H	61	ASN
3	H	69	THR
3	H	71	THR
3	H	77	SER
3	H	83	LEU
3	H	97	VAL
3	H	108	THR
3	H	110	THR
3	H	124	LEU
3	H	138	LEU
3	H	141	LEU
3	H	142	VAL
3	H	148	GLU
3	H	153	THR
3	H	155	ASN
3	H	170	LEU
3	H	174	LEU
3	H	177	LEU
3	H	185	SER
3	H	195	CYS
3	H	206	VAL
3	H	213	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	69	ASN
1	A	148	ASN
1	A	231	GLN
2	L	6	GLN
2	L	30	ASN
2	L	37	GLN
2	L	38	GLN
2	L	52	ASN
2	L	137	ASN
2	L	161	ASN
2	L	190	ASN
2	L	198	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	212	ASN
3	H	6	GLN
3	H	35	ASN
3	H	133	ASN
3	H	155	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 oligosaccharides 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	216/342 (63%)	0.93	28 (12%) 7 8	58, 192, 250, 290	0
2	L	214/214 (100%)	0.22	10 (4%) 36 27	44, 86, 138, 179	0
3	H	217/217 (100%)	0.37	11 (5%) 33 25	44, 88, 154, 232	0
All	All	647/773 (83%)	0.51	49 (7%) 20 17	44, 104, 228, 290	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	5	THR	7.0
1	A	116	CYS	4.3
1	A	316	TYR	4.0
3	H	74	LYS	3.9
3	H	105	GLN	3.8
2	L	31	SER	3.7
1	A	63	ARG	3.5
1	A	331	ASP	3.3
1	A	112	ILE	3.3
2	L	214	CYS	3.2
2	L	65	THR	3.1
1	A	335	ALA	3.0
3	H	7	SER	2.9
1	A	68	THR	2.9
2	L	212	ASN	2.8
1	A	225	GLU	2.6
2	L	152	GLY	2.6
3	H	173	ASP	2.6
2	L	19	VAL	2.6
1	A	346	SER	2.6
1	A	242	VAL	2.6
1	A	274	THR	2.6
1	A	288	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	319	SER	2.5
1	A	61	PHE	2.5
1	A	145	LEU	2.5
1	A	311	LEU	2.5
1	A	133	PHE	2.5
1	A	318	ASN	2.4
3	H	43	GLN	2.4
1	A	77	CYS	2.4
2	L	71	TYR	2.4
3	H	11	LEU	2.4
1	A	141	TYR	2.3
1	A	81	VAL	2.2
1	A	291	ILE	2.2
3	H	20	LEU	2.2
1	A	279	MET	2.2
1	A	113	ASP	2.2
1	A	313	TRP	2.1
3	H	82	GLN	2.1
3	H	162	GLY	2.1
3	H	161	SER	2.1
3	H	98	ARG	2.0
2	L	62	PHE	2.0
1	A	144	LEU	2.0
1	A	158	TRP	2.0
1	A	223	PHE	2.0
2	L	48	ILE	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 oligosaccharides 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.