



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:38 AM GMT

PDB ID : 2B5F
Title : Crystal structure of the spinach aquaporin SoPIP2;1 in an open conformation to 3.9 resolution
Authors : Tornroth-Horsefield, S.; Wang, Y.; Hedfalk, K.; Johanson, U.; Karlsson, M.; Tajkhorshid, E.; Neutze, R.; Kjellbom, P.
Deposited on : 2005-09-28
Resolution : 3.90 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

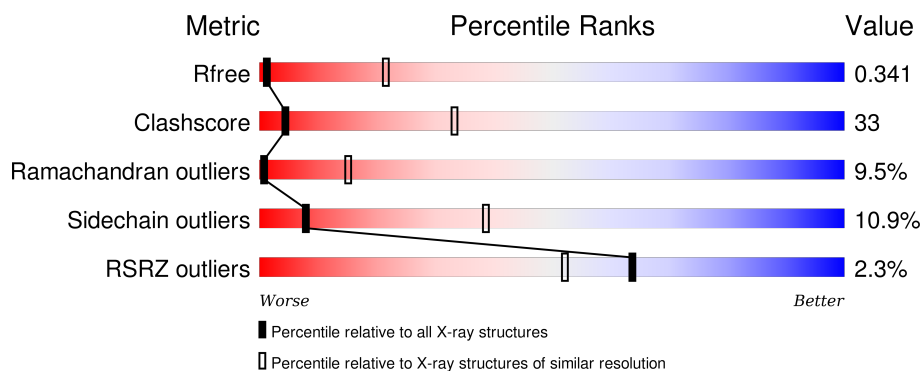
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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	303	<div> <div>4%</div> <div>39%</div> <div>29%</div> <div>9%</div> <div>22%</div> </div>
1	B	303	<div> <div>%</div> <div>39%</div> <div>26%</div> <div>8%</div> <div>26%</div> </div>
1	C	303	<div> <div>2%</div> <div>36%</div> <div>28%</div> <div>9%</div> <div>25%</div> </div>
1	D	303	<div> <div></div> <div>40%</div> <div>27%</div> <div>8%</div> <div>24%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6854 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 aquaporin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1767	1175	288	296	8			
1	B	224	Total	C	N	O	S	0	0	0
			1671	1116	267	280	8			
1	C	227	Total	C	N	O	S	0	0	0
			1696	1134	271	283	8			
1	D	230	Total	C	N	O	S	0	0	0
			1720	1150	276	286	8			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	LEU	-	EXPRESSION TAG	UNP Q41372
A	283	GLU	-	EXPRESSION TAG	UNP Q41372
A	284	GLN	-	EXPRESSION TAG	UNP Q41372
A	285	LYS	-	EXPRESSION TAG	UNP Q41372
A	286	LEU	-	EXPRESSION TAG	UNP Q41372
A	287	ILE	-	EXPRESSION TAG	UNP Q41372
A	288	SER	-	EXPRESSION TAG	UNP Q41372
A	289	GLU	-	EXPRESSION TAG	UNP Q41372
A	290	GLU	-	EXPRESSION TAG	UNP Q41372
A	291	ASP	-	EXPRESSION TAG	UNP Q41372
A	292	LEU	-	EXPRESSION TAG	UNP Q41372
A	293	ASN	-	EXPRESSION TAG	UNP Q41372
A	294	SER	-	EXPRESSION TAG	UNP Q41372
A	295	ALA	-	EXPRESSION TAG	UNP Q41372
A	296	VAL	-	EXPRESSION TAG	UNP Q41372
A	297	ASP	-	EXPRESSION TAG	UNP Q41372
A	298	HIS	-	EXPRESSION TAG	UNP Q41372
A	299	HIS	-	EXPRESSION TAG	UNP Q41372
A	300	HIS	-	EXPRESSION TAG	UNP Q41372
A	301	HIS	-	EXPRESSION TAG	UNP Q41372
A	302	HIS	-	EXPRESSION TAG	UNP Q41372

Continued on next page...

Continued from previous page...

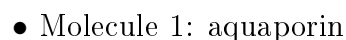
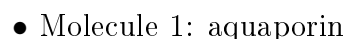
Chain	Residue	Modelled	Actual	Comment	Reference
A	303	HIS	-	EXPRESSION TAG	UNP Q41372
B	282	LEU	-	EXPRESSION TAG	UNP Q41372
B	283	GLU	-	EXPRESSION TAG	UNP Q41372
B	284	GLN	-	EXPRESSION TAG	UNP Q41372
B	285	LYS	-	EXPRESSION TAG	UNP Q41372
B	286	LEU	-	EXPRESSION TAG	UNP Q41372
B	287	ILE	-	EXPRESSION TAG	UNP Q41372
B	288	SER	-	EXPRESSION TAG	UNP Q41372
B	289	GLU	-	EXPRESSION TAG	UNP Q41372
B	290	GLU	-	EXPRESSION TAG	UNP Q41372
B	291	ASP	-	EXPRESSION TAG	UNP Q41372
B	292	LEU	-	EXPRESSION TAG	UNP Q41372
B	293	ASN	-	EXPRESSION TAG	UNP Q41372
B	294	SER	-	EXPRESSION TAG	UNP Q41372
B	295	ALA	-	EXPRESSION TAG	UNP Q41372
B	296	VAL	-	EXPRESSION TAG	UNP Q41372
B	297	ASP	-	EXPRESSION TAG	UNP Q41372
B	298	HIS	-	EXPRESSION TAG	UNP Q41372
B	299	HIS	-	EXPRESSION TAG	UNP Q41372
B	300	HIS	-	EXPRESSION TAG	UNP Q41372
B	301	HIS	-	EXPRESSION TAG	UNP Q41372
B	302	HIS	-	EXPRESSION TAG	UNP Q41372
B	303	HIS	-	EXPRESSION TAG	UNP Q41372
C	282	LEU	-	EXPRESSION TAG	UNP Q41372
C	283	GLU	-	EXPRESSION TAG	UNP Q41372
C	284	GLN	-	EXPRESSION TAG	UNP Q41372
C	285	LYS	-	EXPRESSION TAG	UNP Q41372
C	286	LEU	-	EXPRESSION TAG	UNP Q41372
C	287	ILE	-	EXPRESSION TAG	UNP Q41372
C	288	SER	-	EXPRESSION TAG	UNP Q41372
C	289	GLU	-	EXPRESSION TAG	UNP Q41372
C	290	GLU	-	EXPRESSION TAG	UNP Q41372
C	291	ASP	-	EXPRESSION TAG	UNP Q41372
C	292	LEU	-	EXPRESSION TAG	UNP Q41372
C	293	ASN	-	EXPRESSION TAG	UNP Q41372
C	294	SER	-	EXPRESSION TAG	UNP Q41372
C	295	ALA	-	EXPRESSION TAG	UNP Q41372
C	296	VAL	-	EXPRESSION TAG	UNP Q41372
C	297	ASP	-	EXPRESSION TAG	UNP Q41372
C	298	HIS	-	EXPRESSION TAG	UNP Q41372
C	299	HIS	-	EXPRESSION TAG	UNP Q41372
C	300	HIS	-	EXPRESSION TAG	UNP Q41372

