



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5GXB / pdb_00005gxb
Title : crystal structure of a LacY/Nanobody complex
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Deposited on : 2016-09-16
Resolution : 3.30 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

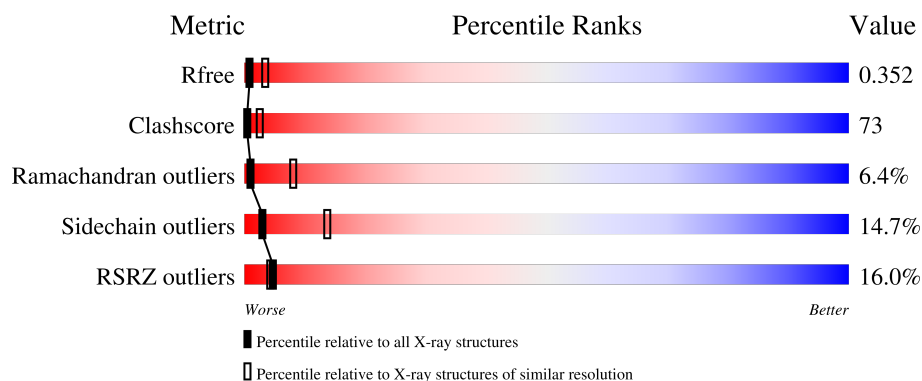
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	423	
2	B	140	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4121 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 Lactose permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			3086	2102	465	498	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	TRP	GLY	conflict	UNP P02920
A	262	TRP	GLY	conflict	UNP P02920
A	418	HIS	-	expression tag	UNP P02920
A	419	HIS	-	expression tag	UNP P02920
A	420	HIS	-	expression tag	UNP P02920
A	421	HIS	-	expression tag	UNP P02920
A	422	HIS	-	expression tag	UNP P02920
A	423	HIS	-	expression tag	UNP P02920

- Molecule 2 is a protein called nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			1035	649	183	198	5			

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	96.54Å 96.54Å 145.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.34 – 3.30 48.34 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.2 (48.34-3.30) 95.2 (48.34-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.33Å)	Xtriage
Refinement program	PHENIX (dev_2405: ???)	Depositor
R, R_{free}	0.340 , 0.346 0.345 , 0.352	Depositor DCC
R_{free} test set	513 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	93.7	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	4121	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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

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	0.76	8/3182 (0.3%)	1.12	30/4312 (0.7%)
2	B	0.91	2/1059 (0.2%)	1.08	3/1433 (0.2%)
All	All	0.80	10/4241 (0.2%)	1.11	33/5745 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	398	PHE	C-N	15.27	1.54	1.33
1	A	27	PHE	C-N	8.20	1.41	1.33
1	A	156	SER	C-N	6.86	1.43	1.33
2	B	73	ASP	CA-C	-6.48	1.47	1.53
1	A	96	GLY	C-N	6.15	1.41	1.34
1	A	88	ALA	C-N	5.71	1.40	1.34
1	A	30	PHE	C-N	5.63	1.41	1.33
2	B	102	PRO	N-CD	5.28	1.55	1.47
1	A	31	PRO	N-CD	5.17	1.54	1.47
1	A	97	PRO	N-CD	5.03	1.54	1.47

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ILE	CB-CA-C	19.70	136.76	111.94
1	A	156	SER	O-C-N	-14.42	103.64	122.39
1	A	170	PHE	CB-CA-C	-11.80	92.36	110.88
1	A	87	PHE	CB-CA-C	11.19	132.16	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	PRO	CB-CA-C	10.69	127.18	111.04
1	A	156	SER	CA-C-N	10.26	140.44	121.97
1	A	156	SER	C-N-CA	10.26	140.44	121.97
1	A	170	PHE	N-CA-C	9.71	121.47	111.07
1	A	97	PRO	N-CA-C	9.13	125.26	114.03
1	A	93	PHE	CB-CA-C	8.68	127.11	109.67
1	A	97	PRO	CB-CA-C	7.78	123.18	111.44
2	B	104	TYR	N-CA-C	7.50	121.10	110.23
1	A	245	ASN	N-CA-C	-6.99	104.23	112.89
1	A	365	MET	N-CA-C	-6.77	103.52	111.03
1	A	27	PHE	CA-C-N	-6.46	113.07	120.89
1	A	27	PHE	C-N-CA	-6.46	113.07	120.89
1	A	96	GLY	CA-C-N	-6.35	113.26	119.87
1	A	96	GLY	C-N-CA	-6.35	113.26	119.87
1	A	286	ILE	N-CA-C	-6.28	103.20	111.05
1	A	144	ARG	N-CA-C	-6.28	104.32	112.23
2	B	2	VAL	N-CA-C	-6.09	99.76	109.20
1	A	88	ALA	CA-C-N	-6.04	113.51	120.04
1	A	88	ALA	C-N-CA	-6.04	113.51	120.04
1	A	160	ILE	N-CA-C	5.84	115.91	110.42
2	B	10	ARG	N-CA-C	-5.78	98.49	110.80
1	A	364	PHE	CA-C-N	-5.71	112.87	120.63
1	A	364	PHE	C-N-CA	-5.71	112.87	120.63
1	A	89	PRO	CA-N-CD	-5.67	104.06	112.00
1	A	30	PHE	CA-C-N	-5.66	113.06	119.28
1	A	30	PHE	C-N-CA	-5.66	113.06	119.28
1	A	23	MET	N-CA-C	-5.24	105.75	111.82
1	A	326	VAL	CA-C-N	-5.13	113.35	119.05
1	A	326	VAL	C-N-CA	-5.13	113.35	119.05

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	SER	Mainchain
1	A	87	PHE	Peptide

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	3086	0	3120	397	1
2	B	1035	0	988	224	1
All	All	4121	0	4108	599	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 73.

