WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 06:33 PM EDT

PDB ID	:	4IU8
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)

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

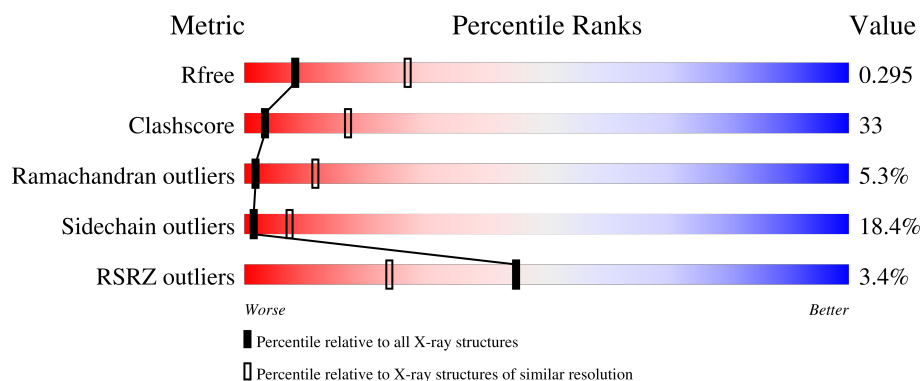|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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	Percentile Ranks	Value
Rfree		0.295
Clashscore		33
Ramachandran outliers		5.3%
Sidechain outliers		18.4%
RSRZ outliers		3.4%

Worse   *Better*

▊ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (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 <=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	2% 41% 38% 11% 10%
1	B	468	4% 39% 43% 9% · 9%

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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

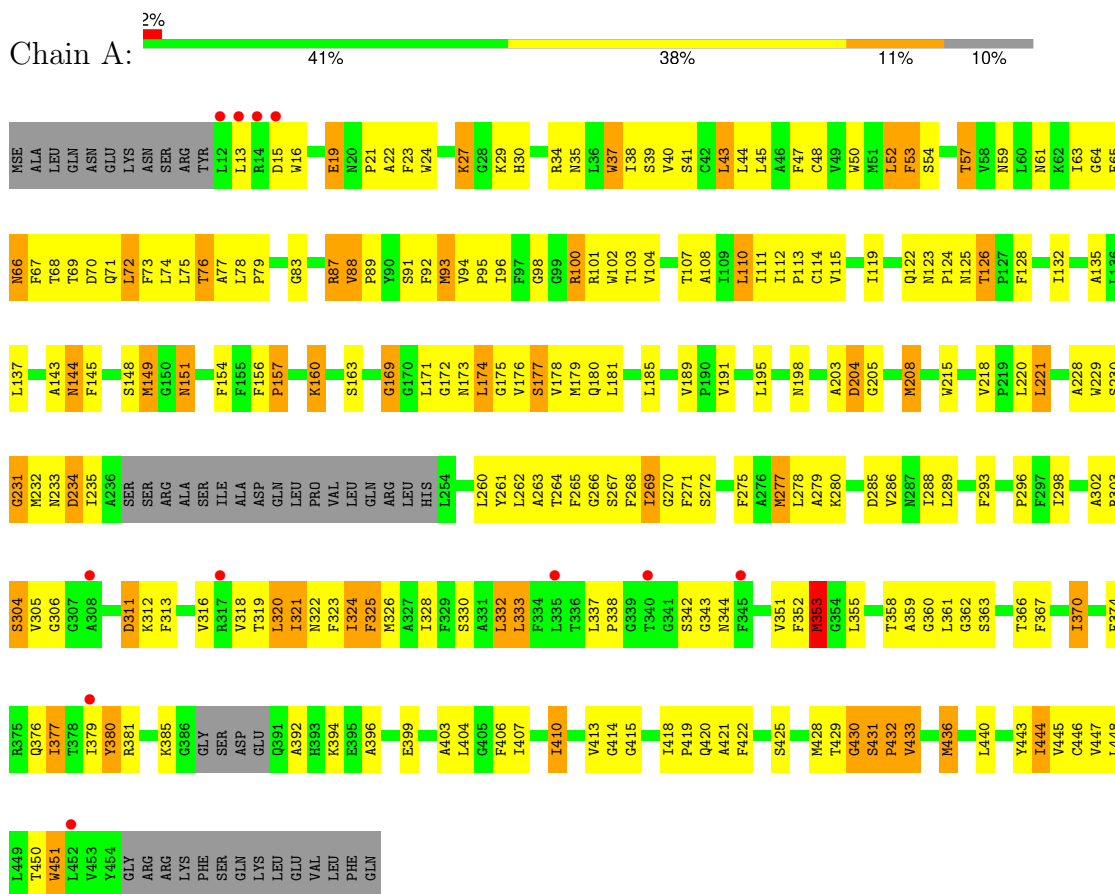- Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO_3).

