



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:48 AM UTC

PDB ID : 4IU8 / pdb_00004iu8
Title : Crystal structure of a membrane transporter (selenomethionine derivative)
Authors : Yan, H.; Huang, W.; Yan, C.; Gong, X.; Jiang, S.; Zhao, Y.; Wang, J.; Shi, Y.
Deposited on : 2013-01-20
Resolution : 3.11 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

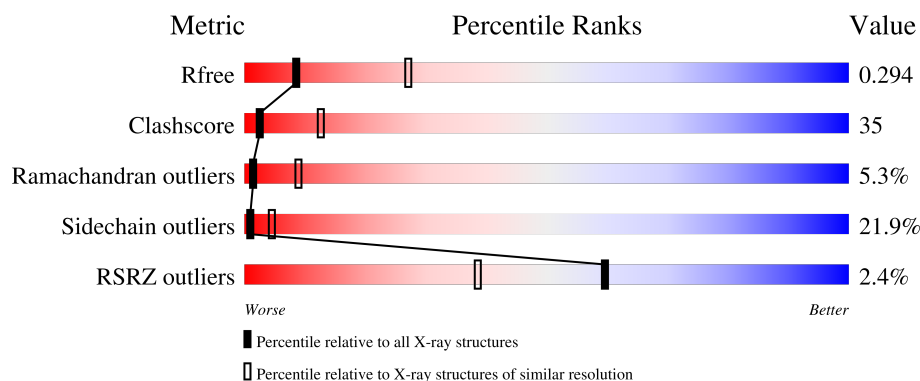
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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	468	40% 36% 14% 10%
1	B	468	3% 36% 44% 11% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6214 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.

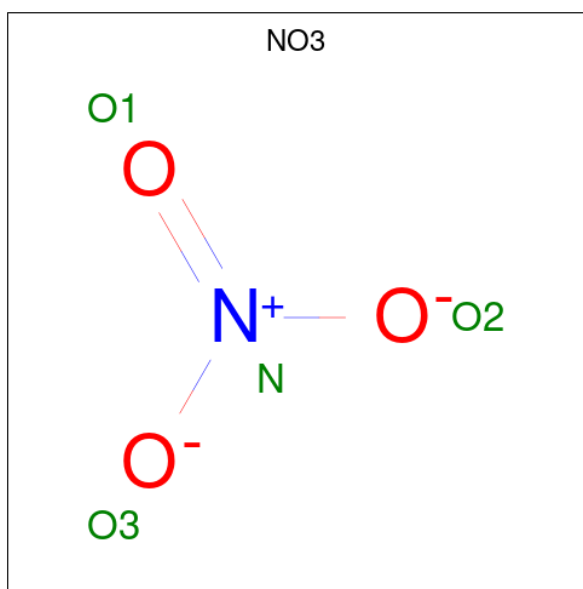
- Molecule 1 is a protein called Nitrite extrusion protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	Se	0	0	0
			3081	2059	490	514	5	13			
1	B	427	Total	C	N	O	S	Se	0	0	0
			3129	2092	500	519	5	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	463	LEU	-	expression tag	UNP P37758
A	464	GLU	-	expression tag	UNP P37758
A	465	VAL	-	expression tag	UNP P37758
A	466	LEU	-	expression tag	UNP P37758
A	467	PHE	-	expression tag	UNP P37758
A	468	GLN	-	expression tag	UNP P37758
B	463	LEU	-	expression tag	UNP P37758
B	464	GLU	-	expression tag	UNP P37758
B	465	VAL	-	expression tag	UNP P37758
B	466	LEU	-	expression tag	UNP P37758
B	467	PHE	-	expression tag	UNP P37758
B	468	GLN	-	expression tag	UNP P37758

- Molecule 2 is NITRATE ION (CCD ID: NO3) (formula: NO₃).