All (599) 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:286:ILE:CD1	1:A:290:ASN:HB2	1.26	1.64
2:B:0:MET:CE	2:B:101:ARG:HD3	1.26	1.59
2:B:0:MET:HE1	2:B:101:ARG:CD	1.31	1.59
1:A:286:ILE:HD11	1:A:290:ASN:CB	1.36	1.55
1:A:247:PHE:HE1	1:A:251:PHE:CE1	1.37	1.41
2:B:22:CYS:SG	2:B:96:CYS:SG	1.42	1.40
1:A:317:ILE:O	1:A:320:THR:CG2	1.75	1.33
1:A:30:PHE:CE1	1:A:33:TRP:HZ3	1.48	1.32
1:A:249:SER:HB3	2:B:115:ARG:NH2	1.44	1.31
2:B:19:ARG:HD2	2:B:82:GLN:NE2	1.44	1.30
1:A:317:ILE:O	1:A:320:THR:HG22	1.19	1.29
1:A:30:PHE:CE1	1:A:33:TRP:CZ3	2.23	1.26
1:A:48:ILE:O	1:A:52:ILE:HD12	1.27	1.26
1:A:247:PHE:CE1	1:A:251:PHE:CE1	2.22	1.25
1:A:158:VAL:O	1:A:162:PHE:CB	1.85	1.24
1:A:286:ILE:HD12	1:A:286:ILE:O	1.35	1.23
2:B:59:TYR:HD2	2:B:110:TYR:CD1	1.58	1.22
2:B:87:LYS:O	2:B:127:VAL:HG11	1.34	1.22
1:A:158:VAL:O	1:A:162:PHE:HB2	1.04	1.20
1:A:282:ILE:O	1:A:286:ILE:HG22	1.37	1.19
2:B:87:LYS:O	2:B:127:VAL:CG1	1.90	1.19
2:B:32:TYR:CZ	2:B:99:ALA:HB1	1.78	1.18
1:A:239:PHE:CE1	1:A:382:TYR:CE1	2.34	1.16
2:B:30:THR:CG2	2:B:100:ALA:HB1	1.77	1.13
1:A:235:THR:HG23	1:A:385:LEU:HD22	1.26	1.13
1:A:282:ILE:O	1:A:286:ILE:CG2	1.97	1.12
1:A:48:ILE:HA	1:A:108:ILE:HD11	1.34	1.10
1:A:99:LEU:HB3	1:A:107:SER:OG	1.49	1.10
1:A:239:PHE:HE1	1:A:382:TYR:CE1	1.69	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ILE:CD1	1:A:290:ASN:CB	2.08	1.08
2:B:22:CYS:SG	2:B:96:CYS:CB	2.40	1.08
1:A:299:MET:HG3	1:A:325:GLU:HG3	1.34	1.08
1:A:89:PRO:O	1:A:93:PHE:HB2	1.54	1.08
1:A:247:PHE:CE1	1:A:251:PHE:HE1	1.65	1.08
1:A:235:THR:CG2	1:A:385:LEU:HD22	1.83	1.07
2:B:40:ALA:HB1	2:B:41:PRO:CD	1.84	1.07
2:B:0:MET:HE1	2:B:101:ARG:NE	1.69	1.05
1:A:48:ILE:O	1:A:52:ILE:CD1	2.04	1.05
1:A:48:ILE:HG22	1:A:52:ILE:HD11	1.37	1.05
1:A:114:LEU:O	1:A:116:PHE:N	1.90	1.05
1:A:312:ALA:HA	1:A:315:VAL:HG22	1.38	1.05
1:A:337:ILE:HG23	1:A:349:ILE:HD11	1.39	1.04
2:B:32:TYR:CZ	2:B:99:ALA:CB	2.40	1.03
2:B:52:ARG:HH11	2:B:52:ARG:HB3	1.22	1.02
2:B:59:TYR:CD2	2:B:110:TYR:CD1	2.45	1.02
1:A:32:ILE:HG21	1:A:162:PHE:CE1	1.93	1.02
1:A:247:PHE:HE1	1:A:251:PHE:CZ	1.76	1.02
1:A:299:MET:O	1:A:303:ILE:HG13	1.60	1.02
2:B:31:THR:HA	2:B:99:ALA:O	1.60	1.02
1:A:271:LEU:O	1:A:275:ILE:HG12	1.59	1.01
2:B:12:VAL:HG22	2:B:16:ASP:HB3	1.43	1.01
1:A:161:MET:HA	1:A:164:ILE:HD11	1.41	1.01
1:A:88:ALA:HB2	1:A:174:SER:HB2	1.40	1.00
2:B:30:THR:O	2:B:31:THR:C	2.02	1.00
1:A:33:TRP:CE3	1:A:34:LEU:HD12	1.97	0.99
1:A:99:LEU:HB2	1:A:104:LEU:HD23	1.45	0.99
2:B:82:GLN:OE1	2:B:84:ASN:ND2	1.96	0.99
1:A:35:HIS:ND1	1:A:42:LYS:HE3	1.78	0.99
1:A:88:ALA:HB2	1:A:174:SER:CB	1.92	0.99
1:A:304:ILE:HG12	1:A:386:GLY:HA3	1.43	0.99
1:A:286:ILE:HD12	1:A:286:ILE:C	1.88	0.98
1:A:29:PHE:CZ	1:A:170:PHE:HE1	1.81	0.98
1:A:312:ALA:HA	1:A:315:VAL:CG2	1.93	0.97
2:B:41:PRO:O	2:B:43:LYS:N	1.98	0.97
2:B:33:LEU:CD2	2:B:116:TYR:HE1	1.77	0.96
1:A:160:ILE:O	1:A:164:ILE:HD11	1.65	0.96
2:B:40:ALA:HB1	2:B:41:PRO:HD2	1.48	0.95
1:A:252:ALA:HA	2:B:110:TYR:CE2	2.00	0.95
2:B:1:GLN:N	2:B:118:TYR:OH	2.00	0.95
1:A:263:TYR:OH	1:A:267:MET:HE2	1.67	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:ARG:CD	2:B:82:GLN:NE2	2.28	0.95
2:B:76:LYS:O	2:B:78:THR:OG1	1.86	0.94
1:A:303:ILE:HG21	1:A:385:LEU:HB3	1.49	0.94
1:A:317:ILE:C	1:A:320:THR:HG22	1.91	0.94
1:A:317:ILE:O	1:A:320:THR:HG23	1.68	0.93
1:A:30:PHE:HE1	1:A:33:TRP:CZ3	1.75	0.93
1:A:268:GLY:O	1:A:323:MET:HG3	1.68	0.93
1:A:114:LEU:O	1:A:115:GLY:C	2.11	0.92
2:B:19:ARG:CD	2:B:82:GLN:HE21	1.82	0.92
1:A:29:PHE:HD2	1:A:158:VAL:HG13	1.33	0.91
1:A:234:CYS:O	1:A:238:VAL:HG13	1.69	0.91
2:B:30:THR:HG22	2:B:100:ALA:CB	1.99	0.91
2:B:1:GLN:HA	2:B:118:TYR:OH	1.68	0.91
2:B:12:VAL:HG11	2:B:86:LEU:CD1	2.00	0.91
1:A:376:ILE:HG12	1:A:380:GLY:HA3	1.50	0.91
2:B:89:GLU:OE1	2:B:89:GLU:N	2.04	0.91
1:A:224:PHE:CD1	1:A:399:THR:HB	2.05	0.91
1:A:106:GLY:O	1:A:109:VAL:HG22	1.70	0.90
1:A:30:PHE:CD1	1:A:33:TRP:CZ3	2.59	0.90
1:A:239:PHE:CD1	1:A:382:TYR:CE1	2.58	0.90
1:A:322:HIS:O	1:A:326:VAL:HG23	1.71	0.90
2:B:0:MET:HE3	2:B:101:ARG:HD3	1.51	0.90
1:A:235:THR:HG23	1:A:385:LEU:CD2	2.00	0.90
2:B:27:ARG:O	2:B:28:THR:OG1	1.89	0.90
1:A:239:PHE:HE1	1:A:382:TYR:CZ	1.90	0.89
1:A:373:TYR:HD2	2:B:102:PRO:HD3	1.35	0.89
2:B:0:MET:HG3	2:B:118:TYR:CE2	2.06	0.89
2:B:33:LEU:HD21	2:B:116:TYR:HE1	1.34	0.89
2:B:59:TYR:HD2	2:B:110:TYR:CE1	1.91	0.89
1:A:312:ALA:O	1:A:314:GLU:N	2.06	0.88
1:A:369:ALA:O	1:A:373:TYR:CD1	2.26	0.88
1:A:48:ILE:HA	1:A:108:ILE:CD1	2.03	0.88
2:B:64:VAL:HG11	2:B:68:PHE:CD2	2.09	0.88
1:A:161:MET:HA	1:A:164:ILE:CD1	2.03	0.87
1:A:312:ALA:O	1:A:315:VAL:N	2.06	0.87
1:A:272:ASN:HB2	1:A:323:MET:HB3	1.56	0.87
2:B:34:MET:SD	2:B:98:ALA:HB2	2.16	0.86
2:B:19:ARG:HD2	2:B:82:GLN:HE21	1.06	0.86
1:A:303:ILE:CG2	1:A:385:LEU:HB3	2.06	0.86
1:A:27:PHE:CD2	1:A:151:TRP:HH2	1.94	0.85
1:A:249:SER:CB	2:B:115:ARG:NH2	2.35	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:MET:O	1:A:113:TYR:OH	1.93	0.85
1:A:48:ILE:CG2	1:A:52:ILE:HD11	2.05	0.85
1:A:252:ALA:CA	2:B:110:TYR:CE2	2.58	0.85
2:B:30:THR:CG2	2:B:100:ALA:CB	2.55	0.85
1:A:167:GLN:NE2	1:A:171:TRP:NE1	2.24	0.84
2:B:12:VAL:HG11	2:B:86:LEU:HD13	1.56	0.84
1:A:46:TRP:HA	1:A:46:TRP:CE3	2.09	0.84
2:B:0:MET:CE	2:B:101:ARG:CD	2.14	0.84
2:B:74:ASN:O	2:B:76:LYS:N	2.11	0.84
1:A:33:TRP:CZ3	1:A:34:LEU:CD1	2.60	0.84
2:B:1:GLN:CA	2:B:118:TYR:OH	2.25	0.83
2:B:59:TYR:CE2	2:B:110:TYR:CG	2.67	0.83
1:A:252:ALA:N	2:B:110:TYR:CE2	2.47	0.82
2:B:88:LEU:HD23	2:B:88:LEU:O	1.79	0.82
1:A:86:MET:O	1:A:90:PHE:HB3	1.79	0.82
1:A:32:ILE:HG21	1:A:162:PHE:CZ	2.15	0.81
1:A:312:ALA:C	1:A:314:GLU:H	1.87	0.81
2:B:32:TYR:OH	2:B:99:ALA:HB1	1.80	0.81
2:B:30:THR:HG22	2:B:100:ALA:HB1	1.55	0.81
1:A:368:LEU:HD12	1:A:368:LEU:O	1.81	0.81
1:A:313:LEU:O	1:A:317:ILE:HD12	1.81	0.80
2:B:40:ALA:CB	2:B:41:PRO:CD	2.57	0.80
2:B:62:ASP:O	2:B:64:VAL:N	2.14	0.80
2:B:102:PRO:O	2:B:103:SER:HB2	1.79	0.80
1:A:27:PHE:CG	1:A:151:TRP:HH2	2.00	0.79
1:A:59:PHE:CZ	1:A:112:ILE:HD11	2.17	0.79
1:A:167:GLN:HE22	1:A:171:TRP:NE1	1.78	0.79
2:B:59:TYR:CD2	2:B:110:TYR:CG	2.70	0.79
1:A:161:MET:HA	1:A:164:ILE:CG1	2.13	0.78
2:B:64:VAL:CG1	2:B:68:PHE:CD2	2.66	0.78
1:A:304:ILE:CG1	1:A:386:GLY:HA3	2.13	0.78
2:B:38:ARG:NH2	2:B:46:GLU:OE1	2.16	0.78
1:A:286:ILE:HD13	1:A:290:ASN:CB	2.12	0.78
1:A:33:TRP:CZ3	1:A:34:LEU:HD11	2.19	0.77
1:A:249:SER:HB3	2:B:115:ARG:CZ	2.13	0.77
1:A:29:PHE:CE1	1:A:170:PHE:CE1	2.72	0.77
1:A:48:ILE:C	1:A:52:ILE:HD12	2.09	0.77
