



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:05 AM UTC

PDB ID : 5FRR / pdb_00005frr
Title : Structure of the Pds5-Scc1 complex and implications for cohesin function
Authors : Muir, K.W.; Kschonsak, M.; Li, Y.; Metz, J.; Haering, C.H.; Panne, D.
Deposited on : 2015-12-22
Resolution : 5.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

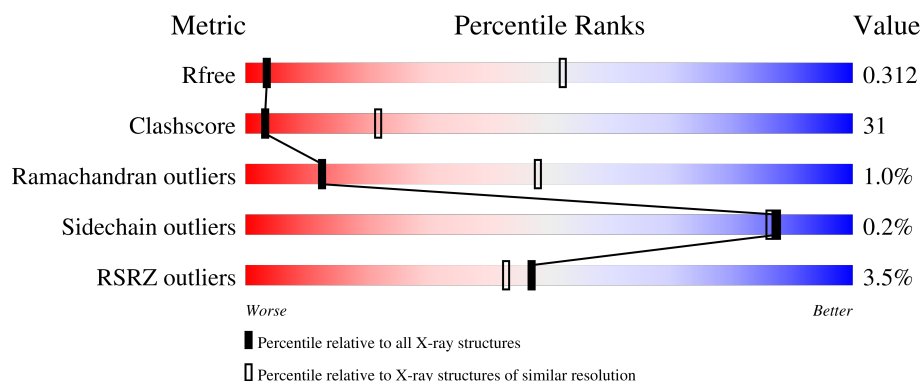
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.80 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	1125 (7.60-4.00)
Clashscore	190562	1190 (7.60-4.00)
Ramachandran outliers	187476	1019 (7.60-4.00)
Sidechain outliers	187428	1009 (7.60-3.98)
RSRZ outliers	180081	1118 (7.60-4.00)

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	703	4% 46% 49% • •
1	B	703	2% 45% 48% • 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10858 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 SISTER CHROMATID COHESION PROTEIN PDS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	677	Total	C	N	O	S	0	0	0
			5494	3526	914	1041	13			
1	B	660	Total	C	N	O	S	0	0	0
			5364	3455	889	1009	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q04264
A	0	ALA	-	expression tag	UNP Q04264
B	-1	GLY	-	expression tag	UNP Q04264
B	0	ALA	-	expression tag	UNP Q04264

- Molecule 1: SISTER CHROMATID COHESION PROTEIN PDS5



Chain B: 2% 45% 48% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	283.69Å 283.69Å 172.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 5.80 50.00 – 5.80	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-5.80) 99.5 (50.00-5.80)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 5.73Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.311 0.251 , 0.312	Depositor DCC
R_{free} test set	518 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	383.9	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 638.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10858	wwPDB-VP
Average B, all atoms (Å ²)	424.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.28	0/5600	0.72	0/7597
1	B	0.27	0/5464	0.71	1/7408 (0.0%)
All	All	0.27	0/11064	0.72	1/15005 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	ILE	CB-CA-C	-5.45	108.52	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5494	0	5551	346	0
1	B	5364	0	5435	338	1
All	All	10858	0	10986	673	1

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 31.

All (673) 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:B:333:ILE:H	1:B:333:ILE:HD12	1.29	0.97
1:A:98:LEU:HD23	1:A:142:LEU:HD21	1.51	0.93
1:B:373:ARG:HA	1:B:376:ARG:HH12	1.36	0.91
1:B:98:LEU:HD23	1:B:142:LEU:HD21	1.52	0.89
1:B:462:LEU:HD13	1:B:559:SER:HA	1.53	0.88
1:A:333:ILE:HD12	1:A:333:ILE:H	1.39	0.86
1:A:483:ASN:HA	1:A:486:ARG:NH1	1.94	0.82
1:B:523:ILE:HD13	1:B:580:PHE:HA	1.63	0.81
1:A:70:VAL:HG12	1:A:73:ARG:HH21	1.46	0.80
1:B:70:VAL:HG12	1:B:73:ARG:HH21	1.47	0.78
1:B:372:PRO:HA	1:B:375:ARG:HE	1.49	0.78
1:B:396:ASN:HB3	1:B:399:ILE:HG12	1.65	0.78
1:A:342:THR:HA	1:A:345:ILE:HD13	1.65	0.78
1:B:308:THR:HA	1:B:351:THR:HG21	1.66	0.78
1:B:105:VAL:HG23	1:B:126:LEU:HD21	1.64	0.77
1:A:682:LEU:H	1:A:682:LEU:HD23	1.50	0.77
1:A:293:GLU:HA	1:A:296:ARG:HE	1.51	0.76
1:A:610:PRO:HG3	1:A:626:PRO:HG2	1.66	0.76
1:A:105:VAL:HG23	1:A:126:LEU:HD21	1.66	0.75
1:B:351:THR:HG22	1:B:352:ARG:HG3	1.67	0.75
1:B:111:GLN:HB2	1:B:123:GLN:HE22	1.53	0.73
1:A:396:ASN:HB3	1:A:399:ILE:HG12	1.70	0.73
1:B:483:ASN:HA	1:B:486:ARG:NH1	2.03	0.73
1:B:242:ILE:HG21	1:B:262:LEU:HD21	1.70	0.73
1:A:480:GLU:HB2	1:A:481:PRO:HA	1.70	0.72
1:A:69:ASP:HB3	1:A:72:ILE:HD13	1.72	0.72
1:A:330:ILE:HG21	1:A:362:ALA:HB1	1.70	0.72
1:A:121:ILE:HD12	1:A:121:ILE:H	1.54	0.71
1:A:154:HIS:HD2	1:A:192:LEU:HD22	1.55	0.70
1:B:633:ILE:HD12	1:B:634:GLN:N	2.07	0.70
1:B:512:GLN:HA	1:B:639:ARG:O	1.92	0.70
1:A:56:ARG:HD2	1:A:92:PRO:HB2	1.74	0.69
1:B:373:ARG:HA	1:B:376:ARG:NH1	2.07	0.69
1:A:380:MET:HA	1:A:383:ASN:HD22	1.55	0.69
1:A:111:GLN:HB2	1:A:123:GLN:HE22	1.57	0.69
1:A:381:ILE:O	1:A:385:VAL:HG12	1.91	0.69
1:B:522:TYR:OH	1:B:572:LYS:HG3	1.93	0.69
1:B:263:HIS:HB3	1:B:302:LEU:HD13	1.74	0.69
1:A:482:ASP:CG	1:A:483:ASN:H	2.00	0.68
1:A:196:LYS:HE3	1:A:216:GLY:HA3	1.74	0.68
1:A:473:PHE:HB3	1:A:479:PHE:HE1	1.57	0.68
