



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:11 AM UTC

PDB ID : 1TQQ / pdb_00001tqq
Title : Structure of TolC in complex with hexamminecobalt
Authors : Higgins, M.K.; Eswaran, J.; Edwards, P.C.; Schertler, G.F.; Hughes, C.; Koronakis, V.
Deposited on : 2004-06-18
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

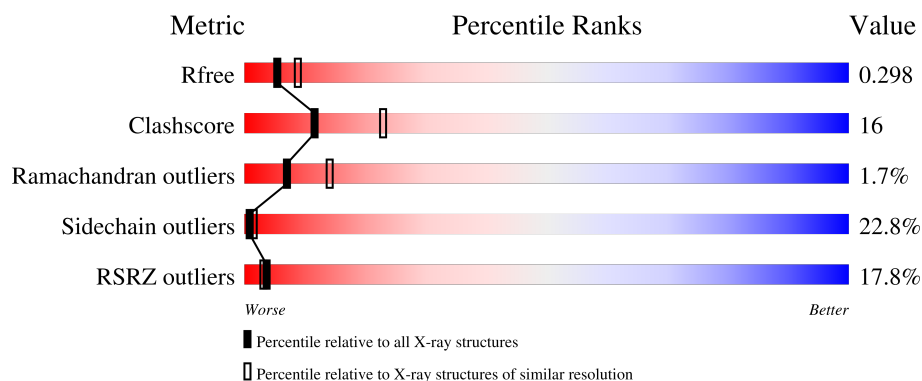
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	471	15% 55% 28% 7% 9%
1	B	471	17% 57% 24% 8% 9%
1	C	471	17% 58% 24% 8% 9%

2 Entry composition [i](#)

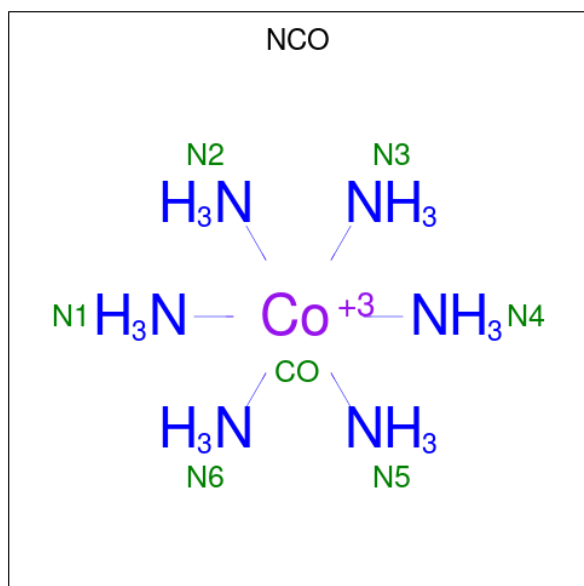
There are 3 unique types of molecules in this entry. The entry contains 10227 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Outer membrane protein tolC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3305	2038	586	676	5			
1	B	428	Total	C	N	O	S	0	0	0
			3305	2038	586	676	5			
1	C	428	Total	C	N	O	S	0	0	0
			3305	2038	586	676	5			

- Molecule 2 is COBALT HEXAMMINE(III) (CCD ID: NCO) (formula: $\text{CoH}_{18}\text{N}_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	Co	N	0	0
			7	1	6		

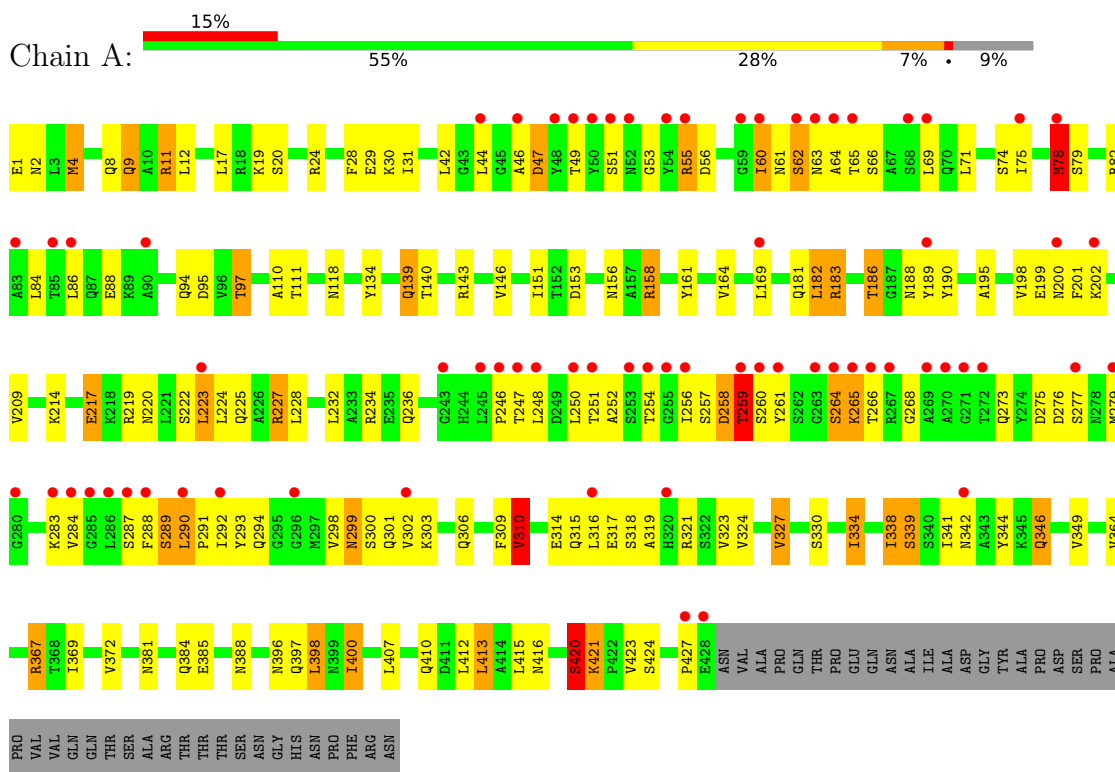
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	97	Total 97	O 97	0	0
3	B	101	Total 101	O 101	0	0
3	C	107	Total 107	O 107	0	0

