



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:55 AM UTC

PDB ID : 4TRY / pdb_00004try
Title : Structure of BACE1 complex with a HEA-type inhibitor
Authors : Akaji, K.; Teruya, K.; Akiyama, T.; Sanjho, A.; Yamashita, E.; Nakagawa, A.
Deposited on : 2014-06-18
Resolution : 2.75 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

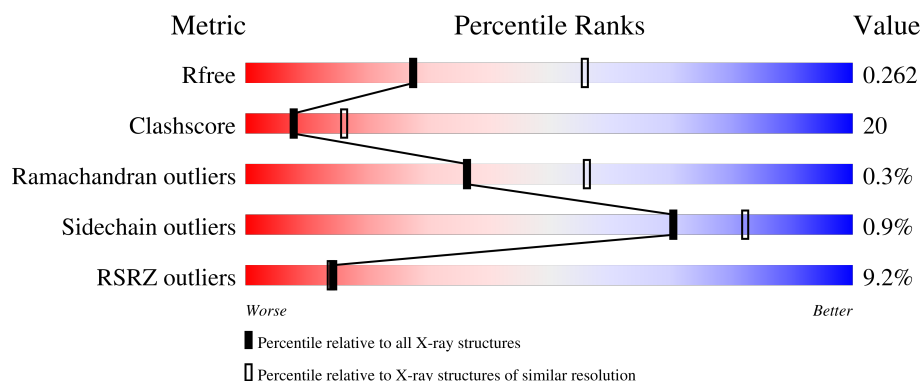
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	388	8% 71% 28% .
1	B	388	9% 70% 29% .
1	C	388	11% 67% 31% .
2	D	4	25% 75%
2	E	4	75% 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	4	 50%50%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9326 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-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			3042	1948	505	575	14			
1	B	388	Total	C	N	O	S	0	0	0
			3050	1954	506	576	14			
1	C	388	Total	C	N	O	S	0	0	0
			3050	1954	506	576	14			

- Molecule 2 is a protein called GLU-ILE-TIH-THC-NVA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	S	0	0	0
			47	31	5	9	2			
2	E	4	Total	C	N	O	S	0	0	0
			47	31	5	9	2			
2	F	4	Total	C	N	O	S	0	0	0
			47	31	5	9	2			

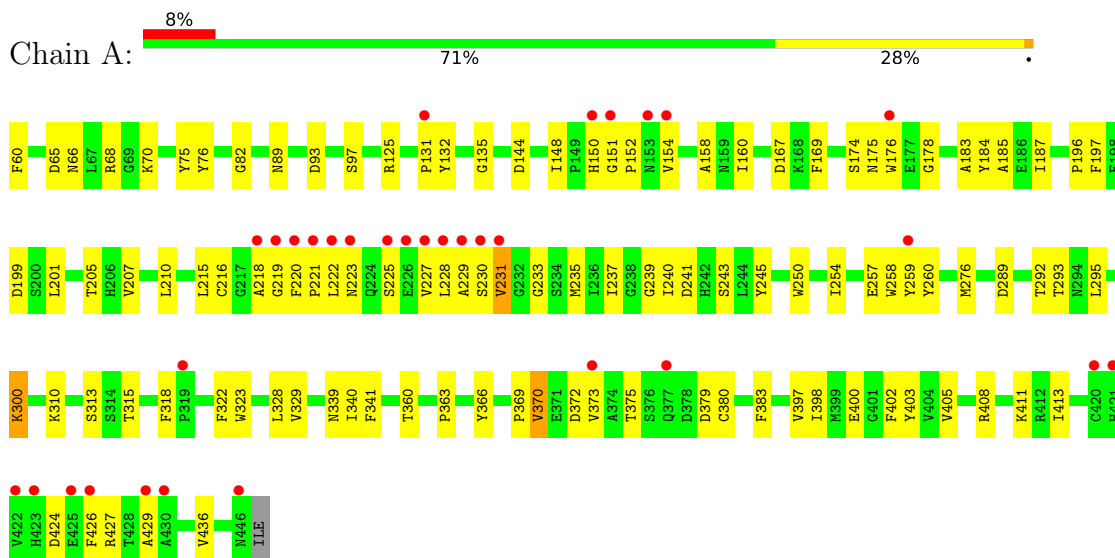
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	15	Total	O	0	0
			15	15		
3	C	16	Total	O	0	0
			16	16		
3	E	1	Total	O	0	0
			1	1		
3	F	1	Total	O	0	0
			1	1		