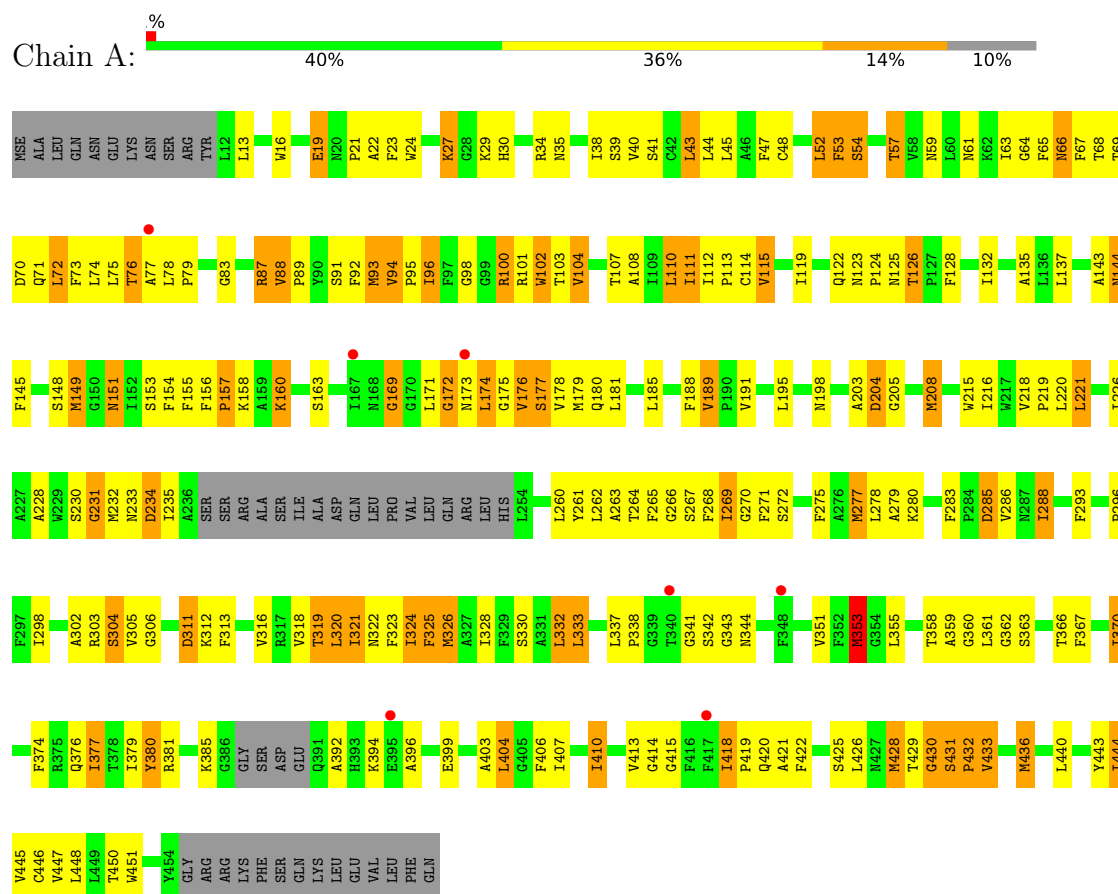


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	N	O	0	0
			4	1	3		

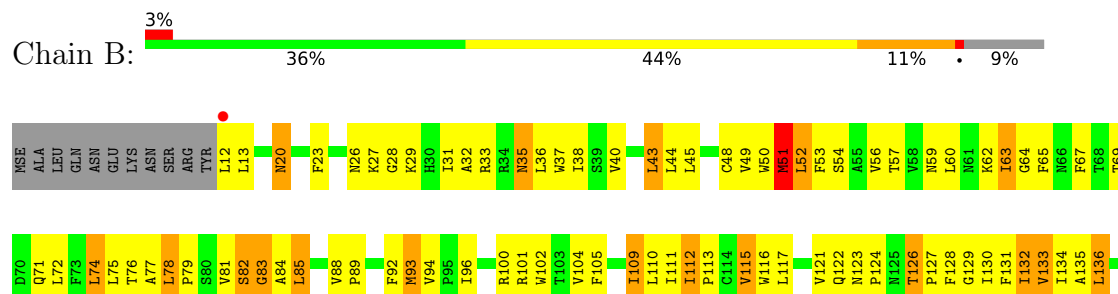
3 Residue-property plots

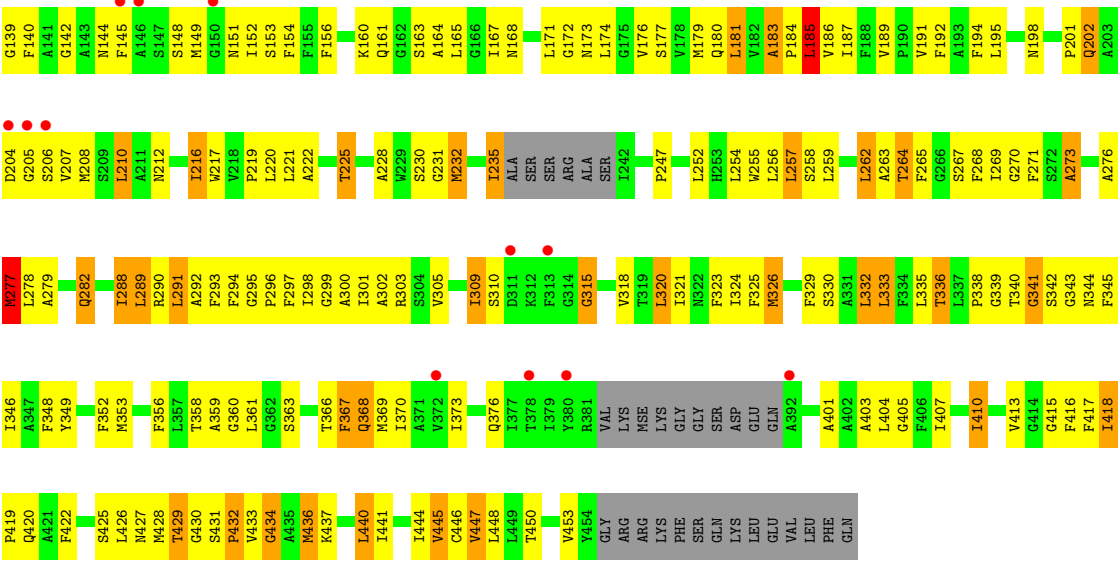
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Nitrite extrusion protein 2



• Molecule 1: Nitrite extrusion protein 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.58Å 117.50Å 127.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.11 40.00 – 3.11	Depositor EDS
% Data completeness (in resolution range)	82.7 (40.00-3.11) 83.0 (40.00-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.239 , 0.299 0.240 , 0.294	Depositor DCC
R_{free} test set	1224 reflections (2.84%)	wwPDB-VP
Wilson B-factor (Å ²)	79.4	Xtriage
Anisotropy	1.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6214	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NO3

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	0.82	2/3150 (0.1%)	1.16	14/4276 (0.3%)
1	B	0.90	1/3202 (0.0%)	1.19	16/4349 (0.4%)
All	All	0.86	3/6352 (0.0%)	1.17	30/8625 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	432	PRO	N-CA	-6.43	1.43	1.47
1	A	189	VAL	CA-CB	5.28	1.58	1.54
1	A	215	TRP	CD2-CE2	5.20	1.50	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	418	ILE	CA-C-N	-8.29	111.18	119.56
1	B	418	ILE	C-N-CA	-8.29	111.18	119.56
1	B	183	ALA	CA-C-N	-7.42	112.39	121.00
1	B	183	ALA	C-N-CA	-7.42	112.39	121.00
1	B	445	VAL	CB-CA-C	-6.76	103.18	112.04
1	B	247	PRO	N-CA-CB	6.72	110.31	103.25
1	A	418	ILE	CA-C-N	-6.52	112.11	119.28
1	A	418	ILE	C-N-CA	-6.52	112.11	119.28
1	A	188	PHE	CA-C-N	-6.24	117.90	123.33
1	A	188	PHE	C-N-CA	-6.24	117.90	123.33
1	A	94	VAL	CB-CA-C	-6.08	107.92	113.70
1	A	353	MSE	CG-SE-CE	6.03	112.19	98.92
1	B	49	VAL	CB-CA-C	-5.94	104.02	112.22
1	A	176	VAL	N-CA-C	-5.87	104.91	110.42
1	A	172	GLY	N-CA-C	-5.81	105.33	112.77
1	B	20	ASN	CA-C-N	5.77	125.24	119.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	ASN	C-N-CA	5.77	125.24	119.24
1	A	52	LEU	N-CA-C	-5.56	106.17	113.12
1	A	54	SER	N-CA-C	-5.47	103.19	111.56
1	B	185	LEU	N-CA-C	-5.43	107.20	113.88
1	B	434	GLY	N-CA-C	-5.42	105.84	112.77
1	B	277	MSE	CA-CB-CG	-5.39	103.32	114.10
1	B	321	ILE	CB-CA-C	-5.38	104.87	112.14
1	B	161	GLN	N-CA-C	5.32	117.16	111.36
1	A	189	VAL	CB-CA-C	5.29	115.26	110.13
1	B	341	GLY	N-CA-C	-5.28	103.08	110.63
1	A	102	TRP	N-CA-C	5.22	116.65	111.07
1	A	158	LYS	N-CA-C	-5.15	106.95	113.18
1	B	273	ALA	N-CA-C	5.09	116.91	111.36
1	A	341	GLY	N-CA-C	-5.08	104.55	112.58

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	3081	0	3049	223	0
1	B	3129	0	3092	206	0
2	A	4	0	0	1	0
All	All	6214	0	6141	427	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 35.