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	301	HIS	-	EXPRESSION TAG	UNP Q41372
C	302	HIS	-	EXPRESSION TAG	UNP Q41372
C	303	HIS	-	EXPRESSION TAG	UNP Q41372
D	282	LEU	-	EXPRESSION TAG	UNP Q41372
D	283	GLU	-	EXPRESSION TAG	UNP Q41372
D	284	GLN	-	EXPRESSION TAG	UNP Q41372
D	285	LYS	-	EXPRESSION TAG	UNP Q41372
D	286	LEU	-	EXPRESSION TAG	UNP Q41372
D	287	ILE	-	EXPRESSION TAG	UNP Q41372
D	288	SER	-	EXPRESSION TAG	UNP Q41372
D	289	GLU	-	EXPRESSION TAG	UNP Q41372
D	290	GLU	-	EXPRESSION TAG	UNP Q41372
D	291	ASP	-	EXPRESSION TAG	UNP Q41372
D	292	LEU	-	EXPRESSION TAG	UNP Q41372
D	293	ASN	-	EXPRESSION TAG	UNP Q41372
D	294	SER	-	EXPRESSION TAG	UNP Q41372
D	295	ALA	-	EXPRESSION TAG	UNP Q41372
D	296	VAL	-	EXPRESSION TAG	UNP Q41372
D	297	ASP	-	EXPRESSION TAG	UNP Q41372
D	298	HIS	-	EXPRESSION TAG	UNP Q41372
D	299	HIS	-	EXPRESSION TAG	UNP Q41372
D	300	HIS	-	EXPRESSION TAG	UNP Q41372
D	301	HIS	-	EXPRESSION TAG	UNP Q41372
D	302	HIS	-	EXPRESSION TAG	UNP Q41372
D	303	HIS	-	EXPRESSION TAG	UNP Q41372

- Molecule 1: aquaporin



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	181.30 Å 103.97 Å 67.07 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.90 32.37 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.90) 89.9 (32.37-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 3.75 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.290 , 0.332 0.283 , 0.341	Depositor DCC
R_{free} test set	519 reflections (4.78%)	DCC
Wilson B-factor (Å ²)	103.8	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 60.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 11748 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6854	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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

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	1.11	4/1817 (0.2%)	0.97	6/2479 (0.2%)
1	B	1.12	4/1718 (0.2%)	1.03	7/2344 (0.3%)
1	C	1.12	4/1743 (0.2%)	1.01	6/2377 (0.3%)
1	D	1.12	5/1769 (0.3%)	1.00	7/2414 (0.3%)
All	All	1.12	17/7047 (0.2%)	1.00	26/9614 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	122	TYR	CE2-CZ	-12.34	1.22	1.38
1	C	122	TYR	CE2-CZ	-12.30	1.22	1.38
1	A	122	TYR	CE2-CZ	-12.30	1.22	1.38
1	B	122	TYR	CE2-CZ	-12.27	1.22	1.38
1	D	122	TYR	CG-CD1	-10.79	1.25	1.39
1	C	122	TYR	CG-CD1	-10.74	1.25	1.39
1	A	122	TYR	CG-CD1	-10.70	1.25	1.39
1	B	122	TYR	CG-CD1	-10.70	1.25	1.39
1	D	122	TYR	CE1-CZ	-8.12	1.27	1.38
1	A	122	TYR	CE1-CZ	-8.06	1.28	1.38
1	C	122	TYR	CE1-CZ	-8.05	1.28	1.38
1	B	122	TYR	CE1-CZ	-8.04	1.28	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	122	TYR	CG-CD2	-7.62	1.29	1.39
1	D	122	TYR	CG-CD2	-7.61	1.29	1.39
1	B	122	TYR	CG-CD2	-7.55	1.29	1.39
1	A	122	TYR	CG-CD2	-7.54	1.29	1.39
1	D	35	TRP	CB-CG	5.39	1.59	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	PRO	CA-N-CD	-15.52	89.77	111.50
1	D	201	PRO	CA-N-CD	-15.52	89.77	111.50
1	C	201	PRO	CA-N-CD	-15.48	89.82	111.50
1	B	201	PRO	CA-N-CD	-15.48	89.83	111.50
1	A	122	TYR	CB-CG-CD1	6.54	124.93	121.00
1	B	122	TYR	CB-CG-CD1	6.50	124.90	121.00
1	D	122	TYR	CB-CG-CD1	6.50	124.90	121.00
1	C	122	TYR	CB-CG-CD1	6.38	124.83	121.00
1	C	199	PRO	N-CA-C	6.11	127.98	112.10
1	D	118	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	118	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	B	118	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	C	118	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	204	PHE	CB-CG-CD1	5.38	124.56	120.80
1	C	204	PHE	CB-CG-CD1	5.36	124.56	120.80
1	D	36	SER	N-CA-C	5.33	125.38	111.00
1	D	204	PHE	CB-CG-CD1	5.33	124.53	120.80
1	B	204	PHE	CB-CG-CD1	5.32	124.52	120.80
1	D	65	GLU	N-CA-C	5.23	125.13	111.00
1	B	70	GLY	N-CA-C	-5.15	100.23	113.10
1	C	213	THR	OG1-CB-CG2	-5.08	98.31	110.00
1	A	213	THR	OG1-CB-CG2	-5.07	98.34	110.00
1	B	213	THR	OG1-CB-CG2	-5.07	98.35	110.00
1	A	122	TYR	CD1-CG-CD2	-5.07	112.33	117.90
1	D	213	THR	OG1-CB-CG2	-5.05	98.38	110.00
1	B	122	TYR	CD1-CG-CD2	-5.05	112.35	117.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	99	HIS	Sidechain
1	B	99	HIS	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	99	HIS	Sidechain
1	D	99	HIS	Sidechain

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	1767	0	1796	126	0
1	B	1671	0	1692	106	0
1	C	1696	0	1727	144	0
1	D	1720	0	1750	121	0
All	All	6854	0	6965	452	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 33.