1:B:381:ILE:O	1:B:385:VAL:HG12	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:HIS:HB3	1:A:302:LEU:HD13	1.77	0.67
1:B:339:VAL:HG13	1:B:377:THR:HG21	1.76	0.67
1:B:513:ILE:HD12	1:B:514:LYS:N	2.10	0.67
1:A:52:LEU:O	1:A:52:LEU:HD23	1.95	0.66
1:A:201:ASN:ND2	1:A:268:ARG:HE	1.93	0.66
1:B:272:THR:HG23	1:B:273:VAL:HG22	1.76	0.66
1:A:513:ILE:HD12	1:A:514:LYS:N	2.09	0.66
1:B:522:TYR:OH	1:B:571:ILE:HG13	1.95	0.66
1:A:411:HIS:HE1	1:A:413:GLU:HB3	1.61	0.65
1:B:164:PRO:HG2	1:B:167:LEU:HD13	1.78	0.65
1:A:349:ILE:HG23	1:A:393:ASN:ND2	2.12	0.65
1:B:99:THR:HG22	1:B:142:LEU:HD13	1.79	0.65
1:B:522:TYR:CE1	1:B:568:LEU:HB3	2.32	0.65
1:B:330:ILE:HG21	1:B:362:ALA:HB1	1.79	0.65
1:A:539:GLN:O	1:A:543:VAL:HG12	1.97	0.64
1:B:604:VAL:O	1:B:608:GLN:HG3	1.98	0.64
1:A:687:ILE:HD13	1:B:687:ILE:HG12	1.78	0.64
1:B:415:ARG:NH1	1:B:464:ILE:HD11	2.13	0.64
1:A:360:ASN:HB3	1:A:396:ASN:HB2	1.79	0.63
1:A:683:PHE:HZ	1:B:690:LEU:HB3	1.61	0.63
1:B:102:PHE:HA	1:B:105:VAL:HG12	1.80	0.63
1:A:333:ILE:HD12	1:A:333:ILE:N	2.13	0.63
1:A:683:PHE:CZ	1:B:690:LEU:HD13	2.33	0.63
1:A:79:CYS:O	1:A:83:ILE:HG12	1.98	0.63
1:A:509:ASN:OD1	1:A:644:ILE:HD11	1.99	0.63
1:B:490:LEU:O	1:B:490:LEU:HD23	1.99	0.63
1:A:551:LEU:HD12	1:A:552:GLN:N	2.14	0.63
1:B:201:ASN:O	1:B:204:GLU:HG2	1.99	0.63
1:B:267:LEU:O	1:B:271:GLU:HG3	1.99	0.63
1:B:522:TYR:HH	1:B:572:LYS:HG3	1.64	0.63
1:A:102:PHE:O	1:A:106:LEU:HG	1.99	0.62
1:B:572:LYS:NZ	1:B:572:LYS:HB3	2.14	0.62
1:B:635:ILE:HD12	1:B:636:LEU:N	2.14	0.62
1:B:449:ILE:O	1:B:453:LEU:HD13	1.99	0.62
1:A:165:ALA:HA	1:A:168:PHE:CD1	2.35	0.62
1:A:151:GLU:O	1:A:155:ILE:HG13	2.00	0.62
1:A:256:LEU:O	1:A:260:VAL:HG23	2.00	0.62
1:B:394:ILE:HD12	1:B:394:ILE:O	2.00	0.62
1:A:568:LEU:HD12	1:A:569:GLU:N	2.14	0.61
1:B:650:ILE:HD12	1:B:651:SER:N	2.14	0.61
1:A:412:LYS:NZ	1:A:412:LYS:HB3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:LEU:HD13	1:A:633:ILE:HD11	1.83	0.61
1:A:283:PHE:O	1:A:287:GLU:HG3	1.99	0.61
1:A:333:ILE:H	1:A:333:ILE:CD1	2.13	0.61
1:A:394:ILE:O	1:A:394:ILE:HD12	2.00	0.61
1:B:462:LEU:HB3	1:B:559:SER:CB	2.30	0.61
1:B:18:THR:HG23	1:B:21:GLN:H	1.65	0.61
1:B:547:TYR:OH	1:B:572:LYS:HE3	2.00	0.61
1:A:686:GLN:O	1:A:690:LEU:HG	2.01	0.61
1:A:3:LYS:HB3	1:A:50:THR:HG21	1.82	0.61
1:A:387:VAL:HA	1:A:390:ILE:HD12	1.82	0.60
1:A:524:ASP:HA	1:A:527:LYS:HE2	1.83	0.60
1:B:80:LEU:HD13	1:B:101:ILE:HG23	1.83	0.60
1:A:415:ARG:NH1	1:A:464:ILE:HD11	2.16	0.60
1:B:513:ILE:HG22	1:B:589:ASN:HD21	1.65	0.60
1:A:483:ASN:HA	1:A:486:ARG:HH12	1.66	0.60
1:B:462:LEU:HB3	1:B:559:SER:HB3	1.83	0.60
1:A:201:ASN:HD22	1:A:268:ARG:HE	1.49	0.60
1:B:655:ASN:OD1	1:B:668:LYS:HD2	2.01	0.60
1:A:290:SER:O	1:A:296:ARG:HD3	2.01	0.60
1:A:22:LEU:C	1:A:23:ILE:HD12	2.27	0.60
1:A:288:LEU:HB3	1:A:329:LYS:HE3	1.83	0.60
1:B:151:GLU:O	1:B:155:ILE:HG13	2.02	0.60
1:B:554:LEU:HD12	1:B:555:ALA:N	2.17	0.60
1:A:635:ILE:HA	1:A:638:PHE:HD2	1.66	0.59
1:A:584:ASN:O	1:A:588:THR:HG23	2.01	0.59
1:B:355:ILE:N	1:B:355:ILE:HD12	2.17	0.59
1:B:467:GLN:O	1:B:471:VAL:HG23	2.03	0.59
1:B:628:ASP:O	1:B:631:LYS:HG2	2.01	0.59
1:A:489:ARG:O	1:A:493:VAL:HG23	2.02	0.59
1:B:648:SER:O	1:B:652:VAL:HG23	2.03	0.59
1:A:49:LEU:HD23	1:A:49:LEU:O	2.02	0.59
1:B:156:PHE:HA	1:B:163:PHE:CE2	2.38	0.59
1:B:333:ILE:H	1:B:333:ILE:CD1	2.07	0.59
1:A:418:CYS:O	1:A:422:MET:HG2	2.02	0.59
1:A:635:ILE:HA	1:A:638:PHE:CD2	2.38	0.59
1:B:70:VAL:HG12	1:B:73:ARG:NH2	2.16	0.59
1:A:70:VAL:HG12	1:A:73:ARG:NH2	2.16	0.59
1:A:673:ASP:OD1	1:A:677:LYS:HE2	2.03	0.59
1:B:654:LEU:C	1:B:655:ASN:HD22	2.11	0.59
1:B:676:SER:HA	1:B:682:LEU:HD11	1.84	0.59
1:B:49:LEU:O	1:B:49:LEU:HD23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:O	1:A:459:ILE:HG13	2.02	0.59
1:B:95:ASP:O	1:B:99:THR:HG23	2.03	0.58
1:B:254:ARG:O	1:B:258:VAL:HG23	2.03	0.58
1:A:644:ILE:HG13	1:A:645:TYR:CD1	2.38	0.58
1:B:523:ILE:HD11	1:B:583:LEU:HD23	1.85	0.58
1:A:121:ILE:HD12	1:A:121:ILE:N	2.17	0.58
1:B:288:LEU:HB3	1:B:329:LYS:CE	2.33	0.58
1:A:509:ASN:CG	1:A:644:ILE:HD11	2.29	0.58
1:B:314:ASN:OD1	1:B:316:VAL:HG22	2.03	0.58
1:A:110:GLU:HG3	1:A:161:LYS:NZ	2.18	0.58
1:B:288:LEU:HB3	1:B:329:LYS:HE3	1.84	0.58
1:B:139:LEU:O	1:B:139:LEU:HD23	2.04	0.58
1:B:22:LEU:HD12	1:B:22:LEU:O	2.04	0.58
1:B:333:ILE:HD12	1:B:333:ILE:N	2.11	0.58
1:B:646:ASN:OD1	1:B:647:VAL:HG13	2.03	0.58