All (427) 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:A:123:ASN:O	1:A:126:THR:HG22	1.47	1.11
1:B:12:LEU:HD23	1:B:13:LEU:H	1.12	1.08
1:A:63:ILE:HG22	1:A:64:GLY:H	1.23	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:VAL:HB	1:A:89:PRO:HD3	1.41	1.01
1:B:93:MSE:HG2	1:B:102:TRP:CH2	1.96	1.00
1:B:74:LEU:HD23	1:B:420:GLN:HE22	1.24	0.98
1:A:269:ILE:HD12	1:A:415:GLY:HA3	1.50	0.94
1:B:123:ASN:O	1:B:126:THR:HB	1.68	0.94
1:A:320:LEU:HD11	1:A:450:THR:HB	1.52	0.91
1:A:374:PHE:HE2	1:A:399:GLU:HG3	1.35	0.90
1:A:323:PHE:CE1	1:A:446:CYS:HB3	2.05	0.90
1:B:12:LEU:HD23	1:B:13:LEU:N	1.86	0.89
1:A:324:ILE:HG12	1:A:447:VAL:HG13	1.54	0.88
1:A:324:ILE:HG12	1:A:447:VAL:CG1	2.04	0.87
1:B:258:SER:HB3	1:B:407:ILE:HG12	1.57	0.87
1:A:44:LEU:HD21	1:A:178:VAL:HG11	1.57	0.86
1:B:74:LEU:HD23	1:B:420:GLN:NE2	1.89	0.86
1:A:64:GLY:HA3	1:A:124:PRO:HB3	1.58	0.83
1:A:374:PHE:CE2	1:A:399:GLU:HG3	2.15	0.81
1:B:100:ARG:HG3	1:B:232:MSE:HB3	1.63	0.81
1:A:433:VAL:H	1:A:436:MSE:HG3	1.46	0.80
1:A:323:PHE:CD1	1:A:446:CYS:HB3	2.17	0.80
1:A:93:MSE:HG2	1:A:102:TRP:CH2	2.18	0.79
1:B:63:ILE:HG22	1:B:64:GLY:H	1.48	0.78
1:A:279:ALA:HB3	1:A:288:ILE:HD13	1.64	0.78
1:A:53:PHE:O	1:A:57:THR:OG1	2.03	0.77
1:A:111:ILE:HG23	1:A:218:VAL:HG22	1.65	0.77
1:A:73:PHE:CZ	1:A:277:MSE:HB3	2.20	0.77
1:B:276:ALA:HA	1:B:288:ILE:HD12	1.66	0.77
1:A:279:ALA:CB	1:A:288:ILE:HD13	2.15	0.76
1:B:320:LEU:HD23	1:B:450:THR:HB	1.65	0.76
1:B:300:ALA:O	1:B:303:ARG:HB3	1.86	0.76
1:B:51:MSE:HE3	1:B:51:MSE:HA	1.69	0.75
1:A:52:LEU:HD23	1:A:179:MSE:HE1	1.69	0.74
1:A:88:VAL:HB	1:A:89:PRO:CD	2.16	0.74
1:B:82:SER:CB	1:B:139:GLY:HA3	2.18	0.74
1:A:304:SER:O	1:A:306:GLY:N	2.20	0.74
1:A:77:ALA:HB2	1:A:419:PRO:HB2	1.69	0.73
1:A:123:ASN:O	1:A:126:THR:CG2	2.32	0.73
1:B:367:PHE:C	1:B:369:MSE:H	1.97	0.73
1:A:396:ALA:HA	1:A:399:GLU:HB3	1.71	0.72
1:B:65:PHE:CD1	1:B:67:PHE:CE2	2.77	0.72
1:B:426:LEU:O	1:B:430:GLY:HA2	1.89	0.72
1:B:35:ASN:HD21	1:B:232:MSE:HA	1.53	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:PHE:O	1:A:149:MSE:HB2	1.89	0.71
1:B:363:SER:O	1:B:366:THR:HG22	1.90	0.71
1:B:81:VAL:O	1:B:85:LEU:HB2	1.91	0.71
1:A:320:LEU:O	1:A:324:ILE:HG13	1.91	0.70
1:A:94:VAL:HB	1:A:95:PRO:HD3	1.73	0.70
1:A:94:VAL:O	1:A:98:GLY:N	2.22	0.70
1:A:304:SER:C	1:A:306:GLY:H	1.99	0.70
1:B:93:MSE:HG2	1:B:102:TRP:CZ3	2.27	0.69
1:A:72:LEU:O	1:A:76:THR:HG23	1.92	0.69
1:A:323:PHE:HB3	1:A:447:VAL:HG22	1.72	0.69
1:B:82:SER:HB2	1:B:139:GLY:HA3	1.74	0.69
1:B:278:LEU:HD22	1:B:422:PHE:CZ	2.28	0.69
1:A:35:ASN:OD1	1:A:232:MSE:HA	1.93	0.68
1:B:258:SER:CB	1:B:407:ILE:HG12	2.23	0.68
1:B:330:SER:OG	1:B:440:LEU:HD23	1.94	0.68
1:A:24:TRP:NE1	1:A:29:LYS:HB3	2.10	0.67
1:B:71:GLN:HB2	1:B:128:PHE:CE2	2.29	0.67
1:A:103:THR:HG21	1:A:232:MSE:SE	2.44	0.67
1:B:425:SER:OG	1:B:432:PRO:HA	1.93	0.67
1:A:111:ILE:HG12	1:A:221:LEU:HD23	1.76	0.67
1:B:67:PHE:CE1	1:B:128:PHE:HD2	2.11	0.67
1:A:370:ILE:HG21	1:A:407:ILE:HD13	1.75	0.67
1:A:433:VAL:N	1:A:436:MSE:HG3	2.10	0.67
1:A:65:PHE:HE1	1:A:126:THR:HG23	1.59	0.67
1:A:425:SER:OG	1:A:432:PRO:O	2.12	0.66
1:B:12:LEU:CD2	1:B:13:LEU:H	2.00	0.66
1:A:65:PHE:HB3	1:A:67:PHE:CE2	2.31	0.66
1:A:323:PHE:HE1	1:A:446:CYS:HB3	1.58	0.66
1:A:63:ILE:HG22	1:A:64:GLY:N	2.03	0.65
1:A:363:SER:O	1:A:367:PHE:HB2	1.96	0.65
1:A:262:LEU:C	1:A:262:LEU:HD23	2.22	0.64
1:A:234:ASP:C	1:A:235:ILE:HG13	2.22	0.64
1:B:302:ALA:HA	1:B:305:VAL:HB	1.79	0.64
1:A:443:TYR:O	1:A:447:VAL:HG23	1.97	0.64
1:B:324:ILE:HD13	1:B:447:VAL:HG21	1.78	0.64
1:A:45:LEU:O	1:A:48:CYS:HB2	1.97	0.64
1:B:35:ASN:ND2	1:B:232:MSE:HA	2.13	0.64
1:A:149:MSE:HE1	1:A:169:GLY:CA	2.28	0.64
1:A:230:SER:O	1:A:232:MSE:N	2.30	0.64
1:A:271:PHE:CE1	1:A:418:ILE:HD13	2.32	0.64