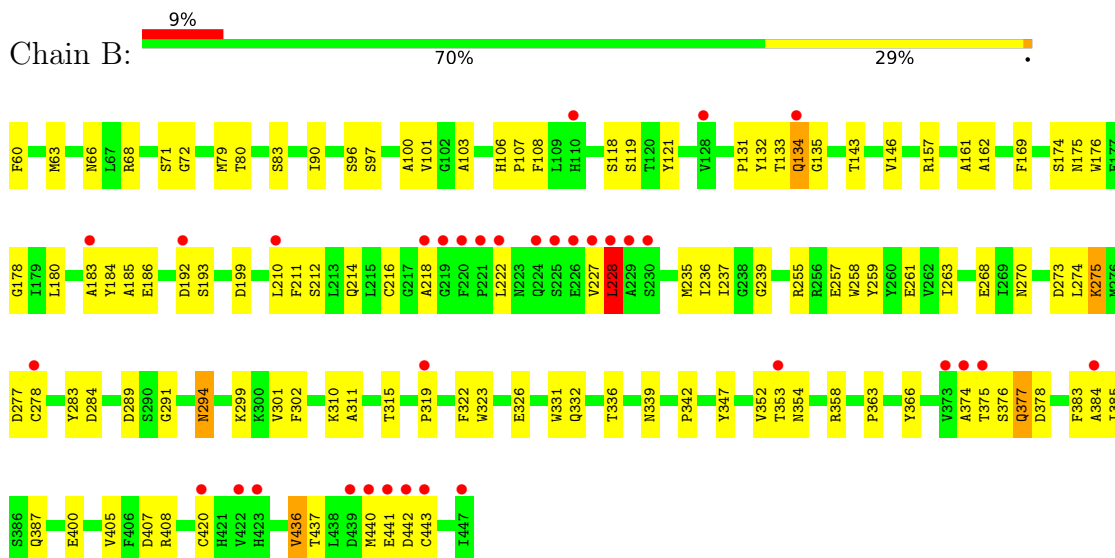
3 Residue-property plots

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

• Molecule 1: Beta-secretase 1

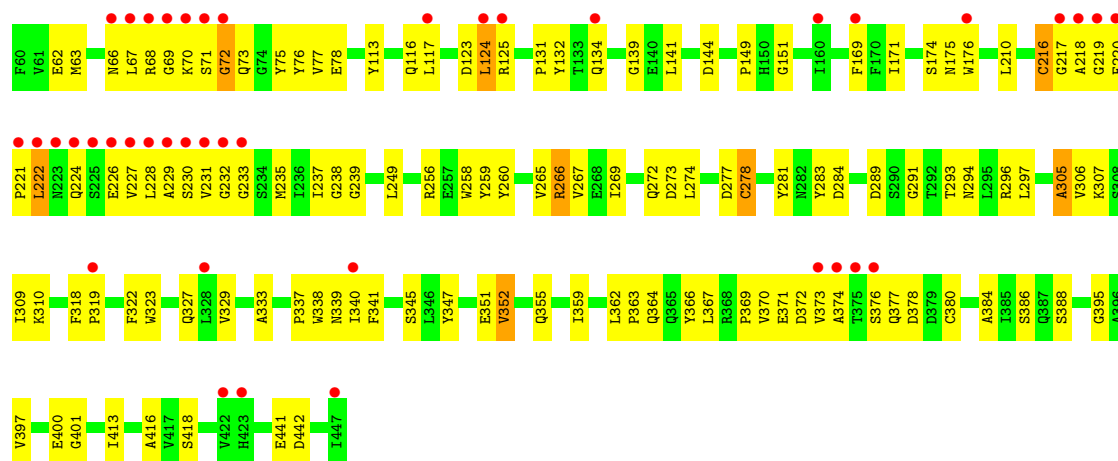


• Molecule 1: Beta-secretase 1



• Molecule 1: Beta-secretase 1

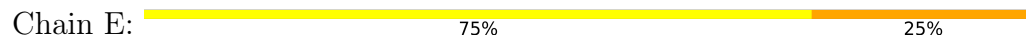




● Molecule 2: GLU-ILE-TIH-THC-NVA



● Molecule 2: GLU-ILE-TIH-THC-NVA



● Molecule 2: GLU-ILE-TIH-THC-NVA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.33Å 102.62Å 101.29Å 90.00° 103.53° 90.00°	Depositor
Resolution (Å)	49.18 – 2.75 49.18 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.18-2.75) 99.7 (49.18-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.179 , 0.252 0.206 , 0.262	Depositor DCC
R_{free} test set	2139 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9326	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TIH, 36D

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	0.80	0/3120	1.06	9/4243 (0.2%)
1	B	0.86	1/3128 (0.0%)	1.08	12/4254 (0.3%)
1	C	0.81	0/3128	1.06	10/4254 (0.2%)
2	D	1.14	0/16	0.50	0/20
2	E	0.01	0/16	0.28	0/20
2	F	0.03	0/16	0.28	0/20
All	All	0.82	1/9424 (0.0%)	1.07	31/12811 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	135	GLY	N-CA	5.77	1.49	1.44

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	LEU	N-CA-C	10.07	122.01	111.14
1	A	257	GLU	N-CA-C	8.98	123.09	109.62
1	C	373	VAL	N-CA-C	-8.89	101.31	111.00
1	A	229	ALA	N-CA-C	7.94	119.57	111.07
1	A	300	LYS	N-CA-C	7.56	119.60	111.36
1	A	233	GLY	N-CA-C	7.38	121.53	110.75
1	C	219	GLY	N-CA-C	-6.92	104.42	112.73
1	A	231	VAL	N-CA-C	6.81	118.85	109.80
1	A	373	VAL	N-CA-C	6.67	117.46	110.72
1	C	373	VAL	N-CA-CB	6.47	121.37	110.56
1	B	377	GLN	N-CA-C	-6.30	104.47	111.71
1	B	134	GLN	N-CA-C	6.27	121.27	112.93
1	A	219	GLY	N-CA-C	-6.25	104.05	111.36
1	A	185	ALA	N-CA-C	6.14	118.78	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	341	PHE	N-CA-C	6.04	117.42	109.93
1	C	124	LEU	N-CA-C	6.02	117.51	111.07
1	C	272	GLN	N-CA-C	6.00	118.50	108.96
1	C	371	GLU	N-CA-C	5.64	118.02	110.35
1	B	294	ASN	N-CA-C	5.61	118.12	110.55
1	B	218	ALA	N-CA-C	5.60	117.38	111.28
1	B	436	VAL	N-CA-CB	5.54	117.64	110.99
1	B	257	GLU	N-CA-C	5.50	119.23	110.70
1	A	402	PHE	N-CA-C	5.40	117.39	109.24
1	B	66	ASN	N-CA-C	5.38	119.71	113.20
1	B	108	PHE	N-CA-C	5.28	119.35	113.01
1	B	275	LYS	N-CA-CB	-5.24	103.78	113.89
1	C	305	ALA	N-CA-C	5.18	116.93	111.28
1	B	326	GLU	N-CA-C	5.09	119.36	112.04
1	B	301	VAL	N-CA-C	-5.06	105.91	110.82
1	C	139	GLY	N-CA-C	5.04	119.81	111.59
1	C	72	GLY	N-CA-C	5.03	118.73	112.64

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	3042	0	2951	110	0
1	B	3050	0	2964	112	0
1	C	3050	0	2962	144	0
2	D	47	0	43	8	0
2	E	47	0	43	13	0
2	F	47	0	43	9	0
3	A	10	0	0	0	0
3	B	15	0	0	0	0
3	C	16	0	0	1	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	9326	0	9006	359	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 20.