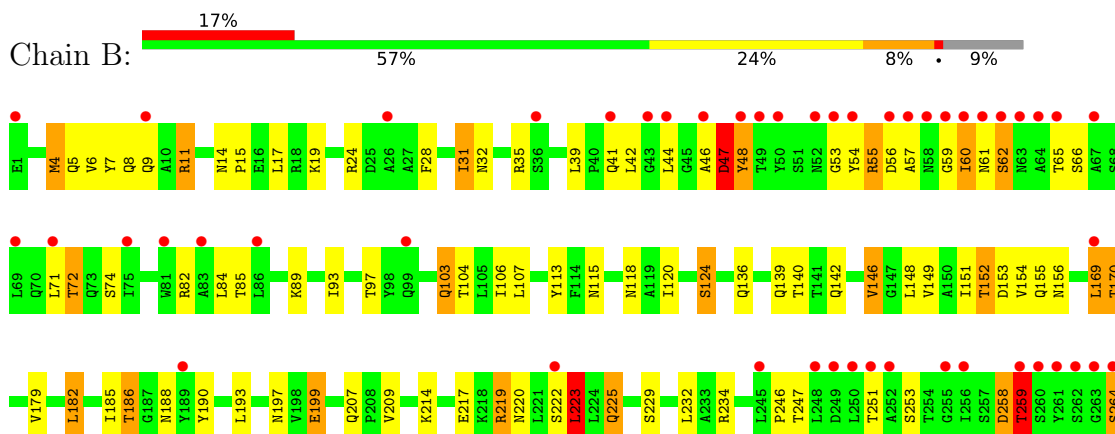
3 Residue-property plots

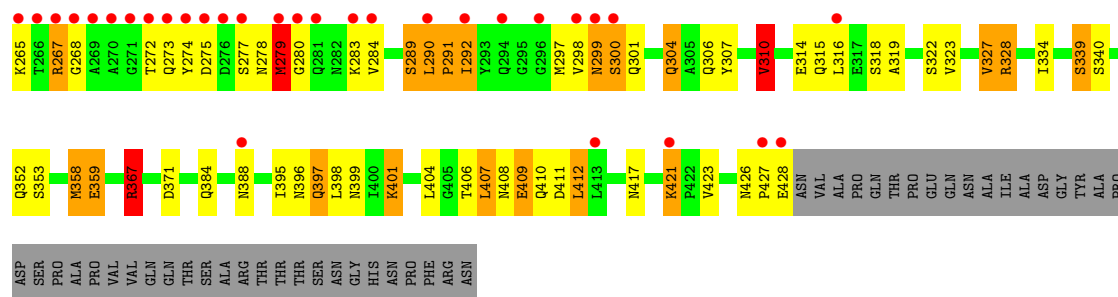
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

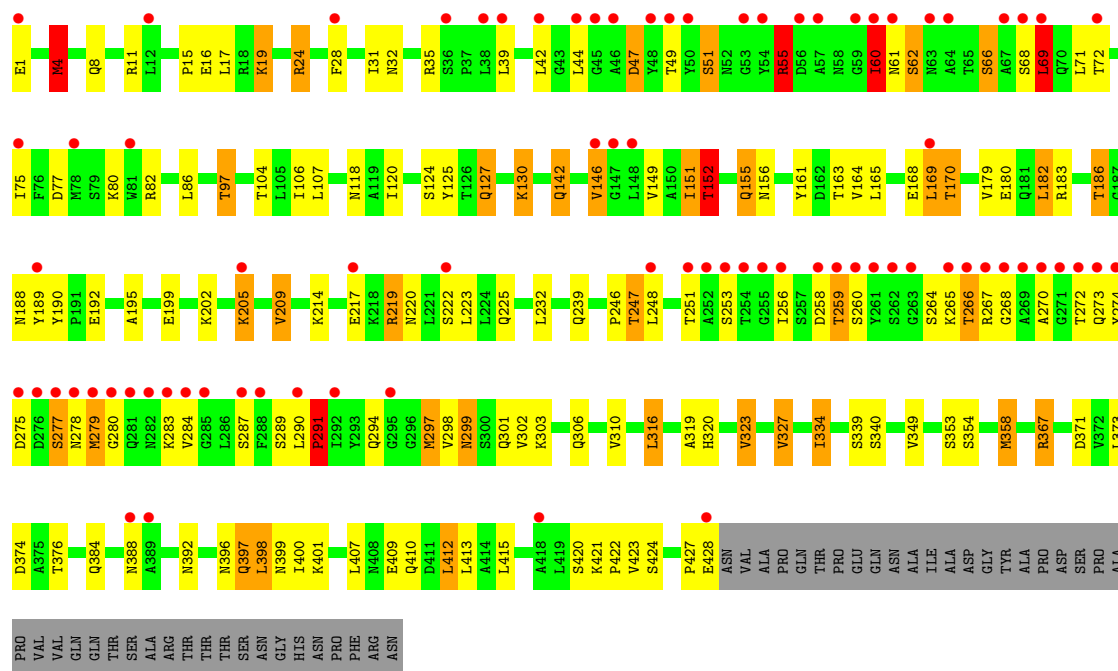


• Molecule 1: Outer membrane protein tolC





• Molecule 1: Outer membrane protein tolC



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	265.28Å 265.28Å 96.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.43 – 2.75 30.43 – 2.75	Depositor EDS
% Data completeness (in resolution range)	95.6 (30.43-2.75) 95.6 (30.43-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.264 , 0.305 0.253 , 0.298	Depositor DCC
R_{free} test set	3174 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10227	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.07	8/3346 (0.2%)	1.28	7/4545 (0.2%)
1	B	1.11	4/3346 (0.1%)	1.29	7/4545 (0.2%)
1	C	1.11	11/3346 (0.3%)	1.28	7/4545 (0.2%)
All	All	1.10	23/10038 (0.2%)	1.28	21/13635 (0.2%)

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
1	B	0	2
1	C	0	2
All	All	0	6

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	MET	SD-CE	9.48	2.03	1.79
1	C	358	MET	SD-CE	-8.59	1.58	1.79
1	A	364	VAL	CA-CB	8.14	1.63	1.54
1	C	75	ILE	CA-CB	7.91	1.63	1.55
1	C	151	ILE	CA-CB	7.29	1.63	1.54
1	B	310	VAL	CA-CB	7.16	1.63	1.54
1	C	152	THR	CA-CB	6.70	1.63	1.53
1	C	272	THR	CA-CB	6.46	1.64	1.53
1	A	338	ILE	CA-CB	6.33	1.61	1.54
1	A	310	VAL	CA-CB	5.90	1.61	1.54
1	C	60	ILE	CA-CB	5.78	1.60	1.54
1	C	284	VAL	CA-CB	5.76	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	349	VAL	CA-CB	5.65	1.60	1.54
1	B	358	MET	SD-CE	-5.59	1.65	1.79
1	A	75	ILE	CA-CB	5.57	1.61	1.55
1	B	279	MET	SD-CE	5.26	1.92	1.79
1	A	341	ILE	CA-CB	5.24	1.60	1.54
1	C	146	VAL	CA-C	5.22	1.59	1.52
1	A	372	VAL	CA-CB	5.20	1.60	1.54
1	C	4	MET	SD-CE	5.16	1.92	1.79
1	A	324	VAL	CA-CB	5.13	1.60	1.54
1	B	149	VAL	CA-CB	5.08	1.63	1.54
1	C	367	ARG	CA-C	5.08	1.58	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	264	SER	N-CA-C	7.80	119.69	111.03
1	C	264	SER	N-CA-C	7.74	121.21	111.69
1	A	264	SER	N-CA-C	6.83	119.73	111.40
1	A	209	VAL	N-CA-C	6.60	117.36	110.62
1	A	47	ASP	N-CA-C	6.15	118.81	109.95
1	C	209	VAL	N-CA-C	6.04	118.61	111.05
1	B	209	VAL	N-CA-C	5.73	116.46	110.62
1	B	47	ASP	N-CA-C	5.72	118.92	110.46
1	C	152	THR	CB-CA-C	5.71	120.26	110.79
1	A	338	ILE	N-CA-C	-5.69	104.96	110.42
1	C	47	ASP	N-CA-C	5.65	118.83	110.46
1	C	69	LEU	CA-CB-CG	5.48	135.48	116.30
1	B	408	ASN	N-CA-C	5.38	115.39	108.34
1	A	140	THR	OG1-CB-CG2	-5.37	98.57	109.30
1	B	291	PRO	N-CA-C	5.36	122.47	113.78
1	C	291	PRO	N-CA-C	5.23	123.24	112.47
1	B	367	ARG	CG-CD-NE	-5.23	100.50	112.00
1	A	201	PHE	N-CA-C	5.22	117.27	109.59
1	C	146	VAL	CB-CA-C	5.13	119.70	111.29
1	B	223	LEU	CA-CB-CG	5.05	133.99	116.30
1	A	293	TYR	N-CA-C	5.02	116.21	107.93

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	427	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	62	SER	Peptide
1	B	427	PRO	Peptide
1	B	62	SER	Peptide
1	C	427	PRO	Peptide
1	C	62	SER	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	3305	0	3256	122	0
1	B	3305	0	3256	123	3
1	C	3305	0	3256	111	0
2	C	7	0	0	1	0
3	A	97	0	0	31	2
3	B	101	0	0	22	4
3	C	107	0	0	35	2
All	All	10227	0	9768	314	6

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 16.