1:A:61:ASN:OD1	1:A:66:ASN:HA	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:SER:HA	1:B:407:ILE:HG23	1.78	0.63
1:B:71:GLN:HB2	1:B:128:PHE:CZ	2.33	0.63
1:B:67:PHE:CD1	1:B:128:PHE:HD2	2.16	0.63
1:B:323:PHE:CE1	1:B:446:CYS:HB3	2.33	0.63
1:B:65:PHE:CD1	1:B:67:PHE:HE2	2.15	0.63
1:B:51:MSE:HA	1:B:51:MSE:CE	2.26	0.62
1:B:100:ARG:HD3	1:B:232:MSE:O	1.99	0.62
1:B:426:LEU:HD21	1:B:432:PRO:HG3	1.80	0.62
1:B:349:TYR:CE2	1:B:353:MSE:HE3	2.35	0.62
1:A:264:THR:OG1	1:A:362:GLY:HA3	1.99	0.62
1:A:43:LEU:HD21	1:A:144:ASN:O	2.00	0.61
1:B:29:LYS:O	1:B:33:ARG:HG2	2.00	0.61
1:B:32:ALA:HB1	1:B:156:PHE:CE2	2.35	0.61
1:B:122:GLN:HG2	1:B:198:ASN:HB2	1.83	0.61
1:B:297:PHE:CZ	1:B:301:ILE:HD11	2.35	0.60
1:B:51:MSE:O	1:B:53:PHE:N	2.31	0.60
1:A:24:TRP:CE2	1:A:29:LYS:HB3	2.37	0.60
1:A:304:SER:C	1:A:306:GLY:N	2.59	0.60
1:B:111:ILE:O	1:B:115:VAL:HG12	2.00	0.60
1:B:116:TRP:CH2	1:B:133:VAL:HG21	2.36	0.60
1:B:174:LEU:O	1:B:177:SER:HB3	2.02	0.60
1:A:59:ASN:HB3	1:A:208:MSE:CE	2.32	0.60
1:B:221:LEU:O	1:B:225:THR:HB	2.01	0.60
1:A:358:THR:C	1:A:360:GLY:H	2.09	0.60
1:B:149:MSE:HE3	1:B:165:LEU:HB3	1.83	0.60
1:B:181:LEU:O	1:B:185:LEU:HD22	2.01	0.59
1:B:184:PRO:HG3	1:B:289:LEU:HD13	1.84	0.59
1:B:326:MSE:HG2	1:B:358:THR:HB	1.84	0.59
1:A:181:LEU:HD13	1:A:293:PHE:CE2	2.37	0.59
1:A:323:PHE:CE1	1:A:446:CYS:CB	2.85	0.59
1:A:265:PHE:HB2	1:A:363:SER:HB3	1.84	0.59
1:A:234:ASP:O	1:A:235:ILE:HG13	2.02	0.59
1:B:302:ALA:O	1:B:361:LEU:HA	2.02	0.59
1:B:434:GLY:O	1:B:437:LYS:HB2	2.02	0.59
1:A:278:LEU:HD22	1:A:422:PHE:CZ	2.38	0.58
1:A:59:ASN:HB3	1:A:208:MSE:HE1	1.84	0.58
1:A:92:PHE:O	1:A:96:ILE:HG12	2.04	0.58
1:B:192:PHE:HB3	1:B:195:LEU:HD12	1.86	0.58
1:A:43:LEU:O	1:A:44:LEU:C	2.47	0.58
1:B:183:ALA:HB3	1:B:184:PRO:HD3	1.85	0.58
1:A:358:THR:C	1:A:360:GLY:N	2.62	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:GLY:O	1:B:363:SER:HB3	2.03	0.57
1:A:38:ILE:HG21	1:A:232:MSE:HG3	1.85	0.57
1:A:52:LEU:C	1:A:54:SER:H	2.12	0.57
1:A:324:ILE:HG12	1:A:447:VAL:HG11	1.84	0.57
1:A:176:VAL:O	1:A:179:MSE:HG3	2.04	0.57
1:B:154:PHE:HB3	1:B:235:ILE:HD11	1.85	0.57
1:B:325:PHE:O	1:B:329:PHE:CD2	2.58	0.57
1:A:271:PHE:O	1:A:275:PHE:HB2	2.05	0.56
1:B:105:PHE:CE2	1:B:109:ILE:HD11	2.41	0.56
1:B:305:VAL:O	1:B:309:ILE:HB	2.05	0.56
1:A:40:VAL:HG23	1:A:41:SER:N	2.21	0.56
1:A:43:LEU:HD13	1:A:172:GLY:HA3	1.88	0.56
1:B:279:ALA:HB3	1:B:288:ILE:CD1	2.36	0.56
1:A:107:THR:O	1:A:110:LEU:HB2	2.05	0.55
1:B:270:GLY:HA3	1:B:418:ILE:HD12	1.86	0.55
1:A:110:LEU:HB3	1:A:221:LEU:HD21	1.89	0.55
1:B:257:LEU:HD22	1:B:370:ILE:HG12	1.89	0.55
1:B:263:ALA:O	1:B:326:MSE:HE1	2.07	0.55
1:B:324:ILE:HD13	1:B:447:VAL:CG2	2.37	0.55
1:B:33:ARG:O	1:B:37:TRP:CD1	2.60	0.55
1:B:76:THR:O	1:B:79:PRO:HD2	2.06	0.54
1:A:101:ARG:O	1:A:104:VAL:HG22	2.08	0.54
1:B:404:LEU:O	1:B:405:GLY:C	2.50	0.54
1:A:270:GLY:HA2	1:A:415:GLY:HA2	1.88	0.54
1:B:44:LEU:HA	1:B:172:GLY:O	2.08	0.54
1:B:117:LEU:HD13	1:B:134:ILE:HG21	1.88	0.54
1:B:216:ILE:O	1:B:219:PRO:HD2	2.07	0.54
1:A:333:LEU:HD23	1:A:436:MSE:HE1	1.89	0.54
1:A:72:LEU:HB3	1:A:277:MSE:HE2	1.88	0.54
1:A:269:ILE:HD12	1:A:415:GLY:CA	2.31	0.54
1:A:52:LEU:HA	1:A:179:MSE:HE1	1.91	0.53
1:B:116:TRP:CZ3	1:B:133:VAL:CG2	2.90	0.53
1:B:335:LEU:H	1:B:335:LEU:HD12	1.74	0.53
1:A:418:ILE:O	1:A:419:PRO:C	2.50	0.53
1:B:128:PHE:CE1	1:B:132:ILE:HD11	2.42	0.53
1:B:401:ALA:HA	1:B:404:LEU:HD12	1.90	0.53
1:A:73:PHE:CE1	1:A:277:MSE:HB3	2.43	0.53
1:B:269:ILE:HG22	1:B:415:GLY:HA3	1.91	0.53
1:A:115:VAL:O	1:A:119:ILE:HG13	2.08	0.53
1:B:335:LEU:HD12	1:B:335:LEU:N	2.24	0.53
1:B:302:ALA:HB1	1:B:361:LEU:HB2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLU:O	1:A:21:PRO:HD3	2.09	0.53
1:B:63:ILE:HG22	1:B:64:GLY:N	2.22	0.53
1:B:126:THR:HG22	1:B:131:PHE:HE2	1.73	0.53