All (452) 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:39:ARG:HD3	1:D:263:VAL:HG13	1.42	1.01
1:C:66:THR:HG23	1:C:67:VAL:H	1.28	0.98
1:C:134:VAL:HG11	1:C:229:ALA:HA	1.48	0.95
1:C:202:ILE:O	1:C:203:GLY:C	2.02	0.95
1:A:202:ILE:O	1:A:203:GLY:C	2.02	0.95
1:B:32:LEU:HA	1:B:38:TRP:HE1	1.33	0.93
1:C:32:LEU:HD22	1:C:38:TRP:CZ2	2.05	0.91
1:B:202:ILE:O	1:B:203:GLY:C	2.02	0.91
1:D:106:PHE:CE2	1:D:110:LEU:HD11	2.04	0.91
1:D:202:ILE:O	1:D:203:GLY:C	2.02	0.90
1:C:32:LEU:HD22	1:C:38:TRP:HZ2	1.38	0.88
1:A:32:LEU:HD22	1:A:38:TRP:CZ2	2.09	0.86
1:B:199:PRO:O	1:B:201:PRO:N	2.08	0.86
1:A:213:THR:HB	1:A:219:THR:OG1	1.77	0.85
1:C:149:GLY:HA2	1:C:233:PHE:CZ	2.13	0.83
1:C:220:GLY:O	1:C:221:ILE:HG12	1.77	0.83
1:A:74:LEU:HD12	1:A:77:ILE:HD12	1.58	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HD21	1:A:117:LEU:HD21	1.61	0.82
1:B:183:THR:HG22	1:B:185:PRO:HD3	1.62	0.81
1:A:64:LYS:O	1:A:64:LYS:HG2	1.81	0.81
1:A:37:PHE:C	1:A:39:ARG:H	1.83	0.81
1:C:210:HIS:CD2	1:C:219:THR:HG21	2.17	0.80
1:A:194:VAL:HG22	1:A:195:PRO:HD2	1.62	0.79
1:C:37:PHE:C	1:C:39:ARG:H	1.84	0.79
1:D:74:LEU:HD23	1:D:214:ILE:HG21	1.65	0.78
1:D:37:PHE:C	1:D:39:ARG:H	1.85	0.77
1:A:35:TRP:O	1:A:37:PHE:N	2.16	0.77
1:C:35:TRP:O	1:C:37:PHE:N	2.17	0.77
1:A:49:LEU:HD22	1:A:50:LEU:HD23	1.67	0.77
1:D:49:LEU:HD22	1:D:50:LEU:HD23	1.67	0.76
1:C:49:LEU:HD22	1:C:50:LEU:HD23	1.67	0.76
1:B:138:LYS:O	1:B:138:LYS:HG2	1.83	0.76
1:B:35:TRP:HB3	1:B:39:ARG:HD2	1.68	0.76
1:C:133:GLY:O	1:C:137:VAL:HG23	1.86	0.75
1:B:32:LEU:CA	1:B:38:TRP:HE1	2.00	0.75
1:D:251:ILE:O	1:D:255:VAL:HG23	1.86	0.75
1:B:99:HIS:CE1	1:B:108:LEU:HD12	2.22	0.75
1:A:74:LEU:HD22	1:B:70:GLY:O	1.87	0.74
1:A:35:TRP:CE3	1:A:39:ARG:NH1	2.48	0.74
1:A:99:HIS:CE1	1:A:108:LEU:HD12	2.22	0.74
1:C:262:TYR:O	1:C:263:VAL:HG23	1.87	0.74
1:C:62:HIS:HD1	1:C:71:SER:HG	1.32	0.74
1:C:99:HIS:CE1	1:C:108:LEU:HD12	2.22	0.74
1:D:99:HIS:CE1	1:D:108:LEU:HD12	2.22	0.74
1:B:49:LEU:HD22	1:B:50:LEU:HD23	1.67	0.74
1:D:97:GLY:O	1:D:197:LEU:HD12	1.88	0.74
1:C:92:THR:O	1:C:94:GLY:N	2.21	0.74
1:B:31:GLU:HG3	1:B:33:LYS:HG2	1.69	0.73
1:B:37:PHE:C	1:B:39:ARG:H	1.91	0.73
1:D:114:VAL:HG22	1:D:194:VAL:HG22	1.70	0.73
1:C:31:GLU:O	1:C:32:LEU:HD23	1.88	0.73
1:A:106:PHE:CE2	1:A:110:LEU:HD11	2.24	0.72
1:C:180:PHE:HB3	1:C:260:HIS:NE2	2.03	0.72
1:B:31:GLU:HG3	1:B:33:LYS:HE2	1.71	0.72
1:B:32:LEU:HA	1:B:38:TRP:NE1	2.05	0.71
1:B:62:HIS:ND1	1:B:71:SER:HB2	2.05	0.71
1:B:258:ALA:O	1:B:261:GLN:HB3	1.92	0.70
1:B:142:LYS:HG3	1:B:146:ASN:HD21	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:PHE:CD1	1:A:199:PRO:HB2	2.26	0.70
1:B:142:LYS:HG3	1:B:146:ASN:ND2	2.08	0.69
1:C:138:LYS:O	1:C:140:PHE:N	2.24	0.68
1:C:140:PHE:HZ	1:D:166:GLY:HA3	1.59	0.68
1:A:180:PHE:HB3	1:A:260:HIS:CD2	2.28	0.68
1:C:37:PHE:C	1:C:39:ARG:N	2.48	0.68
1:C:62:HIS:ND1	1:C:71:SER:OG	2.20	0.68
1:C:50:LEU:HD22	1:D:170:ILE:CD1	2.24	0.67
1:D:63:SER:C	1:D:65:GLU:H	1.97	0.67
1:D:86:PHE:HD1	1:D:199:PRO:HB2	1.60	0.67
1:D:35:TRP:CE3	1:D:39:ARG:NH1	2.63	0.67
1:C:93:ALA:HA	1:C:97:GLY:C	2.15	0.67
1:C:86:PHE:CZ	1:D:201:PRO:HD3	2.31	0.66
1:B:210:HIS:HA	1:B:219:THR:HG21	1.76	0.66
1:C:86:PHE:CD1	1:C:199:PRO:HB2	2.30	0.66
1:C:141:MET:CE	1:D:216:ILE:HD11	2.26	0.66
1:D:37:PHE:C	1:D:39:ARG:N	2.48	0.65
1:A:37:PHE:C	1:A:39:ARG:N	2.47	0.65
1:B:73:GLY:O	1:B:76:GLY:N	2.30	0.65
1:B:32:LEU:HD22	1:B:38:TRP:HZ2	1.62	0.65
1:B:60:ILE:HD12	1:B:145:TYR:HA	1.79	0.65
1:C:60:ILE:HD12	1:C:145:TYR:HA	1.77	0.65
1:B:35:TRP:O	1:B:37:PHE:N	2.25	0.64
1:A:32:LEU:HD22	1:A:38:TRP:HZ2	1.59	0.64
1:C:86:PHE:HD1	1:C:199:PRO:HB2	1.62	0.64
1:A:28:ASP:OD1	1:A:29:LEU:N	2.31	0.64
1:C:92:THR:HB	1:C:96:SER:OG	1.98	0.64
1:A:106:PHE:CZ	1:A:110:LEU:HD11	2.33	0.64
1:D:130:ALA:O	1:D:134:VAL:HG23	1.98	0.64
1:C:184:ASP:CG	1:C:186:LYS:HE2	2.19	0.63
1:B:37:PHE:C	1:B:39:ARG:N	2.50	0.63
1:C:50:LEU:HD22	1:D:170:ILE:HD13	1.79	0.63
1:C:72:VAL:HG11	1:D:211:LEU:HD22	1.80	0.62
1:C:72:VAL:HB	1:C:76:GLY:HA3	1.82	0.62
1:D:33:LYS:O	1:D:34:LEU:O	2.17	0.62
1:D:65:GLU:HG3	1:D:67:VAL:O	1.99	0.62
1:C:56:VAL:HG12	1:C:137:VAL:HG11	1.82	0.62
1:C:86:PHE:HZ	1:D:201:PRO:HD3	1.65	0.62
1:D:136:LEU:H	1:D:136:LEU:HD12	1.65	0.62
1:B:220:GLY:O	1:B:221:ILE:HG12	1.99	0.62
1:D:143:GLY:O	1:D:147:GLN:HB2	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ILE:O	1:C:197:LEU:HD23	2.00	0.61
1:C:142:LYS:HE3	1:C:146:ASN:HD22	1.65	0.61
1:A:39:ARG:HH21	1:A:39:ARG:HG2	1.64	0.61
1:C:64:LYS:HA	1:C:148:PHE:HE2	1.64	0.61
1:C:210:HIS:CG	1:C:219:THR:HG21	2.36	0.61
1:B:68:VAL:O	1:B:69:CYS:HB2	2.01	0.61
1:C:263:VAL:O	1:C:263:VAL:HG12	2.01	0.61
1:B:253:ALA:O	1:B:256:ALA:HB3	2.00	0.60
1:C:35:TRP:C	1:C:37:PHE:H	2.03	0.60
1:C:39:ARG:HG2	1:C:39:ARG:HH21	1.64	0.60
1:A:201:PRO:HD3	1:B:86:PHE:CZ	2.36	0.60
1:B:149:GLY:HA2	1:B:233:PHE:CZ	2.36	0.60
1:B:64:LYS:HG2	1:B:64:LYS:O	2.01	0.60
1:C:58:THR:OG1	1:D:212:ALA:HA	2.01	0.60
1:C:182:ALA:O	1:C:197:LEU:HA	2.02	0.60
1:A:52:LEU:HD21	1:A:225:ARG:HA	1.84	0.60
1:D:86:PHE:CD1	1:D:199:PRO:HB2	2.37	0.60
1:C:52:LEU:HD21	1:C:225:ARG:HA	1.84	0.60
1:D:52:LEU:HD21	1:D:225:ARG:HA	1.84	0.60
1:C:50:LEU:HD11	1:D:173:PHE:CD2	2.37	0.59
1:B:52:LEU:HD21	1:B:225:ARG:HA	1.84	0.59
1:C:220:GLY:O	1:C:221:ILE:CG1	2.48	0.59
1:D:196:ILE:HG22	1:D:197:LEU:N	2.17	0.59
1:C:130:ALA:O	1:C:134:VAL:HG23	2.03	0.59
1:C:70:GLY:O	1:D:74:LEU:HD13	2.03	0.59
1:D:106:PHE:CZ	1:D:110:LEU:HD11	2.38	0.59
1:A:32:LEU:CD2	1:A:117:LEU:HD21	2.30	0.59
1:C:50:LEU:CD2	1:D:170:ILE:HD11	2.34	0.58
1:B:31:GLU:CG	1:B:33:LYS:HE2	2.33	0.58
1:B:32:LEU:HD13	1:B:38:TRP:NE1	2.18	0.58
1:A:164:ALA:HB1	1:A:217:THR:HG21	1.85	0.58
1:C:66:THR:HG23	1:C:67:VAL:HG23	1.86	0.58
1:A:197:LEU:O	1:A:199:PRO:N	2.35	0.58
1:A:99:HIS:CE1	1:A:108:LEU:CD1	2.87	0.58
1:A:114:VAL:HG12	1:A:118:ARG:HD2	1.85	0.58
1:C:99:HIS:CE1	1:C:108:LEU:CD1	2.87	0.58
1:B:99:HIS:CE1	1:B:108:LEU:CD1	2.87	0.58
1:C:72:VAL:HG11	1:D:211:LEU:CD2	2.33	0.58
1:A:72:VAL:HG23	1:A:76:GLY:HA3	1.86	0.58
1:A:251:ILE:O	1:A:255:VAL:HG23	2.04	0.58
1:D:183:THR:O	1:D:185:PRO:HD3	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ASP:HB2	1:D:196:ILE:HB	1.85	0.57
1:D:99:HIS:CE1	1:D:108:LEU:CD1	2.87	0.57
1:A:166:GLY:HA3	1:B:140:PHE:HE1	1.68	0.57
1:D:159:TYR:CE2	1:D:216:ILE:HG12	2.39	0.57
1:D:99:HIS:C	1:D:100:ILE:HG12	2.25	0.57
1:C:66:THR:HG23	1:C:67:VAL:N	2.10	0.57
1:B:29:LEU:O	1:B:31:GLU:N	2.38	0.57
1:C:183:THR:CG2	1:C:184:ASP:N	2.68	0.56
1:A:65:GLU:CD	1:A:66:THR:H	2.07	0.56
1:C:141:MET:HE3	1:D:216:ILE:HD11	1.86	0.56
1:B:32:LEU:HD13	1:B:38:TRP:CE2	2.40	0.56