1:A:355:ILE:HD12	1:A:355:ILE:N	2.19	0.57
1:B:116:GLU:HA	1:B:120:HIS:CE1	2.39	0.57
1:B:186:PRO:HG2	1:B:189:VAL:HG23	1.86	0.57
1:B:256:LEU:O	1:B:260:VAL:HG23	2.04	0.57
1:B:355:ILE:HG22	1:B:359:LEU:HG	1.84	0.57
1:B:554:LEU:HD11	1:B:568:LEU:HD11	1.86	0.57
1:A:139:LEU:HD23	1:A:139:LEU:O	2.04	0.57
1:B:523:ILE:HG21	1:B:580:PHE:HB3	1.85	0.57
1:B:251:ASN:HB3	1:B:254:ARG:HB2	1.85	0.57
1:A:624:ILE:HG12	1:A:625:MET:N	2.19	0.57
1:A:571:ILE:HA	1:A:574:PHE:CD2	2.39	0.57
1:B:519:ILE:O	1:B:522:TYR:HB3	2.04	0.57
1:B:22:LEU:C	1:B:23:ILE:HD12	2.29	0.57
1:B:481:PRO:HG2	1:B:482:ASP:H	1.70	0.57
1:A:288:LEU:HB3	1:A:329:LYS:CE	2.35	0.57
1:A:187:LEU:HG	1:A:191:ARG:NH1	2.20	0.57
1:B:509:ASN:HD21	1:B:644:ILE:HD11	1.69	0.57
1:A:293:GLU:HA	1:A:296:ARG:NE	2.19	0.56
1:A:449:ILE:N	1:A:450:PRO:HD2	2.19	0.56
1:A:376:ARG:O	1:A:380:MET:HG2	2.03	0.56
1:A:446:ILE:N	1:A:446:ILE:HD12	2.21	0.56
1:B:449:ILE:HB	1:B:450:PRO:HD3	1.87	0.56
1:B:633:ILE:O	1:B:637:LEU:HG	2.04	0.56
1:B:645:TYR:CE2	1:B:678:VAL:HG21	2.41	0.56
1:B:175:LEU:HD12	1:B:219:VAL:HG11	1.88	0.56
1:B:513:ILE:HG22	1:B:589:ASN:ND2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:686:GLN:O	1:B:690:LEU:HG	2.04	0.56
1:A:397:LYS:NZ	1:A:445:ILE:HD11	2.21	0.56
1:B:78:CYS:SG	1:B:122:GLN:HB3	2.46	0.56
1:B:17:SER:HA	1:B:23:ILE:HD13	1.88	0.56
1:B:579:ILE:HG23	1:B:603:LEU:HD11	1.87	0.56
1:A:459:ILE:C	1:A:459:ILE:HD12	2.31	0.56
1:A:560:ASP:OD1	1:A:563:LYS:HB2	2.06	0.56
1:B:62:ARG:NH1	1:B:66:LYS:HD2	2.21	0.56
1:B:187:LEU:O	1:B:187:LEU:HD23	2.06	0.56
1:B:273:VAL:HB	1:B:276:LEU:HD13	1.86	0.56
1:A:453:LEU:HA	1:A:456:LEU:HD13	1.86	0.55
1:B:23:ILE:HD12	1:B:23:ILE:N	2.22	0.55
1:B:110:GLU:HG3	1:B:161:LYS:NZ	2.21	0.55
1:A:14:PRO:HG2	1:A:31:ARG:NH1	2.21	0.55
1:B:584:ASN:HA	1:B:587:VAL:HG12	1.88	0.55
1:A:633:ILE:O	1:A:637:LEU:HG	2.07	0.55
1:B:386:PRO:O	1:B:390:ILE:HG13	2.06	0.55
1:A:459:ILE:HD12	1:A:460:ASN:N	2.21	0.55
1:A:95:ASP:O	1:A:99:THR:HG23	2.07	0.55
1:B:131:LEU:HB2	1:B:174:ILE:HD11	1.89	0.55
1:B:283:PHE:O	1:B:287:GLU:HG3	2.07	0.55
1:A:565:ILE:HG13	1:A:566:ASP:OD1	2.06	0.55
1:B:51:GLY:C	1:B:52:LEU:HD12	2.32	0.55
1:B:110:GLU:HG3	1:B:161:LYS:HZ1	1.72	0.55
1:B:592:PRO:O	1:B:595:THR:HG22	2.07	0.55
1:A:568:LEU:HA	1:A:571:ILE:HD12	1.88	0.55
1:A:664:GLN:HG2	1:A:668:LYS:HE3	1.88	0.55
1:B:219:VAL:O	1:B:223:LEU:HD13	2.07	0.55
1:B:663:LYS:O	1:B:667:LEU:HD13	2.07	0.55
1:B:188:GLU:O	1:B:192:LEU:HG	2.08	0.54
1:A:270:TRP:HE3	1:A:277:ILE:HG13	1.73	0.54
1:B:102:PHE:O	1:B:106:LEU:HG	2.08	0.54
1:B:288:LEU:HD12	1:B:299:ALA:HB1	1.89	0.54
1:A:335:PRO:HA	1:A:338:ARG:HD2	1.90	0.54
1:A:628:ASP:O	1:A:632:VAL:HG23	2.07	0.54
1:A:635:ILE:C	1:A:635:ILE:HD12	2.32	0.54
1:B:372:PRO:HB3	1:B:375:ARG:HH21	1.71	0.54
1:A:219:VAL:O	1:A:223:LEU:HD13	2.08	0.54
1:B:102:PHE:O	1:B:105:VAL:HG12	2.08	0.54
1:B:238:TYR:O	1:B:242:ILE:HG12	2.07	0.54
1:B:418:CYS:O	1:B:422:MET:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:LEU:HD22	1:B:476:LEU:HD21	1.90	0.54
1:B:560:ASP:OD1	1:B:563:LYS:HG3	2.07	0.54
1:A:690:LEU:HD13	1:B:683:PHE:CE2	2.43	0.54
1:B:376:ARG:O	1:B:380:MET:HG2	2.08	0.54
1:A:668:LYS:O	1:A:672:LEU:HD13	2.08	0.54
1:A:683:PHE:CZ	1:B:690:LEU:HB3	2.43	0.54
1:A:22:LEU:O	1:A:22:LEU:HD12	2.08	0.54
1:A:467:GLN:O	1:A:471:VAL:HG23	2.07	0.54
1:A:526:SER:C	1:A:528:PHE:H	2.14	0.54
1:B:544:MET:HE3	1:B:544:MET:O	2.08	0.53
1:B:165:ALA:HA	1:B:168:PHE:CD1	2.43	0.53
1:B:205:ILE:N	1:B:206:PRO:CD	2.71	0.53
1:B:316:VAL:HG11	1:B:355:ILE:HD11	1.90	0.53
1:B:572:LYS:HB3	1:B:572:LYS:HZ3	1.73	0.53
1:A:157:TYR:HB2	1:A:192:LEU:HD21	1.89	0.53
1:A:585:ALA:O	1:A:591:ILE:HD13	2.07	0.53
1:B:396:ASN:HB3	1:B:399:ILE:CG1	2.37	0.53
1:B:411:HIS:HE1	1:B:413:GLU:HB3	1.72	0.53
1:A:23:ILE:HD12	1:A:23:ILE:N	2.23	0.53
1:A:84:LEU:O	1:A:88:ALA:HB2	2.08	0.53
1:B:650:ILE:HD12	1:B:650:ILE:C	2.33	0.53
1:A:635:ILE:HD12	1:A:636:LEU:N	2.24	0.53
1:B:156:PHE:HA	1:B:163:PHE:HE2	1.73	0.53
1:A:215:CYS:O	1:A:219:VAL:HG23	2.08	0.53
1:B:292:ASN:HB3	1:B:295:PHE:HD2	1.73	0.53
1:B:344:SER:O	1:B:348:ILE:HG13	2.09	0.53
1:B:516:SER:OG	1:B:587:VAL:HG22	2.09	0.53
1:A:154:HIS:O	1:A:158:ASP:HB2	2.09	0.53
1:A:646:ASN:OD1	1:A:647:VAL:HG13	2.09	0.53
1:B:479:PHE:HB3	1:B:597:LYS:HD3	1.90	0.53
1:A:571:ILE:HA	1:A:574:PHE:HD2	1.72	0.53
