



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:35 PM UTC

PDB ID : 1WC7 / pdb_00001wc7
Title : FAB FRAGMENT OF PLP-DEPENDENT CATALYTIC ANTIBODY 15A9
IN COMPLEX WITH PHOSPHOPYRIDOXYL-L-ALANINE
Authors : Golinelli-Pimpaneau, B.; Christen, P.
Deposited on : 2004-11-09
Resolution : 2.33 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

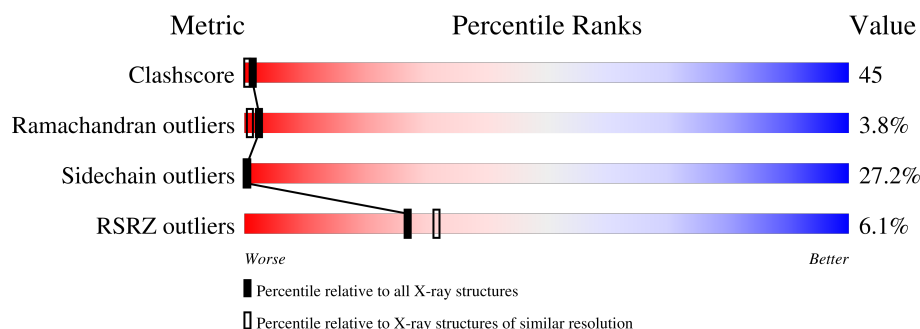
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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))
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	213	5% 31% 53% 13% .
1	L	213	5% 33% 50% 15% .
2	B	226	5% 31% 47% 20% ..
2	H	226	9% 30% 50% 19% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	H	1214	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6610 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 FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	1
			1596	991	267	330	8			
1	L	212	Total	C	N	O	S	0	0	1
			1599	996	268	327	8			

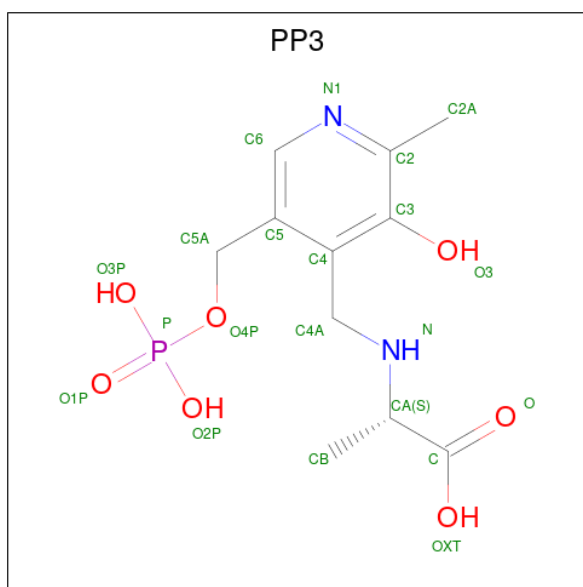
- Molecule 2 is a protein called FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	224	Total	C	N	O	S	0	0	1
			1640	1045	273	315	7			
2	H	224	Total	C	N	O	S	0	0	1
			1630	1041	272	310	7			

- Molecule 3 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	I	0	0
			1	1		
3	B	1	Total	I	0	0
			1	1		
3	H	2	Total	I	0	0
			2	2		
3	L	1	Total	I	0	0
			1	1		

- Molecule 4 is ALANYL-PYRIDOXAL-5'-PHOSPHATE (CCD ID: PP3) (formula: C₁₁H₁₇N₂O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

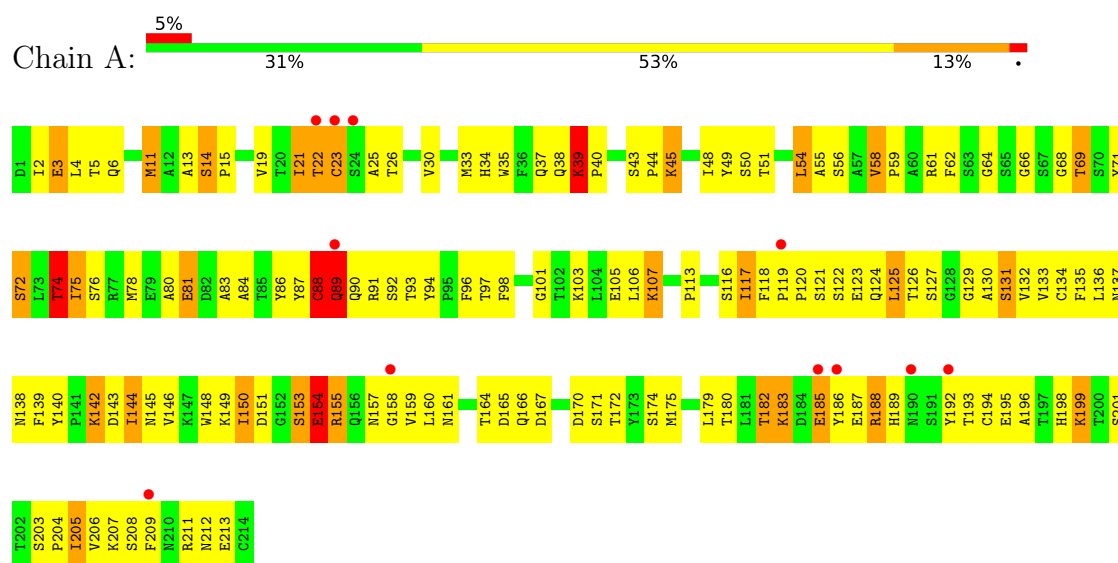
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		
5	B	25	Total	O	0	0
			25	25		
5	H	33	Total	O	0	0
			33	33		
5	L	30	Total	O	0	0
			30	30		

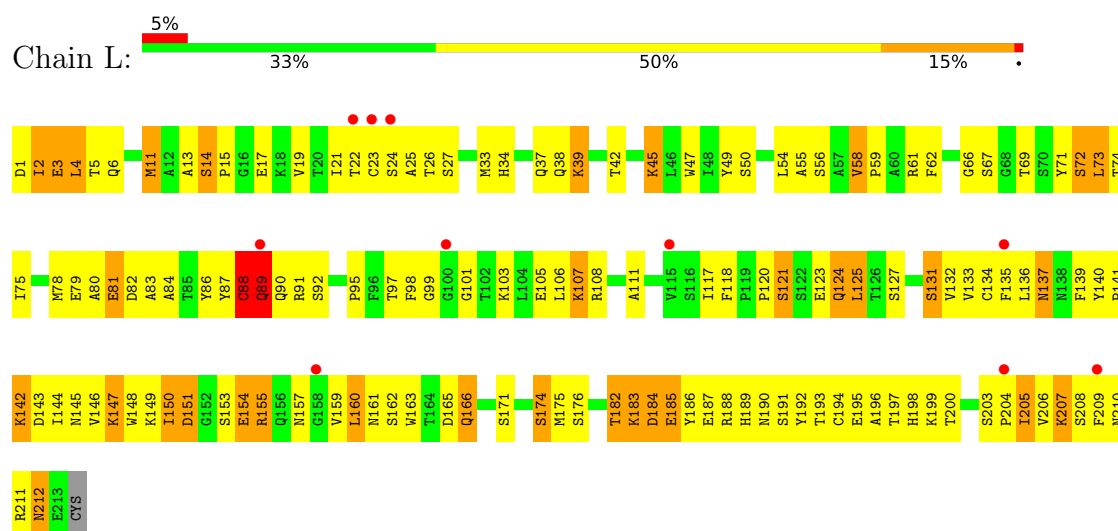
3 Residue-property plots

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: FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, LIGHT CHAIN

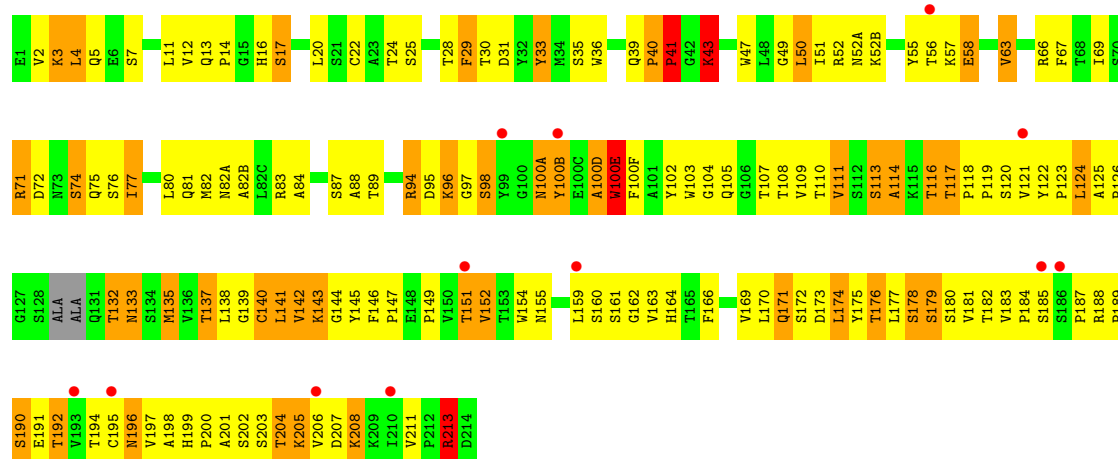


• Molecule 1: FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, LIGHT CHAIN