1:B:145:TYR:CE1	1:B:150:GLY:HA2	2.40	0.56
1:C:132:CYS:O	1:C:136:LEU:HB2	2.04	0.56
1:A:262:TYR:O	1:A:263:VAL:HG23	2.05	0.56
1:C:259:TYR:O	1:C:263:VAL:HB	2.05	0.56
1:A:194:VAL:HG13	1:A:195:PRO:CD	2.36	0.56
1:A:99:HIS:C	1:A:100:ILE:HG12	2.25	0.56
1:B:112:ARG:O	1:B:112:ARG:HG3	2.06	0.56
1:C:111:ALA:O	1:C:113:LYS:HG3	2.05	0.56
1:C:184:ASP:OD2	1:C:186:LYS:HE2	2.05	0.56
1:B:134:VAL:HB	1:B:232:ILE:HG13	1.88	0.55
1:C:37:PHE:O	1:C:39:ARG:N	2.40	0.55
1:D:138:LYS:HD2	1:D:232:ILE:CG2	2.36	0.55
1:C:50:LEU:HD13	1:D:174:VAL:HG22	1.88	0.55
1:C:99:HIS:C	1:C:100:ILE:HG12	2.25	0.55
1:A:150:GLY:HA3	1:A:233:PHE:CD1	2.41	0.55
1:D:159:TYR:CZ	1:D:216:ILE:HG12	2.41	0.55
1:A:166:GLY:HA3	1:B:140:PHE:CE1	2.42	0.55
1:A:201:PRO:HD3	1:B:86:PHE:HZ	1.72	0.55
1:D:139:ALA:O	1:D:140:PHE:C	2.45	0.55
1:A:37:PHE:O	1:A:39:ARG:N	2.40	0.55
1:A:113:LYS:O	1:A:114:VAL:HG22	2.07	0.55
1:B:99:HIS:C	1:B:100:ILE:HG12	2.25	0.54
1:D:202:ILE:O	1:D:203:GLY:O	2.26	0.54
1:D:72:VAL:CG2	1:D:76:GLY:HA3	2.37	0.54
1:A:86:PHE:HD1	1:A:199:PRO:HB2	1.72	0.54
1:B:202:ILE:O	1:B:203:GLY:O	2.26	0.54
1:C:62:HIS:HA	1:C:71:SER:CB	2.37	0.54
1:B:49:LEU:CD2	1:B:50:LEU:HD23	2.38	0.54
1:A:194:VAL:CG2	1:A:195:PRO:HD2	2.35	0.53
1:A:49:LEU:CD2	1:A:50:LEU:HD23	2.37	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:ALA:C	1:C:259:TYR:H	2.12	0.53
1:C:58:THR:HG1	1:D:211:LEU:C	2.12	0.53
1:A:95:ILE:HG22	1:A:95:ILE:O	2.07	0.53
1:A:212:ALA:HA	1:B:58:THR:OG1	2.09	0.53
1:A:50:LEU:HD22	1:C:170:ILE:CD1	2.39	0.53
1:C:46:ILE:HG21	1:D:259:TYR:CE2	2.44	0.53
1:A:138:LYS:HG3	1:A:145:TYR:HD2	1.74	0.53
1:D:196:ILE:CG2	1:D:197:LEU:N	2.72	0.52
1:A:95:ILE:O	1:A:96:SER:HB3	2.09	0.52
1:A:194:VAL:O	1:A:196:ILE:N	2.42	0.52
1:C:111:ALA:O	1:C:113:LYS:N	2.41	0.52
1:A:202:ILE:O	1:A:203:GLY:O	2.25	0.52
1:C:202:ILE:O	1:C:203:GLY:O	2.26	0.52
1:A:86:PHE:CE1	1:A:199:PRO:HB2	2.45	0.52
1:D:49:LEU:CD2	1:D:50:LEU:HD23	2.38	0.52
1:D:150:GLY:C	1:D:152:ALA:H	2.12	0.52
1:A:28:ASP:CG	1:A:29:LEU:N	2.63	0.52
1:A:31:GLU:C	1:A:33:LYS:H	2.12	0.52
1:A:202:ILE:HA	1:A:205:ALA:HB3	1.92	0.51
1:C:49:LEU:HD22	1:C:50:LEU:CD2	2.39	0.51
1:D:133:GLY:C	1:D:135:GLY:H	2.13	0.51
1:D:92:THR:OG1	1:D:98:GLY:HA2	2.10	0.51
1:C:202:ILE:HA	1:C:205:ALA:HB3	1.92	0.51
1:D:49:LEU:HD22	1:D:50:LEU:CD2	2.40	0.51
1:B:65:GLU:OE2	1:B:67:VAL:HG23	2.11	0.51
1:D:37:PHE:O	1:D:39:ARG:N	2.42	0.51
1:B:37:PHE:O	1:B:39:ARG:N	2.43	0.51
1:C:141:MET:HE2	1:D:216:ILE:HD11	1.91	0.51
1:C:217:THR:C	1:C:219:THR:N	2.63	0.51
1:B:202:ILE:HA	1:B:205:ALA:HB3	1.92	0.51
1:D:34:LEU:O	1:D:35:TRP:C	2.48	0.51
1:B:147:GLN:HG2	1:B:147:GLN:O	2.11	0.51
1:C:34:LEU:O	1:C:35:TRP:HB2	2.10	0.51
1:C:49:LEU:CD2	1:C:50:LEU:HD23	2.37	0.51
1:C:29:LEU:H	1:C:29:LEU:HD12	1.76	0.51
1:A:174:VAL:HG22	1:B:50:LEU:HD13	1.93	0.51
1:C:58:THR:HG1	1:D:212:ALA:HA	1.74	0.51
1:B:153:ASN:HD21	1:B:218:GLY:HA3	1.76	0.50
1:C:85:ILE:HG21	1:C:202:ILE:CG2	2.41	0.50
1:A:60:ILE:HD12	1:A:145:TYR:HA	1.92	0.50
1:A:50:LEU:HD13	1:C:174:VAL:HG22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HD22	1:B:50:LEU:CD2	2.40	0.50
1:D:202:ILE:HA	1:D:205:ALA:HB3	1.92	0.50
1:A:217:THR:C	1:A:219:THR:H	2.13	0.50
1:A:85:ILE:HG21	1:A:202:ILE:CG2	2.41	0.50
1:D:85:ILE:HG21	1:D:202:ILE:CG2	2.41	0.50
1:A:144:PRO:O	1:A:145:TYR:C	2.50	0.50
1:D:137:VAL:O	1:D:141:MET:HG2	2.12	0.50
1:D:156:ALA:HB2	1:D:216:ILE:C	2.32	0.50
1:A:153:ASN:OD1	1:A:225:ARG:CZ	2.60	0.50
1:B:155:VAL:HG23	1:B:241:ASP:OD2	2.12	0.50
1:C:257:ALA:O	1:C:259:TYR:N	2.45	0.49
1:D:114:VAL:HG12	1:D:115:SER:N	2.27	0.49
1:D:145:TYR:CD1	1:D:150:GLY:HA2	2.47	0.49
1:A:211:LEU:C	1:B:58:THR:HG1	2.16	0.49
1:A:113:LYS:C	1:A:114:VAL:HG22	2.32	0.49
1:A:28:ASP:CG	1:A:29:LEU:H	2.15	0.49
1:D:72:VAL:HG23	1:D:76:GLY:HA3	1.93	0.49
1:B:262:TYR:O	1:B:263:VAL:CG2	2.59	0.49
1:B:85:ILE:HG21	1:B:202:ILE:CG2	2.41	0.49
1:B:213:THR:HB	1:B:219:THR:HG23	1.94	0.49
1:C:142:LYS:HE3	1:C:146:ASN:ND2	2.26	0.49
1:B:109:PHE:C	1:B:111:ALA:H	2.15	0.49
1:D:63:SER:O	1:D:65:GLU:N	2.46	0.49
1:C:199:PRO:O	1:C:201:PRO:N	2.46	0.49
1:C:111:ALA:O	1:C:112:ARG:C	2.51	0.49
1:C:155:VAL:HG23	1:C:241:ASP:OD2	2.13	0.49
1:D:213:THR:HB	1:D:219:THR:HG23	1.94	0.49
1:C:35:TRP:O	1:C:39:ARG:HG3	2.13	0.49
1:C:66:THR:CG2	1:C:67:VAL:H	2.09	0.49
1:C:142:LYS:HA	1:C:145:TYR:HB3	1.95	0.48
1:B:31:GLU:CG	1:B:33:LYS:HG2	2.40	0.48
1:D:95:ILE:HG22	1:D:96:SER:N	2.27	0.48
1:C:134:VAL:HG21	1:C:228:GLY:C	2.34	0.48
1:A:62:HIS:C	1:A:62:HIS:ND1	2.66	0.48
1:D:35:TRP:O	1:D:39:ARG:CG	2.61	0.48
1:A:211:LEU:HD22	1:B:72:VAL:HG11	1.96	0.48
1:C:86:PHE:HD1	1:C:199:PRO:CB	2.25	0.48
1:D:138:LYS:HD2	1:D:232:ILE:HG23	1.94	0.48
1:C:183:THR:HG22	1:C:184:ASP:N	2.27	0.48
1:D:64:LYS:HG3	1:D:64:LYS:O	2.13	0.48
1:D:64:LYS:CG	1:D:64:LYS:O	2.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:VAL:O	1:B:182:ALA:N	2.47	0.48
1:B:108:LEU:O	1:B:111:ALA:HB3	2.14	0.48
1:B:33:LYS:O	1:B:34:LEU:C	2.53	0.48
1:A:141:MET:CE	1:C:216:ILE:HD11	2.44	0.48
1:D:135:GLY:O	1:D:138:LYS:HB3	2.14	0.47
1:A:258:ALA:O	1:A:261:GLN:HB3	2.14	0.47
1:A:259:TYR:O	1:A:263:VAL:HB	2.14	0.47
1:C:217:THR:C	1:C:219:THR:H	2.17	0.47
1:A:64:LYS:O	1:A:64:LYS:CG	2.54	0.47
1:D:179:VAL:O	1:D:182:ALA:N	2.47	0.47
1:A:66:THR:HG23	1:A:67:VAL:HG23	1.95	0.47
1:A:179:VAL:O	1:A:182:ALA:N	2.47	0.47
1:B:199:PRO:O	1:B:202:ILE:N	2.47	0.47
1:B:199:PRO:O	1:B:200:LEU:C	2.53	0.47
1:A:49:LEU:HD22	1:A:50:LEU:CD2	2.40	0.47
1:B:73:GLY:O	1:B:74:LEU:C	2.52	0.47
1:C:58:THR:OG1	1:D:211:LEU:C	2.53	0.47
1:B:180:PHE:CE2	1:B:257:ALA:HA	2.50	0.47
1:A:72:VAL:CG2	1:A:76:GLY:HA3	2.44	0.47
1:A:39:ARG:NH2	1:A:39:ARG:HG2	2.29	0.47
1:A:187:ARG:HG3	1:A:191:ASP:HB2	1.97	0.47
1:A:191:ASP:O	1:A:192:SER:HB3	2.15	0.47
1:D:35:TRP:O	1:D:37:PHE:N	2.48	0.47
1:A:170:ILE:CD1	1:B:50:LEU:HD22	2.45	0.47
1:C:50:LEU:CD2	1:D:170:ILE:CD1	2.91	0.46
1:B:48:THR:HG21	1:B:126:GLN:O	2.15	0.46
1:B:137:VAL:O	1:B:141:MET:HG3	2.15	0.46
1:C:110:LEU:HD12	1:C:254:ALA:HA	1.97	0.46
1:B:220:GLY:O	1:B:221:ILE:CG1	2.64	0.46
1:A:138:LYS:HG3	1:A:145:TYR:CD2	2.51	0.46
1:C:251:ILE:O	1:C:255:VAL:HG23	2.16	0.46
1:D:159:TYR:CD2	1:D:216:ILE:HG23	2.51	0.46
1:A:48:THR:HG21	1:A:126:GLN:O	2.16	0.46
1:A:68:VAL:HG13	1:A:69:CYS:SG	2.56	0.46
1:B:145:TYR:CE1	1:B:150:GLY:CA	2.99	0.46
1:D:134:VAL:O	1:D:232:ILE:HG21	2.16	0.46
1:C:39:ARG:HG2	1:C:39:ARG:NH2	2.29	0.46
1:D:156:ALA:CB	1:D:216:ILE:O	2.63	0.46
1:A:144:PRO:O	1:A:145:TYR:O	2.34	0.46
1:D:113:LYS:HE3	1:D:113:LYS:HA	1.98	0.46
1:D:48:THR:HG21	1:D:126:GLN:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:C	1:A:62:HIS:H	2.19	0.46
1:B:113:LYS:HA	1:B:113:LYS:HE3	1.98	0.46