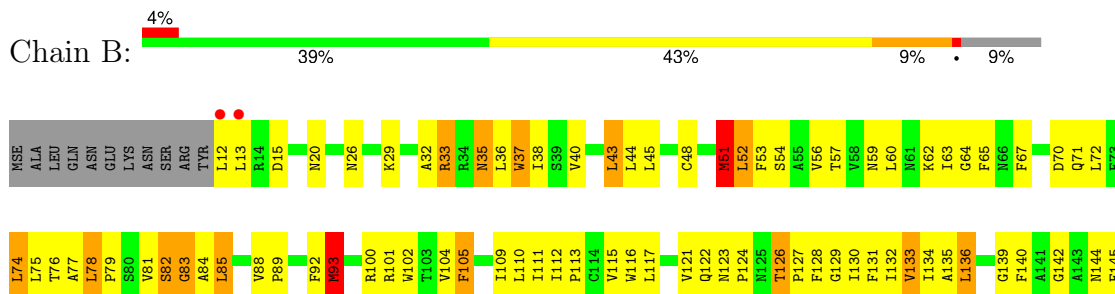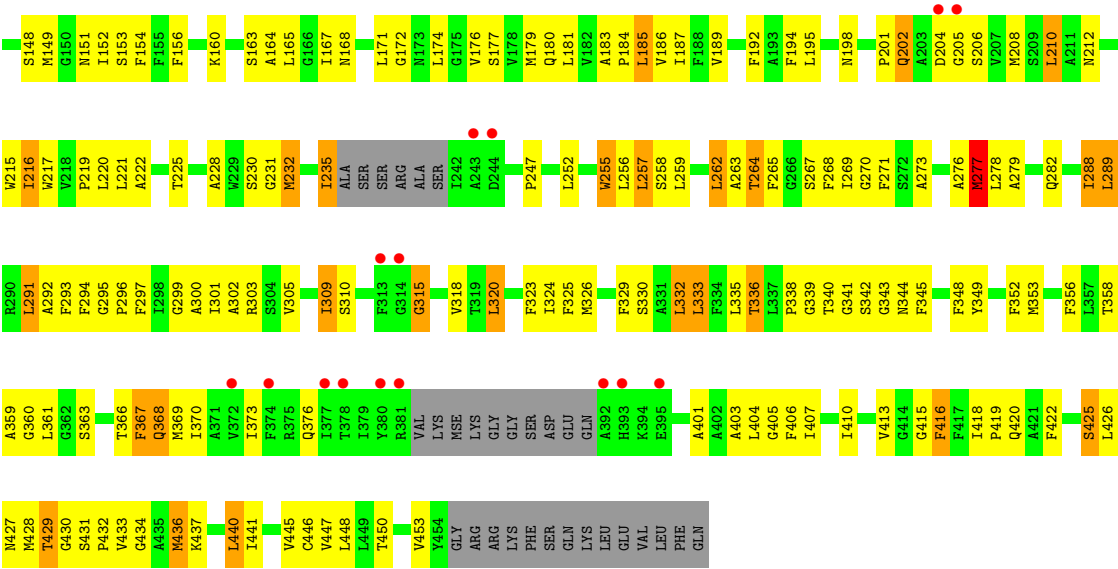| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
2	A	1	4	1	3	0	0

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

Chain A:

• Molecule 1: Nitrite extrusion protein 2

Chain B:

4 Data and refinement statistics (i)

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 40.03 – 3.11	Depositor EDS
% Data completeness (in resolution range)	82.7 (40.00-3.11) 82.9 (40.03-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.239 , 0.299 0.240 , 0.295	Depositor DCC
R_{free} test set	1224 reflections (5.01%)	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)	0.27 , 45.8	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.67	5/3150 (0.2%)	0.79	3/4276 (0.1%)
1	B	0.71	3/3202 (0.1%)	0.83	4/4349 (0.1%)
All	All	0.69	8/6352 (0.1%)	0.81	7/8625 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	TRP	CD2-CE2	7.37	1.50	1.41
1	B	215	TRP	CD2-CE2	6.32	1.49	1.41
1	A	229	TRP	CD2-CE2	5.53	1.48	1.41
1	A	451	TRP	CD2-CE2	5.34	1.47	1.41
1	A	50	TRP	CD2-CE2	5.20	1.47	1.41
1	A	37	TRP	CD2-CE2	5.11	1.47	1.41
1	B	255	TRP	CD2-CE2	5.08	1.47	1.41
1	B	37	TRP	CD2-CE2	5.08	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	MSE	CG-SE-CE	6.04	112.19	98.90
1	A	52	LEU	CA-CB-CG	6.02	129.14	115.30
1	B	277	MSE	CA-CB-CG	-5.87	103.32	113.30
1	B	247	PRO	N-CA-CB	5.84	110.31	103.30
1	B	33	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	93	MSE	CA-CB-CG	-5.16	104.52	113.30
1	A	289	LEU	CA-CB-CG	5.03	126.86	115.30