All (314) 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:78:MET:SD	1:A:78:MET:CE	2.03	1.46
1:B:423:VAL:HB	3:B:479:HOH:O	1.38	1.22
1:A:156:ASN:ND2	1:B:367:ARG:NH1	1.90	1.18
1:A:156:ASN:ND2	1:B:367:ARG:HH11	1.42	1.12
1:A:323:VAL:O	1:A:327:VAL:HG12	1.52	1.09
1:A:384:GLN:HB3	3:A:532:HOH:O	1.56	1.06
1:B:352:GLN:HB3	3:B:537:HOH:O	1.56	1.03
1:A:217:GLU:HG3	3:A:530:HOH:O	1.56	1.03
1:A:186:THR:HG21	1:A:190:TYR:HE1	1.26	1.01
1:A:367:ARG:NH1	1:C:156:ASN:ND2	2.09	1.00
1:C:247:THR:HB	3:C:559:HOH:O	1.61	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ARG:HH11	1:C:156:ASN:ND2	1.63	0.97
1:A:11:ARG:HD3	3:A:523:HOH:O	1.64	0.97
1:A:146:VAL:O	1:A:146:VAL:HG22	1.62	0.96
1:B:156:ASN:HD21	1:C:358:MET:HE1	1.28	0.96
1:A:156:ASN:HD21	1:B:367:ARG:NH1	1.58	0.95
1:B:186:THR:HG21	1:B:190:TYR:HE1	1.29	0.93
1:A:367:ARG:HH11	1:C:156:ASN:HD21	1.14	0.92
1:A:156:ASN:HD21	1:B:367:ARG:HH11	0.91	0.91
1:C:219:ARG:HG3	1:C:219:ARG:HH11	1.34	0.91
1:B:156:ASN:ND2	1:C:367:ARG:NH1	2.21	0.89
1:A:60:ILE:HD11	1:A:261:TYR:HD2	1.37	0.88
1:A:181:GLN:HG2	3:A:493:HOH:O	1.73	0.88
1:C:60:ILE:C	1:C:61:ASN:HD22	1.82	0.87
1:B:169:LEU:HG	1:C:339:SER:HB3	1.55	0.87
1:A:156:ASN:HD22	1:B:367:ARG:NH1	1.73	0.85
1:B:156:ASN:OD1	1:C:358:MET:HE3	1.75	0.85
1:B:186:THR:HG21	1:B:190:TYR:CE1	2.11	0.85
1:A:60:ILE:HD11	1:A:261:TYR:CD2	2.10	0.85
1:A:298:VAL:O	1:A:299:ASN:HB2	1.73	0.85
1:B:274:TYR:HE2	3:B:543:HOH:O	1.60	0.84
1:C:298:VAL:O	1:C:299:ASN:HB2	1.78	0.84
1:A:186:THR:HG22	1:A:188:ASN:H	1.40	0.84
1:B:59:GLY:HA2	3:B:539:HOH:O	1.77	0.83
1:B:298:VAL:O	1:B:299:ASN:HB2	1.77	0.83
1:A:186:THR:HG21	1:A:190:TYR:CE1	2.14	0.82
1:A:139:GLN:O	1:A:143:ARG:HG3	1.80	0.81
1:A:146:VAL:O	1:A:146:VAL:CG2	2.28	0.80
1:C:397:GLN:HE21	1:C:397:GLN:HA	1.43	0.80
1:A:97:THR:HG22	1:A:225:GLN:NE2	1.97	0.79
1:A:156:ASN:HD21	1:B:358:MET:HE1	1.48	0.79
1:C:69:LEU:HD22	3:C:575:HOH:O	1.81	0.79
1:A:323:VAL:O	1:A:327:VAL:CG1	2.31	0.79
1:C:274:TYR:HB3	3:C:533:HOH:O	1.82	0.79
1:B:358:MET:HE2	1:B:358:MET:HA	1.64	0.79
1:A:342:ASN:HB3	3:A:484:HOH:O	1.82	0.79
1:B:156:ASN:HD21	1:C:367:ARG:HH11	1.31	0.77
1:B:182:LEU:O	1:B:186:THR:HB	1.86	0.76
1:B:289:SER:HB2	3:B:515:HOH:O	1.84	0.76
1:C:274:TYR:CB	3:C:533:HOH:O	2.35	0.75
3:A:474:HOH:O	1:B:279:MET:SD	2.45	0.74
1:C:168:GLU:OE2	3:C:531:HOH:O	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:MET:HE1	1:B:367:ARG:HD2	1.69	0.74
1:B:60:ILE:HG21	3:B:516:HOH:O	1.88	0.73
1:B:48:TYR:HD1	1:B:48:TYR:O	1.71	0.73
1:C:182:LEU:O	1:C:186:THR:HB	1.88	0.73
1:B:48:TYR:CD1	1:B:48:TYR:C	2.66	0.72
1:A:195:ALA:HB2	1:A:423:VAL:CG2	2.19	0.72
1:B:156:ASN:HD21	1:C:367:ARG:NH1	1.86	0.71
1:A:228:LEU:HD11	3:A:508:HOH:O	1.89	0.71
1:A:367:ARG:NH1	1:C:156:ASN:HD22	1.86	0.70
1:C:358:MET:HE1	1:C:367:ARG:HH11	1.56	0.70
1:C:219:ARG:HG3	1:C:219:ARG:NH1	1.96	0.70
1:B:334:ILE:HG13	1:B:396:ASN:HB3	1.73	0.70
1:B:136:GLN:NE2	1:B:359:GLU:OE2	2.21	0.70
1:C:260:SER:HB2	3:C:516:HOH:O	1.93	0.69
1:C:247:THR:HG23	1:C:289:SER:HB3	1.75	0.69
1:A:413:LEU:HD22	3:A:564:HOH:O	1.92	0.68
1:C:186:THR:HG21	1:C:190:TYR:HE1	1.57	0.68
1:A:181:GLN:CG	3:A:493:HOH:O	2.34	0.68
1:A:346:GLN:HA	1:A:346:GLN:NE2	2.09	0.68
1:A:234:ARG:HG3	3:A:563:HOH:O	1.91	0.68
1:B:186:THR:HG22	1:B:188:ASN:H	1.58	0.68
1:B:328:ARG:HG2	1:B:328:ARG:HH11	1.58	0.67
1:C:256:ILE:O	3:C:534:HOH:O	2.11	0.67
1:C:16:GLU:CG	3:C:512:HOH:O	2.43	0.67
1:A:4:MET:O	1:A:8:GLN:HG2	1.95	0.67
1:B:358:MET:CE	1:B:367:ARG:HD2	2.24	0.67
1:C:55:ARG:HB3	3:C:527:HOH:O	1.93	0.67
1:A:195:ALA:HB2	1:A:423:VAL:HG21	1.75	0.67
1:A:9:GLN:HG3	3:A:552:HOH:O	1.95	0.67
1:A:319:ALA:O	1:A:323:VAL:HG13	1.94	0.66
1:B:97:THR:OG1	1:B:225:GLN:NE2	2.28	0.66
1:B:323:VAL:O	1:B:327:VAL:HG13	1.96	0.66
1:A:156:ASN:ND2	1:B:367:ARG:HH12	1.89	0.66
1:C:66:SER:HB3	3:C:534:HOH:O	1.96	0.66
1:A:349:VAL:HG13	3:A:498:HOH:O	1.96	0.65
1:B:32:ASN:HD22	1:B:35:ARG:HH22	1.45	0.65
1:B:156:ASN:ND2	1:C:358:MET:HE1	2.06	0.64
1:A:42:LEU:O	1:B:291:PRO:O	2.16	0.64
1:C:4:MET:O	1:C:8:GLN:HG2	1.98	0.64
1:A:182:LEU:O	1:A:186:THR:HB	1.97	0.64
1:C:319:ALA:O	1:C:323:VAL:HG13	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:HG3	1:A:265:LYS:O	1.98	0.63
1:C:195:ALA:HB2	1:C:423:VAL:HG21	1.80	0.63
1:A:84:LEU:O	1:A:88:GLU:HG3	1.99	0.62
1:B:152:THR:HG21	3:C:482:HOH:O	1.99	0.62
1:B:153:ASP:OD1	1:C:367:ARG:NH2	2.30	0.62
1:C:277:SER:HB3	1:C:279:MET:HE3	1.82	0.62
1:A:71:LEU:HB3	1:A:252:ALA:HB3	1.82	0.62
1:C:28:PHE:O	1:C:31:ILE:HG13	1.99	0.62
1:C:44:LEU:HG	3:C:526:HOH:O	2.01	0.61
1:B:274:TYR:CE2	3:B:543:HOH:O	2.39	0.61