1:A:624:ILE:HG12	1:A:625:MET:H	1.73	0.53
1:B:205:ILE:O	1:B:207:GLU:HG2	2.09	0.53
1:B:513:ILE:HD12	1:B:513:ILE:C	2.34	0.53
1:A:380:MET:SD	1:A:417:LEU:HD21	2.49	0.52
1:A:411:HIS:CE1	1:A:413:GLU:HB3	2.43	0.52
1:A:673:ASP:O	1:A:677:LYS:HG3	2.09	0.52
1:A:104:LEU:C	1:A:104:LEU:HD23	2.34	0.52
1:B:566:ASP:O	1:B:570:THR:HG23	2.08	0.52
1:B:671:ILE:HG22	1:B:675:ILE:HD11	1.90	0.52
1:A:664:GLN:O	1:A:668:LYS:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:O	1:B:88:ALA:HB2	2.10	0.52
1:B:589:ASN:HA	1:B:642:PRO:HG3	1.91	0.52
1:B:635:ILE:HD12	1:B:635:ILE:C	2.34	0.52
1:A:339:VAL:O	1:A:343:GLU:HG3	2.09	0.52
1:A:449:ILE:O	1:A:453:LEU:HD13	2.09	0.52
1:A:551:LEU:HD22	1:A:568:LEU:HD11	1.91	0.52
1:B:254:ARG:HE	1:B:254:ARG:HA	1.74	0.52
1:B:643:ILE:HD12	1:B:643:ILE:N	2.25	0.52
1:A:72:ILE:N	1:A:72:ILE:HD12	2.25	0.52
1:A:644:ILE:HG13	1:A:645:TYR:HD1	1.75	0.52
1:B:521:LYS:HB3	1:B:525:PHE:CE2	2.44	0.52
1:B:3:LYS:HE3	1:B:50:THR:HG21	1.91	0.52
1:B:380:MET:SD	1:B:417:LEU:HD21	2.50	0.52
1:B:565:ILE:HG13	1:B:566:ASP:OD1	2.09	0.52
1:A:262:LEU:O	1:A:266:VAL:HG23	2.08	0.52
1:A:527:LYS:HA	1:A:530:ASN:OD1	2.10	0.52
1:A:121:ILE:H	1:A:121:ILE:CD1	2.20	0.52
1:A:99:THR:HG22	1:A:142:LEU:HD13	1.92	0.52
1:A:238:TYR:O	1:A:242:ILE:HG12	2.10	0.52
1:A:396:ASN:HB3	1:A:399:ILE:CG1	2.40	0.52
1:A:355:ILE:HG22	1:A:359:LEU:HG	1.92	0.51
1:B:48:ASP:C	1:B:50:THR:H	2.18	0.51
1:A:27:GLU:O	1:A:31:ARG:HG3	2.10	0.51
1:A:523:ILE:HG23	1:A:580:PHE:HD2	1.75	0.51
1:B:649:ASN:O	1:B:653:LEU:HG	2.10	0.51
1:A:314:ASN:OD1	1:A:316:VAL:HG22	2.11	0.51
1:A:513:ILE:HD12	1:A:513:ILE:C	2.35	0.51
1:A:643:ILE:N	1:A:643:ILE:HD12	2.25	0.51
1:B:464:ILE:O	1:B:468:VAL:HG23	2.10	0.51
1:B:547:TYR:HH	1:B:572:LYS:HE3	1.75	0.51
1:A:301:LYS:O	1:A:305:GLN:HG3	2.10	0.51
1:A:506:PHE:HA	1:A:509:ASN:HD22	1.74	0.51
1:B:215:CYS:O	1:B:219:VAL:HG23	2.11	0.51
1:B:607:LEU:HD23	1:B:633:ILE:HG12	1.92	0.51
1:B:693:ILE:HD12	1:B:694:ILE:N	2.26	0.51
1:A:87:TYR:HB3	1:A:92:PRO:HD3	1.92	0.51
1:A:265:LEU:O	1:A:269:LEU:HG	2.11	0.51
1:A:634:GLN:HG2	1:A:638:PHE:CE2	2.46	0.51
1:B:136:ILE:HG12	1:B:174:ILE:HG23	1.90	0.51
1:A:528:PHE:CE2	1:A:543:VAL:HG11	2.45	0.51
1:A:539:GLN:C	1:A:543:VAL:HG12	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:TRP:HE3	1:B:277:ILE:HG13	1.74	0.51
1:B:526:SER:CB	1:B:572:LYS:HE2	2.40	0.51
1:A:105:VAL:HG22	1:A:109:PHE:CE2	2.46	0.51
1:A:388:THR:O	1:A:392:LYS:HG2	2.10	0.51
1:A:576:ASP:OD2	1:A:578:ARG:HB3	2.10	0.51
1:B:415:ARG:HH11	1:B:464:ILE:HD11	1.74	0.51
1:B:594:LEU:HD13	1:B:594:LEU:C	2.35	0.51
1:A:663:LYS:O	1:A:667:LEU:HD13	2.11	0.51
1:B:360:ASN:HB3	1:B:396:ASN:HB2	1.92	0.51
1:B:397:LYS:HE3	1:B:401:THR:HG21	1.93	0.51
1:A:357:LYS:HB3	1:A:358:GLU:OE1	2.11	0.51
1:A:59:LEU:O	1:A:80:LEU:HD21	2.11	0.50
1:A:116:GLU:HG2	1:A:118:GLY:H	1.75	0.50
1:A:529:LEU:N	1:A:529:LEU:HD12	2.26	0.50
1:B:693:ILE:HD12	1:B:693:ILE:C	2.36	0.50
1:A:56:ARG:HD3	1:A:87:TYR:CE2	2.45	0.50
1:A:479:PHE:HA	1:A:593:PHE:HZ	1.75	0.50
1:A:523:ILE:HG23	1:A:580:PHE:CD2	2.46	0.50
1:B:97:GLN:O	1:B:101:ILE:HG13	2.11	0.50
1:A:273:VAL:HB	1:A:276:LEU:HD13	1.94	0.50
1:A:566:ASP:O	1:A:570:THR:HG23	2.12	0.50
1:A:650:ILE:HG21	1:B:650:ILE:HD13	1.93	0.50
1:B:339:VAL:O	1:B:343:GLU:HG3	2.11	0.50
1:B:430:LEU:HD12	1:B:431:ASN:OD1	2.11	0.50
1:B:578:ARG:NE	1:B:582:LEU:HD11	2.27	0.50
1:B:584:ASN:O	1:B:587:VAL:HG12	2.11	0.50
1:A:592:PRO:HB2	1:A:595:THR:HG22	1.93	0.50
1:A:110:GLU:HG3	1:A:161:LYS:HZ1	1.75	0.50
1:A:366:THR:HG22	1:A:378:SER:OG	2.11	0.50
1:A:487:VAL:O	1:A:491:LEU:HG	2.12	0.50
1:B:104:LEU:HD23	1:B:104:LEU:C	2.36	0.50
1:A:72:ILE:HD12	1:A:72:ILE:H	1.77	0.50
1:A:387:VAL:HG23	1:A:425:PHE:CE1	2.47	0.50
1:B:209:LEU:N	1:B:209:LEU:HD12	2.26	0.50
1:B:262:LEU:O	1:B:266:VAL:HG23	2.12	0.50
1:A:468:VAL:O	1:A:472:ILE:HG13	2.12	0.50
1:B:105:VAL:HG22	1:B:109:PHE:CE2	2.47	0.50
1:B:167:LEU:O	1:B:171:ILE:HG13	2.12	0.50
1:B:354:ASP:HB3	1:B:355:ILE:HD12	1.94	0.50
1:B:690:LEU:O	1:B:694:ILE:HG13	2.12	0.50
1:A:134:ARG:HG2	1:A:134:ARG:HH11	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ILE:O	1:A:394:ILE:HG13	2.11	0.49
1:B:6:VAL:CG1	1:B:46:ASN:HD21	2.24	0.49
1:A:102:PHE:HA	1:A:105:VAL:HG12	1.93	0.49
1:B:482:ASP:O	1:B:486:ARG:HG3	2.12	0.49
1:A:683:PHE:HZ	1:B:690:LEU:HD13	1.78	0.49
1:B:265:LEU:O	1:B:269:LEU:HG	2.11	0.49