All (359) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:GLY:O	1:C:231:VAL:HB	1.32	1.28
1:C:229:ALA:CA	1:C:230:SER:OG	1.81	1.27
1:C:229:ALA:HA	1:C:230:SER:CB	1.57	1.24
1:B:134:GLN:OE1	2:E:3:TIH:HD	1.40	1.20
1:A:70:LYS:NZ	1:A:222:LEU:HD13	1.65	1.12
1:C:229:ALA:HA	1:C:230:SER:OG	0.92	1.09
1:C:217:GLY:HA2	1:C:231:VAL:HG13	1.32	1.08
1:C:67:LEU:HD11	1:C:77:VAL:HB	1.26	1.07
1:A:235:MET:HE3	1:A:237:ILE:CD1	1.85	1.06
1:A:235:MET:CE	1:A:237:ILE:HD11	1.88	1.03
1:C:67:LEU:HB2	1:C:233:GLY:O	1.59	1.01
1:C:217:GLY:HA2	1:C:231:VAL:CG1	1.95	0.96
1:C:210:LEU:HD11	1:C:239:GLY:HA2	1.48	0.96
1:B:310:LYS:HE3	1:B:323:TRP:CD1	2.00	0.95
1:A:65:ASP:OD1	1:A:231:VAL:HG11	1.66	0.95
1:A:70:LYS:HZ2	1:A:222:LEU:HD13	1.17	0.95
1:C:229:ALA:HB1	1:C:231:VAL:N	1.83	0.92
1:C:210:LEU:HD11	1:C:239:GLY:CA	1.99	0.92
1:C:76:TYR:HE1	1:C:224:GLN:NE2	1.69	0.91
1:C:66:ASN:HD21	1:C:235:MET:H	1.11	0.91
1:A:125:ARG:HG3	1:A:125:ARG:HH11	1.34	0.90
1:C:76:TYR:HE1	1:C:224:GLN:HE21	0.99	0.90
1:A:235:MET:HE3	1:A:237:ILE:HD11	0.92	0.89
1:B:212:SER:OG	1:B:236:ILE:HB	1.73	0.87
1:C:216:CYS:O	1:C:231:VAL:HG12	1.75	0.87
1:C:221:PRO:C	1:C:222:LEU:HD23	2.00	0.87
1:B:169:PHE:CD1	2:E:4:36D:H9	2.11	0.85
1:C:229:ALA:HB1	1:C:231:VAL:H	1.40	0.85
1:B:270:ASN:ND2	1:B:342:PRO:HB3	1.92	0.84
1:C:305:ALA:O	1:C:309:ILE:HG13	1.78	0.84
1:B:294:ASN:HB3	1:B:384:ALA:O	1.78	0.83
1:C:218:ALA:CB	1:C:220:PHE:O	2.26	0.83
1:A:97:SER:OG	1:A:187:ILE:HD11	1.79	0.83
1:C:222:LEU:HB2	1:C:229:ALA:O	1.78	0.82
1:C:67:LEU:CB	1:C:233:GLY:O	2.28	0.81
1:C:218:ALA:HB3	1:C:220:PHE:O	1.80	0.81
1:C:66:ASN:ND2	1:C:235:MET:H	1.77	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:PHE:CD1	1:B:311:ALA:HB1	2.16	0.80
1:C:351:GLU:H	1:C:355:GLN:HE21	1.30	0.80
1:C:210:LEU:HD11	1:C:239:GLY:N	1.97	0.80
1:A:65:ASP:OD1	1:A:231:VAL:CG1	2.29	0.79
1:B:210:LEU:HD23	1:B:211:PHE:N	1.98	0.79
1:C:67:LEU:CD1	1:C:77:VAL:HB	2.11	0.79
1:B:210:LEU:HD11	1:B:405:VAL:CG1	2.13	0.78
1:C:217:GLY:CA	1:C:231:VAL:HG13	2.14	0.78
1:A:426:PHE:CD2	1:A:427:ARG:HG3	2.18	0.78
1:A:183:ALA:HB3	1:A:187:ILE:HD11	1.66	0.77
1:C:226:GLU:HB3	1:C:227:VAL:HA	1.67	0.76
1:C:372:ASP:HB3	1:C:374:ALA:O	1.85	0.76
1:C:66:ASN:HD21	1:C:235:MET:N	1.83	0.75
1:A:424:ASP:HB3	1:A:427:ARG:O	1.86	0.75
1:C:174:SER:HB2	1:C:176:TRP:CD1	2.20	0.75
1:C:67:LEU:HD11	1:C:77:VAL:CB	2.10	0.75
1:B:222:LEU:HD13	1:B:227:VAL:HA	1.67	0.74
1:A:97:SER:OG	1:A:187:ILE:CD1	2.35	0.74
1:C:123:ASP:OD2	1:C:125:ARG:HD3	1.87	0.74
1:C:70:LYS:HG3	1:C:73:GLN:H	1.52	0.73
1:C:352:VAL:HB	1:C:355:GLN:HG2	1.71	0.73
1:C:70:LYS:HD2	1:C:73:GLN:HG3	1.72	0.72
1:A:339:ASN:OD1	1:A:340:ILE:HG23	1.89	0.71
1:B:210:LEU:HD23	1:B:210:LEU:C	2.14	0.71
1:B:274:LEU:O	1:B:275:LYS:HB2	1.90	0.71
1:C:351:GLU:H	1:C:355:GLN:NE2	1.89	0.71
1:C:229:ALA:CA	1:C:230:SER:CB	2.38	0.71
1:A:125:ARG:HG3	1:A:125:ARG:NH1	2.01	0.71
1:A:176:TRP:HE3	1:A:178:GLY:H	1.38	0.71
1:C:228:LEU:O	1:C:230:SER:HB3	1.90	0.70
1:A:97:SER:OG	1:A:187:ILE:CG1	2.39	0.70
1:C:337:PRO:HB2	1:C:340:ILE:CD1	2.22	0.70
1:B:294:ASN:ND2	1:B:384:ALA:O	2.25	0.70
1:A:97:SER:OG	1:A:187:ILE:HG13	1.93	0.69
1:B:310:LYS:CE	1:B:323:TRP:CD1	2.74	0.69
1:C:67:LEU:O	1:C:233:GLY:N	2.22	0.69
1:A:315:THR:HG23	1:B:339:ASN:HD21	1.58	0.68
1:B:100:ALA:HB2	1:B:161:ALA:HB3	1.75	0.68
1:A:254:ILE:O	1:A:411:LYS:HE2	1.95	0.67
1:C:123:ASP:CG	1:C:125:ARG:HB2	2.19	0.67
1:C:337:PRO:HB2	1:C:340:ILE:HD12	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:MET:HE3	1:B:237:ILE:HD11	1.76	0.67
