



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:11 PM UTC

PDB ID : 1H54 / pdb_00001h54
Title : Maltose phosphorylase from Lactobacillus brevis
Authors : Van Tilbeurgh, H.; Egloff, M.-P.
Deposited on : 2001-05-18
Resolution : 2.15 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

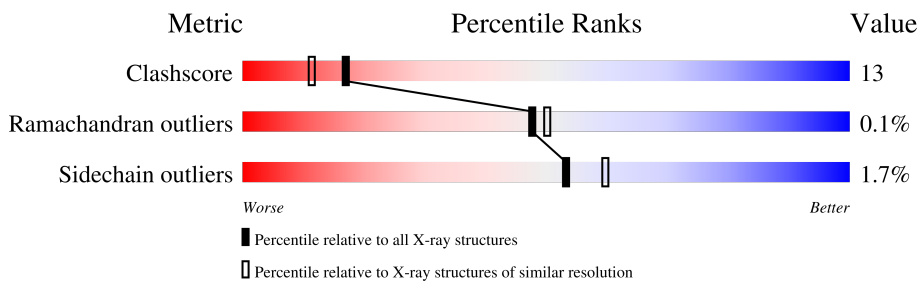
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	754	
1	B	754	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13699 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.

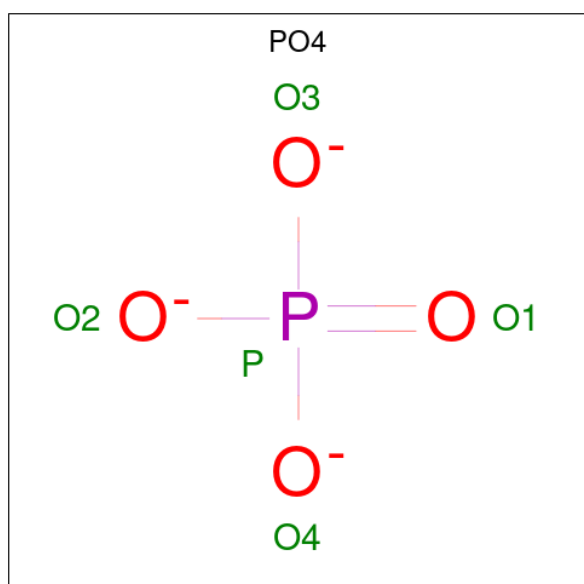
- Molecule 1 is a protein called MALTOSE PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	753	Total	C	N	O	S	0	0	1
			6045	3843	1020	1165	17			
1	B	754	Total	C	N	O	S	0	0	0
			6055	3848	1020	1170	17			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

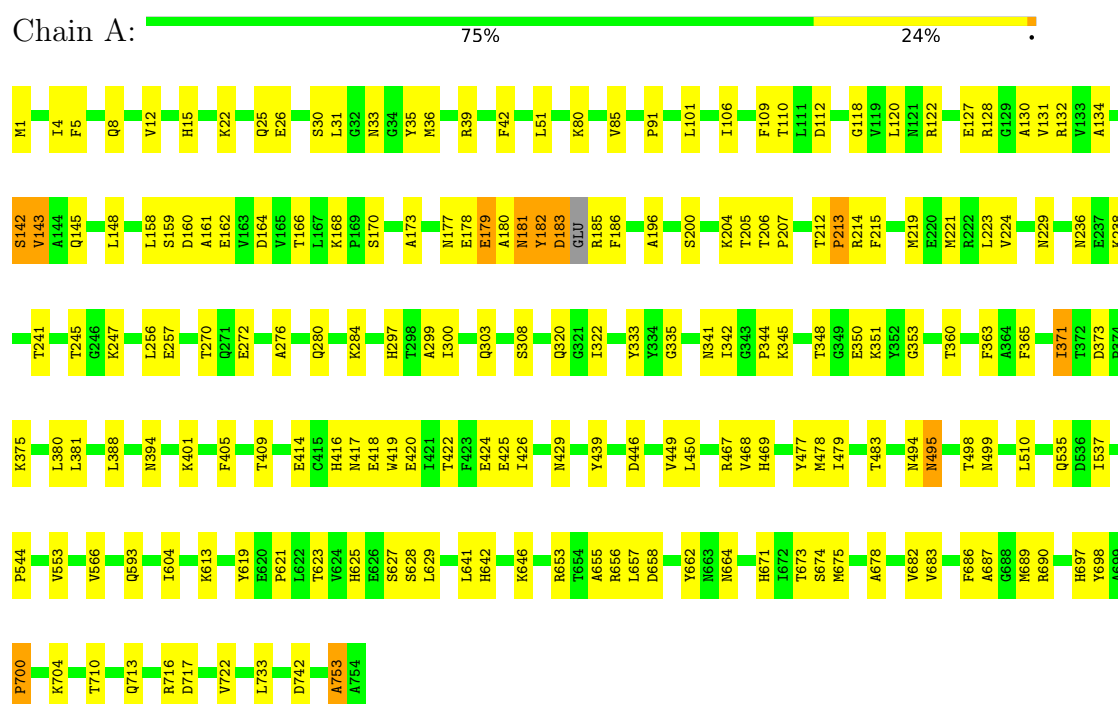
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	723	Total	O	0	0
			723	723		
4	B	869	Total	O	0	0
			869	869		