1:A:508:PHE:HE1	1:A:639:ARG:HG2	1.77	0.49
1:B:154:HIS:O	1:B:158:ASP:HB2	2.11	0.49
1:B:366:THR:HG22	1:B:378:SER:OG	2.13	0.49
1:A:594:LEU:C	1:A:594:LEU:HD13	2.37	0.49
1:A:628:ASP:HA	1:A:631:LYS:HG2	1.94	0.49
1:A:97:GLN:O	1:A:101:ILE:HG13	2.12	0.49
1:A:102:PHE:HZ	1:A:138:LEU:HB2	1.77	0.49
1:B:145:SER:HB3	1:B:182:PHE:HZ	1.76	0.49
1:B:579:ILE:HG23	1:B:603:LEU:CD1	2.43	0.49
1:A:515:ILE:HD12	1:A:639:ARG:O	2.13	0.49
1:B:301:LYS:HD3	1:B:340:GLU:OE2	2.12	0.49
1:A:52:LEU:HD22	1:A:87:TYR:HE1	1.78	0.49
1:A:276:LEU:HD12	1:A:276:LEU:N	2.27	0.49
1:A:482:ASP:CG	1:A:483:ASN:N	2.70	0.49
1:A:678:VAL:O	1:A:679:ASN:CB	2.61	0.49
1:A:687:ILE:HA	1:A:690:LEU:HD12	1.95	0.49
1:B:276:LEU:N	1:B:276:LEU:HD12	2.28	0.49
1:B:25:THR:O	1:B:29:LEU:HG	2.13	0.49
1:B:387:VAL:HG23	1:B:425:PHE:CE1	2.48	0.49
1:B:515:ILE:HG22	1:B:519:ILE:HD13	1.93	0.49
1:A:29:LEU:C	1:A:29:LEU:HD23	2.37	0.48
1:A:292:ASN:HB3	1:A:295:PHE:HD2	1.77	0.48
1:A:534:SER:OG	1:A:538:SER:HB3	2.13	0.48
1:B:461:ASP:HB3	1:B:464:ILE:HB	1.95	0.48
1:B:588:THR:HG22	1:B:588:THR:O	2.13	0.48
1:B:218:GLU:O	1:B:222:ILE:HG13	2.13	0.48
1:B:442:ILE:HG22	1:B:446:ILE:HD13	1.94	0.48
1:B:523:ILE:CD1	1:B:583:LEU:HD23	2.43	0.48
1:B:551:LEU:C	1:B:551:LEU:HD23	2.37	0.48
1:A:6:VAL:HG13	1:A:7:THR:HG23	1.94	0.48
1:A:515:ILE:HG22	1:A:519:ILE:HD13	1.94	0.48
1:A:554:LEU:HD12	1:A:554:LEU:C	2.39	0.48
1:B:452:THR:O	1:B:456:LEU:HG	2.14	0.48
1:B:582:LEU:HD23	1:B:599:CYS:O	2.13	0.48
1:A:266:VAL:HG13	1:A:277:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:SER:O	1:B:148:LEU:HD13	2.13	0.48
1:B:165:ALA:HA	1:B:168:PHE:CE1	2.48	0.48
1:A:211:VAL:HG22	1:A:211:VAL:O	2.12	0.48
1:A:357:LYS:HG2	1:A:361:GLN:HE21	1.77	0.48
1:A:473:PHE:CE2	1:A:638:PHE:HB3	2.49	0.48
1:B:56:ARG:HD3	1:B:87:TYR:CE2	2.48	0.48
1:B:166:ARG:HG3	1:B:167:LEU:CD1	2.43	0.48
1:A:139:LEU:HD23	1:A:139:LEU:C	2.38	0.48
1:A:354:ASP:HB3	1:A:355:ILE:HD12	1.96	0.48
1:A:511:ARG:O	1:A:515:ILE:HG13	2.14	0.48
1:B:589:ASN:C	1:B:591:ILE:HD12	2.37	0.48
1:A:102:PHE:CZ	1:A:138:LEU:HB2	2.48	0.48
1:A:131:LEU:HB2	1:A:174:ILE:HD11	1.95	0.48
1:A:523:ILE:CD1	1:A:584:ASN:HB2	2.44	0.48
1:B:515:ILE:O	1:B:519:ILE:HD13	2.13	0.48
1:B:468:VAL:O	1:B:472:ILE:HG13	2.13	0.48
1:B:681:THR:HA	1:B:684:LYS:HE3	1.96	0.48
1:A:48:ASP:C	1:A:50:THR:H	2.22	0.48
1:A:104:LEU:HD23	1:A:104:LEU:O	2.13	0.48
1:A:452:THR:HA	1:A:455:ASN:HD22	1.79	0.48
1:A:109:PHE:HE1	1:A:127:ILE:HB	1.79	0.48
1:A:464:ILE:O	1:A:468:VAL:HG23	2.14	0.48
1:B:249:ASP:C	1:B:251:ASN:H	2.22	0.48
1:B:411:HIS:CE1	1:B:413:GLU:HB3	2.49	0.48
1:B:676:SER:CB	1:B:682:LEU:HD11	2.44	0.48
1:A:107:SER:O	1:A:111:GLN:HG3	2.14	0.47
1:B:153:PHE:CE1	1:B:175:LEU:HB3	2.49	0.47
1:B:293:GLU:HA	1:B:296:ARG:HD2	1.95	0.47
1:A:551:LEU:HB2	1:A:568:LEU:HD21	1.96	0.47
1:A:544:MET:HE3	1:A:544:MET:O	2.14	0.47
1:A:569:GLU:O	1:A:572:LYS:HB3	2.14	0.47
1:B:139:LEU:HD23	1:B:139:LEU:C	2.38	0.47
1:B:487:VAL:O	1:B:491:LEU:HG	2.15	0.47
1:B:509:ASN:ND2	1:B:644:ILE:HD11	2.28	0.47
1:A:436:THR:HG23	1:A:439:ASN:HD21	1.80	0.47
1:B:448:THR:O	1:B:452:THR:HG23	2.14	0.47
1:B:564:ALA:O	1:B:568:LEU:HG	2.15	0.47
1:A:412:LYS:HB3	1:A:412:LYS:HZ3	1.77	0.47
1:B:402:SER:O	1:B:406:LEU:HG	2.15	0.47
1:B:582:LEU:H	1:B:582:LEU:HD12	1.79	0.47
1:A:565:ILE:O	1:A:569:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:LEU:H	1:A:682:LEU:CD2	2.25	0.47
1:B:60:VAL:HA	1:B:65:LEU:HD11	1.96	0.47
1:B:131:LEU:HB2	1:B:174:ILE:CD1	2.45	0.47
1:B:149:LEU:HD22	1:B:182:PHE:CE2	2.50	0.47
1:B:201:ASN:ND2	1:B:268:ARG:HE	2.13	0.47
1:B:314:ASN:HD21	1:B:352:ARG:HH22	1.63	0.47
1:A:567:ALA:O	1:A:571:ILE:HG13	2.15	0.47
1:B:404:LEU:N	1:B:404:LEU:HD12	2.29	0.47
1:B:554:LEU:HD12	1:B:554:LEU:C	2.39	0.47
1:A:36:HIS:CE1	1:A:78:CYS:HB3	2.50	0.47
1:A:218:GLU:O	1:A:222:ILE:HG13	2.15	0.47
1:A:569:GLU:OE2	1:A:572:LYS:HD3	2.15	0.47
1:B:49:LEU:HD23	1:B:49:LEU:C	2.40	0.47
1:B:607:LEU:CD2	1:B:633:ILE:HG12	2.45	0.47
1:A:157:TYR:HB3	1:A:192:LEU:HD11	1.98	0.47
1:A:232:SER:OG	1:A:279:ALA:HB2	2.15	0.47
1:A:690:LEU:HD13	1:B:683:PHE:CD2	2.50	0.47
1:B:36:HIS:CE1	1:B:78:CYS:HB3	2.50	0.47
1:B:647:VAL:O	1:B:650:ILE:HG13	2.15	0.47
1:A:80:LEU:HD13	1:A:101:ILE:HG23	1.96	0.46
1:A:369:ASP:HB3	1:A:374:VAL:HG21	1.96	0.46
1:A:568:LEU:HD12	1:A:568:LEU:C	2.40	0.46
1:B:126:LEU:O	1:B:130:LEU:HG	2.15	0.46