1:A:312:ALA:C	1:A:314:GLU:N	2.40	0.77
1:A:33:TRP:CZ3	1:A:34:LEU:HD12	2.18	0.77
2:B:33:LEU:HD21	2:B:116:TYR:CE1	2.20	0.77
1:A:29:PHE:CZ	1:A:170:PHE:CE1	2.69	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:O	1:A:108:ILE:HG22	1.85	0.77
1:A:239:PHE:C	1:A:241:GLN:H	1.92	0.76
2:B:32:TYR:CE1	2:B:99:ALA:CB	2.68	0.76
1:A:161:MET:CA	1:A:164:ILE:HD11	2.16	0.76
1:A:249:SER:HB3	2:B:115:ARG:HH22	1.48	0.76
1:A:46:TRP:HA	1:A:46:TRP:HE3	1.50	0.76
1:A:167:GLN:NE2	1:A:171:TRP:HE1	1.82	0.76
1:A:26:TYR:CD2	1:A:118:PHE:CD2	2.74	0.76
1:A:263:TYR:OH	1:A:267:MET:CE	2.33	0.76
2:B:115:ARG:HD2	2:B:115:ARG:O	1.86	0.75
2:B:0:MET:HE1	2:B:101:ARG:HD3	0.76	0.75
2:B:10:ARG:HG2	2:B:11:LEU:O	1.86	0.75
1:A:167:GLN:O	1:A:171:TRP:CD1	2.39	0.75
1:A:25:ALA:O	1:A:29:PHE:HB3	1.86	0.75
1:A:49:PHE:HA	1:A:52:ILE:CD1	2.17	0.74
2:B:12:VAL:CG2	2:B:16:ASP:HB3	2.17	0.74
1:A:167:GLN:O	1:A:171:TRP:HD1	1.68	0.74
2:B:33:LEU:HD23	2:B:33:LEU:O	1.87	0.74
2:B:52:ARG:HH11	2:B:52:ARG:CB	1.98	0.74
2:B:32:TYR:CE1	2:B:99:ALA:HB3	2.23	0.74
2:B:16:ASP:OD1	2:B:17:SER:N	2.20	0.74
1:A:372:MET:O	1:A:376:ILE:N	2.15	0.74
1:A:49:PHE:HA	1:A:52:ILE:HD13	1.68	0.74
2:B:16:ASP:CG	2:B:17:SER:H	1.96	0.74
1:A:247:PHE:CE1	1:A:251:PHE:CZ	2.63	0.73
2:B:59:TYR:CD2	2:B:110:TYR:CE1	2.72	0.73
1:A:210:LEU:O	1:A:214:LEU:HD13	1.88	0.73
1:A:33:TRP:HZ3	1:A:34:LEU:HD11	1.54	0.72
1:A:42:LYS:HD2	2:B:104:TYR:CE2	2.24	0.72
1:A:373:TYR:O	1:A:377:GLY:N	2.21	0.72
2:B:33:LEU:HD23	2:B:33:LEU:C	2.15	0.72
1:A:86:MET:O	1:A:90:PHE:CB	2.37	0.72
1:A:252:ALA:HA	2:B:110:TYR:CD2	2.23	0.72
2:B:87:LYS:O	2:B:127:VAL:CB	2.37	0.72
1:A:368:LEU:HD12	1:A:368:LEU:C	2.14	0.72
2:B:51:ILE:HG12	2:B:52:ARG:N	2.05	0.72
1:A:160:ILE:HD12	1:A:160:ILE:C	2.14	0.71
1:A:239:PHE:O	1:A:241:GLN:N	2.22	0.71
1:A:163:THR:C	1:A:164:ILE:HD13	2.16	0.71
1:A:112:ILE:HD13	1:A:112:ILE:O	1.89	0.71
1:A:90:PHE:HD2	1:A:91:PHE:CE1	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PHE:O	1:A:166:ASN:ND2	2.24	0.71
1:A:252:ALA:HA	2:B:110:TYR:CZ	2.25	0.70
2:B:0:MET:HG3	2:B:118:TYR:HE2	1.55	0.70
2:B:27:ARG:C	2:B:27:ARG:HD3	2.15	0.70
2:B:52:ARG:HB3	2:B:52:ARG:NH1	2.02	0.70
1:A:35:HIS:ND1	1:A:42:LYS:CE	2.55	0.70
1:A:160:ILE:HD12	1:A:161:MET:N	2.06	0.70
1:A:27:PHE:CD2	1:A:151:TRP:CH2	2.78	0.70
2:B:27:ARG:C	2:B:28:THR:HG1	1.97	0.70
1:A:27:PHE:CG	1:A:151:TRP:CH2	2.79	0.70
2:B:10:ARG:HG2	2:B:11:LEU:N	2.06	0.69
1:A:373:TYR:HA	1:A:377:GLY:O	1.92	0.69
1:A:167:GLN:NE2	1:A:171:TRP:CD1	2.59	0.69
2:B:58:THR:C	2:B:59:TYR:HD1	2.01	0.69
1:A:378:PHE:O	1:A:381:ALA:N	2.27	0.68
2:B:3:GLN:HA	2:B:3:GLN:NE2	2.07	0.68
2:B:30:THR:O	2:B:31:THR:O	2.11	0.68
2:B:40:ALA:HB1	2:B:41:PRO:HD3	1.71	0.68
1:A:225:LEU:HD11	1:A:354:PHE:CZ	2.29	0.68
1:A:365:MET:O	1:A:368:LEU:N	2.26	0.68
1:A:59:PHE:CE2	1:A:112:ILE:HD11	2.29	0.68
1:A:167:GLN:HE22	1:A:171:TRP:HE1	1.39	0.68
2:B:59:TYR:HE2	2:B:110:TYR:CG	2.10	0.68
1:A:168:PHE:O	1:A:172:LEU:N	2.20	0.67
1:A:32:ILE:HG21	1:A:162:PHE:HE1	1.57	0.67
1:A:48:ILE:C	1:A:52:ILE:CD1	2.65	0.67
2:B:19:ARG:HG3	2:B:19:ARG:HH11	1.58	0.67
2:B:33:LEU:CD2	2:B:116:TYR:CE1	2.69	0.67
2:B:44:GLU:OE2	2:B:44:GLU:N	2.28	0.67
1:A:42:LYS:CD	2:B:104:TYR:CE2	2.78	0.66
2:B:32:TYR:CZ	2:B:99:ALA:HB3	2.31	0.66
1:A:239:PHE:CD1	1:A:382:TYR:HE1	2.13	0.66
2:B:0:MET:HE2	2:B:101:ARG:HD3	1.65	0.66
1:A:29:PHE:CE1	1:A:170:PHE:HE1	2.12	0.66
1:A:48:ILE:HG22	1:A:52:ILE:CD1	2.20	0.66
2:B:0:MET:HE1	2:B:101:ARG:CZ	2.24	0.66
1:A:235:THR:O	1:A:238:VAL:HG22	1.95	0.66
1:A:286:ILE:CD1	1:A:290:ASN:HB3	2.22	0.66
2:B:73:ASP:OD1	2:B:75:ALA:HB3	1.95	0.66
1:A:294:LEU:HD23	1:A:328:PHE:CE2	2.31	0.66
1:A:114:LEU:C	1:A:116:PHE:N	2.52	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:ALA:CB	2:B:41:PRO:HD2	2.21	0.65
2:B:104:TYR:O	2:B:105:SER:HB2	1.95	0.65
2:B:19:ARG:HD2	2:B:82:GLN:HE22	1.57	0.65
2:B:3:GLN:C	2:B:4:LEU:HD23	2.22	0.65
2:B:64:VAL:CG1	2:B:68:PHE:CG	2.80	0.65
2:B:93:VAL:HG22	2:B:124:GLN:HE21	1.62	0.65
1:A:99:LEU:CB	1:A:107:SER:OG	2.38	0.64
1:A:239:PHE:CE1	1:A:382:TYR:CD1	2.85	0.64
2:B:32:TYR:CE2	2:B:99:ALA:HB1	2.32	0.64
1:A:30:PHE:HE1	1:A:33:TRP:CH2	2.15	0.64
2:B:67:ARG:NH1	2:B:90:ASP:OD2	2.30	0.64
2:B:30:THR:HG21	2:B:100:ALA:HB1	1.78	0.64
1:A:337:ILE:HG23	1:A:349:ILE:CD1	2.23	0.64
1:A:168:PHE:HA	1:A:171:TRP:HB2	1.79	0.64
1:A:272:ASN:CB	1:A:323:MET:HB3	2.26	0.63
1:A:378:PHE:O	1:A:379:GLN:C	2.39	0.63
1:A:29:PHE:HZ	1:A:170:PHE:HE1	1.39	0.63
1:A:238:VAL:O	1:A:241:GLN:HB2	1.98	0.63
1:A:259:ARG:O	1:A:262:TRP:HD1	1.81	0.63
1:A:408:LEU:H	1:A:408:LEU:HD23	1.63	0.63
2:B:110:TYR:HD1	2:B:110:TYR:O	1.82	0.63
1:A:26:TYR:CE2	1:A:118:PHE:CD2	2.87	0.62
2:B:108:TYR:O	2:B:115:ARG:NH1	2.32	0.62
1:A:239:PHE:CE1	1:A:382:TYR:CZ	2.77	0.62
1:A:32:ILE:CG2	1:A:162:PHE:CE1	2.76	0.62
1:A:299:MET:CG	1:A:325:GLU:HG3	2.22	0.62
2:B:130:HIS:HB3	2:B:131:HIS:HD2	1.64	0.62
2:B:12:VAL:CG1	2:B:86:LEU:HD13	2.27	0.62
1:A:156:SER:O	1:A:160:ILE:HG23	1.99	0.62
1:A:238:VAL:O	1:A:241:GLN:CG	2.48	0.62
1:A:286:ILE:CD1	1:A:286:ILE:C	2.56	0.62
1:A:38:ASN:O	1:A:40:ILE:N	2.33	0.61
2:B:88:LEU:HD12	2:B:129:SER:HA	1.82	0.61
1:A:303:ILE:HD12	1:A:389:ALA:CB	2.31	0.61
2:B:30:THR:HG22	2:B:100:ALA:HB2	1.83	0.61
1:A:99:LEU:HB3	1:A:107:SER:HG	1.63	0.61
1:A:259:ARG:O	1:A:262:TRP:CD1	2.54	0.61
2:B:4:LEU:HD23	2:B:4:LEU:N	2.16	0.61
1:A:313:LEU:O	1:A:313:LEU:HD12	2.01	0.61
2:B:34:MET:HG3	2:B:79:VAL:HG21	1.82	0.61
2:B:38:ARG:CZ	2:B:46:GLU:OE1	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:ARG:HH11	2:B:19:ARG:CG	2.14	0.60
1:A:369:ALA:O	1:A:373:TYR:HD1	1.82	0.60
1:A:59:PHE:HZ	1:A:112:ILE:HD11	1.63	0.60
2:B:123:THR:HG23	2:B:123:THR:O	2.00	0.60
1:A:106:GLY:O	1:A:109:VAL:CG2	2.45	0.60
1:A:30:PHE:CE1	1:A:34:LEU:HD11	2.37	0.60
1:A:48:ILE:HG12	1:A:108:ILE:HD13	1.83	0.59
2:B:38:ARG:NE	2:B:46:GLU:OE1	2.35	0.59
2:B:63:SER:C	2:B:64:VAL:HG23	2.26	0.59
1:A:112:ILE:O	1:A:113:TYR:C	2.45	0.59
2:B:16:ASP:CG	2:B:17:SER:N	2.60	0.59
1:A:373:TYR:CD2	1:A:378:PHE:HE1	2.21	0.59
2:B:12:VAL:HG23	2:B:16:ASP:OD2	2.03	0.59
2:B:59:TYR:CE2	2:B:110:TYR:CD2	2.90	0.59
2:B:75:ALA:O	2:B:76:LYS:HG2	2.02	0.59
1:A:373:TYR:O	1:A:377:GLY:CA	2.51	0.58
2:B:88:LEU:HD11	2:B:129:SER:HB3	1.84	0.58
2:B:65:LYS:C	2:B:67:ARG:H	2.11	0.58
2:B:47:PHE:HD2	2:B:61:ALA:HB2	1.68	0.58
1:A:286:ILE:HG13	1:A:287:GLY:O	2.03	0.58
2:B:28:THR:O	2:B:28:THR:HG22	2.02	0.58
1:A:40:ILE:HG22	1:A:44:ASP:HB2	1.86	0.58
1:A:158:VAL:HG22	1:A:169:VAL:HG11	1.86	0.58