3 Residue-property plots [i](#)

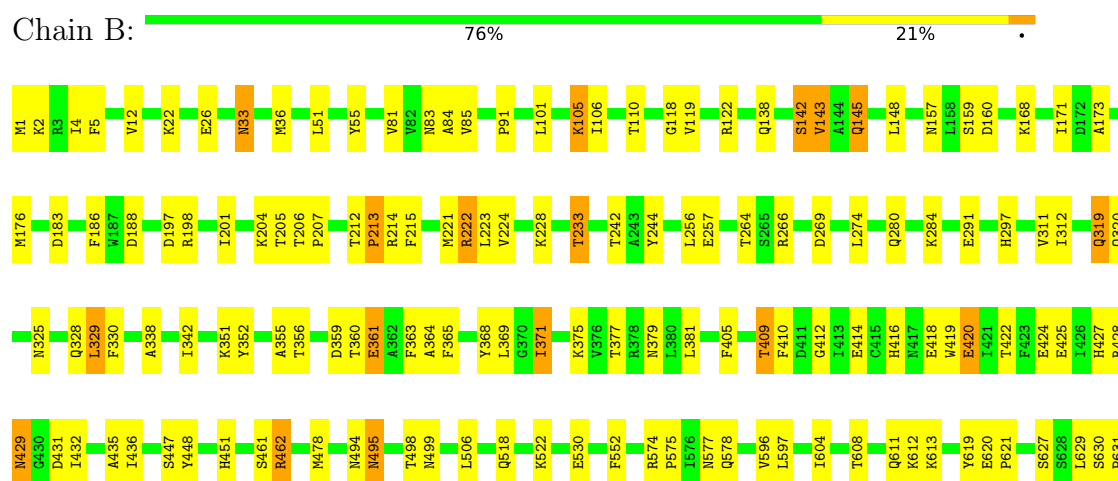
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

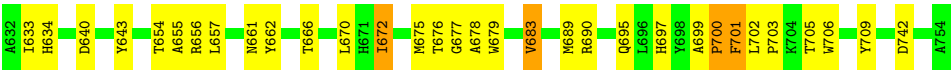
Note EDS was not executed.