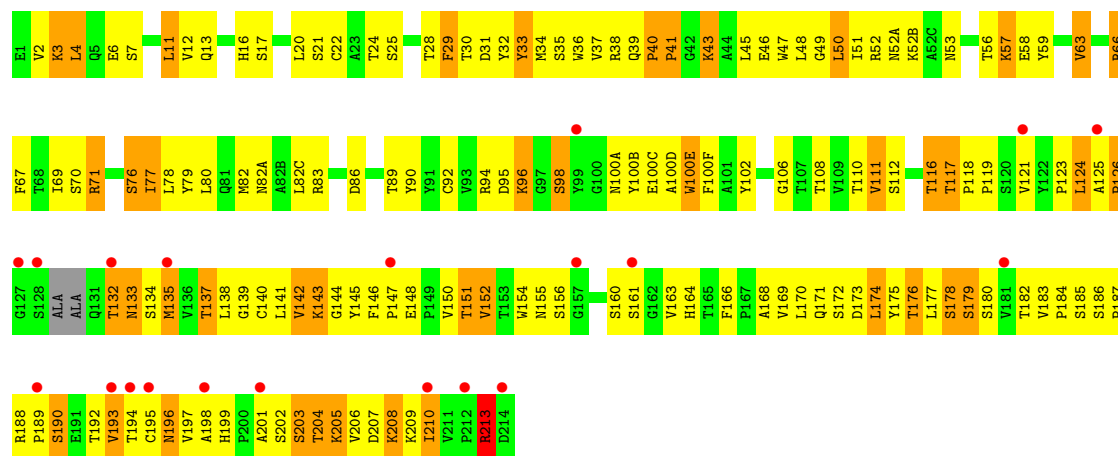


• Molecule 2: FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, HEAVY CHAIN





● Molecule 2: FAB FRAGMENT OF CATALYTIC ANTIBODY 15A9, HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.48Å 81.69Å 79.33Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	20.00 – 2.33 20.00 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.33) 95.1 (20.00-2.33)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.33Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.223 , 0.309 0.212 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 159.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-l,-k 0.000 for -h,l,k 0.048 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6610	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: PP3, IOD

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	0.39	1/1634 (0.1%)	1.29	16/2228 (0.7%)
1	L	0.40	1/1638 (0.1%)	1.25	8/2231 (0.4%)
2	B	0.40	1/1685 (0.1%)	1.17	5/2308 (0.2%)
2	H	0.39	1/1675 (0.1%)	1.13	3/2296 (0.1%)
All	All	0.40	4/6632 (0.1%)	1.21	32/9063 (0.4%)