1:C:69:GLY:HA3	1:C:75:TYR:HA	1.76	0.67
1:A:220:PHE:CE2	1:A:379:ASP:OD1	2.48	0.67
1:B:258:TRP:CG	1:B:259:TYR:H	2.12	0.66
1:C:71:SER:HB2	1:C:400:GLU:OE1	1.96	0.66
1:A:68:ARG:O	1:A:76:TYR:CD1	2.49	0.66
1:B:294:ASN:CB	1:B:384:ALA:O	2.44	0.66
1:A:220:PHE:HE2	1:A:379:ASP:OD1	1.78	0.65
1:B:174:SER:HG	1:B:176:TRP:CD1	2.13	0.65
1:A:154:VAL:CG2	1:A:205:THR:HG21	2.26	0.65
1:A:292:THR:HA	2:D:2:ILE:O	1.95	0.65
1:C:218:ALA:HB1	1:C:220:PHE:O	1.96	0.65
1:A:175:ASN:HB3	1:A:228:LEU:HD22	1.79	0.64
1:B:255:ARG:HE	1:B:440:MET:HE3	1.62	0.64
1:B:210:LEU:HD23	1:B:211:PHE:CA	2.26	0.64
1:C:210:LEU:CD1	1:C:239:GLY:N	2.60	0.64
1:C:318:PHE:HB3	1:C:319:PRO:HD2	1.79	0.64
1:C:66:ASN:OD1	1:C:67:LEU:N	2.30	0.64
1:A:148:ILE:HB	1:A:151:GLY:HA3	1.78	0.64
1:A:68:ARG:HD2	1:A:228:LEU:O	1.99	0.63
1:A:68:ARG:O	1:A:76:TYR:CE1	2.51	0.63
1:A:154:VAL:HG21	1:A:205:THR:HG21	1.79	0.62
1:B:354:ASN:CB	1:B:436:VAL:HG12	2.29	0.62
1:A:295:LEU:HD22	1:A:398:ILE:HD11	1.81	0.62
1:A:222:LEU:HD12	1:A:222:LEU:O	2.00	0.62
1:C:319:PRO:O	1:C:322:PHE:HB3	2.00	0.62
1:B:134:GLN:CD	2:E:3:TIH:HD	2.22	0.62
1:C:70:LYS:HE3	1:C:224:GLN:HB2	1.81	0.61
1:A:210:LEU:HD11	1:A:239:GLY:CA	2.30	0.61
1:B:227:VAL:HG23	1:B:228:LEU:HD23	1.82	0.61
1:A:176:TRP:HE3	1:A:178:GLY:N	1.98	0.60
1:A:328:LEU:HD11	1:A:370:VAL:HG21	1.82	0.60
1:C:76:TYR:CE1	1:C:224:GLN:NE2	2.52	0.60
1:C:222:LEU:HD23	1:C:222:LEU:N	2.17	0.60
1:B:332:GLN:HA	1:B:378:ASP:OD1	2.01	0.60
1:C:289:ASP:OD2	2:F:4:36D:O2	2.20	0.60
1:A:436:VAL:HB	1:B:436:VAL:HG13	1.84	0.59
1:A:223:ASN:O	1:A:227:VAL:HG23	2.01	0.59
1:A:175:ASN:CB	1:A:228:LEU:HD22	2.32	0.59
1:B:83:SER:HB2	1:B:119:SER:HB3	1.84	0.59
1:B:294:ASN:CG	1:B:384:ALA:O	2.45	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ARG:NH1	1:B:228:LEU:HD22	2.17	0.59
1:B:216:CYS:HG	1:B:420:CYS:HG	0.62	0.59
1:C:305:ALA:O	1:C:309:ILE:CG1	2.50	0.59
1:B:319:PRO:O	1:B:322:PHE:HB3	2.03	0.58
1:C:66:ASN:OD1	1:C:67:LEU:HD13	2.02	0.58
1:B:100:ALA:CB	1:B:161:ALA:HB3	2.34	0.58
1:C:70:LYS:O	1:C:71:SER:C	2.46	0.58
1:B:263:ILE:HG23	1:B:443:CYS:O	2.04	0.58
1:B:353:THR:OG1	1:B:437:THR:O	2.21	0.57
1:A:184:TYR:O	1:A:187:ILE:HG12	2.04	0.57
1:B:258:TRP:HD1	1:B:258:TRP:H	1.52	0.57
1:B:96:SER:O	1:B:183:ALA:HB3	2.05	0.57
1:C:132:TYR:CG	2:F:4:36D:H10	2.40	0.57
1:B:352:VAL:HG12	1:B:354:ASN:OD1	2.05	0.57
1:C:174:SER:HB2	1:C:176:TRP:NE1	2.19	0.57
1:C:291:GLY:C	2:F:2:ILE:HD12	2.30	0.56
1:A:360:THR:O	1:A:429:ALA:HB1	2.05	0.56
1:B:255:ARG:HG3	1:B:440:MET:HE3	1.87	0.56
1:B:258:TRP:H	1:B:258:TRP:CD1	2.23	0.56
1:A:154:VAL:HG23	1:A:154:VAL:O	2.05	0.56
1:A:339:ASN:HD21	1:B:315:THR:HG23	1.70	0.56
1:C:210:LEU:CD1	1:C:239:GLY:CA	2.80	0.56
1:A:240:ILE:HG23	1:A:403:TYR:HE2	1.71	0.56
1:B:71:SER:HB3	1:B:400:GLU:OE1	2.06	0.55
1:C:67:LEU:CD1	1:C:77:VAL:CB	2.80	0.55
1:A:210:LEU:HD11	1:A:239:GLY:HA2	1.88	0.55
1:B:383:PHE:CZ	1:B:385:ILE:HB	2.41	0.55
1:A:175:ASN:HD22	1:A:228:LEU:HD22	1.72	0.55
1:B:210:LEU:HD12	1:B:407:ASP:HA	1.89	0.55
1:C:66:ASN:CG	1:C:67:LEU:HD13	2.31	0.55
1:A:218:ALA:HB1	1:A:369:PRO:HG2	1.89	0.55
1:A:174:SER:HB2	1:A:176:TRP:CD1	2.41	0.55
1:C:329:VAL:O	1:C:380:CYS:HA	2.07	0.55
1:B:310:LYS:HE2	1:B:323:TRP:NE1	2.23	0.54
1:C:226:GLU:HA	1:C:227:VAL:C	2.32	0.54
1:A:66:ASN:HB2	1:A:150:HIS:CG	2.42	0.54
1:A:329:VAL:O	1:A:380:CYS:HA	2.07	0.54
1:C:123:ASP:OD1	1:C:125:ARG:HG3	2.06	0.54
1:A:205:THR:OG1	1:A:207:VAL:HG23	2.08	0.54
1:B:310:LYS:CE	1:B:323:TRP:NE1	2.71	0.54