1:C:257:ALA:C	1:C:259:TYR:N	2.70	0.45
1:D:150:GLY:C	1:D:152:ALA:N	2.69	0.45
1:C:179:VAL:O	1:C:182:ALA:N	2.47	0.45
1:D:60:ILE:HD13	1:D:60:ILE:HA	1.77	0.45
1:D:74:LEU:HD23	1:D:214:ILE:CG2	2.41	0.45
1:D:156:ALA:HB3	1:D:159:TYR:HD2	1.81	0.45
1:C:29:LEU:HD12	1:C:29:LEU:N	2.32	0.45
1:C:48:THR:HG21	1:C:126:GLN:O	2.16	0.45
1:C:106:PHE:CZ	1:C:110:LEU:HD21	2.51	0.45
1:B:201:PRO:HD3	1:D:86:PHE:CZ	2.51	0.45
1:B:199:PRO:C	1:B:201:PRO:N	2.66	0.45
1:A:74:LEU:CD1	1:A:77:ILE:HD12	2.40	0.45
1:D:35:TRP:O	1:D:39:ARG:HG2	2.17	0.45
1:A:64:LYS:HA	1:A:148:PHE:CZ	2.52	0.45
1:C:62:HIS:HA	1:C:71:SER:HB2	1.97	0.45
1:A:196:ILE:O	1:A:197:LEU:HG	2.17	0.45
1:A:50:LEU:CD2	1:C:170:ILE:HD11	2.47	0.45
1:A:190:ARG:HG3	1:A:193:HIS:HD2	1.82	0.45
1:C:199:PRO:O	1:C:200:LEU:C	2.55	0.45
1:A:64:LYS:HA	1:A:148:PHE:CE1	2.52	0.45
1:D:196:ILE:CG2	1:D:197:LEU:H	2.30	0.45
1:C:140:PHE:CZ	1:D:166:GLY:HA3	2.46	0.45
1:A:60:ILE:O	1:A:62:HIS:N	2.50	0.45
1:A:256:ALA:C	1:A:258:ALA:H	2.21	0.45
1:A:213:THR:CB	1:A:219:THR:OG1	2.56	0.44
1:B:99:HIS:HE1	1:B:108:LEU:HD12	1.78	0.44
1:C:196:ILE:C	1:C:197:LEU:HD23	2.38	0.44
1:A:52:LEU:HG	1:A:134:VAL:HG23	1.99	0.44
1:C:93:ALA:O	1:C:95:ILE:N	2.50	0.44
1:C:99:HIS:HE1	1:C:108:LEU:HD12	1.78	0.44
1:B:65:GLU:HG3	1:B:67:VAL:H	1.82	0.44
1:C:50:LEU:HD13	1:D:174:VAL:CG2	2.48	0.44
1:C:259:TYR:CE2	1:C:263:VAL:HG21	2.52	0.44
1:D:86:PHE:HE1	1:D:199:PRO:HG2	1.83	0.44
1:A:99:HIS:HE1	1:A:108:LEU:HD12	1.78	0.44
1:B:138:LYS:HB2	1:B:145:TYR:CD2	2.52	0.44
1:C:74:LEU:N	1:C:74:LEU:HD12	2.32	0.44
1:C:95:ILE:HG23	1:C:95:ILE:O	2.18	0.44
1:B:212:ALA:HA	1:D:58:THR:OG1	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:GLY:O	1:C:71:SER:O	2.36	0.43
1:D:99:HIS:HE1	1:D:108:LEU:HD12	1.78	0.43
1:C:64:LYS:HA	1:C:148:PHE:CE2	2.49	0.43
1:B:262:TYR:O	1:B:263:VAL:HG22	2.17	0.43
1:A:259:TYR:CE1	1:A:263:VAL:HG21	2.53	0.43
1:C:58:THR:OG1	1:D:212:ALA:CA	2.64	0.43
1:C:142:LYS:O	1:C:145:TYR:HB3	2.19	0.43
1:C:32:LEU:O	1:C:34:LEU:N	2.51	0.43
1:A:191:ASP:O	1:A:192:SER:CB	2.66	0.43
1:C:149:GLY:O	1:C:151:GLY:N	2.52	0.43
1:A:156:ALA:O	1:A:157:LEU:C	2.57	0.43
1:C:206:VAL:O	1:C:210:HIS:HD2	2.02	0.43
1:C:262:TYR:HA	1:C:262:TYR:HD1	1.71	0.43
1:C:93:ALA:C	1:C:95:ILE:H	2.22	0.43
1:A:194:VAL:HG13	1:A:195:PRO:HD2	2.00	0.43
1:C:155:VAL:HG12	1:C:156:ALA:N	2.33	0.43
1:B:262:TYR:C	1:B:263:VAL:HG23	2.39	0.42
1:C:259:TYR:CD2	1:C:263:VAL:HG21	2.55	0.42
1:D:206:VAL:O	1:D:210:HIS:HD2	2.02	0.42
1:B:31:GLU:HG3	1:B:33:LYS:CE	2.47	0.42
1:A:95:ILE:CG2	1:A:95:ILE:O	2.66	0.42
1:D:95:ILE:CG2	1:D:96:SER:N	2.82	0.42
1:B:41:ALA:HB2	1:B:121:VAL:HG12	2.01	0.42
1:B:206:VAL:O	1:B:210:HIS:HD2	2.02	0.42
1:D:54:ILE:O	1:D:57:ALA:HB3	2.20	0.42
1:A:206:VAL:O	1:A:210:HIS:HD2	2.02	0.42
1:B:145:TYR:CD1	1:B:150:GLY:HA2	2.55	0.42
1:A:53:TYR:O	1:A:54:ILE:C	2.58	0.42
1:B:54:ILE:O	1:B:57:ALA:HB3	2.20	0.42
1:C:54:ILE:O	1:C:57:ALA:HB3	2.20	0.42
1:C:50:LEU:HD11	1:D:173:PHE:CE2	2.55	0.42
1:D:72:VAL:HG23	1:D:73:GLY:O	2.18	0.42
1:B:53:TYR:O	1:B:54:ILE:C	2.58	0.42
1:D:31:GLU:O	1:D:31:GLU:HG2	2.19	0.42
1:A:136:LEU:CD2	1:A:140:PHE:CE2	3.02	0.42
1:A:137:VAL:C	1:A:139:ALA:N	2.68	0.42
1:C:85:ILE:HG21	1:C:202:ILE:HG21	2.01	0.42
1:B:85:ILE:HG21	1:B:202:ILE:HG21	2.01	0.42
1:D:85:ILE:HG21	1:D:202:ILE:HG21	2.01	0.42
1:B:157:LEU:O	1:B:157:LEU:HD22	2.19	0.42
1:D:145:TYR:HE2	1:D:232:ILE:HG22	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:OG1	1:C:212:ALA:HA	2.20	0.42
1:C:85:ILE:HG21	1:C:202:ILE:HG22	2.02	0.42
1:C:156:ALA:O	1:C:158:GLY:N	2.53	0.42
1:D:85:ILE:HG21	1:D:202:ILE:HG22	2.02	0.42
1:A:85:ILE:HG21	1:A:202:ILE:HG21	2.01	0.41
1:A:32:LEU:HB3	1:A:38:TRP:HE1	1.85	0.41
1:A:49:LEU:C	1:A:49:LEU:HD23	2.41	0.41
1:D:184:ASP:OD2	1:D:196:ILE:HG22	2.19	0.41
1:B:64:LYS:HD2	1:B:144:PRO:CG	2.50	0.41
1:A:113:LYS:HD3	1:A:113:LYS:HA	1.73	0.41
1:A:146:ASN:HA	1:A:233:PHE:HE1	1.85	0.41
1:B:31:GLU:HG3	1:B:33:LYS:CG	2.46	0.41
1:A:211:LEU:CD2	1:B:72:VAL:HG11	2.49	0.41
1:A:136:LEU:CD2	1:A:140:PHE:HE2	2.33	0.41
1:C:85:ILE:HA	1:C:85:ILE:HD13	1.84	0.41
1:C:49:LEU:C	1:C:49:LEU:HD23	2.41	0.41
1:D:99:HIS:HE1	1:D:108:LEU:CD1	2.33	0.41
1:A:109:PHE:C	1:A:111:ALA:H	2.23	0.41
1:B:85:ILE:HG21	1:B:202:ILE:HG22	2.02	0.41
1:A:54:ILE:O	1:A:57:ALA:HB3	2.20	0.41
1:C:35:TRP:C	1:C:37:PHE:N	2.69	0.41
1:A:63:SER:O	1:A:148:PHE:CD1	2.73	0.41
1:D:35:TRP:O	1:D:39:ARG:HG3	2.20	0.41
1:D:49:LEU:C	1:D:49:LEU:HD23	2.41	0.41
1:D:92:THR:O	1:D:94:GLY:N	2.54	0.41
1:A:85:ILE:HA	1:A:85:ILE:HD13	1.84	0.41
1:B:201:PRO:HD3	1:D:86:PHE:HZ	1.85	0.41
1:D:53:TYR:O	1:D:54:ILE:C	2.58	0.41
1:A:198:ALA:HB3	1:A:199:PRO:HD3	2.03	0.41
1:B:67:VAL:O	1:B:68:VAL:C	2.59	0.41
1:A:259:TYR:O	1:A:263:VAL:CG2	2.69	0.41
1:B:134:VAL:O	1:B:135:GLY:C	2.59	0.41
1:C:53:TYR:O	1:C:54:ILE:C	2.58	0.41
1:A:194:VAL:CB	1:A:195:PRO:HD2	2.51	0.41
1:A:85:ILE:HG21	1:A:202:ILE:HG22	2.02	0.41
1:B:198:ALA:HB3	1:B:199:PRO:HD3	2.03	0.41
1:D:85:ILE:HD13	1:D:85:ILE:HA	1.84	0.41
1:C:55:THR:HG21	1:C:81:PHE:CD1	2.56	0.41
1:D:63:SER:C	1:D:65:GLU:N	2.66	0.41
1:B:72:VAL:HB	1:B:76:GLY:HA3	2.02	0.41
1:C:179:VAL:HA	1:C:182:ALA:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:VAL:O	1:A:135:GLY:C	2.58	0.41
1:B:134:VAL:HG12	1:B:232:ILE:HG21	2.03	0.41
1:A:55:THR:HG21	1:A:81:PHE:CD1	2.56	0.41
1:B:216:ILE:HG22	1:B:217:THR:CG2	2.51	0.41
1:D:156:ALA:CB	1:D:216:ILE:HA	2.51	0.41
1:A:179:VAL:HA	1:A:182:ALA:HB3	2.03	0.41
1:A:37:PHE:O	1:A:40:ALA:N	2.55	0.40
1:A:163:THR:HA	1:B:140:PHE:HD1	1.86	0.40
1:D:210:HIS:HA	1:D:219:THR:HG21	2.03	0.40
1:D:55:THR:HG21	1:D:81:PHE:CD1	2.56	0.40
1:D:179:VAL:HA	1:D:182:ALA:HB3	2.03	0.40
1:C:39:ARG:O	1:C:42:ILE:N	2.45	0.40
1:B:49:LEU:C	1:B:49:LEU:HD23	2.41	0.40
1:A:81:PHE:CG	1:A:210:HIS:CE1	3.10	0.40
1:C:66:THR:HG23	1:C:67:VAL:CG2	2.52	0.40
1:D:202:ILE:C	1:D:204:PHE:N	2.70	0.40
1:D:81:PHE:CG	1:D:210:HIS:CE1	3.10	0.40
1:A:86:PHE:HB2	1:A:203:GLY:HA3	2.04	0.40
1:B:55:THR:HG21	1:B:81:PHE:CD1	2.56	0.40
1:B:81:PHE:CG	1:B:210:HIS:CE1	3.09	0.40
1:B:216:ILE:HG22	1:B:217:THR:HG23	2.03	0.40
1:C:86:PHE:HB2	1:C:203:GLY:HA3	2.04	0.40
1:C:81:PHE:CG	1:C:210:HIS:CE1	3.10	0.40
1:C:92:THR:OG1	1:C:98:GLY:HA2	2.21	0.40
1:D:41:ALA:HB2	1:D:121:VAL:HG12	2.03	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	234/303 (77%)	170 (73%)	42 (18%)	22 (9%)	1 15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	220/303 (73%)	173 (79%)	29 (13%)	18 (8%)	1	18
1	C	223/303 (74%)	175 (78%)	21 (9%)	27 (12%)	0	8
1	D	226/303 (75%)	180 (80%)	27 (12%)	19 (8%)	1	17
All	All	903/1212 (74%)	698 (77%)	119 (13%)	86 (10%)	1	15