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	207	0
1	B	3129	0	3092	197	0
2	A	4	0	0	1	0
All	All	6214	0	6141	402	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 (402) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:A:63:ILE:HG22	1:A:64:GLY:N	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:PHE:C	1:B:369:MSE:H	1.97	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:304:SER:C	1:A:306:GLY:H	1.99	0.65
1:A:363:SER:O	1:A:367:PHE:HB2	1.96	0.65
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
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:B:425:SER:HG	1:B:432:PRO:HA	1.64	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:262:LEU:C	1:A:262:LEU:HD23	2.22	0.60
1:A:59:ASN:HB3	1:A:208:MSE:CE	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:O	1:B:225:THR:HB	2.01	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:A:234:ASP:C	1:A:235:ILE:HG13	2.22	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:B:183:ALA:HB3	1:B:184:PRO:HD3	1.85	0.58
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: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:A:358:THR:C	1:A:360:GLY:H	2.09	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:52:LEU:C	1:A:54:SER:H	2.12	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: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:43:LEU:O	1:A:44:LEU:C	2.47	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
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: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: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:304:SER:C	1:A:306:GLY:N	2.59	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:A:93:MSE:HG2	1:A:102:TRP:CZ2	2.45	0.51
1:A:358:THR:C	1:A:360:GLY:N	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:404:LEU:O	1:B:405:GLY:C	2.50	0.50
1:B:432:PRO:HB2	1:B:436:MSE:CE	2.41	0.50
1:A:367:PHE:CZ	1:A:404:LEU:HG	2.48	0.49
1:B:186:VAL:HG21	1:B:216:ILE:HG13	1.95	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:A:174:LEU:O	1:A:178:VAL:HG12	2.13	0.48
1:A:418:ILE:O	1:A:419:PRO:C	2.50	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:151:ASN:C	1:A:151:ASN:ND2	2.67	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:78:LEU:O	1:B:79:PRO:C	2.52	0.48
1:B:154:PHE:CB	1:B:235:ILE:HD11	2.44	0.48
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: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:82:SER:HB3	1:B:139:GLY:HA3	1.92	0.46
1:A:376:GLN:O	1:A:377:ILE:C	2.54	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: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:392:ALA:C	1:A:394:LYS:H	2.18	0.46
1:B:367:PHE:C	1:B:369:MSE:N	2.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:43:LEU:HD23	1:B:43:LEU:HA	1.86	0.45
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:A:108:ALA:C	1:A:110:LEU:H	2.20	0.45
1:B:255:TRP:C	1:B:257:LEU:N	2.69	0.45
1:A:22:ALA:O	1:A:23:PHE:C	2.56	0.45
1:A:176:VAL:HG13	1:A:177:SER:H	1.81	0.45
1:A:320:LEU:O	1:A:321:ILE:C	2.54	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:23:PHE:C	1:A:23:PHE:CD2	2.90	0.44
1:A:362:GLY:O	1:A:366:THR:N	2.36	0.44
1:A:143:ALA:C	1:A:145:PHE:H	2.20	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: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: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:339:GLY:C	1:B:341:GLY:H	2.21	0.44
1:B:342:SER:O	1:B:344:ASN:N	2.50	0.44
1:A:175:GLY:HA2	1:A:178:VAL:CG1	2.47	0.43
1:A:262:LEU:C	1:A:262:LEU:CD2	2.86	0.43
1:A:444:ILE:HG22	1:A:445:VAL:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ILE:O	1:B:133:VAL:C	2.53	0.43
1:A:57:THR:HG21	1:A:72:LEU:O	2.18	0.43
1:A:151:ASN:C	1:A:151:ASN:HD22	2.20	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
1:B:293:PHE:O	1:B:294:PHE:C	2.56	0.43
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: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:203:ALA:C	1:A:205:GLY:H	2.21	0.43
1:A:270:GLY:HA3	1:A:418:ILE:HD12	2.00	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:48:CYS:SG	1:B:217:TRP:CZ3	3.04	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:A:108:ALA:C	1:A:110:LEU:N	2.72	0.43
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:73:PHE:O	1:A:74:LEU:C	2.57	0.42
1:A:266:GLY:HA3	1:A:414:GLY:HA3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:140:PHE:C	1:B:142:GLY:H	2.23	0.42
1:B:180:GLN:OE1	1:B:296:PRO:HG2	2.20	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: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:B:64:GLY:O	1:B:124:PRO:HB3	2.21	0.41
1:B:112:ILE:O	1:B:113:PRO:C	2.57	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:B:171:LEU:O	1:B:174:LEU:HB2	2.21	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:A:100:ARG:O	1:A:101:ARG:C	2.59	0.41
1:B:93:MSE:CG	1:B:102:TRP:CZ3	3.02	0.41
1:B:255:TRP:O	1:B:256:LEU:C	2.58	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: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
1:B:282:GLN:HG3	1:B:338:PRO:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:LEU:O	1:B:336:THR:HG23	2.21	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:171:LEU:HD23	1:B:174:LEU:HD12	2.04	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	9
1	B	421/468 (90%)	327 (78%)	75 (18%)	19 (4%)	2	14
All	All	837/936 (89%)	635 (76%)	158 (19%)	44 (5%)	2	12