1:B:416:GLU:HB3	1:B:467:GLN:HE22	1.80	0.46
1:A:112:LEU:HD21	1:A:167:LEU:HD13	1.97	0.46
1:A:386:PRO:O	1:A:390:ILE:HG13	2.14	0.46
1:A:592:PRO:O	1:A:595:THR:HG22	2.15	0.46
1:B:59:LEU:O	1:B:80:LEU:HD21	2.15	0.46
1:B:107:SER:O	1:B:111:GLN:HG3	2.14	0.46
1:B:630:ALA:O	1:B:634:GLN:HG3	2.15	0.46
1:A:462:LEU:HD13	1:A:558:LEU:O	2.15	0.46
1:B:109:PHE:HE1	1:B:127:ILE:HB	1.80	0.46
1:B:174:ILE:O	1:B:178:VAL:HG23	2.15	0.46
1:A:167:LEU:O	1:A:171:ILE:HG13	2.15	0.46
1:A:246:ALA:CB	1:A:258:VAL:HG21	2.46	0.46
1:A:243:ILE:HD11	1:A:262:LEU:HD12	1.97	0.46
1:A:394:ILE:HD12	1:A:394:ILE:C	2.41	0.46
1:A:678:VAL:HG23	1:A:679:ASN:N	2.30	0.46
1:B:582:LEU:HD12	1:B:582:LEU:N	2.30	0.46
1:A:10:LYS:HB2	1:A:38:GLU:OE2	2.15	0.46
1:A:153:PHE:HB3	1:A:192:LEU:HD23	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:O	1:A:271:GLU:HG3	2.16	0.46
1:B:102:PHE:HZ	1:B:138:LEU:HB2	1.80	0.46
1:B:345:ILE:HD13	1:B:363:LEU:HD21	1.97	0.46
1:B:357:LYS:O	1:B:361:GLN:HG3	2.15	0.46
1:A:404:LEU:N	1:A:404:LEU:HD12	2.30	0.46
1:B:476:LEU:HD12	1:B:476:LEU:N	2.29	0.46
1:B:526:SER:OG	1:B:572:LYS:HG2	2.15	0.46
1:B:687:ILE:HA	1:B:690:LEU:HD12	1.97	0.46
1:A:131:LEU:HB2	1:A:174:ILE:CD1	2.45	0.46
1:A:207:GLU:HG2	1:A:210:ASN:OD1	2.16	0.46
1:A:523:ILE:HD12	1:A:584:ASN:HB2	1.97	0.46
1:A:453:LEU:HD22	1:A:476:LEU:HD21	1.98	0.46
1:A:512:GLN:HA	1:A:639:ARG:O	2.16	0.46
1:B:166:ARG:NH1	1:B:167:LEU:HD11	2.31	0.46
1:A:288:LEU:HD12	1:A:299:ALA:HB1	1.97	0.45
1:A:532:GLN:HE22	1:A:535:MET:HB2	1.81	0.45
1:A:686:GLN:CD	1:A:686:GLN:H	2.24	0.45
1:B:24:SER:HB3	1:B:27:GLU:HG3	1.98	0.45
1:A:125:TYR:CZ	1:A:129:LYS:HG3	2.51	0.45
1:A:168:PHE:CE2	1:A:215:CYS:HA	2.51	0.45
1:B:49:LEU:CA	1:B:52:LEU:HD13	2.46	0.45
1:B:292:ASN:O	1:B:296:ARG:HG3	2.17	0.45
1:A:83:ILE:HG21	1:A:93:TYR:OH	2.16	0.45
1:A:390:ILE:HG22	1:A:394:ILE:HD11	1.97	0.45
1:A:476:LEU:N	1:A:476:LEU:HD12	2.31	0.45
1:A:542:ILE:HG13	1:A:543:VAL:N	2.31	0.45
1:B:263:HIS:CG	1:B:302:LEU:HD22	2.51	0.45
1:A:145:SER:HB3	1:A:182:PHE:HZ	1.81	0.45
1:A:116:GLU:HA	1:A:120:HIS:NE2	2.32	0.45
1:A:347:GLN:CD	1:A:347:GLN:H	2.24	0.45
1:A:629:ILE:O	1:A:633:ILE:HG22	2.16	0.45
1:A:165:ALA:HA	1:A:168:PHE:CE1	2.52	0.45
1:A:273:VAL:C	1:A:275:GLU:H	2.25	0.45
1:B:256:LEU:O	1:B:259:VAL:HG12	2.16	0.45
1:B:284:ILE:O	1:B:288:LEU:HD13	2.15	0.45
1:A:49:LEU:HD23	1:A:49:LEU:C	2.41	0.45
1:A:560:ASP:CG	1:A:563:LYS:HB2	2.42	0.45
1:B:79:CYS:O	1:B:83:ILE:HD13	2.17	0.45
1:B:268:ARG:O	1:B:272:THR:HG22	2.16	0.45
1:B:635:ILE:HA	1:B:638:PHE:HD2	1.82	0.45
1:A:400:TYR:HB3	1:A:445:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:LYS:HD2	1:B:133:TYR:CE2	2.52	0.45
1:B:166:ARG:C	1:B:167:LEU:HD12	2.42	0.45
1:B:301:LYS:O	1:B:305:GLN:HG3	2.17	0.45
1:B:422:MET:HE2	1:B:453:LEU:HD11	1.97	0.45
1:B:633:ILE:HD12	1:B:633:ILE:C	2.42	0.45
1:B:238:TYR:CE1	1:B:242:ILE:HD11	2.52	0.45
1:A:347:GLN:O	1:A:351:THR:HG23	2.17	0.44
1:A:411:HIS:CE1	1:A:414:VAL:HG23	2.52	0.44
1:A:519:ILE:O	1:A:522:TYR:HB3	2.17	0.44
1:A:551:LEU:HD12	1:A:551:LEU:C	2.41	0.44
1:A:558:LEU:HD13	1:A:632:VAL:HG13	2.00	0.44
1:A:149:LEU:HD22	1:A:182:PHE:CE2	2.52	0.44
1:A:191:ARG:HB3	1:A:195:ASN:HD21	1.82	0.44
1:B:61:SER:O	1:B:65:LEU:HD13	2.18	0.44
1:B:243:ILE:HG23	1:B:255:LEU:HD11	1.99	0.44
1:A:153:PHE:CE1	1:A:175:LEU:HB3	2.52	0.44
1:A:174:ILE:O	1:A:178:VAL:HG23	2.16	0.44
1:A:519:ILE:HD12	1:A:519:ILE:N	2.33	0.44
1:A:28:LEU:O	1:A:32:LEU:HG	2.18	0.44
1:A:345:ILE:HD12	1:A:345:ILE:N	2.32	0.44
1:B:345:ILE:HB	1:B:346:PRO:HD3	2.00	0.44
1:B:676:SER:CA	1:B:682:LEU:HD11	2.48	0.44
1:A:52:LEU:HD22	1:A:87:TYR:CE1	2.52	0.44
1:A:436:THR:OG1	1:A:439:ASN:ND2	2.51	0.44
1:B:22:LEU:HD12	1:B:22:LEU:C	2.42	0.44
1:B:387:VAL:HA	1:B:390:ILE:HD12	2.00	0.44
1:A:43:ASP:HB2	1:A:46:ASN:OD1	2.18	0.44
1:B:29:LEU:HD23	1:B:72:ILE:HD13	1.98	0.44
1:B:482:ASP:OD1	1:B:484:ASP:HB2	2.17	0.44
1:B:589:ASN:N	1:B:591:ILE:HD11	2.32	0.44
1:B:646:ASN:OD1	1:B:647:VAL:N	2.50	0.44
1:A:273:VAL:O	1:A:273:VAL:HG23	2.17	0.44
1:A:358:GLU:OE1	1:A:358:GLU:N	2.48	0.44
1:A:374:VAL:HG23	1:A:375:ARG:N	2.32	0.44
1:B:239:TYR:CE1	1:B:243:ILE:HD11	2.53	0.44
1:B:645:TYR:CD2	1:B:678:VAL:HG21	2.52	0.44
1:A:35:LEU:O	1:A:39:LEU:HG	2.18	0.44
1:A:646:ASN:OD1	1:A:647:VAL:N	2.51	0.44
1:A:683:PHE:CZ	1:B:690:LEU:HD22	2.52	0.44
1:A:506:PHE:HA	1:A:509:ASN:ND2	2.33	0.44