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	SER
1	A	96	SER
1	A	145	TYR
1	A	187	ARG
1	A	195	PRO
1	A	196	ILE
1	A	198	ALA
1	B	30	GLY
1	B	36	SER
1	B	199	PRO
1	B	200	LEU
1	C	33	LYS
1	C	34	LEU
1	C	36	SER
1	C	67	VAL
1	C	71	SER
1	C	93	ALA
1	C	112	ARG
1	C	157	LEU
1	D	29	LEU
1	D	34	LEU
1	D	35	TRP
1	D	36	SER
1	D	64	LYS
1	D	93	ALA
1	D	199	PRO
1	A	34	LEU
1	A	114	VAL
1	A	197	LEU
1	B	34	LEU
1	B	93	ALA
1	C	37	PHE
1	C	139	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	149	GLY
1	C	219	THR
1	C	258	ALA
1	D	143	GLY
1	D	149	GLY
1	A	45	PHE
1	A	61	GLY
1	B	33	LYS
1	B	45	PHE
1	C	45	PHE
1	C	94	GLY
1	C	138	LYS
1	D	45	PHE
1	D	62	HIS
1	D	139	ALA
1	A	29	LEU
1	A	38	TRP
1	A	192	SER
1	A	219	THR
1	B	96	SER
1	C	35	TRP
1	C	38	TRP
1	C	145	TYR
1	D	140	PHE
1	D	219	THR
1	A	53	TYR
1	A	199	PRO
1	B	53	TYR
1	B	69	CYS
1	B	72	VAL
1	B	150	GLY
1	B	219	THR
1	C	53	TYR
1	C	66	THR
1	C	140	PHE
1	C	221	ILE
1	D	53	TYR
1	D	142	LYS
1	A	54	ILE
1	B	54	ILE
1	C	54	ILE
1	C	95	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	158	GLY
1	D	54	ILE
1	A	100	ILE
1	B	100	ILE
1	C	100	ILE
1	D	100	ILE
1	A	218	GLY
1	A	221	ILE
1	B	221	ILE
1	C	199	PRO
1	D	134	VAL