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
1	A	432	PRO
1	B	52	LEU
1	B	54	SER
1	B	230	SER
1	B	291	LEU

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Mol	Chain	Res	Type
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%)	246 (82%)	53 (18%)	2	8
1	B	304/356 (85%)	246 (81%)	58 (19%)	1	6
All	All	603/712 (85%)	492 (82%)	111 (18%)	1	7

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	19	GLU
1	A	37	TRP
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	110	LEU
1	A	112	ILE
1	A	114	CYS
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
1	A	195	LEU
1	A	204	ASP
1	A	208	MSE
1	A	221	LEU
1	A	233	ASN
1	A	234	ASP
1	A	269	ILE
1	A	277	MSE
1	A	280	LYS

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Mol	Chain	Res	Type
1	A	285	ASP
1	A	286	VAL
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	332	LEU
1	A	352	PHE
1	A	353	MSE
1	A	370	ILE
1	A	406	PHE
1	A	410	ILE
1	A	413	VAL
1	A	431	SER
1	A	436	MSE
1	A	448	LEU
1	A	451	TRP
1	B	15	ASP
1	B	20	ASN
1	B	35	ASN
1	B	40	VAL
1	B	43	LEU
1	B	51	MSE
1	B	56	VAL
1	B	70	ASP
1	B	74	LEU
1	B	78	LEU
1	B	82	SER
1	B	85	LEU
1	B	93	MSE
1	B	105	PHE
1	B	121	VAL
1	B	126	THR
1	B	133	VAL
1	B	136	LEU
1	B	151	ASN
1	B	160	LYS
1	B	163	SER
1	B	176	VAL
1	B	185	LEU

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Mol	Chain	Res	Type
1	B	202	GLN
1	B	204	ASP
1	B	206	SER
1	B	210	LEU
1	B	216	ILE
1	B	235	ILE
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	288	ILE
1	B	289	LEU
1	B	291	LEU
1	B	309	ILE
1	B	318	VAL
1	B	320	LEU
1	B	332	LEU
1	B	333	LEU
1	B	336	THR
1	B	340	THR
1	B	352	PHE
1	B	367	PHE
1	B	368	GLN
1	B	373	ILE
1	B	406	PHE
1	B	413	VAL
1	B	416	PHE
1	B	425	SER
1	B	427	ASN
1	B	429	THR
1	B	436	MSE
1	B	440	LEU
1	B	448	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	122	GLN
1	A	168	ASN

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Mol	Chain	Res	Type
1	A	173	ASN
1	A	287	ASN
1	B	173	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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

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(Å²)	Q<0.9
1	A	408/468 (87%)	-0.27	11 (2%)	54	31	18, 43, 91, 145	0
1	B	414/468 (88%)	-0.18	17 (4%)	37	18	16, 33, 96, 141	0
All	All	822/936 (87%)	-0.23	28 (3%)	45	24	16, 37, 94, 145	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	378	THR	4.7
1	B	393	HIS	4.5
1	B	244	ASP	4.4
1	A	12	LEU	4.4
1	B	12	LEU	3.8
1	B	392	ALA	3.7
1	B	380	TYR	3.6
1	A	340	THR	3.5
1	B	313	PHE	3.5
1	A	13	LEU	3.4
1	B	204	ASP	3.4
1	A	14	ARG	3.3
1	B	13	LEU	3.3
1	B	314	GLY	3.1
1	B	243	ALA	2.9
1	A	345	PHE	2.9
1	B	205	GLY	2.6
1	A	15	ASP	2.6
1	B	381	ARG	2.6
1	A	379	ILE	2.5
1	A	317	ARG	2.5
1	B	372	VAL	2.5
1	A	452	LEU	2.5
1	A	335	LEU	2.4

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W O R L D W I D E
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PROTEIN DATA BANK

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Mol	Chain	Res	Type	RSRZ
1	B	395	GLU	2.4
1	B	374	PHE	2.3
1	B	377	ILE	2.1
1	A	308	ALA	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	NO3	A	501	4/4	0.85	0.85	64,68,68,70	0

6.5 Other polymers ⓘ

There are no such residues in this entry.