1:A:528:PHE:HB3	1:A:529:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:ILE:HG13	1:B:645:TYR:CD1	2.53	0.44
1:A:529:LEU:HD11	1:A:572:LYS:HE3	1.98	0.43
1:B:208:GLY:C	1:B:209:LEU:HD12	2.43	0.43
1:B:514:LYS:HE2	1:B:553:TRP:CZ2	2.53	0.43
1:A:22:LEU:C	1:A:22:LEU:HD12	2.43	0.43
1:B:201:ASN:OD1	1:B:203:ASN:ND2	2.51	0.43
1:B:394:ILE:HD12	1:B:394:ILE:C	2.43	0.43
1:B:446:ILE:N	1:B:446:ILE:HD12	2.33	0.43
1:A:48:ASP:O	1:A:49:LEU:HB3	2.18	0.43
1:A:224:CYS:O	1:A:276:LEU:HD11	2.17	0.43
1:A:227:TYR:O	1:A:231:MET:HG2	2.18	0.43
1:A:567:ALA:CB	1:A:629:ILE:HG12	2.48	0.43
1:B:369:ASP:CG	1:B:374:VAL:HG11	2.44	0.43
1:B:522:TYR:CZ	1:B:568:LEU:HD22	2.53	0.43
1:B:672:LEU:N	1:B:672:LEU:HD12	2.33	0.43
1:A:526:SER:C	1:A:528:PHE:N	2.76	0.43
1:A:582:LEU:N	1:A:582:LEU:HD12	2.34	0.43
1:B:35:LEU:O	1:B:39:LEU:HG	2.18	0.43
1:B:430:LEU:HD12	1:B:430:LEU:C	2.44	0.43
1:B:642:PRO:C	1:B:643:ILE:HD12	2.43	0.43
1:A:126:LEU:O	1:A:130:LEU:HG	2.18	0.43
1:B:341:TRP:CZ3	1:B:345:ILE:HD11	2.53	0.43
1:B:582:LEU:H	1:B:582:LEU:CD1	2.32	0.43
1:A:72:ILE:H	1:A:72:ILE:CD1	2.31	0.43
1:A:355:ILE:CG2	1:A:359:LEU:HG	2.49	0.43
1:B:104:LEU:HD23	1:B:104:LEU:O	2.17	0.43
1:B:499:LYS:O	1:B:503:THR:HG23	2.17	0.43
1:B:591:ILE:HD12	1:B:591:ILE:N	2.34	0.43
1:A:157:TYR:CD2	1:A:192:LEU:HG	2.54	0.43
1:B:33:LYS:O	1:B:37:GLU:HG3	2.19	0.43
1:B:442:ILE:O	1:B:446:ILE:HD13	2.19	0.43
1:B:593:PHE:O	1:B:596:PHE:HB3	2.19	0.43
1:A:82:ASP:O	1:A:85:ARG:HB3	2.18	0.43
1:A:99:THR:O	1:A:103:LYS:HB2	2.18	0.43
1:A:116:GLU:HA	1:A:120:HIS:CD2	2.54	0.43
1:A:263:HIS:CG	1:A:302:LEU:HD22	2.54	0.43
1:A:567:ALA:HB1	1:A:629:ILE:HG23	2.00	0.43
1:B:355:ILE:CG2	1:B:359:LEU:HG	2.47	0.43
1:B:80:LEU:O	1:B:84:LEU:HG	2.19	0.42
1:B:273:VAL:HG23	1:B:273:VAL:O	2.18	0.42
1:B:686:GLN:OE1	1:B:686:GLN:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ILE:HG13	1:A:185:VAL:HG21	2.01	0.42
1:A:667:LEU:O	1:A:671:ILE:HG13	2.19	0.42
1:B:320:SER:O	1:B:324:LYS:HG3	2.19	0.42
1:A:508:PHE:O	1:A:512:GLN:HG3	2.20	0.42
1:A:522:TYR:OH	1:A:568:LEU:HB2	2.18	0.42
1:A:539:GLN:O	1:A:540:GLY:C	2.62	0.42
1:A:671:ILE:HG22	1:A:675:ILE:HD11	2.02	0.42
1:B:292:ASN:HB3	1:B:295:PHE:CD2	2.51	0.42
1:B:490:LEU:HD23	1:B:490:LEU:C	2.43	0.42
1:A:383:ASN:OD1	1:A:424:LYS:HE2	2.19	0.42
1:A:480:GLU:HB2	1:A:481:PRO:CA	2.46	0.42
1:B:52:LEU:HD12	1:B:52:LEU:N	2.34	0.42
1:A:650:ILE:HD13	1:B:650:ILE:HB	2.01	0.42
1:B:249:ASP:O	1:B:250:ASP:HB3	2.20	0.42
1:A:307:LEU:HD21	1:A:315:PHE:HD2	1.84	0.42
1:A:539:GLN:HB3	1:A:542:ILE:HG13	2.01	0.42
1:B:652:VAL:HG12	1:B:672:LEU:HD11	2.02	0.42
1:A:497:PHE:CD2	1:A:501:ALA:HB1	2.55	0.42
1:A:525:PHE:O	1:A:528:PHE:HB2	2.19	0.42
1:B:481:PRO:HG2	1:B:482:ASP:N	2.33	0.42
1:A:112:LEU:HD21	1:A:167:LEU:CD1	2.49	0.42
1:A:292:ASN:HB3	1:A:295:PHE:CD2	2.54	0.42
1:A:462:LEU:O	1:A:466:GLU:HG3	2.19	0.42
1:A:499:LYS:O	1:A:503:THR:HG23	2.18	0.42
1:A:547:TYR:CD1	1:A:547:TYR:C	2.98	0.42
1:A:678:VAL:O	1:A:679:ASN:HB2	2.19	0.42
1:B:273:VAL:C	1:B:275:GLU:H	2.27	0.42
1:B:376:ARG:NH1	1:B:376:ARG:HB3	2.35	0.42
1:A:345:ILE:HB	1:A:346:PRO:HD3	2.02	0.42
1:A:397:LYS:HZ3	1:A:445:ILE:HD11	1.83	0.42
1:A:671:ILE:O	1:A:675:ILE:HG13	2.20	0.42
1:A:678:VAL:O	1:A:679:ASN:ND2	2.52	0.42
1:B:154:HIS:CD2	1:B:192:LEU:HD11	2.54	0.42
1:B:509:ASN:O	1:B:512:GLN:HB3	2.19	0.42
1:B:511:ARG:HG2	1:B:515:ILE:HG13	2.00	0.42
1:A:191:ARG:HB3	1:A:195:ASN:ND2	2.34	0.42
1:A:679:ASN:C	1:A:681:THR:H	2.28	0.42
1:B:381:ILE:C	1:B:383:ASN:H	2.28	0.42
1:A:376:ARG:HG2	1:A:376:ARG:HH11	1.85	0.41
1:A:671:ILE:HG22	1:A:675:ILE:CD1	2.49	0.41
1:B:48:ASP:O	1:B:49:LEU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:CYS:O	1:B:276:LEU:HD11	2.20	0.41
1:B:49:LEU:HA	1:B:52:LEU:HD13	2.01	0.41
1:B:125:TYR:CZ	1:B:129:LYS:HG3	2.55	0.41
1:B:164:PRO:CG	1:B:167:LEU:HD13	2.46	0.41
1:B:191:ARG:HB2	1:B:195:ASN:ND2	2.35	0.41
1:B:230:ARG:HG3	1:B:230:ARG:HH11	1.85	0.41
1:A:3:LYS:HB3	1:A:50:THR:CG2	2.48	0.41
1:A:411:HIS:ND1	1:A:414:VAL:HG23	2.36	0.41
1:A:529:LEU:CD1	1:A:572:LYS:HE3	2.50	0.41
1:A:591:ILE:H	1:A:646:ASN:HD21	1.67	0.41
1:B:185:VAL:HG13	1:B:186:PRO:HD2	2.01	0.41
1:B:236:THR:HG23	1:B:283:PHE:CE2	2.56	0.41
1:B:270:TRP:HB2	1:B:277:ILE:HG13	2.01	0.41
1:B:523:ILE:HD13	1:B:580:PHE:CA	2.43	0.41
1:A:458:TYR:CE2	1:A:500:LYS:HB3	2.55	0.41