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	176/234 (75%)	157 (89%)	19 (11%)	8	39
1	B	165/234 (70%)	147 (89%)	18 (11%)	8	39
1	C	168/234 (72%)	151 (90%)	17 (10%)	9	41
1	D	171/234 (73%)	151 (88%)	20 (12%)	7	35
All	All	680/936 (73%)	606 (89%)	74 (11%)	8	39

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	52	LEU
1	A	71	SER
1	A	100	ILE
1	A	114	VAL
1	A	120	LEU
1	A	136	LEU
1	A	147	GLN
1	A	157	LEU
1	A	170	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	188	SER
1	A	190	ARG
1	A	191	ASP
1	A	193	HIS
1	A	194	VAL
1	A	201	PRO
1	A	225	ARG
1	A	235	SER
1	A	260	HIS
1	B	32	LEU
1	B	39	ARG
1	B	52	LEU
1	B	66	THR
1	B	68	VAL
1	B	72	VAL
1	B	74	LEU
1	B	100	ILE
1	B	113	LYS
1	B	120	LEU
1	B	153	ASN
1	B	157	LEU
1	B	170	ILE
1	B	185	PRO
1	B	201	PRO
1	B	225	ARG
1	B	235	SER
1	B	262	TYR
1	C	52	LEU
1	C	68	VAL
1	C	72	VAL
1	C	95	ILE
1	C	100	ILE
1	C	120	LEU
1	C	136	LEU
1	C	140	PHE
1	C	141	MET
1	C	154	SER
1	C	170	ILE
1	C	184	ASP
1	C	201	PRO
1	C	225	ARG
1	C	235	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	260	HIS
1	C	262	TYR
1	D	28	ASP
1	D	29	LEU
1	D	39	ARG
1	D	52	LEU
1	D	63	SER
1	D	66	THR
1	D	95	ILE
1	D	100	ILE
1	D	113	LYS
1	D	120	LEU
1	D	147	GLN
1	D	157	LEU
1	D	170	ILE
1	D	193	HIS
1	D	201	PRO
1	D	225	ARG
1	D	235	SER
1	D	260	HIS
1	D	262	TYR
1	D	263	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	A	147	GLN
1	A	193	HIS
1	A	210	HIS
1	A	260	HIS
1	B	99	HIS
1	B	147	GLN
1	B	153	ASN
1	B	210	HIS
1	C	99	HIS
1	C	146	ASN
1	C	210	HIS
1	D	99	HIS
1	D	210	HIS