1:B:32:ASN:ND2	1:B:35:ARG:HH22	1.99	0.61
1:A:290:LEU:HD13	1:A:292:ILE:HG13	1.84	0.60
1:A:415:LEU:HD21	3:A:494:HOH:O	2.01	0.60
1:B:53:GLY:HA2	1:C:280:GLY:O	2.01	0.60
1:B:265:LYS:HD3	3:B:555:HOH:O	2.02	0.60
1:C:97:THR:HG22	1:C:225:GLN:NE2	2.16	0.60
1:C:195:ALA:HB2	1:C:423:VAL:CG2	2.32	0.60
1:C:323:VAL:O	1:C:327:VAL:HG12	2.01	0.59
1:A:219:ARG:NH1	1:A:219:ARG:HG3	2.18	0.59
1:A:60:ILE:C	1:A:61:ASN:HD22	2.10	0.59
1:C:107:LEU:HD11	1:C:399:ASN:ND2	2.16	0.59
1:C:32:ASN:HD22	1:C:35:ARG:HH22	1.52	0.58
1:A:183:ARG:NH1	3:A:534:HOH:O	2.35	0.58
1:C:16:GLU:HG2	3:C:512:HOH:O	2.00	0.58
1:A:28:PHE:O	1:A:31:ILE:HB	2.03	0.58
1:A:303:LYS:HD2	3:A:502:HOH:O	2.03	0.58
1:B:32:ASN:HD22	1:B:35:ARG:NH2	2.02	0.58
1:A:330:SER:HB3	1:A:400:ILE:HG13	1.84	0.58
1:B:207:GLN:HG3	3:B:519:HOH:O	2.04	0.58
1:B:56:ASP:HB3	1:C:278:ASN:O	2.04	0.57
1:A:156:ASN:OD1	1:B:358:MET:HE3	2.03	0.57
1:B:106:ILE:HG23	1:B:412:LEU:HD13	1.85	0.57
1:B:9:GLN:OE1	1:B:188:ASN:ND2	2.38	0.57
1:A:156:ASN:HD22	1:B:367:ARG:HH12	1.49	0.57
1:C:127:GLN:HG2	3:C:569:HOH:O	2.05	0.57
1:C:120:ILE:HG22	3:C:578:HOH:O	2.05	0.57
1:A:97:THR:HG22	1:A:225:GLN:HE22	1.70	0.56
1:A:183:ARG:NH1	1:A:189:TYR:HB2	2.20	0.56
1:A:219:ARG:HG3	1:A:219:ARG:HH11	1.71	0.56
1:B:28:PHE:O	1:B:31:ILE:HB	2.06	0.56
1:B:156:ASN:ND2	1:C:367:ARG:HH12	2.01	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ALA:HB2	1:A:423:VAL:HG23	1.88	0.55
1:A:232:LEU:O	1:A:236:GLN:HG3	2.06	0.55
1:C:118:ASN:HD21	1:C:388:ASN:ND2	2.04	0.55
1:A:44:LEU:HD13	1:A:69:LEU:HD23	1.89	0.55
1:A:53:GLY:HA2	1:B:280:GLY:O	2.07	0.55
1:A:339:SER:HB3	1:C:169:LEU:HG	1.89	0.54
1:C:130:LYS:HD3	3:C:531:HOH:O	2.07	0.54
1:A:367:ARG:HH12	1:C:156:ASN:ND2	2.03	0.54
1:A:298:VAL:O	1:A:299:ASN:CB	2.50	0.54
1:C:16:GLU:HG3	3:C:512:HOH:O	2.05	0.54
1:B:93:ILE:HD13	3:B:542:HOH:O	2.06	0.54
1:A:220:ASN:ND2	1:A:323:VAL:HG11	2.22	0.54
1:B:409:GLU:HG2	3:B:501:HOH:O	2.08	0.54
1:A:220:ASN:O	1:A:223:LEU:HD12	2.08	0.54
1:A:11:ARG:HG2	3:A:548:HOH:O	2.07	0.53
1:B:156:ASN:OD1	1:C:358:MET:CE	2.53	0.53
1:B:258:ASP:O	1:B:259:THR:OG1	2.20	0.53
1:A:310:VAL:O	1:A:314:GLU:HG2	2.09	0.53
1:B:423:VAL:CB	3:B:479:HOH:O	2.20	0.52
1:C:32:ASN:ND2	1:C:35:ARG:HH22	2.06	0.52
1:C:189:TYR:HE2	3:C:555:HOH:O	1.91	0.52
1:C:323:VAL:O	1:C:327:VAL:CG1	2.57	0.52
1:A:346:GLN:HA	1:A:346:GLN:HE21	1.75	0.52
1:B:397:GLN:HE21	1:B:397:GLN:HA	1.73	0.52
1:A:315:GLN:NE2	1:C:19:LYS:HE2	2.25	0.52
1:B:169:LEU:CG	1:C:339:SER:HB3	2.36	0.51
1:A:334:ILE:HG12	1:A:396:ASN:HB3	1.92	0.51
1:C:266:THR:HA	3:C:533:HOH:O	2.11	0.51
1:A:169:LEU:CD1	1:B:339:SER:HB3	2.42	0.50
1:A:156:ASN:ND2	1:B:358:MET:HE1	2.24	0.50
1:B:103:GLN:HE21	1:B:407:LEU:H	1.58	0.50
1:B:59:GLY:CA	3:B:539:HOH:O	2.47	0.50
1:B:54:TYR:HD2	1:B:55:ARG:HB3	1.77	0.50
1:B:290:LEU:HD13	1:B:292:ILE:HG13	1.94	0.50
1:B:151:ILE:O	1:B:155:GLN:HG3	2.12	0.49
1:C:374:ASP:OD2	2:C:472:NCO:N2	2.45	0.49
1:A:19:LYS:HE2	1:B:315:GLN:NE2	2.27	0.49
1:B:220:ASN:ND2	1:B:223:LEU:H	2.10	0.49
1:C:220:ASN:ND2	1:C:323:VAL:HG11	2.27	0.49
1:A:56:ASP:OD1	1:A:56:ASP:O	2.30	0.49
1:B:358:MET:SD	1:B:367:ARG:HD2	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:LYS:HB2	3:C:517:HOH:O	2.11	0.49
1:A:258:ASP:O	1:A:259:THR:OG1	2.22	0.49
1:B:42:LEU:O	1:C:291:PRO:O	2.30	0.49
1:C:397:GLN:HA	1:C:397:GLN:NE2	2.20	0.49
1:C:398:LEU:HD11	1:C:415:LEU:HD11	1.95	0.49
1:C:183:ARG:NH1	1:C:189:TYR:HB2	2.27	0.49
1:A:410:GLN:HA	1:A:410:GLN:NE2	2.28	0.49
1:B:113:TYR:CE2	1:B:193:LEU:HD22	2.48	0.49
1:B:6:VAL:HG22	1:B:190:TYR:CZ	2.48	0.48
1:A:299:ASN:H	1:A:302:VAL:HG23	1.77	0.48
1:C:277:SER:CB	1:C:279:MET:HE3	2.42	0.48
1:A:60:ILE:C	1:A:60:ILE:HD13	2.38	0.48
1:A:265:LYS:O	1:A:265:LYS:CG	2.60	0.48
1:A:306:GLN:O	1:A:309:PHE:HB3	2.13	0.48
1:B:328:ARG:HH11	1:B:328:ARG:CG	2.24	0.48
1:A:134:TYR:HB2	1:A:161:TYR:CE1	2.49	0.48
1:C:125:TYR:CE1	3:C:500:HOH:O	2.65	0.48
1:C:358:MET:SD	1:C:371:ASP:HB3	2.53	0.48
1:A:183:ARG:CZ	3:A:534:HOH:O	2.61	0.48
1:B:170:THR:HG22	3:C:485:HOH:O	2.14	0.48
1:B:4:MET:SD	1:B:412:LEU:HD23	2.54	0.48
1:A:29:GLU:OE1	1:B:300:SER:HB2	2.13	0.48
3:A:486:HOH:O	1:C:169:LEU:HD12	2.13	0.48
1:B:358:MET:HE1	1:B:367:ARG:HH11	1.78	0.48
1:A:95:ASP:HB3	3:A:499:HOH:O	2.13	0.47
1:C:205:LYS:HA	1:C:205:LYS:HD3	1.75	0.47
1:A:169:LEU:HG	1:B:339:SER:HB3	1.97	0.47
1:A:294:GLN:NE2	3:A:568:HOH:O	2.47	0.47
1:A:161:TYR:O	1:A:164:VAL:HG12	2.14	0.47
1:B:47:ASP:HB3	3:B:524:HOH:O	2.14	0.47
1:A:64:ALA:HB1	3:A:514:HOH:O	2.14	0.47
1:B:41:GLN:HB2	1:B:72:THR:OG1	2.13	0.47
1:B:103:GLN:NE2	1:B:407:LEU:H	2.13	0.47