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	1
1	L	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	213	ARG	C-N	-5.86	1.25	1.33
2	H	213	ARG	C-N	-5.81	1.25	1.33
1	L	212	ASN	C-N	-5.81	1.25	1.33
1	A	213	GLU	C-N	-5.69	1.25	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	89	GLN	CB-CG-CD	16.62	140.85	112.60
1	L	89	GLN	CA-C-N	10.87	138.85	122.65
1	L	89	GLN	C-N-CA	10.87	138.85	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	GLN	CB-CG-CD	10.31	130.13	112.60
1	A	89	GLN	CA-C-N	8.96	136.00	122.65
1	A	89	GLN	C-N-CA	8.96	136.00	122.65
1	A	74	THR	CA-C-N	7.70	131.06	122.59
1	A	74	THR	C-N-CA	7.70	131.06	122.59
2	B	43	LYS	CA-C-N	6.79	132.66	121.39
2	B	43	LYS	C-N-CA	6.79	132.66	121.39
1	A	137	ASN	CA-C-N	6.77	134.48	121.54
1	A	137	ASN	C-N-CA	6.77	134.48	121.54
2	H	40	PRO	O-C-N	6.50	129.13	121.46
1	A	23	CYS	CA-CB-SG	6.27	128.82	114.40
1	L	137	ASN	CA-C-N	5.91	132.82	121.54
1	L	137	ASN	C-N-CA	5.91	132.82	121.54
1	A	88	CYS	CA-C-N	5.89	132.79	121.54
1	A	88	CYS	C-N-CA	5.89	132.79	121.54
1	L	88	CYS	CA-C-N	5.78	132.58	121.54
1	L	88	CYS	C-N-CA	5.78	132.58	121.54
2	B	40	PRO	O-C-N	5.78	128.27	121.46
1	A	39	LYS	O-C-N	5.77	126.52	121.39
1	A	88	CYS	CA-C-O	-5.76	115.47	121.98
2	H	40	PRO	CA-C-N	5.48	126.69	119.84
2	H	40	PRO	C-N-CA	5.48	126.69	119.84
1	A	22	THR	N-CA-C	5.19	116.88	108.26
1	L	58	VAL	CA-C-O	5.18	122.56	119.19
2	B	113	SER	CA-C-N	5.13	131.33	121.54
2	B	113	SER	C-N-CA	5.13	131.33	121.54
1	A	58	VAL	CA-C-O	5.06	122.48	119.19
1	A	89	GLN	N-CA-C	5.00	121.46	110.80
1	A	89	GLN	OE1-CD-NE2	-5.00	117.60	122.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88	CYS	Peptide
1	L	88	CYS	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	1596	0	1477	155	0
1	L	1599	0	1502	130	0
2	B	1640	0	1545	147	0
2	H	1630	0	1521	157	0
3	A	1	0	0	1	0
3	B	1	0	0	1	0
3	H	2	0	0	3	0
3	L	1	0	0	0	0
4	A	21	0	14	4	0
5	A	31	0	0	5	0
5	B	25	0	0	0	0
5	H	33	0	0	6	0
5	L	30	0	0	2	0
All	All	6610	0	6059	567	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (567) 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)
2:B:125:ALA:CB	2:B:213:ARG:O	1.88	1.22
2:B:125:ALA:HB1	2:B:213:ARG:O	1.42	1.20
1:L:89:GLN:HG2	1:L:98:PHE:HA	1.40	1.04
1:A:182:THR:HG23	1:A:185:GLU:HB2	1.46	0.95
2:B:125:ALA:HB3	2:B:213:ARG:O	1.67	0.94
2:H:184:PRO:HD2	2:H:187:PRO:HG2	1.50	0.92
2:H:33:TYR:HB2	2:H:95:ASP:HB3	1.48	0.91
1:A:66:GLY:HA3	1:A:71:TYR:HA	1.55	0.88
1:A:193:THR:HG23	1:A:208:SER:HB3	1.55	0.88
1:L:193:THR:HG23	1:L:208:SER:HB3	1.53	0.87
2:B:33:TYR:HB2	2:B:95:ASP:HB3	1.56	0.86
1:L:66:GLY:HA3	1:L:71:TYR:HA	1.57	0.86
1:A:91:ARG:HH11	4:A:1214:PP3:H2A1	1.42	0.84
2:B:119:PRO:HD2	2:B:204:THR:HG21	1.57	0.84
1:L:15:PRO:HG3	1:L:106:LEU:HD11	1.62	0.82
1:L:80:ALA:HA	1:L:106:LEU:HD22	1.61	0.81
2:B:184:PRO:HD2	2:B:187:PRO:HG2	1.62	0.80
2:B:100(E):TRP:NE1	3:B:1214:IOD:I	2.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:TRP:HZ2	2:B:50:LEU:HD13	1.46	0.80
1:L:54:LEU:HD11	1:L:62:PHE:O	1.84	0.78
1:L:4:LEU:HD23	1:L:25:ALA:HA	1.67	0.77
2:B:184:PRO:O	2:B:187:PRO:HD2	1.84	0.76
1:A:157:ASN:O	1:A:159:VAL:HG23	1.86	0.76
2:H:121:VAL:HG22	2:H:142:VAL:HG13	1.68	0.76
2:H:188:ARG:HA	2:H:190:SER:H	1.50	0.76
1:A:6:GLN:HA	1:A:22:THR:O	1.86	0.75
1:L:145:ASN:HB3	1:L:197:THR:OG1	1.87	0.74
1:A:81:GLU:OE2	2:H:57:LYS:HG3	1.87	0.74
2:B:66:ARG:HD2	2:B:82(A):ASN:O	1.87	0.74
2:H:11:LEU:HD12	2:H:110:THR:HG22	1.68	0.73
2:H:125:ALA:HB1	2:H:213:ARG:O	1.89	0.73
2:H:205:LYS:HE2	5:H:2032:HOH:O	1.87	0.73
2:B:75:GLN:O	2:B:77:ILE:HG12	1.89	0.73
1:A:150:ILE:HD12	1:A:192:TYR:HD2	1.53	0.73
1:A:125:LEU:HA	1:A:129:GLY:O	1.88	0.72
1:L:121:SER:O	1:L:125:LEU:HB2	1.88	0.72
2:H:30:THR:HG23	5:H:2004:HOH:O	1.89	0.72
2:H:124:LEU:HD21	1:L:133:VAL:HG21	1.71	0.72
2:B:52(B):LYS:HE2	2:B:55:TYR:OH	1.90	0.72
2:B:119:PRO:HA	2:B:144:GLY:O	1.90	0.72
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.70	0.71
2:H:119:PRO:HB2	2:H:142:VAL:HG12	1.71	0.71
1:A:149:LYS:HA	1:A:154:GLU:HA	1.72	0.71
1:A:13:ALA:O	1:A:107:LYS:HB2	1.90	0.71
1:A:195:GLU:HA	1:A:206:VAL:HG12	1.72	0.71
2:B:13:GLN:O	2:B:16:HIS:HB2	1.91	0.71
1:L:23:CYS:O	1:L:33:MET:HE3	1.90	0.71
1:A:19:VAL:HB	1:A:75:ILE:HB	1.72	0.71
1:A:69:THR:HG23	5:A:2013:HOH:O	1.90	0.70
1:A:155:ARG:HG3	1:A:179:LEU:HD11	1.74	0.70
1:A:125:LEU:HG	1:A:183:LYS:HE3	1.71	0.70
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.73	0.70
1:L:3:GLU:O	1:L:26:THR:HG23	1.92	0.70
1:L:38:GLN:O	1:L:84:ALA:HB1	1.92	0.70
1:L:120:PRO:HB2	1:L:125:LEU:HD12	1.73	0.69
1:A:80:ALA:HB3	2:H:57:LYS:HD3	1.73	0.69
2:H:169:VAL:HG21	1:L:161:ASN:O	1.92	0.69
1:A:39:LYS:HG3	1:A:84:ALA:HB2	1.74	0.69
1:L:33:MET:SD	1:L:89:GLN:HA	2.32	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:120:PRO:HD3	1:L:132:VAL:HG22	1.73	0.69
1:L:184:ASP:O	1:L:188:ARG:HG3	1.94	0.68
2:B:11:LEU:HD12	2:B:110:THR:O	1.93	0.68
2:B:137:THR:HG23	2:B:182:THR:OG1	1.93	0.68
1:A:4:LEU:HD23	1:A:25:ALA:HB2	1.74	0.67
1:A:122:SER:O	1:A:126:THR:HG23	1.94	0.67
2:H:47:TRP:HZ2	2:H:50:LEU:HD13	1.60	0.67
2:B:118:PRO:HA	2:B:199:HIS:ND1	2.09	0.67
2:H:184:PRO:O	2:H:187:PRO:HD2	1.95	0.67
1:A:91:ARG:HD2	4:A:1214:PP3:O3	1.95	0.66
1:A:89:GLN:HG2	1:A:98:PHE:HA	1.77	0.66
1:L:39:LYS:NZ	1:L:39:LYS:HB3	2.11	0.66
2:B:166:PHE:O	2:B:177:LEU:HD22	1.96	0.65
2:H:4:LEU:HD12	2:H:24:THR:HG22	1.77	0.65
2:H:100(A):ASN:N	3:H:1214:IOD:I	3.00	0.65
1:L:1:ASP:HA	1:L:95:PRO:HD2	1.78	0.65
1:L:79:GLU:HB2	1:L:82:ASP:OD2	1.97	0.65
2:B:20:LEU:HG	2:B:82:MET:HE2	1.79	0.65
2:B:198:ALA:HA	2:B:204:THR:O	1.97	0.65
2:H:100(F):PHE:HB2	1:L:91:ARG:NH1	2.11	0.64
1:A:59:PRO:O	1:A:62:PHE:HB2	1.96	0.64
2:B:164:HIS:HB2	2:B:180:SER:OG	1.97	0.64
2:H:135:MET:SD	2:H:184:PRO:HA	2.38	0.64
2:B:144:GLY:HA2	2:B:174:LEU:HD13	1.80	0.64
1:A:131:SER:HB3	1:A:180:THR:HA	1.80	0.64
2:H:36:TRP:CE2	2:H:80:LEU:HB2	2.33	0.64
2:H:155:ASN:OD1	2:H:193:VAL:HG13	1.98	0.64
1:L:121:SER:OG	1:L:124:GLN:HB3	1.98	0.64
1:A:21:ILE:O	1:A:72:SER:HA	1.97	0.64
2:H:100(C):GLU:HA	1:L:49:TYR:CZ	2.33	0.63
2:H:100(E):TRP:NE1	3:H:1214:IOD:I	2.99	0.63
1:A:150:ILE:HD12	1:A:192:TYR:CD2	2.34	0.63
1:A:80:ALA:HA	1:A:106:LEU:HD22	1.81	0.62
2:B:51:ILE:HD13	2:B:71:ARG:HG2	1.81	0.62
2:H:20:LEU:HG	2:H:82:MET:HE2	1.79	0.62
2:H:123:PRO:HD3	2:H:208:LYS:HZ2	1.63	0.62
1:L:59:PRO:HB3	1:L:61:ARG:NH1	2.13	0.62
1:L:192:TYR:HB2	1:L:209:PHE:CE2	2.35	0.62
1:A:185:GLU:HG2	5:A:2026:HOH:O	2.00	0.61
2:H:34:MET:HB2	2:H:78:LEU:HD13	1.82	0.61
1:L:34:HIS:CE1	1:L:50:SER:H	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:TRP:CZ3	2:B:195:CYS:HB2	2.35	0.61
1:A:149:LYS:O	1:A:150:ILE:HD13	2.00	0.61
2:B:96:LYS:HA	2:B:100(E):TRP:CG	2.36	0.61
2:B:14:PRO:HD3	2:B:113:SER:N	2.16	0.61
2:B:33:TYR:CE2	2:B:52:ARG:HG2	2.36	0.60
1:L:108:ARG:HD3	1:L:171:SER:O	2.00	0.60
1:L:61:ARG:NE	1:L:79:GLU:HG3	2.17	0.60
2:B:117:THR:O	2:B:145:TYR:HA	2.00	0.60
1:L:162:SER:HB3	1:L:176:SER:HB3	1.84	0.60
2:B:67:PHE:CD1	2:B:82:MET:HA	2.37	0.60
1:A:124:GLN:OE1	1:A:130:ALA:HA	2.02	0.60
2:B:121:VAL:HG22	2:B:142:VAL:HG13	1.83	0.59
1:L:204:PRO:O	1:L:206:VAL:HG13	2.02	0.59
1:A:34:HIS:CG	1:A:91:ARG:HH21	2.21	0.59
2:H:11:LEU:HG	2:H:12:VAL:N	2.18	0.59
1:A:23:CYS:HB3	1:A:33:MET:CE	2.33	0.58
2:H:154:TRP:HA	2:H:194:THR:O	2.03	0.58
1:L:21:ILE:O	1:L:72:SER:HA	2.03	0.58
1:A:48:ILE:HD13	1:A:64:GLY:HA3	1.84	0.58
1:A:161:ASN:HB3	1:A:175:MET:HE3	1.84	0.58
2:B:11:LEU:HB2	2:B:147:PRO:HG3	1.86	0.58
2:H:188:ARG:HA	2:H:190:SER:N	2.18	0.58
2:B:188:ARG:HA	2:B:190:SER:H	1.68	0.58
2:B:47:TRP:CZ2	2:B:50:LEU:HD13	2.34	0.58
2:B:170:LEU:HD13	2:B:175:TYR:CE1	2.39	0.58
2:H:196:ASN:HB3	2:H:207:ASP:OD2	2.02	0.58
2:B:144:GLY:HA2	2:B:174:LEU:CD1	2.34	0.57
2:H:69:ILE:HG12	2:H:80:LEU:HD12	1.85	0.57
2:H:142:VAL:HG11	2:H:197:VAL:HG11	1.86	0.57
2:B:5:GLN:O	2:B:22:CYS:HA	2.03	0.57
1:L:6:GLN:HA	1:L:22:THR:O	2.04	0.57
2:H:3:LYS:HZ3	2:H:3:LYS:HB2	1.69	0.57
2:H:143:LYS:HB2	2:H:176:THR:OG1	2.05	0.57
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.40	0.57
1:L:182:THR:HG23	1:L:185:GLU:HB2	1.86	0.57
2:B:35:SER:HA	2:B:50:LEU:HA	1.87	0.57
2:H:29:PHE:CD2	2:H:76:SER:HA	2.40	0.57
2:H:194:THR:HG23	2:H:209:LYS:CA	2.34	0.57
1:A:4:LEU:HD13	1:A:89:GLN:HB2	1.87	0.56
2:H:96:LYS:HA	2:H:100(E):TRP:CD1	2.40	0.56
2:H:135:MET:HB3	2:H:182:THR:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:178:SER:HB2	1:L:135:PHE:HE1	1.70	0.56
2:B:149:PRO:O	2:B:200:PRO:HD2	2.04	0.56
2:H:100(F):PHE:HB2	1:L:91:ARG:HH12	1.70	0.56
2:H:100(A):ASN:HB2	3:H:1214:IOD:I	2.76	0.56
2:B:69:ILE:HG12	2:B:80:LEU:CD1	2.36	0.56
1:L:149:LYS:O	1:L:150:ILE:HD13	2.05	0.56
1:A:185:GLU:HA	1:A:188:ARG:NE	2.21	0.56
1:A:119:PRO:HB3	1:A:209:PHE:CE1	2.40	0.56
2:H:100(C):GLU:HA	1:L:49:TYR:CE1	2.40	0.56
1:L:37:GLN:HG3	1:L:86:TYR:CZ	2.40	0.56
1:L:55:ALA:O	1:L:58:VAL:HG23	2.05	0.56
2:H:63:VAL:HB	2:H:67:PHE:CD2	2.41	0.56
1:L:147:LYS:O	1:L:195:GLU:HB3	2.06	0.56