1:A:224:PHE:CD2	1:A:399:THR:O	2.56	0.58
1:A:263:TYR:CZ	1:A:267:MET:HE2	2.38	0.58
1:A:406:LEU:H	1:A:406:LEU:HD23	1.69	0.57
1:A:238:VAL:HG23	1:A:239:PHE:N	2.20	0.57
2:B:29:PHE:CD1	2:B:29:PHE:N	2.73	0.57
1:A:239:PHE:HD1	1:A:382:TYR:HE1	1.52	0.57
2:B:110:TYR:CD1	2:B:110:TYR:O	2.58	0.57
1:A:275:ILE:CG2	1:A:327:PRO:HG2	2.34	0.57
1:A:91:PHE:CD1	1:A:91:PHE:N	2.73	0.57
1:A:365:MET:O	1:A:366:SER:C	2.47	0.57
1:A:391:GLY:O	1:A:395:ILE:HG13	2.04	0.57
2:B:91:THR:O	2:B:92:ALA:HB2	2.05	0.57
1:A:238:VAL:O	1:A:241:GLN:CB	2.53	0.56
1:A:312:ALA:CA	1:A:315:VAL:HG22	2.25	0.56
1:A:365:MET:O	1:A:367:VAL:N	2.37	0.56
2:B:2:VAL:O	2:B:3:GLN:NE2	2.38	0.56
2:B:59:TYR:CD1	2:B:59:TYR:N	2.72	0.56
1:A:112:ILE:HD13	1:A:112:ILE:C	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:TYR:O	1:A:377:GLY:HA2	2.05	0.56
2:B:30:THR:HG23	2:B:100:ALA:HB1	1.81	0.56
2:B:128:SER:HG	2:B:130:HIS:C	2.12	0.56
1:A:90:PHE:HD2	1:A:91:PHE:CD1	2.23	0.56
1:A:251:PHE:CD1	1:A:251:PHE:N	2.73	0.56
2:B:45:ARG:HD2	2:B:45:ARG:O	2.06	0.56
1:A:88:ALA:CB	1:A:174:SER:CB	2.77	0.56
2:B:44:GLU:HG2	2:B:45:ARG:O	2.05	0.56
2:B:62:ASP:HA	2:B:65:LYS:HE3	1.88	0.56
1:A:142:ARG:O	1:A:143:ALA:HB3	2.05	0.56
1:A:268:GLY:C	1:A:323:MET:HG3	2.30	0.56
1:A:34:LEU:HD23	1:A:48:ILE:HD12	1.87	0.55
1:A:142:ARG:HE	1:A:277:PHE:HE1	1.53	0.55
1:A:279:ALA:O	1:A:283:ILE:HG12	2.06	0.55
1:A:44:ASP:O	1:A:47:ILE:HG12	2.06	0.55
1:A:81:THR:O	1:A:85:VAL:HG23	2.07	0.55
1:A:143:ALA:HA	1:A:146:PHE:HD2	1.71	0.55
1:A:225:LEU:HD11	1:A:354:PHE:CE1	2.41	0.55
2:B:64:VAL:HG12	2:B:64:VAL:O	2.07	0.55
2:B:128:SER:OG	2:B:130:HIS:O	2.24	0.55
1:A:42:LYS:HD3	2:B:104:TYR:HE2	1.71	0.55
1:A:30:PHE:CD1	1:A:33:TRP:CE3	2.94	0.55
1:A:160:ILE:O	1:A:164:ILE:CD1	2.47	0.55
1:A:247:PHE:HD1	1:A:247:PHE:O	1.90	0.55
2:B:67:ARG:HD3	2:B:85:SER:O	2.06	0.55
1:A:236:TYR:CE1	1:A:299:MET:HG2	2.43	0.54
1:A:247:PHE:CD1	1:A:247:PHE:C	2.85	0.54
2:B:60:TYR:CE2	2:B:70:ILE:HG22	2.42	0.54
1:A:26:TYR:CD1	1:A:26:TYR:C	2.86	0.54
2:B:0:MET:HG2	2:B:1:GLN:H	1.73	0.54
1:A:251:PHE:C	2:B:110:TYR:CD2	2.86	0.54
2:B:88:LEU:HD23	2:B:88:LEU:C	2.33	0.54
1:A:247:PHE:CD1	1:A:251:PHE:CE1	2.93	0.54
1:A:251:PHE:HB3	1:A:256:GLN:NE2	2.23	0.54
1:A:247:PHE:HD1	1:A:247:PHE:C	2.16	0.54
2:B:65:LYS:O	2:B:67:ARG:N	2.40	0.54
1:A:164:ILE:HD13	1:A:164:ILE:N	2.22	0.53
2:B:28:THR:C	2:B:29:PHE:CG	2.85	0.53
2:B:130:HIS:HB3	2:B:131:HIS:CD2	2.43	0.53
2:B:37:PHE:CE2	2:B:113:ALA:HB2	2.44	0.53
2:B:112:GLU:O	2:B:115:ARG:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:PHE:HD2	1:A:256:GLN:HE22	1.54	0.53
1:A:251:PHE:CE2	1:A:260:VAL:HG11	2.43	0.53
2:B:87:LYS:O	2:B:127:VAL:HB	2.07	0.53
1:A:151:TRP:CD1	1:A:151:TRP:C	2.85	0.53
1:A:373:TYR:HD1	1:A:373:TYR:H	1.57	0.53
1:A:114:LEU:O	1:A:117:CYS:N	2.42	0.53
1:A:166:ASN:OD1	1:A:166:ASN:N	2.39	0.53
1:A:238:VAL:HA	1:A:241:GLN:HG3	1.91	0.53
1:A:242:GLN:HG3	1:A:373:TYR:CE2	2.44	0.53
1:A:251:PHE:HE2	1:A:260:VAL:HG11	1.74	0.53
1:A:303:ILE:CG2	1:A:385:LEU:CB	2.83	0.53
2:B:62:ASP:C	2:B:64:VAL:H	2.14	0.53
1:A:217:PHE:O	1:A:223:TRP:CZ2	2.61	0.53
1:A:241:GLN:CB	1:A:242:GLN:HE21	2.21	0.53
1:A:242:GLN:O	1:A:245:ASN:N	2.39	0.53
1:A:167:GLN:HE21	1:A:171:TRP:CD1	2.26	0.52
1:A:88:ALA:HB2	1:A:174:SER:HB3	1.88	0.52
2:B:34:MET:SD	2:B:98:ALA:CB	2.94	0.52
2:B:108:TYR:HD1	2:B:112:GLU:HG2	1.74	0.52
2:B:91:THR:HG23	2:B:126:THR:HA	1.92	0.52
2:B:110:TYR:CD1	2:B:110:TYR:C	2.88	0.52
1:A:42:LYS:HD3	2:B:104:TYR:CE2	2.44	0.52
1:A:49:PHE:HA	1:A:52:ILE:HD12	1.92	0.52
2:B:52:ARG:O	2:B:53:TRP:C	2.51	0.52
1:A:229:VAL:HG11	1:A:353:CYS:O	2.09	0.52
1:A:350:TYR:HD1	1:A:351:LEU:HD22	1.75	0.52
2:B:30:THR:HG22	2:B:31:THR:N	2.24	0.52
1:A:242:GLN:O	1:A:243:PHE:C	2.51	0.51
1:A:373:TYR:CD2	2:B:102:PRO:HD3	2.28	0.51
1:A:317:ILE:C	1:A:320:THR:CG2	2.66	0.51
1:A:373:TYR:HD1	1:A:373:TYR:N	2.09	0.51
1:A:238:VAL:CG2	1:A:239:PHE:N	2.73	0.51
1:A:38:ASN:C	1:A:40:ILE:H	2.18	0.51
2:B:19:ARG:CG	2:B:19:ARG:NH1	2.72	0.51
1:A:299:MET:HG3	1:A:325:GLU:CG	2.24	0.51
2:B:128:SER:CB	2:B:130:HIS:O	2.59	0.51
1:A:86:MET:HA	1:A:89:PRO:HD2	1.93	0.51
1:A:372:MET:HE1	1:A:384:VAL:HG11	1.92	0.51
1:A:34:LEU:HD21	1:A:48:ILE:HD13	1.93	0.51
1:A:34:LEU:CD2	1:A:48:ILE:HD12	2.40	0.51
1:A:113:TYR:O	1:A:116:PHE:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ALA:HA	1:A:146:PHE:CD2	2.46	0.51
1:A:26:TYR:O	1:A:30:PHE:HB2	2.11	0.50
1:A:35:HIS:CE1	1:A:42:LYS:HE3	2.45	0.50
1:A:239:PHE:HB2	1:A:385:LEU:CD1	2.42	0.50
2:B:89:GLU:CD	2:B:89:GLU:H	2.13	0.50
1:A:91:PHE:N	1:A:91:PHE:HD1	2.08	0.50
1:A:175:GLY:O	1:A:178:LEU:HG	2.11	0.50
1:A:38:ASN:HB3	1:A:40:ILE:HD11	1.93	0.50
1:A:122:ALA:N	1:A:123:PRO:HD2	2.25	0.50
1:A:88:ALA:H	1:A:89:PRO:CD	2.25	0.50
1:A:99:LEU:HD12	1:A:100:GLN:N	2.27	0.50
1:A:252:ALA:CA	2:B:110:TYR:CZ	2.93	0.50
1:A:32:ILE:CG2	1:A:162:PHE:CZ	2.90	0.50
1:A:32:ILE:CG2	1:A:162:PHE:HE1	2.18	0.50
2:B:29:PHE:HD1	2:B:30:THR:H	1.58	0.50
1:A:217:PHE:O	1:A:223:TRP:HZ2	1.95	0.50
1:A:38:ASN:ND2	1:A:100:GLN:CD	2.70	0.49
1:A:156:SER:HA	1:A:262:TRP:HZ3	1.76	0.49
1:A:252:ALA:O	2:B:110:TYR:N	2.45	0.49
1:A:29:PHE:CD2	1:A:158:VAL:HG13	2.26	0.49
1:A:90:PHE:O	1:A:94:ILE:HB	2.12	0.49
1:A:48:ILE:HG12	1:A:108:ILE:CD1	2.43	0.49
1:A:109:VAL:O	1:A:112:ILE:HG22	2.12	0.49
1:A:251:PHE:CG	1:A:257:GLY:HA2	2.48	0.49
1:A:24:GLY:HA3	1:A:154:CYS:SG	2.52	0.49
1:A:160:ILE:CD1	1:A:161:MET:N	2.76	0.49
1:A:161:MET:C	1:A:163:THR:H	2.21	0.49
1:A:130:GLU:HG3	1:A:334:PHE:CD1	2.48	0.49
1:A:29:PHE:HB2	1:A:158:VAL:HG11	1.94	0.49
2:B:74:ASN:O	2:B:77:ASN:N	2.46	0.48
2:B:39:GLN:C	2:B:92:ALA:HB1	2.37	0.48
2:B:113:ALA:C	2:B:115:ARG:H	2.20	0.48
1:A:251:PHE:CE2	1:A:260:VAL:HG21	2.48	0.48
2:B:45:ARG:HE	2:B:113:ALA:HB3	1.78	0.48
1:A:104:LEU:O	1:A:106:GLY:N	2.47	0.48
1:A:373:TYR:CD1	1:A:373:TYR:N	2.79	0.48
2:B:27:ARG:NE	2:B:28:THR:HA	2.28	0.48
1:A:161:MET:HA	1:A:164:ILE:HG12	1.93	0.48
1:A:49:PHE:N	1:A:49:PHE:CD1	2.82	0.48
1:A:103:ILE:HG23	1:A:103:ILE:O	2.14	0.48
1:A:251:PHE:N	1:A:251:PHE:HD1	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ILE:HD13	1:A:290:ASN:HB3	1.92	0.48
1:A:323:MET:O	1:A:327:PRO:HD3	2.14	0.48
2:B:63:SER:C	2:B:64:VAL:CG2	2.86	0.48
1:A:247:PHE:CD1	1:A:251:PHE:HE1	2.23	0.48
1:A:316:VAL:O	1:A:317:ILE:C	2.57	0.48
2:B:128:SER:HB3	2:B:130:HIS:O	2.14	0.48
1:A:373:TYR:CD2	1:A:378:PHE:CE1	3.02	0.48
1:A:33:TRP:CE3	1:A:34:LEU:CD1	2.78	0.47
1:A:343:VAL:C	1:A:345:PHE:H	2.21	0.47