1:B:184:PRO:CG	1:B:289:LEU:HD13	2.39	0.53
1:B:276:ALA:O	1:B:288:ILE:HD11	2.07	0.53
1:B:416:PHE:O	1:B:419:PRO:HD2	2.09	0.53
1:A:151:ASN:C	1:A:151:ASN:ND2	2.67	0.52
1:A:261:TYR:HA	1:A:264:THR:HG22	1.91	0.52
1:A:370:ILE:CG2	1:A:407:ILE:HD13	2.38	0.52
1:B:78:LEU:O	1:B:79:PRO:C	2.52	0.52
1:B:202:GLN:O	1:B:205:GLY:N	2.38	0.52
1:B:277:MSE:CE	1:B:277:MSE:HA	2.39	0.52
1:B:323:PHE:CD1	1:B:446:CYS:HB3	2.44	0.52
1:A:333:LEU:HD23	1:A:436:MSE:CE	2.39	0.52
1:B:93:MSE:HG2	1:B:102:TRP:CZ2	2.43	0.52
1:A:63:ILE:CG2	1:A:64:GLY:H	2.05	0.52
1:A:52:LEU:HA	1:A:179:MSE:CE	2.40	0.52
1:A:265:PHE:HB2	1:A:363:SER:CB	2.40	0.52
1:A:279:ALA:HB3	1:A:288:ILE:CD1	2.37	0.52
1:B:59:ASN:HB3	1:B:208:MSE:CE	2.40	0.52
1:B:323:PHE:HB3	1:B:447:VAL:HG23	1.93	0.52
1:B:367:PHE:C	1:B:369:MSE:N	2.65	0.52
1:A:93:MSE:HG2	1:A:102:TRP:CZ2	2.45	0.51
1:B:297:PHE:CE2	1:B:301:ILE:HD11	2.45	0.51
1:B:422:PHE:HE2	1:B:436:MSE:CE	2.23	0.51
1:A:323:PHE:HE1	1:A:446:CYS:CB	2.23	0.51
1:B:36:LEU:HA	1:B:152:ILE:HD11	1.91	0.51
1:B:145:PHE:O	1:B:149:MSE:HB2	2.11	0.51
1:A:333:LEU:HB2	1:A:351:VAL:HG11	1.93	0.51
1:A:392:ALA:C	1:A:394:LYS:H	2.18	0.51
1:B:38:ILE:HG21	1:B:228:ALA:HA	1.92	0.51
1:B:78:LEU:HB3	1:B:136:LEU:HD13	1.91	0.51
1:A:122:GLN:HG2	1:A:198:ASN:ND2	2.26	0.51
1:B:325:PHE:O	1:B:329:PHE:HD2	1.92	0.51
1:A:320:LEU:CD1	1:A:450:THR:HB	2.35	0.51
1:A:13:LEU:HB2	1:A:234:ASP:O	2.11	0.51
1:A:100:ARG:HG3	1:A:232:MSE:O	2.11	0.51
1:A:370:ILE:HD13	1:A:407:ILE:HG21	1.93	0.51
1:A:376:GLN:O	1:A:377:ILE:C	2.54	0.51
1:A:330:SER:OG	1:A:440:LEU:HA	2.10	0.51
1:B:100:ARG:CD	1:B:232:MSE:O	2.59	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:PHE:HE2	1:B:436:MSE:HE2	1.76	0.50
1:A:83:GLY:O	1:A:87:ARG:HG3	2.11	0.50
1:A:110:LEU:O	1:A:113:PRO:HD2	2.11	0.50
1:A:177:SER:HB2	1:A:296:PRO:HB2	1.92	0.50
1:B:51:MSE:HE2	1:B:273:ALA:HB2	1.94	0.50
1:B:65:PHE:HD1	1:B:67:PHE:CE2	2.29	0.50
1:B:432:PRO:HB2	1:B:436:MSE:CE	2.41	0.50
1:A:108:ALA:C	1:A:110:LEU:H	2.20	0.49
1:A:22:ALA:O	1:A:23:PHE:C	2.56	0.49
1:A:320:LEU:O	1:A:321:ILE:C	2.54	0.49
1:A:367:PHE:CZ	1:A:404:LEU:HG	2.48	0.49
1:A:23:PHE:C	1:A:23:PHE:CD2	2.90	0.49
1:A:151:ASN:C	1:A:151:ASN:HD22	2.20	0.49
1:B:186:VAL:HG21	1:B:216:ILE:HG13	1.95	0.49
1:A:143:ALA:C	1:A:145:PHE:H	2.20	0.49
1:B:78:LEU:HD13	1:B:78:LEU:N	2.28	0.49
1:A:265:PHE:CZ	2:A:501:NO3:O2	2.65	0.49
1:B:167:ILE:HG23	1:B:171:LEU:HD12	1.95	0.49
1:A:65:PHE:CE1	1:A:126:THR:HG23	2.45	0.49
1:A:366:THR:O	1:A:370:ILE:HD12	2.12	0.49
1:B:36:LEU:HA	1:B:152:ILE:CD1	2.43	0.49
1:A:71:GLN:HB3	1:A:128:PHE:CZ	2.48	0.49
1:B:132:ILE:O	1:B:133:VAL:C	2.53	0.49
1:A:174:LEU:O	1:A:178:VAL:HG12	2.13	0.48
1:B:75:LEU:O	1:B:79:PRO:HD3	2.13	0.48
1:B:52:LEU:H	1:B:179:MSE:HE2	1.78	0.48
1:A:262:LEU:C	1:A:262:LEU:CD2	2.86	0.48
1:B:339:GLY:C	1:B:341:GLY:H	2.21	0.48
1:A:175:GLY:HA2	1:A:178:VAL:HG12	1.96	0.48
1:A:260:LEU:O	1:A:263:ALA:HB3	2.14	0.48
1:A:269:ILE:HD11	1:A:415:GLY:H	1.79	0.48
1:A:302:ALA:O	1:A:361:LEU:HA	2.12	0.48
1:B:428:MSE:O	1:B:429:THR:HG22	2.13	0.48
1:A:52:LEU:HD23	1:A:179:MSE:CE	2.41	0.48
1:A:78:LEU:HD13	1:A:132:ILE:HG23	1.94	0.48
1:A:264:THR:O	1:A:363:SER:HB3	2.14	0.48
1:B:293:PHE:O	1:B:294:PHE:C	2.56	0.48
1:B:403:ALA:O	1:B:407:ILE:HG13	2.13	0.48
1:A:47:PHE:HE1	1:A:173:ASN:ND2	2.11	0.48
1:A:358:THR:O	1:A:360:GLY:N	2.46	0.48
1:B:154:PHE:CB	1:B:235:ILE:HD11	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ALA:C	1:A:205:GLY:H	2.21	0.47
1:B:279:ALA:HB3	1:B:288:ILE:HD13	1.95	0.47
1:B:359:ALA:O	1:B:363:SER:HB2	2.14	0.47
1:B:36:LEU:HD12	1:B:152:ILE:HG12	1.96	0.47
1:B:264:THR:HB	1:B:363:SER:HA	1.95	0.47
1:A:40:VAL:O	1:A:44:LEU:N	2.47	0.47
1:A:171:LEU:HA	1:A:174:LEU:HB2	1.95	0.47