1:A:30:LYS:HE2	1:B:304:GLN:OE1	2.15	0.47
1:B:199:GLU:H	1:B:199:GLU:HG2	1.46	0.47
1:B:401:LYS:HG3	1:B:411:ASP:OD2	2.14	0.47
1:A:224:LEU:HD13	1:A:227:ARG:HH21	1.79	0.47
1:C:130:LYS:HE2	1:C:130:LYS:HB3	1.55	0.47
1:A:334:ILE:O	1:A:338:ILE:HD12	2.15	0.47
1:C:180:GLU:HA	1:C:180:GLU:OE1	2.15	0.47
1:A:153:ASP:HA	1:A:369:ILE:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:HD13	1:A:61:ASN:N	2.30	0.46
1:A:158:ARG:HE	1:A:158:ARG:HB2	1.54	0.46
1:C:51:SER:HB2	3:C:515:HOH:O	2.15	0.46
1:A:421:LYS:HB3	3:A:476:HOH:O	2.15	0.46
1:A:227:ARG:NH1	3:A:550:HOH:O	2.24	0.46
1:C:319:ALA:HA	3:C:579:HOH:O	2.15	0.46
1:C:320:HIS:HB2	3:C:479:HOH:O	2.15	0.46
1:C:270:ALA:HB1	1:C:274:TYR:CD2	2.52	0.45
1:B:197:ASN:C	1:B:197:ASN:HD22	2.23	0.45
1:C:77:ASP:HA	3:C:559:HOH:O	2.15	0.45
1:A:291:PRO:O	1:C:42:LEU:O	2.35	0.45
1:B:283:LYS:O	1:B:284:VAL:HG13	2.16	0.45
1:C:24:ARG:HE	1:C:24:ARG:HB3	1.46	0.45
1:C:163:THR:HG23	3:C:492:HOH:O	2.15	0.45
1:C:165:LEU:O	1:C:169:LEU:HD22	2.17	0.45
1:A:234:ARG:CZ	3:A:546:HOH:O	2.65	0.45
1:B:358:MET:SD	1:B:371:ASP:HB3	2.57	0.45
1:B:140:THR:HG22	1:B:154:VAL:HG22	1.99	0.45
1:C:170:THR:HG21	3:C:502:HOH:O	2.17	0.45
1:C:186:THR:CG2	1:C:188:ASN:H	2.29	0.45
1:B:7:TYR:CE1	1:B:106:ILE:HG13	2.52	0.45
1:B:421:LYS:HG2	3:B:490:HOH:O	2.17	0.45
1:B:85:THR:HG22	1:B:89:LYS:HD2	1.99	0.44
1:B:358:MET:HE2	1:B:358:MET:CA	2.39	0.44
1:A:234:ARG:CD	3:A:546:HOH:O	2.65	0.44
1:B:234:ARG:NE	3:B:541:HOH:O	2.48	0.44
1:A:276:ASP:OD1	3:A:485:HOH:O	2.21	0.44
3:A:496:HOH:O	1:B:297:MET:HG3	2.17	0.44
1:C:373:LEU:O	1:C:376:THR:HB	2.18	0.44
1:A:246:PRO:HA	1:A:289:SER:O	2.17	0.44
1:C:106:ILE:HG23	1:C:412:LEU:HD13	1.99	0.44
1:B:265:LYS:CG	1:B:265:LYS:O	2.65	0.44
1:B:118:ASN:HD21	1:B:388:ASN:HD22	1.65	0.44
1:B:267:ARG:NH1	3:B:529:HOH:O	2.48	0.44
1:B:289:SER:CB	3:B:515:HOH:O	2.57	0.44
1:C:374:ASP:OD1	3:C:495:HOH:O	2.21	0.44
1:A:315:GLN:HE21	1:C:19:LYS:HE2	1.82	0.44
1:B:57:ALA:O	1:B:60:ILE:HG22	2.18	0.44
1:A:118:ASN:HD21	1:A:388:ASN:ND2	2.16	0.43
1:B:310:VAL:O	1:B:314:GLU:HG2	2.18	0.43
1:C:55:ARG:CG	1:C:55:ARG:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ASN:HD22	1:B:223:LEU:H	1.67	0.43
1:B:401:LYS:HA	1:B:401:LYS:HD2	1.52	0.43
1:C:334:ILE:HG13	1:C:396:ASN:HB3	1.99	0.43
1:A:317:GLU:O	1:A:321:ARG:HG3	2.18	0.43
1:C:297:MET:HE2	1:C:297:MET:HB3	2.00	0.43
1:B:107:LEU:HD11	1:B:399:ASN:ND2	2.34	0.43
1:B:246:PRO:HA	1:B:289:SER:O	2.18	0.43
1:A:288:PHE:HE1	3:C:526:HOH:O	2.02	0.43
1:C:151:ILE:HG13	1:C:155:GLN:NE2	2.33	0.43
1:C:161:TYR:HA	1:C:164:VAL:HG12	2.01	0.43
1:C:192:GLU:OE1	1:C:422:PRO:HB3	2.19	0.43
1:B:14:ASN:HA	1:B:15:PRO:HD3	1.80	0.42
1:C:306:GLN:HG2	3:C:556:HOH:O	2.18	0.42
1:A:186:THR:HG22	1:A:188:ASN:N	2.20	0.42
1:C:186:THR:HG22	1:C:188:ASN:H	1.84	0.42
1:B:44:LEU:HG	3:B:558:HOH:O	2.19	0.42
1:B:120:ILE:O	1:B:124:SER:HB2	2.19	0.42
1:C:220:ASN:HD21	1:C:222:SER:HB2	1.84	0.42
1:A:381:ASN:HB3	3:A:475:HOH:O	2.19	0.42
1:C:130:LYS:NZ	3:C:531:HOH:O	2.26	0.42
1:C:142:GLN:HB3	3:C:474:HOH:O	2.19	0.42
1:A:2:ASN:CG	1:A:416:ASN:HD21	2.27	0.42
1:B:219:ARG:HD2	1:B:406:THR:CG2	2.48	0.42
1:B:423:VAL:CG1	3:B:479:HOH:O	2.62	0.42
1:A:250:LEU:HG	3:A:527:HOH:O	2.19	0.42
1:A:318:SER:OG	1:C:15:PRO:HB2	2.20	0.42
1:C:55:ARG:O	1:C:55:ARG:HG3	2.19	0.42
1:A:110:ALA:HB3	1:A:398:LEU:HD23	2.01	0.42
1:C:61:ASN:HD22	1:C:61:ASN:N	2.15	0.42
1:B:115:ASN:HD22	1:B:115:ASN:HA	1.62	0.41
1:C:66:SER:CB	3:C:534:HOH:O	2.63	0.41
1:A:60:ILE:HD11	1:A:261:TYR:CE2	2.54	0.41
3:A:554:HOH:O	1:C:152:THR:HB	2.19	0.41
1:B:186:THR:HG22	1:B:188:ASN:N	2.32	0.41
1:B:417:ASN:ND2	3:B:567:HOH:O	2.52	0.41
1:B:41:GLN:O	1:B:71:LEU:HA	2.20	0.41
1:B:11:ARG:HE	1:B:11:ARG:HB3	1.82	0.41
1:C:316:LEU:HD13	3:C:537:HOH:O	2.20	0.41
1:C:354:SER:O	1:C:358:MET:HG2	2.21	0.41
1:B:55:ARG:O	1:C:278:ASN:O	2.39	0.41
1:A:60:ILE:C	1:A:61:ASN:ND2	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:CD1	1:A:261:TYR:HD2	2.22	0.40
1:A:169:LEU:HD13	1:A:169:LEU:HA	1.90	0.40
1:A:420:SER:OG	1:A:421:LYS:N	2.54	0.40
1:B:220:ASN:ND2	1:B:323:VAL:HG11	2.36	0.40
1:A:346:GLN:NE2	1:A:346:GLN:CA	2.79	0.40
1:B:113:TYR:HE2	1:B:193:LEU:HD22	1.86	0.40
1:B:319:ALA:O	1:B:323:VAL:HG13	2.21	0.40
1:A:183:ARG:NH2	3:A:534:HOH:O	2.54	0.40
1:B:307:TYR:HA	1:B:310:VAL:HG13	2.02	0.40
1:B:426:ASN:ND2	3:B:553:HOH:O	2.54	0.40
1:C:334:ILE:HD11	1:C:396:ASN:O	2.21	0.40
1:A:258:ASP:O	1:A:259:THR:CB	2.69	0.40
1:A:344:TYR:CE2	1:A:385:GLU:HG3	2.57	0.40
1:B:146:VAL:CG1	1:B:148:LEU:HD12	2.51	0.40
1:C:246:PRO:HA	1:C:289:SER:O	2.22	0.40
1:C:279:MET:H	1:C:279:MET:HG2	1.77	0.40