1:A:49:PHE:CA	1:A:52:ILE:HD12	2.44	0.47
1:A:86:MET:C	1:A:89:PRO:HD2	2.39	0.47
1:A:236:TYR:CD1	1:A:299:MET:HG2	2.49	0.47
1:A:251:PHE:HB2	1:A:257:GLY:CA	2.43	0.47
1:A:41:SER:C	1:A:43:SER:H	2.22	0.47
1:A:251:PHE:HB2	1:A:257:GLY:HA2	1.96	0.47
1:A:317:ILE:CA	1:A:320:THR:HG22	2.42	0.47
1:A:337:ILE:O	1:A:341:PHE:HB2	2.14	0.47
2:B:22:CYS:SG	2:B:96:CYS:HB3	2.48	0.47
2:B:10:ARG:CG	2:B:11:LEU:N	2.75	0.47
1:A:38:ASN:C	1:A:40:ILE:N	2.73	0.47
1:A:86:MET:O	1:A:90:PHE:HB2	2.13	0.47
1:A:104:LEU:C	1:A:106:GLY:N	2.72	0.47
1:A:239:PHE:HD1	1:A:382:TYR:CE1	2.19	0.47
1:A:241:GLN:HB2	1:A:242:GLN:HE21	1.79	0.47
1:A:326:VAL:HG12	1:A:330:LEU:HD23	1.97	0.47
1:A:373:TYR:CE2	1:A:378:PHE:HE1	2.33	0.47
1:A:376:ILE:O	1:A:376:ILE:HG23	2.15	0.47
2:B:53:TRP:O	2:B:72:ARG:NE	2.47	0.47
2:B:124:GLN:HG3	2:B:125:VAL:N	2.28	0.47
2:B:19:ARG:CD	2:B:82:GLN:HE22	2.22	0.47
1:A:105:VAL:C	1:A:108:ILE:HG22	2.39	0.47
2:B:0:MET:HE3	2:B:0:MET:HB3	1.69	0.47
2:B:27:ARG:O	2:B:27:ARG:HD3	2.13	0.47
2:B:31:THR:HB	2:B:98:ALA:HB1	1.97	0.47
2:B:3:GLN:NE2	2:B:3:GLN:CA	2.73	0.46
1:A:41:SER:C	1:A:43:SER:N	2.72	0.46
1:A:49:PHE:CA	1:A:52:ILE:CD1	2.92	0.46
1:A:114:LEU:C	1:A:116:PHE:H	2.22	0.46
1:A:264:VAL:HG11	1:A:319:LYS:HB3	1.97	0.46
1:A:314:GLU:O	1:A:318:LEU:HG	2.15	0.46
1:A:320:THR:O	1:A:321:LEU:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ALA:N	1:A:280:PRO:HD2	2.31	0.46
2:B:101:ARG:N	2:B:117:ASP:OD2	2.34	0.46
2:B:64:VAL:HG11	2:B:68:PHE:CE2	2.49	0.46
1:A:34:LEU:HD21	1:A:48:ILE:CD1	2.46	0.46
2:B:93:VAL:HG22	2:B:124:GLN:NE2	2.30	0.46
2:B:0:MET:HG3	2:B:118:TYR:CZ	2.48	0.46
2:B:58:THR:C	2:B:59:TYR:CD1	2.89	0.46
2:B:108:TYR:CD1	2:B:112:GLU:HG2	2.51	0.46
2:B:10:ARG:NE	2:B:11:LEU:O	2.48	0.45
2:B:74:ASN:C	2:B:76:LYS:N	2.72	0.45
1:A:114:LEU:H	1:A:114:LEU:HG	1.55	0.45
1:A:243:PHE:O	1:A:246:PHE:N	2.48	0.45
2:B:23:ALA:HA	2:B:77:ASN:O	2.17	0.45
2:B:59:TYR:HE2	2:B:110:TYR:CD2	2.33	0.45
2:B:92:ALA:O	2:B:94:TYR:CD1	2.70	0.45
1:A:252:ALA:CA	2:B:110:TYR:CD2	2.95	0.45
1:A:311:SER:O	1:A:314:GLU:HB2	2.16	0.45
1:A:160:ILE:HD11	1:A:161:MET:HG3	1.97	0.45
2:B:102:PRO:O	2:B:103:SER:CB	2.51	0.45
2:B:115:ARG:HD2	2:B:115:ARG:C	2.39	0.45
1:A:24:GLY:O	1:A:28:PRO:HD2	2.16	0.45
1:A:49:PHE:N	1:A:49:PHE:HD1	2.14	0.45
1:A:286:ILE:HD11	1:A:290:ASN:CA	2.30	0.45
1:A:369:ALA:O	1:A:373:TYR:CE1	2.68	0.45
1:A:29:PHE:CD1	1:A:29:PHE:C	2.95	0.45
1:A:130:GLU:HG3	1:A:334:PHE:CG	2.52	0.45
2:B:67:ARG:C	2:B:68:PHE:HD1	2.25	0.45
1:A:238:VAL:O	1:A:241:GLN:HG3	2.15	0.45
1:A:294:LEU:HD23	1:A:328:PHE:CD2	2.51	0.45
2:B:1:GLN:HA	2:B:118:TYR:CZ	2.51	0.44
2:B:28:THR:O	2:B:29:PHE:CG	2.70	0.44
2:B:65:LYS:C	2:B:67:ARG:N	2.75	0.44
1:A:161:MET:C	1:A:163:THR:N	2.73	0.44
2:B:2:VAL:HG12	2:B:3:GLN:N	2.32	0.44
1:A:34:LEU:CD2	1:A:48:ILE:CD1	2.95	0.44
1:A:312:ALA:O	1:A:313:LEU:C	2.60	0.44
2:B:51:ILE:HD11	2:B:56:GLY:HA2	2.00	0.44
1:A:321:LEU:O	1:A:324:PHE:N	2.39	0.44
1:A:55:PHE:O	1:A:58:LEU:HG	2.18	0.44
1:A:109:VAL:C	1:A:111:GLY:N	2.76	0.44
1:A:248:THR:OG1	2:B:107:ASP:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ILE:HD11	2:B:72:ARG:HD3	1.99	0.43
1:A:37:ILE:HG22	1:A:37:ILE:O	2.17	0.43
1:A:134:ARG:NH1	1:A:343:VAL:HG11	2.33	0.43
2:B:32:TYR:CE2	2:B:99:ALA:CB	2.96	0.43
2:B:128:SER:OG	2:B:130:HIS:N	2.43	0.43
1:A:178:LEU:O	1:A:182:VAL:HG23	2.18	0.43
2:B:0:MET:HG2	2:B:118:TYR:OH	2.18	0.43
2:B:27:ARG:C	2:B:27:ARG:CD	2.85	0.43
1:A:276:MET:HA	1:A:279:ALA:HB2	1.99	0.43
1:A:326:VAL:N	1:A:327:PRO:CD	2.82	0.43
1:A:251:PHE:CB	1:A:257:GLY:HA2	2.49	0.43
2:B:41:PRO:C	2:B:43:LYS:N	2.72	0.43
1:A:112:ILE:O	1:A:113:TYR:O	2.37	0.43
1:A:216:LEU:HD11	1:A:345:PHE:CG	2.54	0.43
2:B:3:GLN:CA	2:B:3:GLN:HE21	2.31	0.43
1:A:11:MET:HA	1:A:11:MET:HE2	2.01	0.43
1:A:230:ILE:O	1:A:234:CYS:HB3	2.18	0.43
1:A:241:GLN:HB3	1:A:242:GLN:NE2	2.34	0.43
1:A:321:LEU:O	1:A:322:HIS:C	2.60	0.43
2:B:88:LEU:CD1	2:B:129:SER:HB3	2.47	0.42
1:A:40:ILE:H	1:A:40:ILE:HG12	1.52	0.42
1:A:376:ILE:HG12	1:A:380:GLY:CA	2.36	0.42
2:B:1:GLN:HA	2:B:118:TYR:HH	1.78	0.42
2:B:32:TYR:CD1	2:B:33:LEU:HB3	2.54	0.42
1:A:161:MET:CA	1:A:164:ILE:HG12	2.50	0.42
1:A:328:PHE:O	1:A:332:GLY:N	2.45	0.42
1:A:151:TRP:CD1	1:A:151:TRP:O	2.72	0.42
1:A:264:VAL:HG22	1:A:316:VAL:HG13	2.00	0.42
1:A:93:PHE:C	1:A:94:ILE:HG12	2.45	0.42
1:A:109:VAL:HG23	1:A:110:GLY:N	2.33	0.42
2:B:62:ASP:C	2:B:64:VAL:N	2.74	0.42
2:B:113:ALA:C	2:B:115:ARG:N	2.78	0.42
1:A:162:PHE:C	1:A:166:ASN:OD1	2.62	0.42
1:A:16:PHE:CZ	1:A:129:ILE:HD12	2.55	0.42
1:A:38:ASN:HD22	1:A:100:GLN:CD	2.28	0.42
1:A:218:ARG:N	1:A:218:ARG:HD3	2.34	0.42
2:B:59:TYR:HE2	2:B:110:TYR:CB	2.33	0.42
2:B:91:THR:HA	2:B:125:VAL:O	2.19	0.42
1:A:365:MET:C	1:A:367:VAL:N	2.75	0.42
1:A:15:PHE:CE2	1:A:180:LEU:HG	2.55	0.42
1:A:94:ILE:O	1:A:98:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:HD23	1:A:385:LEU:HA	1.81	0.42
2:B:12:VAL:CG2	2:B:16:ASP:CB	2.95	0.42
2:B:62:ASP:HA	2:B:65:LYS:HG3	2.02	0.42
1:A:30:PHE:CZ	1:A:34:LEU:HD11	2.55	0.41
1:A:38:ASN:ND2	1:A:100:GLN:OE1	2.53	0.41
1:A:162:PHE:O	1:A:162:PHE:CG	2.72	0.41
1:A:255:GLU:CD	1:A:255:GLU:C	2.88	0.41
1:A:266:THR:O	1:A:270:LEU:HD23	2.20	0.41
1:A:235:THR:HG21	1:A:385:LEU:HD22	1.88	0.41
1:A:251:PHE:C	2:B:110:TYR:CE2	2.98	0.41
1:A:59:PHE:CE2	1:A:112:ILE:CD1	3.02	0.41
1:A:84:LEU:O	1:A:87:PHE:HB2	2.21	0.41
2:B:28:THR:C	2:B:29:PHE:CD1	2.98	0.41
1:A:48:ILE:O	1:A:52:ILE:HD11	2.12	0.41
1:A:153:LEU:O	1:A:157:ILE:HG12	2.20	0.41
1:A:170:PHE:HD1	1:A:170:PHE:H	1.67	0.41
1:A:90:PHE:CD2	1:A:91:PHE:CE1	2.97	0.41
1:A:104:LEU:O	1:A:105:VAL:C	2.63	0.41
1:A:239:PHE:C	1:A:241:GLN:N	2.60	0.41
1:A:24:GLY:O	1:A:28:PRO:CD	2.69	0.41
1:A:162:PHE:O	1:A:166:ASN:CG	2.64	0.41
1:A:217:PHE:C	1:A:218:ARG:HD3	2.44	0.41
1:A:278:PHE:C	1:A:280:PRO:HD2	2.46	0.41
1:A:66:LEU:HD23	1:A:66:LEU:HA	1.88	0.41
2:B:60:TYR:HE2	2:B:70:ILE:HG22	1.86	0.41
1:A:253:THR:O	1:A:254:GLY:C	2.63	0.41
1:A:283:ILE:HD12	1:A:291:ALA:HB1	2.03	0.41
2:B:60:TYR:CD1	2:B:60:TYR:N	2.90	0.41
1:A:325:GLU:O	1:A:325:GLU:HG2	2.21	0.40
1:A:68:ASP:OD2	1:A:347:ALA:HB3	2.22	0.40
1:A:252:ALA:N	2:B:110:TYR:CD2	2.89	0.40
1:A:38:ASN:HB3	1:A:40:ILE:CD1	2.51	0.40
1:A:87:PHE:HE1	1:A:118:PHE:HE2	1.68	0.40
1:A:229:VAL:CG1	1:A:358:LYS:HB2	2.51	0.40
1:A:312:ALA:O	1:A:314:GLU:C	2.63	0.40
1:A:378:PHE:O	1:A:380:GLY:N	2.54	0.40
1:A:236:TYR:OH	1:A:302:ARG:NH1	2.55	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:A:39:HIS:O	2:B:130:HIS:NE2[7_556]	1.83	0.37