• Molecule 1: MALTOSE PHOSPHORYLASE



• Molecule 1: MALTOSE PHOSPHORYLASE





4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.75Å 102.50Å 114.00Å 90.00° 111.30° 90.00°	Depositor
Resolution (Å)	29.10 – 2.15	Depositor
% Data completeness (in resolution range)	98.0 (29.10-2.15)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.186 , 0.225	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13699	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, PO4

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	0.37	1/6195 (0.0%)	0.90	19/8419 (0.2%)
1	B	0.37	0/6205	0.89	26/8432 (0.3%)
All	All	0.37	1/12400 (0.0%)	0.89	45/16851 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	753	ALA	C-N	-5.67	1.25	1.33

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	655	ALA	N-CA-C	9.88	121.65	111.07
1	B	424	GLU	N-CA-C	7.96	123.28	113.50
1	A	424	GLU	N-CA-C	7.86	123.16	113.50
1	A	148	LEU	N-CA-C	7.46	121.39	109.24
1	A	181	ASN	N-CA-C	-7.32	103.51	114.64
1	B	148	LEU	N-CA-C	7.12	120.84	109.24
1	B	672	ILE	N-CA-C	6.89	117.59	110.36
1	A	619	TYR	N-CA-C	6.66	119.88	111.69
1	B	83	ASN	N-CA-C	-6.42	100.16	109.59
1	A	143	VAL	N-CA-C	-6.24	106.65	112.83
1	B	142	SER	N-CA-C	6.23	119.39	110.10
1	B	677	GLY	N-CA-C	6.22	120.17	112.64
1	A	142	SER	N-CA-C	6.17	119.30	110.24
1	A	8	GLN	CA-C-N	6.14	125.36	118.97
1	A	8	GLN	C-N-CA	6.14	125.36	118.97
1	B	143	VAL	N-CA-C	-5.92	105.99	112.80
1	B	84	ALA	N-CA-C	5.80	118.01	110.53
1	A	185	ARG	N-CA-C	5.77	119.23	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	THR	N-CA-C	5.77	117.61	108.79
1	A	700	PRO	N-CA-C	5.71	120.46	111.38
1	B	619	TYR	N-CA-C	5.71	118.71	111.69
1	A	495	ASN	N-CA-C	-5.65	101.29	109.59
1	A	12	VAL	N-CA-C	-5.62	97.66	109.34
1	A	112	ASP	N-CA-C	5.52	117.85	108.02
1	B	213	PRO	N-CA-C	5.47	119.67	111.14
1	B	495	ASN	N-CA-C	-5.43	101.61	109.59
1	B	627	SER	N-CA-C	-5.43	99.59	108.76
1	B	409	THR	N-CA-C	5.42	116.76	108.42
1	A	683	VAL	N-CA-C	5.40	116.06	110.82
1	B	683	VAL	N-CA-C	5.39	115.65	110.74
1	B	701	PHE	N-CA-C	-5.35	101.22	109.52
1	B	105	LYS	N-CA-C	-5.35	100.98	109.96
1	B	371	ILE	N-CA-C	5.29	118.24	113.10
1	B	596	VAL	N-CA-C	-5.29	105.22	110.62
1	B	342	ILE	N-CA-C	5.29	115.13	106.72
1	B	552	PHE	N-CA-C	-5.24	100.76	109.46
1	B	700	PRO	N-CA-C	5.20	119.65	111.38
1	B	269	ASP	N-CA-C	5.20	119.33	112.89
1	B	12	VAL	N-CA-C	-5.17	98.58	109.34
1	A	417	ASN	N-CA-C	5.15	118.67	111.30
1	B	145	GLN	CA-C-N	5.12	126.24	119.84
1	B	145	GLN	C-N-CA	5.12	126.24	119.84
1	A	371	ILE	N-CA-C	5.08	119.91	109.34
1	B	643	TYR	N-CA-C	-5.07	102.01	109.62
1	A	213	PRO	N-CA-C	5.05	119.02	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6045	0	5809	170	0
1	B	6055	0	5809	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	5	0	0	0	0
4	A	723	0	0	22	0
4	B	869	0	0	18	0
All	All	13699	0	11618	302	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 13.