2:B:83:ARG:O	2:B:111:VAL:HG21	2.06	0.55
2:B:118:PRO:HB3	2:B:202:SER:OG	2.06	0.55
2:B:66:ARG:CD	2:B:82(B):ALA:HB3	2.37	0.55
2:B:100(A):ASN:O	2:B:100(D):ALA:HB3	2.06	0.55
2:B:147:PRO:HD2	2:B:201:ALA:CB	2.36	0.55
2:B:119:PRO:CB	2:B:145:TYR:HB3	2.36	0.55
2:B:11:LEU:HG	2:B:12:VAL:N	2.20	0.55
2:B:89:THR:HA	2:B:107:THR:O	2.07	0.55
1:A:199:LYS:O	1:A:199:LYS:HG3	2.06	0.54
2:H:52:ARG:HB3	2:H:53:ASN:HB2	1.89	0.54
1:A:204:PRO:O	1:A:206:VAL:HG13	2.08	0.54
1:L:195:GLU:HG3	1:L:204:PRO:HB2	1.89	0.54
1:A:123:GLU:HA	1:A:126:THR:OG1	2.07	0.54
2:H:151:THR:HG22	2:H:198:ALA:HB3	1.89	0.54
2:H:145:TYR:CE1	2:H:150:VAL:HG13	2.42	0.54
2:B:116:THR:HG22	2:B:146:PHE:O	2.08	0.54
2:H:20:LEU:HG	2:H:82:MET:CE	2.38	0.54
1:L:163:TRP:CE2	1:L:175:MET:HE3	2.43	0.54
2:B:69:ILE:HG12	2:B:80:LEU:HD12	1.90	0.54
1:L:193:THR:CG2	1:L:208:SER:HB3	2.33	0.54
2:B:87:SER:HA	2:B:109:VAL:O	2.08	0.53
1:A:185:GLU:O	1:A:188:ARG:HD2	2.08	0.53
2:H:40:PRO:O	2:H:43:LYS:HB2	2.09	0.53
1:A:195:GLU:CG	1:A:204:PRO:HB2	2.37	0.53
2:B:140:CYS:O	2:B:178:SER:HA	2.08	0.53
2:B:151:THR:HG22	2:B:198:ALA:HB3	1.89	0.53
1:L:136:LEU:HD12	1:L:175:MET:O	2.07	0.53
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:PRO:HD2	2:B:204:THR:CG2	2.35	0.53
2:B:184:PRO:HD2	2:B:187:PRO:CG	2.34	0.53
1:A:4:LEU:CD2	1:A:25:ALA:HB2	2.38	0.53
1:L:88:CYS:SG	1:L:99:GLY:HA3	2.48	0.53
1:A:35:TRP:CH2	1:A:88:CYS:HB3	2.44	0.53
2:H:125:ALA:O	2:H:126:PRO:O	2.27	0.53
1:A:187:GLU:HA	1:A:211:ARG:CZ	2.39	0.52
1:A:195:GLU:HG3	1:A:204:PRO:HB2	1.91	0.52
2:H:66:ARG:HD2	2:H:82(A):ASN:O	2.09	0.52
1:L:123:GLU:O	1:L:127:SER:HB2	2.10	0.52
1:L:145:ASN:O	1:L:196:ALA:HA	2.09	0.52
2:B:17:SER:OG	2:B:82(A):ASN:OD1	2.27	0.52
2:B:31:ASP:HB3	2:B:98:SER:OG	2.10	0.52
2:B:84:ALA:HA	2:B:111:VAL:HB	1.90	0.52
2:H:11:LEU:HD11	2:H:112:SER:HB3	1.91	0.52
2:H:199:HIS:NE2	2:H:201:ALA:HB3	2.25	0.52
1:A:48:ILE:HD13	1:A:64:GLY:CA	2.39	0.52
1:A:39:LYS:HG3	1:A:84:ALA:CB	2.40	0.52
1:L:190:ASN:OD1	1:L:211:ARG:O	2.28	0.52
2:B:118:PRO:HB3	2:B:204:THR:OG1	2.10	0.52
2:B:146:PHE:H	2:B:199:HIS:CE1	2.28	0.52
1:A:135:PHE:HE1	2:B:178:SER:HB2	1.75	0.51
2:H:117:THR:O	2:H:145:TYR:HA	2.10	0.51
2:H:195:CYS:O	2:H:207:ASP:HA	2.10	0.51
2:B:89:THR:HG23	2:B:107:THR:C	2.36	0.51
1:A:33:MET:SD	1:A:89:GLN:HA	2.50	0.51
1:A:49:TYR:HD1	1:A:50:SER:HG	1.56	0.51
1:A:91:ARG:HA	1:A:96:PHE:CD2	2.45	0.51
1:L:88:CYS:O	1:L:89:GLN:HG3	2.11	0.51
1:A:113:PRO:CA	1:A:139:PHE:HB3	2.41	0.51
2:B:124:LEU:HB2	2:B:139:GLY:C	2.36	0.51
2:B:183:VAL:HB	2:B:187:PRO:HG2	1.91	0.51
2:H:168:ALA:HB2	2:H:177:LEU:HD23	1.93	0.51
1:L:19:VAL:HB	1:L:75:ILE:HB	1.92	0.51
2:H:194:THR:HG23	2:H:209:LYS:HA	1.93	0.51
2:H:204:THR:HG22	2:H:204:THR:O	2.11	0.51
2:B:118:PRO:O	2:B:144:GLY:O	2.29	0.51
2:H:152:VAL:HG11	2:H:179:SER:OG	2.10	0.51
1:A:13:ALA:C	1:A:107:LYS:HB2	2.35	0.51
2:B:135:MET:HB3	2:B:182:THR:CG2	2.41	0.50
1:L:163:TRP:CZ2	1:L:175:MET:HE3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLU:HA	1:A:188:ARG:HD2	1.92	0.50
1:A:38:GLN:O	1:A:84:ALA:HB1	2.12	0.50
2:B:29:PHE:CD2	2:B:76:SER:HA	2.46	0.50
2:H:63:VAL:HG23	2:H:63:VAL:O	2.11	0.50
2:H:124:LEU:HB2	2:H:139:GLY:C	2.36	0.50
2:H:170:LEU:HD21	2:H:173:ASP:HA	1.94	0.50
1:A:19:VAL:O	1:A:74:THR:HA	2.10	0.50
1:A:185:GLU:HA	1:A:188:ARG:CD	2.41	0.50
2:B:191:GLU:O	2:B:192:THR:HB	2.12	0.50
1:A:89:GLN:OE1	1:A:97:THR:O	2.30	0.50
2:B:113:SER:O	2:B:114:ALA:O	2.30	0.50
2:H:52:ARG:HD3	2:H:53:ASN:HB3	1.93	0.50
2:H:118:PRO:O	2:H:144:GLY:O	2.29	0.50
1:A:145:ASN:OD1	1:A:146:VAL:O	2.30	0.50
1:A:54:LEU:HD11	1:A:62:PHE:O	2.11	0.50
2:B:50:LEU:HD12	2:B:95:ASP:OD2	2.12	0.50
2:B:184:PRO:C	2:B:187:PRO:HD2	2.36	0.50
1:L:166:GLN:HG2	1:L:171:SER:HA	1.93	0.50
1:A:75:ILE:O	1:A:75:ILE:HG22	2.12	0.50
1:A:34:HIS:CE1	1:A:50:SER:H	2.30	0.49
2:B:30:THR:O	2:B:52(A):ASN:HB2	2.11	0.49
2:H:123:PRO:HD3	2:H:208:LYS:NZ	2.27	0.49
2:H:124:LEU:HD21	1:L:133:VAL:HG11	1.93	0.49
2:H:203:SER:O	2:H:203:SER:OG	2.30	0.49
1:L:34:HIS:HD2	1:L:91:ARG:HG3	1.76	0.49
1:L:210:ASN:OD1	1:L:212:ASN:OD1	2.30	0.49
2:B:63:VAL:HG23	2:B:63:VAL:O	2.11	0.49
2:B:185:SER:HA	2:B:188:ARG:O	2.12	0.49
2:H:33:TYR:CE2	2:H:52:ARG:HG2	2.47	0.49
1:L:157:ASN:O	1:L:159:VAL:HG23	2.12	0.49
1:A:23:CYS:O	1:A:33:MET:HE3	2.13	0.49
1:A:140:TYR:O	1:A:198:HIS:HE1	1.95	0.49
2:H:100(B):TYR:HA	2:H:100(E):TRP:CD2	2.48	0.49
2:H:116:THR:HG22	2:H:146:PHE:O	2.13	0.49
1:A:133:VAL:HG21	2:B:124:LEU:HD11	1.94	0.49
2:B:66:ARG:HD2	2:B:82(B):ALA:HB3	1.93	0.49
2:H:28:THR:HG22	2:H:28:THR:O	2.11	0.49
1:L:185:GLU:O	1:L:189:HIS:HD2	1.96	0.49
1:L:187:GLU:HA	1:L:211:ARG:CZ	2.42	0.49
1:A:50:SER:O	1:A:51:THR:HB	2.11	0.49
2:H:90:TYR:O	2:H:106:GLY:HA2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:154:TRP:HZ2	2:H:179:SER:O	1.96	0.49
2:H:184:PRO:C	2:H:187:PRO:HD2	2.37	0.49
1:L:34:HIS:HB2	1:L:89:GLN:O	2.13	0.49
2:B:132:THR:O	2:B:133:ASN:O	2.30	0.49
2:H:194:THR:HG23	2:H:209:LYS:N	2.28	0.49
1:A:35:TRP:CZ3	1:A:88:CYS:HB3	2.47	0.49
1:A:94:TYR:CD2	2:B:58:GLU:HG2	2.48	0.49
1:A:167:ASP:HB3	1:A:170:ASP:OD1	2.12	0.49
2:H:145:TYR:OH	2:H:148:GLU:OE1	2.30	0.49
2:H:168:ALA:HA	2:H:177:LEU:HB3	1.95	0.49
1:L:120:PRO:HA	1:L:131:SER:O	2.13	0.49
1:A:136:LEU:HD13	1:A:175:MET:HB3	1.94	0.49
2:B:124:LEU:HD11	2:B:141:LEU:HB2	1.95	0.49
1:A:61:ARG:HG2	3:A:1213:IOD:I	2.83	0.48
1:A:117:ILE:HG13	1:A:134:CYS:HB2	1.95	0.48
1:A:151:ASP:OD2	1:A:189:HIS:HB3	2.14	0.48
1:A:155:ARG:HG3	1:A:179:LEU:CD1	2.43	0.48
1:A:145:ASN:ND2	5:A:2019:HOH:O	2.47	0.48
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.95	0.48
2:H:132:THR:O	2:H:133:ASN:O	2.31	0.48
1:L:111:ALA:C	1:L:200:THR:HG21	2.38	0.48
2:B:3:LYS:HB2	2:B:3:LYS:HZ3	1.78	0.48
2:B:154:TRP:HE1	2:B:163:VAL:HG13	1.78	0.48
1:L:150:ILE:HD12	1:L:192:TYR:CD2	2.48	0.48
1:L:3:GLU:HB3	1:L:26:THR:HG21	1.95	0.48
1:L:111:ALA:HB3	1:L:140:TYR:N	2.28	0.48
4:A:1214:PP3:H2A3	2:B:95:ASP:OD1	2.14	0.48
1:L:90:GLN:HE21	1:L:97:THR:H	1.62	0.48
1:A:93:THR:HG22	1:A:94:TYR:O	2.13	0.48
1:A:195:GLU:HG3	1:A:206:VAL:HG12	1.95	0.48
2:H:30:THR:O	2:H:52(A):ASN:HB2	2.13	0.48
1:A:44:PRO:HD2	2:B:103:TRP:CE3	2.49	0.48
2:B:170:LEU:HB2	2:B:175:TYR:HE1	1.79	0.48
2:H:12:VAL:HG21	2:H:82(C):LEU:HD13	1.96	0.48
2:B:33:TYR:CB	2:B:95:ASP:HB3	2.37	0.48
2:H:173:ASP:O	2:H:174:LEU:HD23	2.14	0.48
1:A:160:LEU:HD11	2:B:171:GLN:CD	2.39	0.48
1:A:196:ALA:O	1:A:204:PRO:HA	2.13	0.47
2:H:83:ARG:O	2:H:111:VAL:HG21	2.14	0.47
2:H:202:SER:OG	2:H:204:THR:HB	2.13	0.47
1:L:75:ILE:HG22	1:L:75:ILE:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:80:ALA:CA	1:L:106:LEU:HD22	2.39	0.47
1:L:106:LEU:HG	1:L:107:LYS:N	2.29	0.47
1:A:90:GLN:HE21	1:A:97:THR:H	1.61	0.47
2:B:39:GLN:O	2:B:88:ALA:HB1	2.15	0.47
1:L:39:LYS:O	1:L:42:THR:OG1	2.30	0.47
1:L:135:PHE:HB3	1:L:137:ASN:HD21	1.78	0.47
1:A:124:GLN:HG2	1:A:125:LEU:N	2.30	0.47
1:L:47:TRP:CE2	1:L:58:VAL:HG13	2.50	0.47
1:A:90:GLN:HE21	1:A:97:THR:N	2.13	0.47
2:B:170:LEU:HB2	2:B:175:TYR:CE1	2.49	0.47
1:A:133:VAL:HG12	1:A:134:CYS:H	1.78	0.47
2:B:143:LYS:HA	2:B:176:THR:OG1	2.15	0.47
2:H:51:ILE:HD13	2:H:71:ARG:HG2	1.96	0.47
2:H:52(B):LYS:HB3	5:H:2005:HOH:O	2.14	0.47
1:L:45:LYS:HE3	5:L:2006:HOH:O	2.15	0.47
2:B:100(B):TYR:HA	2:B:100(E):TRP:CG	2.49	0.47
2:B:199:HIS:HB3	2:B:204:THR:HB	1.97	0.47
2:H:33:TYR:CE2	2:H:96:LYS:HD3	2.50	0.47
2:H:69:ILE:HG23	2:H:79:TYR:O	2.14	0.47
1:L:125:LEU:O	1:L:183:LYS:NZ	2.46	0.47
1:A:6:GLN:OE1	1:A:87:TYR:HA	2.15	0.47
1:L:139:PHE:HD2	1:L:198:HIS:HE2	1.62	0.47
1:A:55:ALA:O	1:A:58:VAL:HG23	2.15	0.46
1:A:149:LYS:HG2	1:A:154:GLU:HA	1.96	0.46
2:B:3:LYS:O	2:B:4:LEU:HD13	2.15	0.46
2:B:11:LEU:HD12	2:B:110:THR:HG22	1.97	0.46
2:H:66:ARG:HG2	2:H:82(A):ASN:O	2.15	0.46
1:A:39:LYS:NZ	1:A:39:LYS:HB2	2.23	0.46
1:A:113:PRO:HA	1:A:139:PHE:HB3	1.97	0.46
1:L:6:GLN:CD	1:L:101:GLY:H	2.22	0.46
1:A:148:TRP:O	1:A:154:GLU:HA	2.15	0.46
1:A:185:GLU:OE1	1:A:189:HIS:NE2	2.48	0.46
2:H:12:VAL:HG21	2:H:82(C):LEU:CD1	2.46	0.46
2:H:124:LEU:HD23	1:L:135:PHE:CZ	2.51	0.46
1:L:4:LEU:HD23	1:L:25:ALA:CA	2.41	0.46
1:L:134:CYS:SG	1:L:194:CYS:CB	3.04	0.46
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.80	0.46
2:H:164:HIS:HB2	2:H:180:SER:OG	2.15	0.46
1:L:4:LEU:HD11	1:L:90:GLN:HG2	1.98	0.46
1:A:4:LEU:HD13	1:A:89:GLN:CB	2.46	0.46
2:B:194:THR:CG2	2:B:207:ASP:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:182:THR:OG1	1:L:184:ASP:OD1	2.30	0.46
2:B:123:PRO:HD3	2:B:208:LYS:NZ	2.31	0.46
2:H:205:LYS:HD3	5:H:2030:HOH:O	2.16	0.46
2:H:208:LYS:HD2	2:H:208:LYS:HA	1.59	0.46
2:B:185:SER:O	2:B:188:ARG:O	2.33	0.46
1:A:170:ASP:OD2	1:A:172:THR:OG1	2.30	0.46
2:H:100(E):TRP:O	2:H:100(F):PHE:HB2	2.16	0.46
2:B:84:ALA:O	2:B:87:SER:HB2	2.15	0.45
2:B:204:THR:O	2:B:204:THR:HG22	2.16	0.45
2:H:69:ILE:HG12	2:H:80:LEU:CD1	2.46	0.45
2:H:116:THR:HG23	2:H:147:PRO:HD3	1.98	0.45
2:H:176:THR:O	2:H:176:THR:HG22	2.16	0.45
1:L:140:TYR:CG	1:L:141:PRO:HA	2.52	0.45
2:B:154:TRP:HZ2	2:B:179:SER:O	1.99	0.45