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	383/423 (90%)	339 (88%)	34 (9%)	10 (3%)	4	23
2	B	130/140 (93%)	89 (68%)	18 (14%)	23 (18%)	0	0
All	All	513/563 (91%)	428 (83%)	52 (10%)	33 (6%)	1	8

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	240	ASP
1	A	252	ALA
1	A	313	LEU
2	B	27	ARG
2	B	28	THR
2	B	30	THR
2	B	40	ALA
2	B	41	PRO
2	B	42	GLY
2	B	63	SER
2	B	75	ALA
2	B	103	SER
2	B	105	SER
2	B	107	ASP
1	A	115	GLY
2	B	1	GLN
2	B	29	PHE
2	B	53	TRP
2	B	100	ALA

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Mol	Chain	Res	Type
1	A	114	LEU
2	B	31	THR
1	A	113	TYR
1	A	165	ASN
2	B	54	SER
2	B	64	VAL
2	B	102	PRO
1	A	105	VAL
2	B	62	ASP
2	B	74	ASN
2	B	92	ALA
1	A	164	ILE
2	B	66	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	325/354 (92%)	293 (90%)	32 (10%)	7	28
2	B	105/112 (94%)	74 (70%)	31 (30%)	0	2
All	All	430/466 (92%)	367 (85%)	63 (15%)	3	14