1:A:649:ASN:O	1:A:653:LEU:HB2	2.19	0.41
1:B:145:SER:HB3	1:B:182:PHE:CZ	2.54	0.41
1:B:680:PRO:C	1:B:682:LEU:H	2.28	0.41
1:B:157:TYR:O	1:B:159:PRO:HD3	2.21	0.41
1:B:523:ILE:CD1	1:B:580:PHE:HA	2.40	0.41
1:A:92:PRO:HG2	1:A:93:TYR:H	1.86	0.41
1:A:154:HIS:CD2	1:A:192:LEU:HD22	2.44	0.41
1:B:65:LEU:O	1:B:73:ARG:HG2	2.21	0.41
1:B:390:ILE:CG2	1:B:394:ILE:HD11	2.51	0.41
1:A:144:SER:O	1:A:148:LEU:HG	2.21	0.41
1:A:161:LYS:HB3	1:A:163:PHE:CE1	2.56	0.41
1:A:335:PRO:HA	1:A:338:ARG:CD	2.50	0.41
1:A:353:GLU:HG2	1:A:353:GLU:O	2.19	0.41
1:A:579:ILE:HG23	1:A:603:LEU:HD11	2.01	0.41
1:B:125:TYR:CD1	1:B:125:TYR:C	2.99	0.41
1:B:522:TYR:OH	1:B:568:LEU:O	2.37	0.41
1:B:588:THR:O	1:B:589:ASN:HB2	2.20	0.41
1:B:671:ILE:O	1:B:675:ILE:HG13	2.21	0.41
1:A:46:ASN:OD1	1:A:46:ASN:O	2.39	0.41
1:A:61:SER:O	1:A:65:LEU:HD13	2.21	0.41
1:B:38:GLU:O	1:B:42:LEU:HG	2.21	0.41
1:B:348:ILE:O	1:B:351:THR:HB	2.21	0.41
1:A:125:TYR:CD1	1:A:125:TYR:C	2.99	0.40
1:A:316:VAL:HG12	1:A:323:PHE:CD1	2.55	0.40
1:A:554:LEU:HD12	1:A:555:ALA:N	2.36	0.40
1:B:27:GLU:O	1:B:31:ARG:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:PHE:HB3	1:B:506:PHE:CE2	2.56	0.40
1:A:12:ASN:HA	1:A:55:TYR:OH	2.21	0.40
1:A:647:VAL:HG12	1:B:654:LEU:HD13	2.04	0.40
1:B:416:GLU:CB	1:B:467:GLN:HE22	2.34	0.40
1:A:145:SER:HB3	1:A:182:PHE:CZ	2.56	0.40
1:A:244:HIS:CE1	1:A:248:ASN:ND2	2.90	0.40
1:A:344:SER:O	1:A:348:ILE:HG13	2.21	0.40
1:A:642:PRO:C	1:A:643:ILE:HD12	2.46	0.40
1:A:683:PHE:C	1:A:685:ASP:H	2.30	0.40
1:B:272:THR:HG23	1:B:273:VAL:N	2.36	0.40
1:B:551:LEU:HD23	1:B:551:LEU:O	2.21	0.40
1:A:385:VAL:CG2	1:A:386:PRO:HD2	2.51	0.40
1:A:385:VAL:HG23	1:A:386:PRO:HD2	2.04	0.40
1:B:422:MET:HE2	1:B:453:LEU:CD1	2.52	0.40
1:B:473:PHE:CE2	1:B:638:PHE:HB3	2.56	0.40
1:B:584:ASN:HA	1:B:587:VAL:CG1	2.50	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:SER:CB	1:B:556:SER:CB[7_555]	2.12	0.08

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	673/703 (96%)	601 (89%)	64 (10%)	8 (1%)	10	43
1	B	650/703 (92%)	582 (90%)	63 (10%)	5 (1%)	16	54
All	All	1323/1406 (94%)	1183 (89%)	127 (10%)	13 (1%)	12	48

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	536	SER
1	A	538	SER
1	A	679	ASN
1	B	682	LEU
1	A	655	ASN
1	A	460	ASN
1	A	660	SER
1	A	684	LYS
1	B	481	PRO
1	B	589	ASN
1	B	587	VAL
1	B	202	PRO
1	A	481	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	629/650 (97%)	628 (100%)	1 (0%)	87	86
1	B	611/650 (94%)	609 (100%)	2 (0%)	86	85
All	All	1240/1300 (95%)	1237 (100%)	3 (0%)	87	86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	412	LYS
1	B	120	HIS
1	B	333	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN

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Mol	Chain	Res	Type
1	A	36	HIS
1	A	154	HIS
1	A	195	ASN
1	A	201	ASN
1	A	244	HIS
1	A	248	ASN
1	A	252	ASN
1	A	305	GLN
1	A	347	GLN
1	A	361	GLN
1	A	393	ASN
1	A	428	ASN
1	A	439	ASN
1	A	455	ASN
1	A	509	ASN
1	A	575	ASN
1	A	598	ASN
1	A	655	ASN
1	A	679	ASN
1	B	36	HIS
1	B	117	ASN
1	B	120	HIS
1	B	123	GLN
1	B	154	HIS
1	B	195	ASN
1	B	203	ASN
1	B	248	ASN
1	B	305	GLN
1	B	393	ASN
1	B	411	HIS
1	B	460	ASN
1	B	467	GLN
1	B	589	ASN
1	B	649	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	677/703 (96%)	0.41	31 (4%) 37 37	217, 391, 564, 683	0
1	B	660/703 (93%)	0.29	16 (2%) 59 51	260, 428, 646, 847	0
All	All	1337/1406 (95%)	0.35	47 (3%) 47 43	217, 407, 606, 847	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	LEU	5.8
1	A	127	ILE	5.0
1	A	55	TYR	3.9
1	A	15	ILE	3.8
1	A	543	VAL	3.7
1	A	124	THR	3.6
1	A	530	ASN	3.4
1	A	590	ASP	3.4
1	B	519	ILE	3.3
1	A	550	THR	3.1
1	A	291	GLU	3.1
1	A	53	ASP	3.0
1	B	113	GLY	3.0
1	B	478	PRO	3.0
1	B	179	ILE	2.9
1	A	480	GLU	2.9
1	B	657	SER	2.8
1	B	350	ALA	2.8
1	A	286	HIS	2.8
1	A	259	VAL	2.8
1	B	353	GLU	2.8
1	A	577	GLU	2.8
1	B	153	PHE	2.7
1	A	531	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	128	THR	2.6
1	B	382	PHE	2.6
1	B	542	ILE	2.5
1	B	515	ILE	2.5
1	B	284	ILE	2.5
1	A	395	THR	2.5
1	A	289	SER	2.4
1	A	33	LYS	2.3
1	A	171	ILE	2.3
1	A	593	PHE	2.3
1	A	252	ASN	2.3
1	B	585	ALA	2.3
1	A	479	PHE	2.3
1	A	594	LEU	2.3
1	B	195	ASN	2.2
1	A	376	ARG	2.2
1	A	51	GLY	2.1
1	B	323	PHE	2.1
1	A	195	ASN	2.1
1	A	49	LEU	2.1
1	B	649	ASN	2.0
1	A	253	SER	2.0
1	A	542	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.