2:H:57:LYS:HB2	2:H:59:TYR:CE2	2.51	0.45
2:H:100(B):TYR:HB3	2:H:100(E):TRP:CE3	2.51	0.45
1:L:83:ALA:O	1:L:84:ALA:HB2	2.16	0.45
1:A:139:PHE:CE1	1:A:174:SER:HA	2.51	0.45
1:A:139:PHE:CZ	1:A:144:ILE:HG21	2.52	0.45
2:H:57:LYS:NZ	2:H:69:ILE:O	2.50	0.45
1:A:30:VAL:HG11	1:A:90:GLN:HB3	1.98	0.45
1:A:33:MET:O	1:A:51:THR:HA	2.17	0.45
1:A:83:ALA:O	1:A:84:ALA:HB2	2.16	0.45
1:A:193:THR:HG23	1:A:207:LYS:O	2.16	0.45
2:H:34:MET:CB	2:H:78:LEU:HD13	2.44	0.45
2:H:183:VAL:HG11	2:H:193:VAL:HG21	1.98	0.45
2:H:199:HIS:HB3	2:H:204:THR:HB	1.99	0.45
1:L:34:HIS:CD2	1:L:91:ARG:HG3	2.52	0.45
1:L:186:TYR:O	1:L:192:TYR:OH	2.30	0.45
1:A:59:PRO:HD2	1:A:62:PHE:CD2	2.52	0.45
1:A:212:ASN:ND2	5:A:2029:HOH:O	2.50	0.45
2:H:31:ASP:HB3	2:H:98:SER:OG	2.16	0.45
2:H:96:LYS:HZ3	2:H:96:LYS:HG3	1.71	0.45
1:L:13:ALA:HB1	1:L:17:GLU:OE2	2.16	0.45
1:L:106:LEU:O	1:L:166:GLN:NE2	2.50	0.45
1:L:150:ILE:HA	1:L:191:SER:O	2.16	0.45
1:A:145:ASN:OD1	1:A:146:VAL:N	2.50	0.45
2:B:39:GLN:NE2	2:B:43:LYS:O	2.50	0.45
2:H:32:TYR:O	2:H:71:ARG:NH2	2.50	0.45
2:H:134:SER:O	2:H:185:SER:N	2.49	0.45
1:A:80:ALA:HA	1:A:106:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.97	0.45
2:H:186:SER:O	2:H:190:SER:OG	2.30	0.45
1:A:15:PRO:HD3	1:A:107:LYS:O	2.17	0.45
1:A:150:ILE:O	1:A:151:ASP:HB2	2.17	0.45
1:A:153:SER:O	1:A:154:GLU:O	2.35	0.45
2:B:96:LYS:NZ	2:B:97:GLY:O	2.50	0.45
2:B:154:TRP:NE1	2:B:163:VAL:HG13	2.32	0.45
2:H:21:SER:OG	2:H:77:ILE:HG21	2.17	0.45
2:H:70:SER:OG	2:H:79:TYR:HB2	2.16	0.45
1:A:33:MET:HB2	1:A:71:TYR:CD2	2.51	0.45
1:A:207:LYS:O	1:A:208:SER:HB3	2.16	0.45
2:H:119:PRO:CB	2:H:145:TYR:HB3	2.43	0.45
1:A:123:GLU:O	1:A:127:SER:N	2.50	0.44
2:B:24:THR:HG21	2:B:29:PHE:CE1	2.52	0.44
2:B:100(B):TYR:HA	2:B:100(E):TRP:CD2	2.53	0.44
1:A:124:GLN:HB2	2:B:122:TYR:CD2	2.51	0.44
2:H:199:HIS:O	2:H:203:SER:N	2.50	0.44
1:L:11:MET:HE2	1:L:11:MET:HB2	1.88	0.44
1:L:89:GLN:HB2	1:L:97:THR:O	2.17	0.44
1:L:195:GLU:CG	1:L:204:PRO:HB2	2.47	0.44
1:A:23:CYS:HB3	1:A:33:MET:SD	2.57	0.44
1:A:133:VAL:HG12	1:A:134:CYS:N	2.32	0.44
2:H:11:LEU:HD12	2:H:110:THR:CG2	2.43	0.44
1:L:75:ILE:HG21	1:L:78:MET:HA	1.99	0.44
1:L:195:GLU:HA	1:L:206:VAL:HG12	1.99	0.44
1:A:3:GLU:OE1	1:A:26:THR:HG23	2.17	0.44
2:B:100(A):ASN:N	2:B:100(A):ASN:OD1	2.50	0.44
2:H:144:GLY:HA2	2:H:174:LEU:HD13	1.99	0.44
1:A:11:MET:HE2	1:A:11:MET:HB2	1.88	0.44
2:B:35:SER:HA	2:B:50:LEU:HB3	1.99	0.44
2:B:40:PRO:HA	2:B:41:PRO:HD2	1.73	0.44
2:B:199:HIS:N	2:B:204:THR:O	2.50	0.44
1:L:67:SER:HA	1:L:71:TYR:CZ	2.53	0.44
1:A:121:SER:OG	1:A:123:GLU:OE2	2.30	0.44
1:A:125:LEU:CG	1:A:183:LYS:HE3	2.45	0.44
1:A:142:LYS:NZ	1:A:164:THR:O	2.50	0.44
1:A:201:SER:HB2	1:A:205:ILE:HD11	2.00	0.44
2:H:38:ARG:NH1	2:H:86:ASP:HB3	2.32	0.44
1:A:30:VAL:HG11	1:A:90:GLN:CB	2.47	0.44
4:A:1214:PP3:O3	4:A:1214:PP3:N	2.50	0.44
2:H:170:LEU:HD12	2:H:174:LEU:C	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:21:ILE:HG13	1:L:73:LEU:HD22	1.99	0.44
1:A:106:LEU:HG	1:A:107:LYS:N	2.32	0.44
2:H:134:SER:O	2:H:184:PRO:HA	2.18	0.44
1:L:3:GLU:N	1:L:26:THR:OG1	2.50	0.44
1:A:34:HIS:O	1:A:89:GLN:N	2.50	0.43
1:A:43:SER:OG	2:B:104:GLY:O	2.29	0.43
2:H:100(B):TYR:HA	2:H:100(E):TRP:CG	2.52	0.43
1:L:193:THR:HG23	1:L:207:LYS:O	2.17	0.43
1:A:23:CYS:HB3	1:A:33:MET:HE3	2.00	0.43
1:A:33:MET:HB2	1:A:71:TYR:CG	2.53	0.43
2:H:13:GLN:O	2:H:16:HIS:HB2	2.18	0.43
1:A:120:PRO:HD3	1:A:132:VAL:HG22	1.99	0.43
2:H:40:PRO:O	2:H:43:LYS:N	2.50	0.43
2:H:139:GLY:O	2:H:210:ILE:HD12	2.19	0.43
2:B:3:LYS:C	2:B:4:LEU:HD13	2.43	0.43
1:A:4:LEU:HB3	1:A:23:CYS:SG	2.59	0.43
1:A:81:GLU:CD	2:H:57:LYS:HG3	2.42	0.43
2:B:105:GLN:CD	2:B:105:GLN:H	2.26	0.43
2:B:140:CYS:O	2:B:179:SER:N	2.50	0.43
2:B:154:TRP:HB2	2:B:159:LEU:CB	2.48	0.43
1:A:37:GLN:HB2	1:A:86:TYR:CE2	2.54	0.43
1:A:39:LYS:HB2	1:A:39:LYS:HE3	1.64	0.43
1:L:151:ASP:N	1:L:151:ASP:OD1	2.50	0.43
1:A:6:GLN:CD	1:A:101:GLY:H	2.27	0.43
1:A:119:PRO:HB3	1:A:209:PHE:CZ	2.52	0.43
2:B:152:VAL:O	2:B:152:VAL:HG12	2.17	0.43
2:B:169:VAL:O	2:B:175:TYR:HA	2.19	0.43
2:B:173:ASP:O	2:B:174:LEU:HD23	2.18	0.43
2:H:151:THR:HG23	5:H:2029:HOH:O	2.17	0.43
1:L:132:VAL:HB	1:L:148:TRP:CZ3	2.54	0.43
1:A:194:CYS:O	1:A:206:VAL:HB	2.18	0.43
2:B:151:THR:O	2:B:197:VAL:HA	2.17	0.43
1:L:2:ILE:O	1:L:97:THR:OG1	2.30	0.43
1:A:193:THR:CG2	1:A:208:SER:HB3	2.38	0.43
2:B:28:THR:O	2:B:28:THR:HG22	2.19	0.43
2:H:57:LYS:NZ	2:H:57:LYS:HB3	2.34	0.43
1:L:34:HIS:N	1:L:89:GLN:O	2.48	0.43
1:A:22:THR:O	1:A:22:THR:OG1	2.36	0.42
1:A:118:PHE:O	1:A:132:VAL:HG13	2.19	0.42
2:B:116:THR:HG23	2:B:147:PRO:HD3	2.00	0.42
2:B:151:THR:HG22	2:B:198:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:143:LYS:HA	2:H:176:THR:OG1	2.18	0.42
1:L:2:ILE:O	1:L:97:THR:HG21	2.18	0.42
1:A:194:CYS:O	1:A:206:VAL:HA	2.18	0.42
1:L:3:GLU:HA	5:L:2001:HOH:O	2.18	0.42
1:L:6:GLN:OE1	1:L:87:TYR:HA	2.19	0.42
1:L:33:MET:HB2	1:L:71:TYR:CG	2.54	0.42
1:A:45:LYS:HE3	5:A:2010:HOH:O	2.19	0.42
1:A:49:TYR:HD1	1:A:50:SER:OG	2.02	0.42
2:B:146:PHE:HA	2:B:147:PRO:HA	1.72	0.42
2:B:208:LYS:HA	2:B:208:LYS:HD2	1.62	0.42
2:H:198:ALA:HB2	5:H:2030:HOH:O	2.19	0.42
1:A:189:HIS:O	1:A:211:ARG:NH2	2.50	0.42
2:B:52:ARG:NH2	2:B:58:GLU:OE2	2.50	0.42
2:H:36:TRP:HD1	2:H:69:ILE:HD13	1.84	0.42
1:L:105:GLU:OE2	1:L:142:LYS:HE3	2.19	0.42
1:L:205:ILE:H	1:L:205:ILE:HG13	1.59	0.42
2:B:162:GLY:O	2:B:181:VAL:HA	2.20	0.42
2:H:166:PHE:HB3	1:L:162:SER:OG	2.19	0.42
2:H:17:SER:HA	2:H:82:MET:O	2.18	0.42
2:H:154:TRP:CD1	2:H:163:VAL:HG11	2.55	0.42
2:H:154:TRP:CZ3	2:H:195:CYS:HB2	2.55	0.42
1:L:4:LEU:HD11	1:L:90:GLN:CG	2.50	0.42
1:A:80:ALA:CA	1:A:106:LEU:HD22	2.49	0.42
2:B:196:ASN:HD22	2:B:207:ASP:CG	2.28	0.42
1:L:34:HIS:O	1:L:89:GLN:N	2.49	0.42
1:L:186:TYR:CE1	1:L:211:ARG:HD3	2.55	0.42
2:B:146:PHE:CE2	2:B:147:PRO:HB3	2.55	0.42
1:L:149:LYS:NZ	1:L:195:GLU:OE1	2.50	0.42
2:B:152:VAL:HG11	2:B:179:SER:OG	2.20	0.42
1:L:81:GLU:H	1:L:81:GLU:HG3	1.38	0.42
2:B:199:HIS:O	2:B:203:SER:N	2.53	0.41
2:H:37:VAL:HG12	2:H:38:ARG:N	2.34	0.41
2:H:57:LYS:HB3	2:H:57:LYS:HZ3	1.83	0.41
1:L:160:LEU:HD23	1:L:160:LEU:N	2.35	0.41
2:H:2:VAL:HB	2:H:102:TYR:CD1	2.54	0.41
1:L:118:PHE:O	1:L:132:VAL:HG13	2.20	0.41
1:A:33:MET:HE3	1:A:71:TYR:HB2	2.01	0.41
2:H:126:PRO:HD3	2:H:138:LEU:CD2	2.51	0.41
1:L:197:THR:HG22	1:L:204:PRO:HB3	2.02	0.41
1:A:14:SER:HA	1:A:107:LYS:HB2	2.03	0.41
1:A:186:TYR:O	1:A:192:TYR:OH	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:133:VAL:HG12	1:L:134:CYS:N	2.34	0.41
1:A:14:SER:O	1:A:78:MET:HB3	2.21	0.41
1:A:62:PHE:CE1	1:A:75:ILE:HG12	2.55	0.41
2:B:2:VAL:HB	2:B:102:TYR:CE1	2.55	0.41
2:B:3:LYS:HB3	2:B:25:SER:OG	2.20	0.41
2:B:96:LYS:HA	2:B:100(E):TRP:CD1	2.56	0.41
1:L:189:HIS:O	1:L:211:ARG:NE	2.50	0.41
2:B:20:LEU:HB2	2:B:80:LEU:HB3	2.01	0.41
2:B:94:ARG:HE	2:B:94:ARG:HB3	1.67	0.41
2:B:187:PRO:O	2:B:191:GLU:N	2.46	0.41
2:H:187:PRO:O	2:H:190:SER:OG	2.39	0.41
1:L:21:ILE:CG1	1:L:73:LEU:HD22	2.51	0.41
1:A:144:ILE:O	1:A:144:ILE:HG23	2.20	0.41
1:A:166:GLN:HG2	1:A:171:SER:C	2.46	0.41
2:B:20:LEU:CG	2:B:82:MET:HE2	2.48	0.41
2:H:170:LEU:CD2	2:H:173:ASP:HA	2.50	0.41
1:L:58:VAL:HA	1:L:59:PRO:HD3	1.95	0.41
1:L:189:HIS:O	1:L:211:ARG:NH2	2.50	0.41
1:A:123:GLU:HB2	2:B:122:TYR:CD1	2.55	0.41
2:B:36:TRP:CD1	2:B:80:LEU:HD13	2.56	0.41
2:B:72:ASP:OD2	2:B:74:SER:OG	2.30	0.41
2:B:100(D):ALA:O	2:B:100(E):TRP:HB2	2.20	0.41
2:H:137:THR:O	2:H:138:LEU:HD23	2.20	0.41
2:H:163:VAL:HG12	2:H:164:HIS:N	2.36	0.41
1:L:23:CYS:SG	1:L:88:CYS:C	3.03	0.41
1:A:96:PHE:HB2	2:B:47:TRP:CD2	2.55	0.41
1:A:122:SER:O	1:A:126:THR:N	2.50	0.41
1:A:150:ILE:HG22	1:A:189:HIS:HB3	2.02	0.41
2:B:194:THR:HG21	2:B:207:ASP:HB3	2.03	0.41
2:B:205:LYS:HB2	2:B:205:LYS:HE3	1.16	0.41
2:H:6:GLU:HG3	2:H:92:CYS:SG	2.61	0.41
2:H:11:LEU:CD1	2:H:112:SER:HB3	2.50	0.41
2:H:32:TYR:HD2	2:H:95:ASP:O	2.04	0.41
2:H:39:GLN:HA	2:H:40:PRO:HD3	1.82	0.41
1:L:4:LEU:HB2	1:L:99:GLY:HA2	2.03	0.41
1:L:75:ILE:HG21	1:L:75:ILE:HD13	1.85	0.41
1:L:137:ASN:HA	1:L:174:SER:HB3	2.02	0.41
2:B:124:LEU:HB2	2:B:139:GLY:CA	2.51	0.41
2:H:38:ARG:HA	2:H:89:THR:O	2.21	0.41
2:H:38:ARG:HB3	2:H:48:LEU:HD11	2.02	0.41
1:L:47:TRP:CZ2	1:L:58:VAL:HG13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:79:GLU:O	1:L:82:ASP:HB2	2.21	0.41
1:A:139:PHE:HD2	1:A:198:HIS:HE2	1.69	0.40
2:H:35:SER:HA	2:H:50:LEU:HA	2.03	0.40
2:H:39:GLN:NE2	2:H:43:LYS:O	2.50	0.40
2:H:40:PRO:HA	2:H:41:PRO:HD2	1.77	0.40
2:H:124:LEU:HB2	2:H:139:GLY:CA	2.51	0.40
2:H:145:TYR:CE2	2:H:175:TYR:HB3	2.57	0.40
2:H:195:CYS:O	2:H:208:LYS:N	2.50	0.40
1:L:14:SER:HA	1:L:107:LYS:HB2	2.02	0.40
2:B:142:VAL:HG23	2:B:177:LEU:HD12	2.03	0.40
1:L:146:VAL:HA	1:L:195:GLU:O	2.22	0.40
1:A:135:PHE:CE1	2:B:178:SER:HB2	2.54	0.40
2:H:39:GLN:HG3	2:H:43:LYS:O	2.22	0.40
2:H:96:LYS:HB2	2:H:100(E):TRP:CE2	2.56	0.40
2:H:170:LEU:HG	2:H:173:ASP:HA	2.03	0.40
1:L:59:PRO:HD2	1:L:62:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