1:A:70:LYS:NZ	1:A:222:LEU:CD1	2.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ASP:OD1	1:A:408:ARG:NH2	2.41	0.53
1:B:277:ASP:OD1	1:B:278:CYS:N	2.41	0.53
1:C:210:LEU:HD11	1:C:238:GLY:C	2.34	0.53
1:A:75:TYR:OH	1:A:400:GLU:OE1	2.20	0.53
1:C:289:ASP:O	1:C:395:GLY:HA2	2.09	0.53
1:B:289:ASP:OD2	2:E:4:36D:O2	2.27	0.53
1:C:124:LEU:N	1:C:125:ARG:HA	2.23	0.53
1:C:277:ASP:OD1	1:C:278:CYS:N	2.42	0.52
1:B:185:ALA:O	1:B:186:GLU:C	2.53	0.52
1:C:69:GLY:O	1:C:231:VAL:CB	2.27	0.52
1:C:293:THR:OG1	2:F:2:ILE:HG13	2.08	0.52
1:B:216:CYS:SG	1:B:420:CYS:CB	2.98	0.52
1:C:258:TRP:CG	1:C:259:TYR:H	2.28	0.51
1:A:151:GLY:O	1:A:152:PRO:C	2.54	0.51
1:B:210:LEU:HD11	1:B:405:VAL:HG13	1.90	0.51
1:C:235:MET:HE3	1:C:237:ILE:HD11	1.92	0.51
1:C:319:PRO:HB2	3:C:506:HOH:O	2.10	0.51
1:A:148:ILE:HG22	1:A:151:GLY:H	1.76	0.51
1:A:222:LEU:HD12	1:A:222:LEU:C	2.35	0.51
1:A:258:TRP:H	1:A:258:TRP:CD1	2.27	0.51
1:C:221:PRO:O	1:C:222:LEU:HD23	2.10	0.51
1:C:78:GLU:O	1:C:149:PRO:HD2	2.11	0.51
1:C:266:ARG:HG2	1:C:266:ARG:HH11	1.76	0.51
1:A:258:TRP:H	1:A:258:TRP:HD1	1.59	0.51
1:A:339:ASN:OD1	1:A:340:ILE:N	2.43	0.51
1:A:93:ASP:OD1	2:D:4:36D:O1	2.29	0.51
1:C:169:PHE:CD1	2:F:4:36D:H9	2.46	0.51
1:C:364:GLN:OE1	1:C:364:GLN:N	2.43	0.51
1:B:255:ARG:CG	1:B:440:MET:HE3	2.41	0.51
1:B:441:GLU:OE1	1:C:273:ASP:OD2	2.28	0.51
1:C:174:SER:O	1:C:175:ASN:HB3	2.11	0.51
1:A:70:LYS:HZ1	1:A:222:LEU:HD13	1.72	0.50
1:A:260:TYR:HB3	1:A:413:ILE:HD11	1.93	0.50
1:C:249:LEU:HD23	1:C:416:ALA:HB2	1.92	0.50
1:B:169:PHE:HD1	2:E:4:36D:H9	1.70	0.50
1:B:376:SER:O	1:B:377:GLN:C	2.53	0.50
1:C:296:ARG:HB3	1:C:388:SER:HB2	1.91	0.50
1:A:293:THR:OG1	2:D:2:ILE:HG12	2.12	0.50
1:B:175:ASN:CG	1:B:175:ASN:O	2.55	0.50
1:A:201:LEU:HD11	1:A:207:VAL:HG21	1.94	0.50
1:B:268:GLU:HG2	1:B:273:ASP:HA	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLY:HA2	1:A:167:ASP:O	2.12	0.49
1:B:103:ALA:CB	1:B:162:ALA:HB1	2.42	0.49
1:B:363:PRO:HA	1:B:366:TYR:CE2	2.47	0.49
1:B:90:ILE:HG21	1:B:180:LEU:HB2	1.94	0.49
1:C:124:LEU:HD12	1:C:141:LEU:HB3	1.95	0.49
1:C:230:SER:C	1:C:231:VAL:HG23	2.37	0.49
1:C:62:GLU:HG3	1:C:63:MET:HG3	1.95	0.49
1:C:124:LEU:HD12	1:C:141:LEU:CB	2.43	0.49
1:B:258:TRP:CG	1:B:259:TYR:N	2.77	0.49
1:C:66:ASN:OD1	1:C:67:LEU:HB2	2.13	0.49
1:A:210:LEU:C	1:A:210:LEU:HD12	2.37	0.49
1:C:68:ARG:O	1:C:76:TYR:CE1	2.66	0.49
1:C:216:CYS:O	1:C:231:VAL:CG1	2.56	0.48
1:B:377:GLN:HA	1:B:377:GLN:NE2	2.28	0.48
1:A:158:ALA:O	1:A:160:ILE:HD12	2.13	0.48
1:A:258:TRP:CG	1:A:259:TYR:H	2.32	0.48
1:B:176:TRP:CE3	1:B:178:GLY:O	2.66	0.48
1:C:333:ALA:HB2	1:C:377:GLN:O	2.12	0.48
1:A:426:PHE:CE2	1:A:427:ARG:HG3	2.49	0.48
1:B:97:SER:OG	1:B:184:TYR:O	2.25	0.48
1:C:294:ASN:ND2	1:C:386:SER:OG	2.41	0.48
1:C:352:VAL:CB	1:C:355:GLN:HG2	2.43	0.48
1:C:310:LYS:HZ1	1:C:323:TRP:CG	2.33	0.47
1:A:322:PHE:CZ	1:A:383:PHE:HB2	2.49	0.47
1:B:331:TRP:CE3	1:B:336:THR:HG23	2.50	0.47
1:B:72:GLY:O	2:E:1:GLU:N	2.40	0.47
1:C:226:GLU:CB	1:C:227:VAL:HA	2.37	0.47
1:A:363:PRO:HA	1:A:366:TYR:CE2	2.50	0.47
1:C:124:LEU:HB2	1:C:125:ARG:HA	1.96	0.47
1:B:274:LEU:O	1:B:275:LYS:CB	2.61	0.47
1:B:352:VAL:CG1	1:B:354:ASN:OD1	2.62	0.47
1:B:118:SER:HB3	1:B:121:TYR:HB2	1.97	0.47
1:A:183:ALA:CB	1:A:187:ILE:HD11	2.41	0.46
1:A:293:THR:O	1:A:397:VAL:HG13	2.15	0.46
1:B:440:MET:O	1:B:442:ASP:O	2.33	0.46
1:A:310:LYS:HG2	1:A:323:TRP:CE2	2.51	0.46
1:A:426:PHE:CG	1:B:311:ALA:HB1	2.51	0.46
1:B:96:SER:C	1:B:183:ALA:HB3	2.40	0.46
1:B:374:ALA:O	1:B:375:THR:C	2.59	0.46