All (6) 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:148:LEU:CD1	3:B:535:HOH:O[9_654]	1.38	0.82
3:A:472:HOH:O	3:C:475:HOH:O[5_545]	1.47	0.73
3:B:483:HOH:O	3:B:484:HOH:O[5_545]	1.51	0.69
3:A:558:HOH:O	3:C:564:HOH:O[5_545]	1.55	0.65
1:B:148:LEU:CG	3:B:535:HOH:O[9_654]	1.96	0.24
1:B:142:GLN:NE2	3:B:534:HOH:O[9_654]	2.17	0.03

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	426/471 (90%)	402 (94%)	16 (4%)	8 (2%)	6	12
1	B	426/471 (90%)	397 (93%)	22 (5%)	7 (2%)	7	14
1	C	426/471 (90%)	400 (94%)	19 (4%)	7 (2%)	7	14
All	All	1278/1413 (90%)	1199 (94%)	57 (4%)	22 (2%)	7	14

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	ASP
1	A	299	ASN
1	B	258	ASP
1	B	299	ASN
1	C	299	ASN
1	A	259	THR
1	A	268	GLY
1	A	275	ASP
1	B	55	ARG
1	B	268	GLY
1	C	55	ARG
1	C	258	ASP
1	C	268	GLY
1	A	55	ARG
1	A	420	SER
1	B	259	THR
1	C	259	THR
1	C	420	SER
1	A	46	ALA
1	C	275	ASP
1	B	46	ALA
1	B	275	ASP

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	358/393 (91%)	281 (78%)	77 (22%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	358/393 (91%)	276 (77%)	82 (23%)	1	1
1	C	358/393 (91%)	272 (76%)	86 (24%)	1	1
All	All	1074/1179 (91%)	829 (77%)	245 (23%)	1	1

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	4	MET
1	A	9	GLN
1	A	11	ARG
1	A	12	LEU
1	A	17	LEU
1	A	20	SER
1	A	24	ARG
1	A	47	ASP
1	A	49	THR
1	A	51	SER
1	A	55	ARG
1	A	60	ILE
1	A	62	SER
1	A	63	ASN
1	A	65	THR
1	A	66	SER
1	A	74	SER
1	A	78	MET
1	A	79	SER
1	A	82	ARG
1	A	86	LEU
1	A	94	GLN
1	A	97	THR
1	A	111	THR
1	A	139	GLN
1	A	151	ILE
1	A	158	ARG
1	A	182	LEU
1	A	183	ARG
1	A	186	THR
1	A	198	VAL
1	A	199	GLU
1	A	200	ASN

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Mol	Chain	Res	Type
1	A	202	LYS
1	A	214	LYS
1	A	217	GLU
1	A	222	SER
1	A	223	LEU
1	A	227	ARG
1	A	247	THR
1	A	248	LEU
1	A	251	THR
1	A	254	THR
1	A	256	ILE
1	A	257	SER
1	A	259	THR
1	A	260	SER
1	A	264	SER
1	A	265	LYS
1	A	266	THR
1	A	273	GLN
1	A	277	SER
1	A	279	MET
1	A	283	LYS
1	A	284	VAL
1	A	287	SER
1	A	289	SER
1	A	290	LEU
1	A	300	SER
1	A	301	GLN
1	A	310	VAL
1	A	316	LEU
1	A	327	VAL
1	A	334	ILE
1	A	339	SER
1	A	346	GLN
1	A	367	ARG
1	A	397	GLN
1	A	398	LEU
1	A	400	ILE
1	A	407	LEU
1	A	412	LEU
1	A	413	LEU
1	A	420	SER
1	A	421	LYS