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	211/213 (99%)	174 (82%)	31 (15%)	6 (3%)	4	2
1	L	210/213 (99%)	180 (86%)	25 (12%)	5 (2%)	4	2
2	B	220/226 (97%)	184 (84%)	25 (11%)	11 (5%)	1	0
2	H	220/226 (97%)	180 (82%)	29 (13%)	11 (5%)	1	0
All	All	861/878 (98%)	718 (83%)	110 (13%)	33 (4%)	2	1

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	154	GLU
2	B	114	ALA
2	B	213	ARG
2	H	126	PRO
2	H	213	ARG
1	L	89	GLN
1	A	68	GLY
1	A	143	ASP
2	B	126	PRO
2	B	132	THR
2	B	133	ASN
2	H	132	THR
2	H	133	ASN
1	L	154	GLU
2	B	41	PRO
2	B	100(D)	ALA
2	H	29	PHE
2	H	41	PRO
2	H	100(D)	ALA
2	H	192	THR
1	L	121	SER
1	L	143	ASP
1	L	155	ARG
2	H	100(E)	TRP
1	A	138	ASN
1	A	158	GLY
2	B	100(E)	TRP
2	B	192	THR
2	B	29	PHE
2	H	189	PRO
2	H	210	ILE
2	B	189	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	174/185 (94%)	135 (78%)	39 (22%)	1	0
1	L	176/185 (95%)	133 (76%)	43 (24%)	1	0
2	B	172/192 (90%)	118 (69%)	54 (31%)	0	0
2	H	166/192 (86%)	115 (69%)	51 (31%)	0	0
All	All	688/754 (91%)	501 (73%)	187 (27%)	0	0