1:B:88:VAL:HG13	1:B:92:PHE:HE1	1.79	0.47
1:B:367:PHE:O	1:B:369:MSE:N	2.47	0.47
1:B:431:SER:OG	1:B:433:VAL:HG23	2.14	0.47
1:A:27:LYS:O	1:A:30:HIS:N	2.46	0.47
1:B:144:ASN:O	1:B:148:SER:HB3	2.15	0.47
1:A:324:ILE:HG13	1:A:324:ILE:H	1.59	0.47
1:A:342:SER:O	1:A:344:ASN:N	2.48	0.47
1:B:53:PHE:CE2	1:B:135:ALA:HA	2.49	0.47
1:B:88:VAL:HB	1:B:89:PRO:HD3	1.96	0.47
1:B:255:TRP:C	1:B:257:LEU:N	2.69	0.47
1:A:149:MSE:HE1	1:A:169:GLY:N	2.30	0.47
1:B:140:PHE:H	1:B:140:PHE:HD2	1.62	0.47
1:A:323:PHE:CD1	1:A:446:CYS:CB	2.92	0.47
1:B:153:SER:HB3	1:B:165:LEU:HD21	1.97	0.47
1:B:441:ILE:O	1:B:445:VAL:HG23	2.15	0.47
1:A:321:ILE:O	1:A:325:PHE:HD2	1.98	0.47
1:B:62:LYS:HB2	1:B:208:MSE:HE1	1.96	0.47
1:A:24:TRP:CZ3	1:A:157:PRO:HD3	2.50	0.46
1:A:264:THR:OG1	1:A:362:GLY:CA	2.64	0.46
1:B:140:PHE:C	1:B:142:GLY:H	2.23	0.46
1:B:82:SER:HB3	1:B:139:GLY:HA3	1.92	0.46
1:A:379:ILE:CG2	1:A:380:TYR:N	2.78	0.46
1:A:425:SER:OG	1:A:431:SER:O	2.33	0.46
1:B:112:ILE:O	1:B:113:PRO:C	2.57	0.46
1:A:271:PHE:O	1:A:275:PHE:CB	2.64	0.46
1:B:110:LEU:O	1:B:113:PRO:HD2	2.16	0.46
1:B:201:PRO:O	1:B:202:GLN:HG3	2.16	0.46
1:A:73:PHE:O	1:A:74:LEU:C	2.57	0.46
1:A:94:VAL:N	1:A:95:PRO:CD	2.78	0.46
1:A:322:ASN:O	1:A:325:PHE:HB2	2.16	0.46
1:A:78:LEU:CD1	1:A:132:ILE:HG23	2.45	0.45
1:A:100:ARG:O	1:A:101:ARG:C	2.59	0.45
1:B:43:LEU:HD23	1:B:43:LEU:HA	1.86	0.45
1:B:255:TRP:O	1:B:256:LEU:C	2.58	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ARG:HG2	1:A:143:ALA:HA	1.98	0.45
1:A:420:GLN:OE1	1:A:420:GLN:HA	2.16	0.45
1:A:65:PHE:HE1	1:A:126:THR:CG2	2.29	0.45
1:B:189:VAL:O	1:B:212:ASN:ND2	2.50	0.45
1:A:125:ASN:HB2	1:B:123:ASN:OD1	2.17	0.45
1:A:403:ALA:O	1:A:407:ILE:HD12	2.16	0.45
1:B:265:PHE:O	1:B:268:PHE:HB3	2.16	0.45
1:B:295:GLY:HA3	1:B:356:PHE:CD2	2.52	0.45
1:A:61:ASN:HA	1:A:65:PHE:O	2.17	0.45
1:B:23:PHE:C	1:B:23:PHE:CD2	2.95	0.45
1:A:176:VAL:HG13	1:A:177:SER:H	1.81	0.45
1:A:220:LEU:O	1:A:221:LEU:C	2.60	0.45
1:B:437:LYS:O	1:B:441:ILE:HG12	2.17	0.45
1:A:16:TRP:CD1	1:A:235:ILE:HD13	2.52	0.44
1:A:362:GLY:O	1:A:366:THR:N	2.36	0.44
1:A:426:LEU:HD12	1:A:431:SER:C	2.41	0.44
1:A:311:ASP:O	1:A:313:PHE:N	2.50	0.44
1:A:75:LEU:HG	1:A:128:PHE:HE2	1.83	0.44
1:A:108:ALA:C	1:A:110:LEU:N	2.72	0.44
1:A:219:PRO:O	1:A:220:LEU:C	2.61	0.44
1:A:322:ASN:ND2	1:A:326:MSE:HE2	2.33	0.44
1:A:325:PHE:O	1:A:328:ILE:HB	2.18	0.44
1:B:116:TRP:CH2	1:B:133:VAL:CG2	3.00	0.44
1:B:149:MSE:SE	1:B:168:ASN:HD22	2.51	0.44
1:A:228:ALA:O	1:A:232:MSE:HB2	2.18	0.44
1:A:275:PHE:O	1:A:278:LEU:N	2.51	0.44
1:B:136:LEU:O	1:B:139:GLY:N	2.50	0.44
1:B:361:LEU:HD23	1:B:361:LEU:C	2.42	0.44
1:B:130:ILE:HD13	1:B:130:ILE:HA	1.86	0.44
1:A:381:ARG:O	1:A:385:LYS:CB	2.66	0.44
1:B:52:LEU:HA	1:B:179:MSE:SE	2.68	0.44
1:B:128:PHE:HE1	1:B:132:ILE:HD11	1.82	0.44
1:B:201:PRO:C	1:B:202:GLN:HG3	2.43	0.44
1:B:342:SER:O	1:B:344:ASN:N	2.50	0.44
1:A:153:SER:C	1:A:155:PHE:H	2.26	0.43
1:A:175:GLY:HA2	1:A:178:VAL:CG1	2.47	0.43
1:A:444:ILE:HG22	1:A:445:VAL:N	2.32	0.43
1:A:57:THR:HG21	1:A:72:LEU:O	2.18	0.43
1:A:179:MSE:HG3	1:A:180:GLN:N	2.33	0.43
1:B:129:GLY:HA2	1:B:132:ILE:HG13	2.00	0.43
1:B:271:PHE:CE2	1:B:418:ILE:HD13	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ARG:HD2	1:A:231:GLY:O	2.18	0.43
1:A:262:LEU:HD23	1:A:262:LEU:O	2.18	0.43
1:B:67:PHE:CE1	1:B:128:PHE:CD2	3.01	0.43
1:A:24:TRP:CD1	1:A:29:LYS:HB3	2.53	0.43
1:A:203:ALA:C	1:A:205:GLY:N	2.76	0.43
1:A:379:ILE:HG23	1:A:380:TYR:N	2.34	0.43
1:B:78:LEU:O	1:B:81:VAL:N	2.47	0.43
1:A:181:LEU:O	1:A:185:LEU:HG	2.19	0.43
1:A:264:THR:OG1	1:A:362:GLY:C	2.61	0.43
1:A:270:GLY:HA3	1:A:418:ILE:HD12	2.00	0.43
1:B:50:TRP:CD1	1:B:50:TRP:C	2.93	0.43
1:B:116:TRP:CZ3	1:B:133:VAL:HG21	2.53	0.43
1:B:288:ILE:O	1:B:292:ALA:N	2.51	0.43