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Mol	Chain	Res	Type
1	A	424	SER
1	B	4	MET
1	B	5	GLN
1	B	8	GLN
1	B	11	ARG
1	B	17	LEU
1	B	19	LYS
1	B	24	ARG
1	B	31	ILE
1	B	39	LEU
1	B	47	ASP
1	B	48	TYR
1	B	60	ILE
1	B	61	ASN
1	B	62	SER
1	B	65	THR
1	B	66	SER
1	B	72	THR
1	B	74	SER
1	B	82	ARG
1	B	84	LEU
1	B	103	GLN
1	B	104	THR
1	B	124	SER
1	B	139	GLN
1	B	146	VAL
1	B	152	THR
1	B	169	LEU
1	B	170	THR
1	B	179	VAL
1	B	182	LEU
1	B	185	ILE
1	B	186	THR
1	B	199	GLU
1	B	214	LYS
1	B	217	GLU
1	B	219	ARG
1	B	222	SER
1	B	223	LEU
1	B	225	GLN
1	B	229	SER
1	B	232	LEU

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Mol	Chain	Res	Type
1	B	247	THR
1	B	251	THR
1	B	253	SER
1	B	259	THR
1	B	264	SER
1	B	267	ARG
1	B	272	THR
1	B	273	GLN
1	B	277	SER
1	B	278	ASN
1	B	279	MET
1	B	289	SER
1	B	290	LEU
1	B	292	ILE
1	B	300	SER
1	B	301	GLN
1	B	304	GLN
1	B	306	GLN
1	B	310	VAL
1	B	316	LEU
1	B	318	SER
1	B	322	SER
1	B	327	VAL
1	B	328	ARG
1	B	339	SER
1	B	340	SER
1	B	353	SER
1	B	359	GLU
1	B	367	ARG
1	B	384	GLN
1	B	395	ILE
1	B	397	GLN
1	B	398	LEU
1	B	401	LYS
1	B	404	LEU
1	B	407	LEU
1	B	409	GLU
1	B	410	GLN
1	B	412	LEU
1	B	421	LYS
1	B	428	GLU
1	C	1	GLU

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Mol	Chain	Res	Type
1	C	4	MET
1	C	11	ARG
1	C	17	LEU
1	C	19	LYS
1	C	24	ARG
1	C	39	LEU
1	C	47	ASP
1	C	49	THR
1	C	51	SER
1	C	55	ARG
1	C	60	ILE
1	C	62	SER
1	C	66	SER
1	C	68	SER
1	C	69	LEU
1	C	71	LEU
1	C	72	THR
1	C	80	LYS
1	C	82	ARG
1	C	86	LEU
1	C	97	THR
1	C	104	THR
1	C	124	SER
1	C	127	GLN
1	C	130	LYS
1	C	142	GLN
1	C	146	VAL
1	C	149	VAL
1	C	152	THR
1	C	155	GLN
1	C	169	LEU
1	C	170	THR
1	C	179	VAL
1	C	182	LEU
1	C	186	THR
1	C	199	GLU
1	C	202	LYS
1	C	205	LYS
1	C	209	VAL
1	C	214	LYS
1	C	217	GLU
1	C	219	ARG

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Mol	Chain	Res	Type
1	C	223	LEU
1	C	232	LEU
1	C	239	GLN
1	C	247	THR
1	C	248	LEU
1	C	251	THR
1	C	253	SER
1	C	259	THR
1	C	265	LYS
1	C	266	THR
1	C	267	ARG
1	C	273	GLN
1	C	277	SER
1	C	279	MET
1	C	283	LYS
1	C	287	SER
1	C	290	LEU
1	C	291	PRO
1	C	294	GLN
1	C	297	MET
1	C	301	GLN
1	C	302	VAL
1	C	303	LYS
1	C	310	VAL
1	C	316	LEU
1	C	323	VAL
1	C	327	VAL
1	C	334	ILE
1	C	340	SER
1	C	353	SER
1	C	384	GLN
1	C	392	ASN
1	C	397	GLN
1	C	398	LEU
1	C	400	ILE
1	C	401	LYS
1	C	407	LEU
1	C	409	GLU
1	C	410	GLN
1	C	412	LEU
1	C	413	LEU
1	C	424	SER

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Mol	Chain	Res	Type
1	C	428	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	9	GLN
1	A	32	ASN
1	A	41	GLN
1	A	61	ASN
1	A	73	GLN
1	A	87	GLN
1	A	99	GLN
1	A	103	GLN
1	A	115	ASN
1	A	118	ASN
1	A	127	GLN
1	A	139	GLN
1	A	155	GLN
1	A	156	ASN
1	A	173	ASN
1	A	174	ASN
1	A	200	ASN
1	A	220	ASN
1	A	225	GLN
1	A	236	GLN
1	A	281	GLN
1	A	282	ASN
1	A	301	GLN
1	A	315	GLN
1	A	332	ASN
1	A	346	GLN
1	A	381	ASN
1	A	388	ASN
1	A	392	ASN
1	A	399	ASN
1	A	410	GLN
1	B	8	GLN
1	B	9	GLN
1	B	32	ASN
1	B	41	GLN
1	B	102	GLN

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Mol	Chain	Res	Type
1	B	103	GLN
1	B	108	ASN
1	B	115	ASN
1	B	118	ASN
1	B	127	GLN
1	B	142	GLN
1	B	155	GLN
1	B	156	ASN
1	B	160	GLN
1	B	173	ASN
1	B	174	ASN
1	B	188	ASN
1	B	197	ASN
1	B	200	ASN
1	B	207	GLN
1	B	220	ASN
1	B	225	GLN
1	B	236	GLN
1	B	273	GLN
1	B	301	GLN
1	B	308	ASN
1	B	315	GLN
1	B	332	ASN
1	B	342	ASN
1	B	352	GLN
1	B	381	ASN
1	B	392	ASN
1	B	397	GLN
1	B	399	ASN
1	B	417	ASN
1	C	14	ASN
1	C	32	ASN
1	C	41	GLN
1	C	52	ASN
1	C	61	ASN
1	C	87	GLN
1	C	94	GLN
1	C	99	GLN
1	C	102	GLN
1	C	118	ASN
1	C	127	GLN
1	C	139	GLN

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Mol	Chain	Res	Type
1	C	155	GLN
1	C	156	ASN
1	C	174	ASN
1	C	210	ASN
1	C	220	ASN
1	C	225	GLN
1	C	241	GLN
1	C	301	GLN
1	C	381	ASN
1	C	388	ASN
1	C	397	GLN
1	C	399	ASN
1	C	417	ASN

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 [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NCO	C	472	-	6,6,6	0.74	0	-		

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	C	472	NCO	1	0

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	428/471 (90%)	1.00	69 (16%) 4 4	15, 50, 72, 83	0
1	B	428/471 (90%)	1.07	80 (18%) 3 2	13, 50, 72, 85	0
1	C	428/471 (90%)	1.06	80 (18%) 3 2	14, 50, 72, 82	0
All	All	1284/1413 (90%)	1.04	229 (17%) 4 3	13, 50, 72, 85	0