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	236/303 (77%)	0.01	11 (4%) 35 26	34, 60, 87, 97	236 (100%)
1	B	224/303 (73%)	-0.11	4 (1%) 71 61	41, 66, 89, 103	224 (100%)
1	C	227/303 (74%)	-0.14	5 (2%) 65 54	44, 68, 94, 103	227 (100%)
1	D	230/303 (75%)	-0.13	1 (0%) 93 90	52, 77, 93, 107	230 (100%)
All	All	917/1212 (75%)	-0.09	21 (2%) 64 52	34, 68, 92, 107	917 (100%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	28	ASP	4.6
1	A	191	ASP	4.3
1	C	31	GLU	3.9
1	A	190	ARG	3.8
1	A	192	SER	3.5
1	A	189	ALA	3.3
1	D	234	ASN	3.2
1	A	195	PRO	2.9
1	A	193	HIS	2.9
1	C	30	GLY	2.9
1	B	35	TRP	2.7
1	C	160	ASN	2.6
1	A	94	GLY	2.4
1	A	183	THR	2.3
1	A	262	TYR	2.2
1	B	33	LYS	2.1
1	C	28	ASP	2.1
1	B	34	LEU	2.1
1	A	233	PHE	2.1
1	A	29	LEU	2.0
1	C	161	LYS	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.