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	MET
1	A	26	TYR
1	A	33	TRP
1	A	36	ASP
1	A	38	ASN
1	A	40	ILE
1	A	46	TRP
1	A	58	LEU
1	A	75	TYR
1	A	92	ILE

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Mol	Chain	Res	Type
1	A	99	LEU
1	A	112	ILE
1	A	160	ILE
1	A	164	ILE
1	A	166	ASN
1	A	167	GLN
1	A	243	PHE
1	A	247	PHE
1	A	251	PHE
1	A	255	GLU
1	A	259	ARG
1	A	286	ILE
1	A	298	ILE
1	A	311	SER
1	A	320	THR
1	A	344	ARG
1	A	365	MET
1	A	368	LEU
1	A	372	MET
1	A	373	TYR
1	A	379	GLN
1	A	408	LEU
2	B	0	MET
2	B	3	GLN
2	B	4	LEU
2	B	7	SER
2	B	10	ARG
2	B	13	GLN
2	B	19	ARG
2	B	25	SER
2	B	29	PHE
2	B	33	LEU
2	B	38	ARG
2	B	43	LYS
2	B	44	GLU
2	B	51	ILE
2	B	52	ARG
2	B	54	SER
2	B	59	TYR
2	B	60	TYR
2	B	62	ASP
2	B	63	SER