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	3	GLU
1	A	5	THR
1	A	11	MET
1	A	14	SER
1	A	21	ILE
1	A	39	LYS
1	A	40	PRO
1	A	45	LYS
1	A	54	LEU
1	A	56	SER
1	A	69	THR
1	A	72	SER
1	A	74	THR
1	A	75	ILE
1	A	76	SER
1	A	81	GLU
1	A	92	SER
1	A	103	LYS
1	A	105	GLU
1	A	107	LYS
1	A	116	SER
1	A	117	ILE
1	A	125	LEU
1	A	131	SER
1	A	142	LYS
1	A	144	ILE
1	A	150	ILE
1	A	153	SER
1	A	154	GLU
1	A	155	ARG
1	A	165	ASP
1	A	182	THR

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Mol	Chain	Res	Type
1	A	183	LYS
1	A	185	GLU
1	A	188	ARG
1	A	199	LYS
1	A	203	SER
1	A	205	ILE
2	B	3	LYS
2	B	4	LEU
2	B	7	SER
2	B	17	SER
2	B	33	TYR
2	B	41	PRO
2	B	43	LYS
2	B	50	LEU
2	B	56	THR
2	B	57	LYS
2	B	58	GLU
2	B	63	VAL
2	B	71	ARG
2	B	74	SER
2	B	77	ILE
2	B	81	GLN
2	B	94	ARG
2	B	96	LYS
2	B	98	SER
2	B	100(A)	ASN
2	B	100(B)	TYR
2	B	100(E)	TRP
2	B	100(F)	PHE
2	B	108	THR
2	B	111	VAL
2	B	116	THR
2	B	117	THR
2	B	120	SER
2	B	124	LEU
2	B	135	MET
2	B	137	THR
2	B	138	LEU
2	B	140	CYS
2	B	141	LEU
2	B	142	VAL
2	B	143	LYS

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Mol	Chain	Res	Type
2	B	151	THR
2	B	152	VAL
2	B	155	ASN
2	B	160	SER
2	B	161	SER
2	B	171	GLN
2	B	172	SER
2	B	174	LEU
2	B	176	THR
2	B	178	SER
2	B	179	SER
2	B	190	SER
2	B	196	ASN
2	B	204	THR
2	B	205	LYS
2	B	206	VAL
2	B	208	LYS
2	B	211	VAL
2	H	3	LYS
2	H	4	LEU
2	H	7	SER
2	H	11	LEU
2	H	22	CYS
2	H	25	SER
2	H	33	TYR
2	H	43	LYS
2	H	46	GLU
2	H	50	LEU
2	H	56	THR
2	H	57	LYS
2	H	58	GLU
2	H	63	VAL
2	H	66	ARG
2	H	71	ARG
2	H	76	SER
2	H	77	ILE
2	H	94	ARG
2	H	96	LYS
2	H	98	SER
2	H	108	THR
2	H	111	VAL
2	H	116	THR

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Mol	Chain	Res	Type
2	H	117	THR
2	H	124	LEU
2	H	135	MET
2	H	137	THR
2	H	140	CYS
2	H	141	LEU
2	H	142	VAL
2	H	143	LYS
2	H	151	THR
2	H	152	VAL
2	H	156	SER
2	H	160	SER
2	H	161	SER
2	H	171	GLN
2	H	172	SER
2	H	174	LEU
2	H	176	THR
2	H	178	SER
2	H	179	SER
2	H	190	SER
2	H	193	VAL
2	H	196	ASN
2	H	203	SER
2	H	204	THR
2	H	205	LYS
2	H	206	VAL
2	H	208	LYS
1	L	2	ILE
1	L	3	GLU
1	L	4	LEU
1	L	5	THR
1	L	11	MET
1	L	14	SER
1	L	24	SER
1	L	27	SER
1	L	39	LYS
1	L	45	LYS
1	L	56	SER
1	L	69	THR
1	L	72	SER
1	L	73	LEU
1	L	74	THR

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Mol	Chain	Res	Type
1	L	81	GLU
1	L	92	SER
1	L	103	LYS
1	L	107	LYS
1	L	117	ILE
1	L	124	GLN
1	L	125	LEU
1	L	131	SER
1	L	142	LYS
1	L	144	ILE
1	L	147	LYS
1	L	150	ILE
1	L	151	ASP
1	L	153	SER
1	L	154	GLU
1	L	155	ARG
1	L	160	LEU
1	L	165	ASP
1	L	166	GLN
1	L	174	SER
1	L	182	THR
1	L	183	LYS
1	L	184	ASP
1	L	185	GLU
1	L	199	LYS
1	L	203	SER
1	L	205	ILE
1	L	207	LYS

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

Mol	Chain	Res	Type
1	A	89	GLN
1	A	90	GLN
1	A	137	ASN
1	A	212	ASN
2	B	53	ASN
2	B	81	GLN
2	H	81	GLN
2	H	164	HIS
1	L	31	ASN
1	L	137	ASN

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Mol	Chain	Res	Type
1	L	189	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 [i](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

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$
4	PP3	A	1214	-	20,21,21	2.33	5 (25%)	26,30,30	4.42	16 (61%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PP3	A	1214	-	-	4/15/15/15	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1214	PP3	C3-C2	5.80	1.47	1.41
4	A	1214	PP3	O-C	5.01	1.37	1.22
4	A	1214	PP3	C5-C4	3.59	1.45	1.40
4	A	1214	PP3	C2-N1	3.41	1.39	1.33
4	A	1214	PP3	C3-C4	2.53	1.43	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1214	PP3	C6-C5-C4	11.56	126.81	118.06
4	A	1214	PP3	C2A-C2-C3	10.79	133.42	120.80
4	A	1214	PP3	C3-C4-C5	-7.29	112.12	118.73
4	A	1214	PP3	C5A-C5-C6	-5.85	109.83	119.36
4	A	1214	PP3	O-C-CA	-4.80	107.59	122.14
4	A	1214	PP3	C2A-C2-N1	-4.67	108.84	117.64
4	A	1214	PP3	C5-C6-N1	-4.11	117.15	123.83
4	A	1214	PP3	OXT-C-CA	3.82	126.42	113.84
4	A	1214	PP3	C4A-C4-C5	3.54	123.61	119.75
4	A	1214	PP3	O4P-C5A-C5	3.53	115.97	109.36
4	A	1214	PP3	O3-C3-C2	-3.52	110.28	117.58
4	A	1214	PP3	C4A-C4-C3	3.23	124.27	119.98
4	A	1214	PP3	O3-C3-C4	3.03	126.96	118.18
4	A	1214	PP3	C3-C2-N1	-2.56	117.73	120.96
4	A	1214	PP3	O2P-P-O1P	2.50	120.58	110.83
4	A	1214	PP3	C6-N1-C2	2.33	123.43	119.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1214	PP3	C5-C4-C4A-N
4	A	1214	PP3	C-CA-N-C4A
4	A	1214	PP3	CB-CA-N-C4A
4	A	1214	PP3	C3-C4-C4A-N