1:C:369:PRO:O	1:C:370:VAL:HG13	2.15	0.46
1:B:299:LYS:HB2	1:B:387:GLN:HE21	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ASP:OD1	1:B:193:SER:N	2.49	0.46
1:B:134:GLN:HB2	2:E:3:TIH:HB3	1.96	0.46
1:B:169:PHE:CE1	2:E:4:36D:C5	2.99	0.46
1:C:70:LYS:C	1:C:72:GLY:N	2.73	0.46
1:A:169:PHE:CD1	2:D:4:36D:H9	2.51	0.46
1:A:220:PHE:CD1	1:A:221:PRO:HA	2.51	0.46
1:A:250:TRP:CZ3	1:C:352:VAL:HG13	2.50	0.46
1:B:176:TRP:HE3	1:B:178:GLY:O	1.98	0.46
1:B:169:PHE:CE1	2:E:4:36D:H9	2.50	0.46
1:B:192:ASP:O	1:B:193:SER:C	2.58	0.46
1:A:405:VAL:O	1:A:413:ILE:HA	2.16	0.46
1:A:60:PHE:CZ	1:A:239:GLY:HA3	2.51	0.45
1:B:354:ASN:HA	1:B:436:VAL:HA	1.98	0.45
1:B:354:ASN:HB3	1:B:436:VAL:HG12	1.98	0.45
1:C:376:SER:HB3	1:C:378:ASP:CG	2.40	0.45
1:A:245:TYR:CD1	1:A:403:TYR:CD2	3.04	0.45
1:C:291:GLY:O	2:F:2:ILE:HD12	2.16	0.45
1:A:426:PHE:CE1	1:B:311:ALA:HB1	2.50	0.45
1:C:401:GLY:O	1:C:418:SER:HB3	2.16	0.45
1:B:134:GLN:OE1	2:E:2:ILE:HA	2.15	0.45
1:B:310:LYS:HE3	1:B:323:TRP:CG	2.48	0.45
1:A:132:TYR:CG	2:D:4:36D:H10	2.52	0.45
1:B:310:LYS:HG3	1:B:323:TRP:CZ2	2.51	0.45
1:B:347:TYR:CZ	1:B:358:ARG:HD2	2.52	0.45
1:C:68:ARG:HA	1:C:232:GLY:HA2	1.98	0.45
1:C:306:VAL:HA	1:C:309:ILE:HD12	1.99	0.45
1:B:132:TYR:CG	2:E:4:36D:H10	2.52	0.45
1:A:176:TRP:CE3	1:A:178:GLY:N	2.84	0.45
1:A:313:SER:HB2	1:A:340:ILE:HD12	1.98	0.45
1:C:305:ALA:O	1:C:309:ILE:CD1	2.65	0.45
1:C:63:MET:HE2	1:C:151:GLY:C	2.42	0.45
1:B:210:LEU:CD2	1:B:211:PHE:N	2.75	0.44
1:A:76:TYR:OH	1:A:228:LEU:CD2	2.65	0.44
1:C:265:VAL:HG23	1:C:347:TYR:HB2	1.98	0.44
1:A:82:GLY:HA2	1:A:144:ASP:OD1	2.18	0.44
1:A:227:VAL:O	1:A:230:SER:O	2.36	0.44
1:B:60:PHE:CZ	1:B:239:GLY:HA3	2.52	0.44
1:C:362:LEU:HB3	1:C:363:PRO:HD2	2.00	0.44
1:A:276:MET:HE1	1:A:300:LYS:HB3	1.99	0.44
1:B:106:HIS:CG	1:B:107:PRO:HD2	2.53	0.44
1:A:196:PRO:O	1:A:197:PHE:C	2.60	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:ALA:CB	1:C:397:VAL:HG11	2.48	0.43
1:B:169:PHE:CD1	2:E:4:36D:C5	2.94	0.43
1:C:123:ASP:OD1	1:C:125:ARG:HB2	2.18	0.43
1:A:89:ASN:HB2	1:A:176:TRP:HA	2.00	0.43
1:B:132:TYR:O	1:B:133:THR:C	2.61	0.43
1:C:116:GLN:HG2	1:C:117:LEU:HD12	1.98	0.43
1:C:124:LEU:CD1	1:C:141:LEU:HB3	2.48	0.43
1:C:174:SER:O	1:C:175:ASN:CB	2.65	0.43
1:C:134:GLN:HB2	2:F:3:TIH:HB3	1.99	0.43
1:C:267:VAL:CG2	1:C:281:TYR:CE1	3.02	0.43
1:A:215:LEU:O	1:A:400:GLU:HA	2.18	0.43
1:A:220:PHE:HA	1:A:221:PRO:HA	1.70	0.43
1:B:79:MET:SD	1:B:90:ILE:HG13	2.58	0.43
1:C:68:ARG:HH11	1:C:232:GLY:HA3	1.84	0.43
1:C:113:TYR:OH	1:C:144:ASP:OD2	2.21	0.43
1:C:229:ALA:CB	1:C:230:SER:OG	2.60	0.43
1:C:294:ASN:ND2	2:F:1:GLU:OE2	2.52	0.43
1:C:310:LYS:HZ1	1:C:323:TRP:CD1	2.36	0.43
1:A:65:ASP:CB	1:A:231:VAL:HG11	2.49	0.43
1:A:313:SER:CB	1:A:340:ILE:HD12	2.49	0.43
1:B:302:PHE:CE1	1:B:385:ILE:HG22	2.54	0.42
1:C:265:VAL:HG23	1:C:266:ARG:N	2.34	0.42
1:B:255:ARG:NE	1:B:440:MET:HE3	2.32	0.42
1:B:289:ASP:OD1	1:B:291:GLY:N	2.24	0.42
1:A:65:ASP:CG	1:A:231:VAL:HG11	2.40	0.42
1:A:341:PHE:HB3	1:A:363:PRO:HB3	2.01	0.42
1:C:306:VAL:HG23	1:C:323:TRP:CE3	2.54	0.42
1:A:372:ASP:OD1	1:A:375:THR:HA	2.19	0.42
1:B:60:PHE:HD1	1:B:63:MET:HE3	1.84	0.42
1:B:174:SER:O	1:B:175:ASN:HB3	2.20	0.42
1:B:259:TYR:O	1:B:261:GLU:N	2.53	0.42
1:B:354:ASN:HB2	1:B:436:VAL:HG12	2.02	0.42
1:C:345:SER:HA	1:C:359:ILE:O	2.20	0.42
1:A:93:ASP:CG	2:D:4:36D:H5	2.27	0.42
1:C:369:PRO:O	1:C:370:VAL:CG1	2.68	0.42
1:B:214:GLN:NE2	1:B:420:CYS:SG	2.93	0.42
1:C:377:GLN:HA	1:C:377:GLN:NE2	2.34	0.42
1:C:78:GLU:HG2	1:C:149:PRO:HG3	2.01	0.42