1:B:417:PHE:CD1	1:B:417:PHE:C	2.97	0.43
1:B:83:GLY:O	1:B:85:LEU:N	2.51	0.43
1:B:116:TRP:CG	1:B:134:ILE:HD11	2.53	0.43
1:B:140:PHE:C	1:B:142:GLY:N	2.74	0.43
1:A:41:SER:C	1:A:43:LEU:N	2.76	0.43
1:A:110:LEU:C	1:A:113:PRO:HD2	2.44	0.43
1:A:41:SER:C	1:A:43:LEU:H	2.27	0.42
1:B:45:LEU:HD23	1:B:45:LEU:HA	1.83	0.42
1:B:51:MSE:HB3	1:B:179:MSE:CE	2.49	0.42
1:B:57:THR:HA	1:B:60:LEU:HD22	2.01	0.42
1:B:323:PHE:HB3	1:B:447:VAL:CG2	2.48	0.42
1:A:125:ASN:H	1:B:123:ASN:HD21	1.67	0.42
1:A:429:THR:OG1	1:A:430:GLY:N	2.51	0.42
1:B:116:TRP:CD1	1:B:134:ILE:HD11	2.55	0.42
1:B:255:TRP:O	1:B:258:SER:N	2.52	0.42
1:A:266:GLY:HA3	1:A:414:GLY:HA3	2.02	0.42
1:A:318:VAL:O	1:A:319:THR:C	2.63	0.42
1:B:323:PHE:HE1	1:B:446:CYS:HB3	1.80	0.42
1:A:72:LEU:HA	1:A:72:LEU:HD12	1.64	0.42
1:A:326:MSE:O	1:A:330:SER:HB2	2.20	0.42
1:B:268:PHE:HE2	1:B:299:GLY:HA3	1.85	0.42
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.78	0.42
1:A:303:ARG:HA	1:A:360:GLY:O	2.20	0.42
1:A:353:MSE:HE3	1:A:353:MSE:N	2.34	0.42
1:B:252:LEU:HA	1:B:255:TRP:HD1	1.85	0.42
1:A:160:LYS:H	1:A:160:LYS:HG2	1.60	0.42
1:B:67:PHE:HB2	1:B:72:LEU:HD21	2.01	0.42
1:B:335:LEU:H	1:B:335:LEU:CD1	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.72	0.42
1:A:267:SER:HB2	1:A:359:ALA:HB1	2.02	0.42
1:B:101:ARG:O	1:B:104:VAL:HG12	2.20	0.42
1:B:180:GLN:OE1	1:B:296:PRO:HG2	2.20	0.42
1:B:288:ILE:C	1:B:290:ARG:N	2.75	0.42
1:A:337:LEU:HB3	1:A:338:PRO:HD2	2.02	0.41
1:B:187:ILE:HG22	1:B:210:LEU:HA	2.02	0.41
1:B:288:ILE:H	1:B:288:ILE:HG12	1.70	0.41
1:A:47:PHE:CD1	1:A:173:ASN:HA	2.55	0.41
1:A:311:ASP:C	1:A:313:PHE:H	2.27	0.41
1:B:255:TRP:O	1:B:257:LEU:N	2.53	0.41
1:A:264:THR:HG21	1:A:366:THR:OG1	2.20	0.41
1:B:109:ILE:H	1:B:109:ILE:HG13	1.53	0.41
1:A:79:PRO:HD3	1:A:135:ALA:HB1	2.01	0.41
1:A:113:PRO:HB3	1:A:137:LEU:HB3	2.01	0.41
1:A:360:GLY:O	1:A:361:LEU:C	2.63	0.41
1:B:64:GLY:O	1:B:124:PRO:HB3	2.21	0.41
1:B:75:LEU:HD23	1:B:75:LEU:HA	1.80	0.41
1:A:16:TRP:NE1	1:A:154:PHE:O	2.53	0.41
1:A:156:PHE:HD1	1:A:160:LYS:HG3	1.85	0.41
1:A:283:PHE:C	1:A:285:ASP:H	2.28	0.41
1:B:171:LEU:O	1:B:174:LEU:HB2	2.21	0.41
1:A:52:LEU:C	1:A:54:SER:N	2.78	0.41
1:B:216:ILE:HD13	1:B:216:ILE:HA	1.92	0.41
1:A:220:LEU:HD23	1:A:220:LEU:HA	1.79	0.41
1:A:318:VAL:O	1:A:321:ILE:HG23	2.21	0.41
1:A:355:LEU:HD23	1:A:355:LEU:HA	1.94	0.41
1:B:57:THR:HA	1:B:60:LEU:HB2	2.02	0.41
1:B:222:ALA:O	1:B:225:THR:HG22	2.20	0.41
1:A:39:SER:OG	1:A:148:SER:OG	2.39	0.41
1:B:93:MSE:CG	1:B:102:TRP:CZ3	3.02	0.41
1:B:310:SER:HB2	1:B:315:GLY:HA2	2.03	0.41
1:A:40:VAL:CG2	1:A:41:SER:N	2.84	0.41
1:A:428:MSE:H	1:A:428:MSE:HG3	1.69	0.41
1:B:45:LEU:HD11	1:B:220:LEU:HB3	2.02	0.41
1:A:59:ASN:HB3	1:A:208:MSE:HE3	2.02	0.40
1:A:93:MSE:HG2	1:A:102:TRP:CZ3	2.55	0.40
1:A:156:PHE:C	1:A:157:PRO:O	2.65	0.40
1:B:28:GLY:O	1:B:29:LYS:C	2.62	0.40
1:B:126:THR:HG22	1:B:131:PHE:CE2	2.55	0.40
1:A:376:GLN:HA	1:A:379:ILE:HG22	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:VAL:C	1:B:96:ILE:H	2.30	0.40
1:B:282:GLN:HG3	1:B:338:PRO:CG	2.51	0.40
1:B:333:LEU:O	1:B:336:THR:HG23	2.21	0.40
1:A:149:MSE:C	1:A:151:ASN:H	2.30	0.40
1:B:12:LEU:CD2	1:B:13:LEU:N	2.71	0.40
1:B:262:LEU:HG	1:B:410:ILE:O	2.21	0.40
1:A:269:ILE:HA	1:A:272:SER:HB2	2.03	0.40
1:B:77:ALA:O	1:B:416:PHE:HA	2.20	0.40
1:B:345:PHE:O	1:B:348:PHE:HB3	2.20	0.40
1:A:265:PHE:O	1:A:268:PHE:N	2.55	0.40
1:A:410:ILE:HD12	1:A:410:ILE:HA	1.87	0.40
1:B:48:CYS:SG	1:B:217:TRP:CZ3	3.04	0.40
1:B:171:LEU:HD23	1:B:174:LEU:HD12	2.04	0.40
1:B:189:VAL:C	1:B:191:VAL:H	2.30	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	416/468 (89%)	308 (74%)	83 (20%)	25 (6%)	1	7
1	B	421/468 (90%)	327 (78%)	75 (18%)	19 (4%)	2	11
All	All	837/936 (89%)	635 (76%)	158 (19%)	44 (5%)	1	9