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Mol	Chain	Res	Type
2	B	78	THR
2	B	87	LYS
2	B	89	GLU
2	B	101	ARG
2	B	103	SER
2	B	105	SER
2	B	111	THR
2	B	112	GLU
2	B	114	LEU
2	B	124	GLN
2	B	129	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	39	HIS
1	A	167	GLN
1	A	242	GLN
2	B	39	GLN
2	B	82	GLN
2	B	84	ASN
2	B	124	GLN
2	B	131	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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(Å ²)	Q<0.9
1	A	387/423 (91%)	1.17	60 (15%) 5 4	55, 69, 91, 108	1 (0%)
2	B	132/140 (94%)	1.20	23 (17%) 4 4	69, 81, 99, 107	0
All	All	519/563 (92%)	1.18	83 (15%) 5 4	55, 72, 94, 108	1 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	342	GLU	6.9
1	A	341	PHE	5.0
1	A	340	GLN	4.4
2	B	105	SER	4.2
2	B	114	LEU	4.0
1	A	339	SER	3.7
2	B	106	GLY	3.5
1	A	101	TYR	3.4
1	A	230	ILE	3.3
1	A	216	LEU	3.3
1	A	408	LEU	3.1
2	B	119	TRP	3.1
1	A	28	PRO	3.1
1	A	297	THR	3.1
2	B	127	VAL	3.1
2	B	79	VAL	2.9
1	A	336	TYR	2.9
1	A	344	ARG	2.9
1	A	345	PHE	2.9
1	A	399	THR	2.8
1	A	179	ILE	2.7
1	A	208	PHE	2.7
2	B	56	GLY	2.7
1	A	8	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	77	LEU	2.7
1	A	221	LYS	2.6
2	B	131	HIS	2.6
1	A	34	LEU	2.6
1	A	81	THR	2.6
1	A	256	GLN	2.5
1	A	70	LEU	2.5
1	A	316	VAL	2.5
1	A	189	THR	2.5
1	A	35	HIS	2.5
2	B	108	TYR	2.5
1	A	219	GLN	2.5
1	A	265	THR	2.5
1	A	97	PRO	2.5
1	A	373	TYR	2.5
1	A	115	GLY	2.5
2	B	66	GLY	2.5
1	A	313	LEU	2.4
1	A	27	PHE	2.4
1	A	243	PHE	2.4
1	A	85	VAL	2.4
1	A	312	ALA	2.4
1	A	217	PHE	2.4
2	B	113	ALA	2.4
1	A	161	MET	2.4
1	A	209	SER	2.4
1	A	50	ALA	2.3
1	A	349	ILE	2.3
2	B	26	GLY	2.3
2	B	22	CYS	2.3
2	B	123	THR	2.3
1	A	62	LEU	2.3
2	B	122	GLY	2.2
1	A	360	LEU	2.2
1	A	173	GLY	2.2
2	B	85	SER	2.2
1	A	330	LEU	2.2
1	A	102	ASN	2.2
2	B	40	ALA	2.2
2	B	61	ALA	2.2
1	A	154	CYS	2.2
2	B	2	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	248	THR	2.1
1	A	218	ARG	2.1
2	B	39	GLN	2.1
2	B	41	PRO	2.1
1	A	162	PHE	2.1
1	A	33	TRP	2.1
1	A	362	MET	2.1
1	A	46	TRP	2.1
2	B	118	TYR	2.1
2	B	121	GLN	2.1
1	A	186	PHE	2.1
1	A	269	GLU	2.1
1	A	43	SER	2.1
1	A	108	ILE	2.1
1	A	321	LEU	2.1
1	A	377	GLY	2.0
1	A	244	ALA	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.