1:C:283:TYR:HA	1:C:284:ASP:HA	1.79	0.42
1:C:319:PRO:HB2	1:C:327:GLN:OE1	2.20	0.42
1:B:103:ALA:HB2	1:B:162:ALA:HB1	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:LEU:O	1:C:230:SER:N	2.45	0.41
1:C:338:TRP:HZ3	1:C:367:LEU:HD12	1.85	0.41
1:C:363:PRO:HA	1:C:366:TYR:CE1	2.55	0.41
1:B:101:VAL:O	1:B:101:VAL:HG23	2.20	0.41
1:C:260:TYR:HB3	1:C:413:ILE:HD11	2.01	0.41
1:B:199:ASP:OD1	1:B:408:ARG:NH2	2.52	0.41
1:B:258:TRP:CD1	1:B:259:TYR:H	2.38	0.41
1:C:256:ARG:HD3	1:C:258:TRP:NE1	2.35	0.41
1:C:338:TRP:O	1:C:339:ASN:C	2.64	0.41
1:C:441:GLU:O	1:C:442:ASP:C	2.63	0.41
1:A:70:LYS:HZ2	1:A:222:LEU:CD1	2.08	0.41
1:A:241:ASP:OD1	1:A:243:SER:OG	2.33	0.41
1:B:175:ASN:O	1:B:175:ASN:OD1	2.39	0.41
1:A:66:ASN:CB	1:A:150:HIS:CG	3.04	0.41
1:A:259:TYR:CE1	2:D:4:36D:H19	2.55	0.41
1:B:80:THR:O	1:B:146:VAL:HA	2.20	0.41
1:C:376:SER:C	1:C:378:ASP:H	2.27	0.41
1:A:258:TRP:CD1	1:A:258:TRP:N	2.89	0.41
1:C:267:VAL:HG23	1:C:281:TYR:CE1	2.55	0.41
1:C:306:VAL:O	1:C:307:LYS:C	2.63	0.41
1:A:97:SER:HG	1:A:187:ILE:CG1	2.33	0.41
1:A:225:SER:HA	1:A:228:LEU:HD12	2.03	0.41
1:C:297:LEU:O	1:C:388:SER:N	2.54	0.41
1:A:76:TYR:OH	1:A:228:LEU:HD22	2.21	0.40
1:A:318:PHE:HD1	1:A:329:VAL:HG11	1.86	0.40
1:B:143:THR:OG1	1:B:157:ARG:NH1	2.54	0.40
1:B:134:GLN:OE1	2:E:3:TIH:CD	2.35	0.40
1:A:289:ASP:OD2	2:D:4:36D:O2	2.40	0.40
1:B:283:TYR:HA	1:B:284:ASP:HA	1.85	0.40
1:C:68:ARG:O	1:C:76:TYR:CD1	2.75	0.40
2:F:2:ILE:C	2:F:3:TIH:CD	2.94	0.40
1:B:210:LEU:C	1:B:210:LEU:CD2	2.86	0.40
1:C:171:ILE:HB	1:C:174:SER:HB3	2.02	0.40
1:C:269:ILE:CG1	1:C:274:LEU:HD21	2.52	0.40
1:C:369:PRO:C	1:C:370:VAL:HG13	2.46	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	385/388 (99%)	381 (99%)	3 (1%)	1 (0%)	36	56
1	B	386/388 (100%)	378 (98%)	7 (2%)	1 (0%)	36	56
1	C	386/388 (100%)	379 (98%)	6 (2%)	1 (0%)	36	56
2	D	1/4 (25%)	1 (100%)	0	0	100	100
2	E	1/4 (25%)	1 (100%)	0	0	100	100
2	F	1/4 (25%)	1 (100%)	0	0	100	100
All	All	1160/1176 (99%)	1141 (98%)	16 (1%)	3 (0%)	36	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	PRO
1	B	131	PRO
1	C	131	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/331 (100%)	328 (99%)	2 (1%)	78	88
1	B	331/331 (100%)	330 (100%)	1 (0%)	86	93
1	C	331/331 (100%)	326 (98%)	5 (2%)	57	74
2	D	2/2 (100%)	2 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	2/2 (100%)	2 (100%)	0	100	100
2	F	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	998/999 (100%)	989 (99%)	9 (1%)	70	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	CYS
1	A	370	VAL
1	B	228	LEU
1	C	216	CYS
1	C	222	LEU
1	C	266	ARG
1	C	278	CYS
1	C	352	VAL
2	F	2	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	365	GLN
1	A	387	GLN
1	B	214	GLN
1	B	270	ASN
1	B	339	ASN
1	B	377	GLN
1	B	387	GLN
1	B	423	HIS
1	C	134	GLN
1	C	223	ASN
1	C	294	ASN
1	C	332	GLN
1	C	355	GLN
1	C	377	GLN
1	C	387	GLN
1	C	446	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TIH	F	3	2	9,10,11	1.08	0	6,12,14	0.98	1 (16%)
2	TIH	D	3	2	9,10,11	1.00	0	6,12,14	1.16	1 (16%)
2	TIH	E	3	2	9,10,11	1.01	1 (11%)	6,12,14	0.91	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TIH	F	3	2	-	0/5/6/8	0/1/1/1
2	TIH	D	3	2	-	0/5/6/8	0/1/1/1
2	TIH	E	3	2	-	0/5/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	TIH	CE1-CD	-2.02	1.32	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	TIH	CE1-CE2-SD	-2.28	107.45	113.02
2	F	3	TIH	CE1-CE2-SD	-2.04	108.03	113.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3	TIH	2	0
2	E	3	TIH	4	0