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	231	GLY
1	A	305	VAL
1	A	312	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	432	PRO
1	B	52	LEU
1	B	54	SER
1	B	230	SER
1	B	291	LEU
1	A	333	LEU
1	A	343	GLY
1	A	380	TYR
1	A	444	ILE
1	B	83	GLY
1	B	194	PHE
1	B	315	GLY
1	B	332	LEU
1	B	368	GLN
1	B	453	VAL
1	A	204	ASP
1	A	304	SER
1	A	421	ALA
1	B	164	ALA
1	B	232	MSE
1	A	27	LYS
1	A	87	ARG
1	A	144	ASN
1	A	311	ASP
1	A	430	GLY
1	B	26	ASN
1	B	51	MSE
1	B	231	GLY
1	A	53	PHE
1	A	332	LEU
1	B	84	ALA
1	B	376	GLN
1	A	88	VAL
1	A	169	GLY
1	A	325	PHE
1	A	377	ILE
1	A	157	PRO
1	A	433	VAL
1	B	127	PRO
1	B	343	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	299/356 (84%)	239 (80%)	60 (20%)	1	5
1	B	304/356 (85%)	232 (76%)	72 (24%)	1	3
All	All	603/712 (85%)	471 (78%)	132 (22%)	1	4

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	43	LEU
1	A	57	THR
1	A	66	ASN
1	A	68	THR
1	A	69	THR
1	A	70	ASP
1	A	72	LEU
1	A	76	THR
1	A	91	SER
1	A	93	MSE
1	A	96	ILE
1	A	104	VAL
1	A	110	LEU
1	A	111	ILE
1	A	112	ILE
1	A	114	CYS
1	A	115	VAL
1	A	126	THR
1	A	149	MSE
1	A	151	ASN
1	A	160	LYS
1	A	163	SER
1	A	174	LEU
1	A	177	SER
1	A	189	VAL
1	A	191	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	195	LEU
1	A	204	ASP
1	A	208	MSE
1	A	216	ILE
1	A	221	LEU
1	A	226	ILE
1	A	233	ASN
1	A	234	ASP
1	A	269	ILE
1	A	277	MSE
1	A	280	LYS
1	A	285	ASP
1	A	286	VAL
1	A	288	ILE
1	A	298	ILE
1	A	316	VAL
1	A	319	THR
1	A	320	LEU
1	A	321	ILE
1	A	324	ILE
1	A	326	MSE
1	A	332	LEU
1	A	353	MSE
1	A	370	ILE
1	A	404	LEU
1	A	406	PHE
1	A	410	ILE
1	A	413	VAL
1	A	428	MSE
1	A	431	SER
1	A	436	MSE
1	A	448	LEU
1	A	451	TRP
1	B	20	ASN
1	B	27	LYS
1	B	31	ILE
1	B	35	ASN
1	B	40	VAL
1	B	43	LEU
1	B	51	MSE
1	B	56	VAL
1	B	63	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	69	THR
1	B	74	LEU
1	B	78	LEU
1	B	82	SER
1	B	85	LEU
1	B	93	MSE
1	B	109	ILE
1	B	112	ILE
1	B	115	VAL
1	B	121	VAL
1	B	126	THR
1	B	132	ILE
1	B	133	VAL
1	B	136	LEU
1	B	151	ASN
1	B	160	LYS
1	B	163	SER
1	B	173	ASN
1	B	176	VAL
1	B	181	LEU
1	B	185	LEU
1	B	202	GLN
1	B	204	ASP
1	B	206	SER
1	B	207	VAL
1	B	210	LEU
1	B	216	ILE
1	B	225	THR
1	B	235	ILE
1	B	254	LEU
1	B	257	LEU
1	B	259	LEU
1	B	262	LEU
1	B	264	THR
1	B	267	SER
1	B	277	MSE
1	B	282	GLN
1	B	288	ILE
1	B	289	LEU
1	B	291	LEU
1	B	298	ILE
1	B	309	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	318	VAL
1	B	320	LEU
1	B	326	MSE
1	B	332	LEU
1	B	333	LEU
1	B	336	THR
1	B	340	THR
1	B	346	ILE
1	B	352	PHE
1	B	367	PHE
1	B	368	GLN
1	B	373	ILE
1	B	410	ILE
1	B	413	VAL
1	B	427	ASN
1	B	429	THR
1	B	436	MSE
1	B	440	LEU
1	B	444	ILE
1	B	447	VAL
1	B	448	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	122	GLN
1	A	144	ASN
1	A	168	ASN
1	A	173	ASN
1	A	287	ASN
1	B	30	HIS
1	B	168	ASN
1	B	173	ASN
1	B	198	ASN
1	B	420	GLN

5.3.3 RNA ⓘ

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](#)

1 ligand is 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	NO3	A	501	-	1,3,3	0.44	0	0,3,3	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NO3	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	408/468 (87%)	-0.17	7 (1%) 69 48	18, 43, 91, 145	0
1	B	414/468 (88%)	-0.21	13 (3%) 51 31	16, 33, 96, 141	0
All	All	822/936 (87%)	-0.19	20 (2%) 59 38	16, 37, 94, 145	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	145	PHE	5.9
1	B	204	ASP	4.0
1	A	340	THR	4.0
1	A	167	ILE	3.6
1	B	313	PHE	3.2
1	B	150	GLY	3.2
1	B	12	LEU	2.9
1	A	348	PHE	2.8
1	B	392	ALA	2.8
1	B	311	ASP	2.8
1	A	173	ASN	2.6
1	A	395	GLU	2.6
1	B	205	GLY	2.6
1	B	372	VAL	2.5
1	A	417	PHE	2.4
1	B	146	ALA	2.2
1	B	206	SER	2.1
1	B	380	TYR	2.1
1	A	77	ALA	2.1
1	B	378	THR	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](#)

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($\text{\AA}^2$)	Q<0.9
2	NO3	A	501	4/4	0.84	0.75	64,68,68,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.