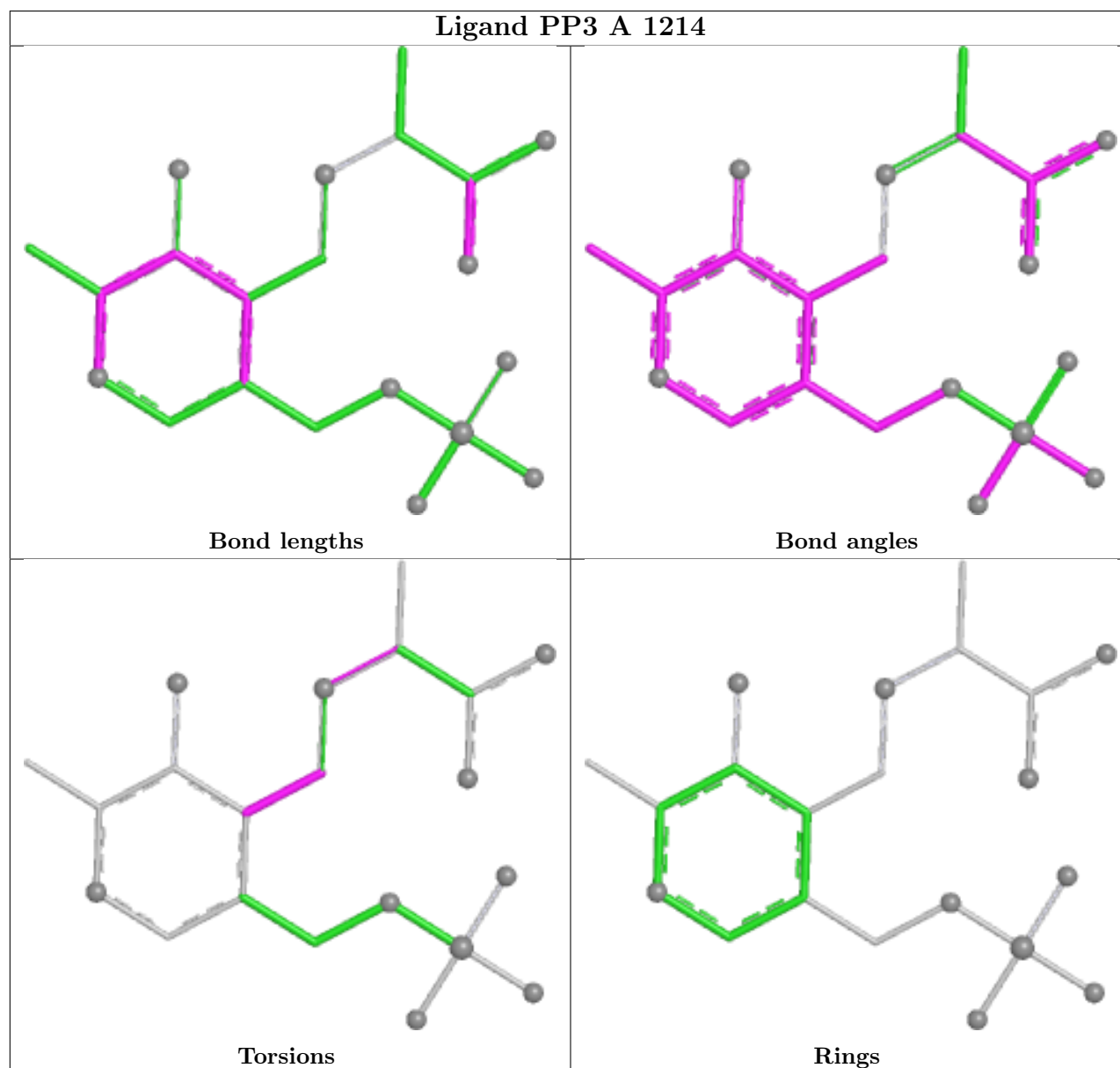
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1214	PP3	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	213/213 (100%)	0.65	11 (5%) 33 39	15, 46, 71, 85	0
1	L	212/213 (99%)	0.70	10 (4%) 36 42	15, 46, 71, 90	0
2	B	224/226 (99%)	0.72	12 (5%) 31 37	21, 50, 91, 110	0
2	H	224/226 (99%)	0.84	20 (8%) 15 18	21, 50, 91, 110	0
All	All	873/878 (99%)	0.73	53 (6%) 27 32	15, 47, 81, 110	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	CYS	7.0
1	L	23	CYS	5.9
1	A	22	THR	4.6
1	L	22	THR	4.3
2	H	214	ASP	3.6
1	A	89	GLN	3.6
2	H	193	VAL	3.3
2	H	125	ALA	3.3
1	L	89	GLN	3.3
1	L	158	GLY	3.1
2	B	195	CYS	3.1
2	B	210	ILE	3.0
2	B	159	LEU	2.9
1	L	115	VAL	2.9
2	H	210	ILE	2.7
2	B	99	TYR	2.7
2	B	121	VAL	2.7
1	A	24	SER	2.7
1	A	185	GLU	2.6
2	H	194	THR	2.6
2	B	186	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	24	SER	2.5
1	A	186	TYR	2.5
2	B	100(B)	TYR	2.5
1	A	190	ASN	2.5
1	L	204	PRO	2.5
1	A	209	PHE	2.4
1	L	135	PHE	2.4
2	B	193	VAL	2.4
1	L	209	PHE	2.4
2	H	121	VAL	2.3
2	B	151	THR	2.3
2	H	161	SER	2.3
2	B	206	VAL	2.3
2	H	198	ALA	2.3
2	H	181	VAL	2.2
1	A	158	GLY	2.2
2	H	135	MET	2.2
1	A	119	PRO	2.1
2	H	212	PRO	2.1
2	H	127	GLY	2.1
2	H	157	GLY	2.1
2	B	185	SER	2.1
2	H	132	THR	2.1
2	H	99	TYR	2.1
2	B	56	THR	2.1
2	H	147	PRO	2.1
2	H	189	PRO	2.1
1	L	100	GLY	2.1
2	H	128	SER	2.1
2	H	195	CYS	2.1
2	H	201	ALA	2.1
1	A	192	TYR	2.1

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

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

6.3 Carbohydrates [i](#)

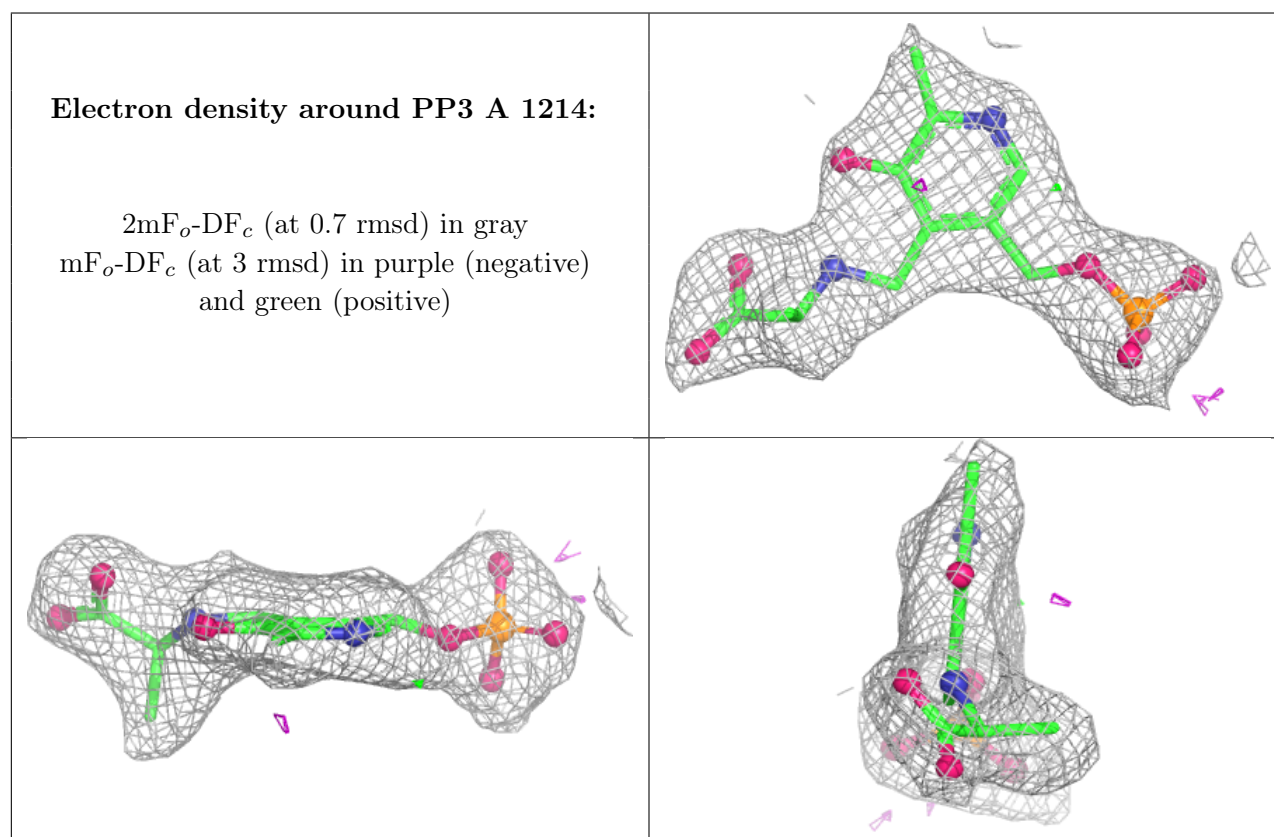
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PP3	A	1214	21/21	0.93	0.10	16,37,59,63	0
3	IOD	H	1214	1/1	0.96	0.08	93,93,93,93	0
3	IOD	A	1213	1/1	0.98	0.04	62,62,62,62	0
3	IOD	H	1215	1/1	0.98	0.05	84,84,84,84	0
3	IOD	L	1213	1/1	0.98	0.06	81,81,81,81	0
3	IOD	B	1214	1/1	0.98	0.04	63,63,63,63	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.