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	268	GLY	8.4
1	B	59	GLY	7.9
1	B	264	SER	7.7
1	C	271	GLY	6.8
1	C	269	ALA	5.9
1	B	263	GLY	5.6
1	B	268	GLY	5.4
1	A	272	THR	5.4
1	A	267	ARG	5.3
1	C	255	GLY	5.2
1	B	270	ALA	5.2
1	B	262	SER	5.2
1	C	59	GLY	5.2
1	C	263	GLY	5.2
1	C	67	ALA	5.1
1	B	260	SER	5.0
1	B	60	ILE	5.0
1	B	267	ARG	4.7
1	B	250	LEU	4.7
1	B	54	TYR	4.6
1	B	272	THR	4.5
1	C	278	ASN	4.5
1	C	274	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	264	SER	4.5
1	C	270	ALA	4.5
1	C	272	THR	4.4
1	A	63	ASN	4.3
1	A	69	LEU	4.3
1	B	269	ALA	4.3
1	C	57	ALA	4.2
1	A	263	GLY	4.2
1	A	248	LEU	4.2
1	C	281	GLN	4.2
1	C	60	ILE	4.1
1	A	50	TYR	4.1
1	A	269	ALA	4.1
1	B	279	MET	4.1
1	C	266	THR	4.0
1	C	277	SER	4.0
1	B	266	THR	3.9
1	B	280	GLY	3.9
1	C	267	ARG	3.9
1	C	56	ASP	3.9
1	B	43	GLY	3.9
1	A	65	THR	3.9
1	B	64	ALA	3.9
1	B	41	GLN	3.8
1	C	273	GLN	3.8
1	A	280	GLY	3.8
1	C	280	GLY	3.7
1	A	243	GLY	3.7
1	C	256	ILE	3.7
1	C	75	ILE	3.6
1	B	274	TYR	3.6
1	A	75	ILE	3.6
1	C	1	GLU	3.6
1	C	253	SER	3.6
1	C	63	ASN	3.6
1	A	271	GLY	3.6
1	A	259	THR	3.5
1	B	61	ASN	3.5
1	C	428	GLU	3.5
1	B	44	LEU	3.5
1	C	262	SER	3.5
1	C	418	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	169	LEU	3.5
1	B	256	ILE	3.5
1	B	292	ILE	3.5
1	B	189	TYR	3.5
1	C	147	GLY	3.5
1	B	71	LEU	3.5
1	C	69	LEU	3.5
1	B	49	THR	3.4
1	B	52	ASN	3.4
1	C	53	GLY	3.4
1	C	282	ASN	3.4
1	B	1	GLU	3.4
1	C	284	VAL	3.4
1	C	292	ILE	3.4
1	B	275	ASP	3.4
1	A	256	ILE	3.4
1	A	260	SER	3.4
1	C	254	THR	3.4
1	B	273	GLN	3.4
1	A	200	ASN	3.4
1	A	48	TYR	3.3
1	B	58	ASN	3.3
1	C	261	TYR	3.3
1	B	265	LYS	3.3
1	C	146	VAL	3.3
1	B	284	VAL	3.2
1	A	270	ALA	3.2
1	A	266	THR	3.1
1	C	54	TYR	3.1
1	B	57	ALA	3.1
1	C	46	ALA	3.1
1	C	78	MET	3.1
1	C	251	THR	3.1
1	C	45	GLY	3.1
1	B	261	TYR	3.1
1	A	255	GLY	3.1
1	B	252	ALA	3.1
1	B	53	GLY	3.0
1	A	284	VAL	3.0
1	B	36	SER	3.0
1	B	83	ALA	3.0
1	A	51	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	62	SER	2.9
1	B	62	SER	2.9
1	C	279	MET	2.9
1	B	69	LEU	2.9
1	C	217	GLU	2.9
1	A	246	PRO	2.9
1	A	78	MET	2.9
1	A	254	THR	2.9
1	A	90	ALA	2.9
1	A	286	LEU	2.9
1	B	251	THR	2.8
1	C	252	ALA	2.8
1	B	277	SER	2.8
1	C	61	ASN	2.8
1	C	388	ASN	2.8
1	A	316	LEU	2.8
1	B	46	ALA	2.8
1	A	49	THR	2.8
1	A	247	THR	2.8
1	A	302	VAL	2.8
1	B	50	TYR	2.8
1	A	283	LYS	2.8
1	A	59	GLY	2.8
1	B	296	GLY	2.7
1	A	265	LYS	2.7
1	A	60	ILE	2.7
1	A	86	LEU	2.7
1	A	251	THR	2.7
1	C	258	ASP	2.7
1	C	48	TYR	2.7
1	C	169	LEU	2.7
1	C	287	SER	2.7
1	C	259	THR	2.7
1	A	287	SER	2.7
1	A	288	PHE	2.7
1	A	279	MET	2.6
1	A	245	LEU	2.6
1	B	255	GLY	2.6
1	C	36	SER	2.6
1	C	275	ASP	2.6
1	C	49	THR	2.6
1	C	42	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	295	GLY	2.6
1	B	428	GLU	2.5
1	A	46	ALA	2.5
1	C	148	LEU	2.5
1	A	296	GLY	2.5
1	C	260	SER	2.5
1	C	276	ASP	2.5
1	C	290	LEU	2.5
1	A	64	ALA	2.5
1	A	253	SER	2.5
1	C	28	PHE	2.5
1	A	292	ILE	2.4
1	B	249	ASP	2.4
1	C	81	TRP	2.4
1	A	428	GLU	2.4
1	C	205	LYS	2.4
1	A	342	ASN	2.4
1	B	86	LEU	2.4
1	B	388	ASN	2.4
1	C	68	SER	2.4
1	A	202	LYS	2.4
1	B	413	LEU	2.4
1	A	277	SER	2.4
1	A	290	LEU	2.4
1	C	72	THR	2.4
1	B	294	GLN	2.4
1	C	64	ALA	2.4
1	A	52	ASN	2.3
1	C	283	LYS	2.3
1	B	9	GLN	2.3
1	B	316	LEU	2.3
1	C	44	LEU	2.3
1	B	48	TYR	2.3
1	C	189	TYR	2.3
1	B	259	THR	2.3
1	C	265	LYS	2.3
1	B	276	ASP	2.3
1	B	271	GLY	2.3
1	B	283	LYS	2.3
1	C	222	SER	2.3
1	C	288	PHE	2.3
1	A	83	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	421	LYS	2.3
1	A	68	SER	2.3
1	A	54	TYR	2.2
1	A	44	LEU	2.2
1	B	245	LEU	2.2
1	A	85	THR	2.2
1	B	298	VAL	2.2
1	B	26	ALA	2.2
1	C	389	ALA	2.2
1	B	222	SER	2.2
1	B	75	ILE	2.2
1	B	299	ASN	2.1
1	A	250	LEU	2.1
1	B	290	LEU	2.1
1	B	81	TRP	2.1
1	A	261	TYR	2.1
1	B	248	LEU	2.1
1	C	285	GLY	2.1
1	B	56	ASP	2.1
1	A	55	ARG	2.1
1	B	427	PRO	2.1
1	B	99	GLN	2.1
1	B	169	LEU	2.1
1	C	38	LEU	2.1
1	C	50	TYR	2.1
1	B	300	SER	2.1
1	A	427	PRO	2.1
1	B	281	GLN	2.1
1	A	223	LEU	2.1
1	C	12	LEU	2.1
1	C	39	LEU	2.1
1	C	248	LEU	2.1
1	A	189	TYR	2.0
1	B	67	ALA	2.0
1	B	65	THR	2.0
1	A	320	HIS	2.0
1	A	285	GLY	2.0
1	B	63	ASN	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NCO	C	472	7/7	0.99	0.07	25,27,28,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.