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	387/388 (99%)	0.31	32 (8%) 17 18	35, 55, 120, 207	0
1	B	388/388 (100%)	0.29	34 (8%) 15 15	33, 56, 106, 189	0
1	C	388/388 (100%)	0.49	41 (10%) 11 10	34, 61, 134, 223	0
2	D	2/4 (50%)	1.19	0 100 100	49, 49, 49, 61	0
2	E	2/4 (50%)	0.36	0 100 100	47, 47, 47, 54	0
2	F	2/4 (50%)	0.98	0 100 100	60, 60, 60, 65	0
All	All	1169/1176 (99%)	0.36	107 (9%) 14 14	33, 57, 123, 223	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	228	LEU	8.2
1	B	227	VAL	7.1
1	A	222	LEU	6.7
1	C	227	VAL	6.6
1	C	219	GLY	6.5
1	A	150	HIS	6.5
1	C	224	GLN	6.5
1	A	221	PRO	6.3
1	A	228	LEU	6.1
1	C	229	ALA	6.1
1	B	447	ILE	6.0
1	C	220	PHE	6.0
1	C	221	PRO	6.0
1	C	222	LEU	5.9
1	C	124	LEU	5.8
1	A	220	PHE	5.7
1	B	228	LEU	5.6
1	C	373	VAL	5.6
1	B	222	LEU	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	422	VAL	5.3
1	A	231	VAL	5.0
1	A	227	VAL	4.7
1	B	221	PRO	4.7
1	A	373	VAL	4.6
1	C	217	GLY	4.5
1	C	134	GLN	4.5
1	A	430	ALA	4.4
1	C	233	GLY	4.4
1	C	218	ALA	4.2
1	B	229	ALA	4.2
1	B	443	CYS	4.2
1	B	220	PHE	4.1
1	C	230	SER	4.1
1	A	154	VAL	4.1
1	B	134	GLN	3.9
1	C	70	LYS	3.9
1	C	71	SER	3.9
1	B	384	ALA	3.8
1	C	226	GLU	3.8
1	C	375	THR	3.7
1	C	422	VAL	3.7
1	B	210	LEU	3.7
1	C	232	GLY	3.5
1	B	375	THR	3.5
1	C	66	ASN	3.4
1	C	117	LEU	3.3
1	C	176	TRP	3.3
1	A	219	GLY	3.2
1	A	153	ASN	3.1
1	A	176	TRP	3.1
1	B	219	GLY	3.1
1	C	68	ARG	3.1
1	A	259	TYR	3.1
1	C	231	VAL	3.1
1	A	218	ALA	3.1
1	A	229	ALA	3.1
1	C	374	ALA	3.0
1	A	225	SER	3.0
1	B	423	HIS	3.0
1	C	125	ARG	3.0
1	A	223	ASN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	319	PRO	3.0
1	A	151	GLY	3.0
1	C	69	GLY	3.0
1	A	423	HIS	2.9
1	A	230	SER	2.9
1	C	447	ILE	2.9
1	C	67	LEU	2.9
1	B	420	CYS	2.8
1	B	373	VAL	2.8
1	A	421	HIS	2.7
1	B	422	VAL	2.7
1	B	442	ASP	2.7
1	C	160	ILE	2.6
1	C	225	SER	2.6
1	B	230	SER	2.6
1	B	353	THR	2.5
1	B	192	ASP	2.5
1	B	440	MET	2.5
1	C	223	ASN	2.5
1	A	420	CYS	2.5
1	C	423	HIS	2.5
1	A	131	PRO	2.5
1	A	426	PHE	2.5
1	A	429	ALA	2.5
1	C	376	SER	2.4
1	A	226	GLU	2.4
1	B	439	ASP	2.4
1	B	218	ALA	2.4
1	B	278	CYS	2.3
1	B	224	GLN	2.3
1	B	110	HIS	2.3
1	B	441	GLU	2.3
1	B	225	SER	2.3
1	C	319	PRO	2.3
1	A	377	GLN	2.2
1	B	374	ALA	2.2
1	B	183	ALA	2.2
1	A	446	ASN	2.2
1	C	340	ILE	2.2
1	C	72	GLY	2.1
1	B	128	VAL	2.1
1	C	169	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	226	GLU	2.1
1	C	328	LEU	2.1
1	A	425	GLU	2.0
1	B	319	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TIH	D	3	10/11	0.94	0.08	35,41,44,58	0
2	TIH	E	3	10/11	0.94	0.08	36,42,45,56	0
2	TIH	F	3	10/11	0.96	0.08	49,56,59,61	0

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.