All (302) 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:179:GLU:OE2	1:A:351:LYS:CE	1.88	1.20
1:A:179:GLU:OE2	1:A:351:LYS:HE3	1.55	1.06
1:A:179:GLU:OE2	1:A:351:LYS:CG	2.05	1.04
1:B:604:ILE:HD13	1:B:690:ARG:HH12	1.19	1.03
1:A:179:GLU:OE1	1:A:179:GLU:HA	1.53	1.03
1:A:128:ARG:HB2	1:A:131:VAL:HG23	1.51	0.93
1:A:426:ILE:HD13	1:A:467:ARG:NH1	1.84	0.92
1:B:604:ILE:HD13	1:B:690:ARG:NH1	1.83	0.92
1:B:328:GLN:HB2	1:B:675:MET:HE3	1.54	0.88
1:A:420:GLU:HG2	1:B:419:TRP:HZ2	1.39	0.88
1:A:420:GLU:HB2	4:A:2441:HOH:O	1.76	0.85
1:A:179:GLU:OE2	1:A:351:LYS:HE2	1.75	0.85
1:A:657:LEU:HD12	1:A:662:TYR:HB2	1.56	0.85
1:A:341:ASN:ND2	1:A:360:THR:HG21	1.92	0.84
1:B:381:LEU:HD22	1:B:436:ILE:HD13	1.57	0.84
1:B:356:THR:HG23	4:B:2518:HOH:O	1.76	0.84
1:B:412:GLY:HA2	4:B:2561:HOH:O	1.75	0.84
1:A:673:THR:HG21	4:A:2674:HOH:O	1.79	0.81
1:B:361:GLU:HG3	1:B:432:ILE:HD13	1.65	0.79
1:B:207:PRO:HA	1:B:214:ARG:HD3	1.63	0.78
1:A:272:GLU:N	4:A:2337:HOH:O	2.16	0.78
1:A:247:LYS:HE2	4:A:2208:HOH:O	1.83	0.78
1:A:419:TRP:HZ2	1:B:420:GLU:HG2	1.49	0.78
1:A:179:GLU:OE2	1:A:351:LYS:HG3	1.83	0.77
1:A:341:ASN:HD22	1:A:342:ILE:H	1.30	0.77
1:B:320:GLN:HE21	1:B:656:ARG:HH12	1.32	0.76
1:A:341:ASN:HD21	1:A:360:THR:HG21	1.48	0.75
1:B:197:ASP:OD2	1:B:198:ARG:HG3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ILE:CD1	1:A:678:ALA:HB1	2.17	0.75
1:A:179:GLU:OE2	1:A:351:LYS:HG2	1.87	0.75
1:A:687:ALA:HA	1:A:700:PRO:HB3	1.69	0.74
1:B:405:PHE:H	1:B:429:ASN:HD21	1.35	0.74
1:A:405:PHE:H	1:A:429:ASN:HD21	1.37	0.73
1:B:325:ASN:HD22	1:B:678:ALA:HB3	1.52	0.73
1:B:613:LYS:HE2	4:B:2785:HOH:O	1.88	0.72
1:B:1:MET:HG2	1:B:661:ASN:O	1.89	0.72
1:A:272:GLU:HG2	4:A:2337:HOH:O	1.89	0.72
1:B:143:VAL:H	1:B:297:HIS:HD2	1.36	0.72
1:A:179:GLU:OE2	1:A:351:LYS:CD	2.36	0.72
1:A:467:ARG:NE	4:A:2469:HOH:O	2.23	0.71
1:B:608:THR:H	1:B:611:GLN:HE21	1.35	0.71
1:A:704:LYS:HE3	4:A:2651:HOH:O	1.89	0.71
1:B:494:ASN:HD22	1:B:499:ASN:HD21	1.39	0.70
1:A:613:LYS:HE2	4:A:2302:HOH:O	1.91	0.70
1:A:179:GLU:HB2	1:A:350:GLU:OE2	1.91	0.70
1:A:468:VAL:HG21	1:A:477:TYR:HB3	1.73	0.70
1:B:222:ARG:HG3	4:B:2351:HOH:O	1.92	0.69
1:A:394:ASN:HD21	1:A:414:GLU:H	1.39	0.69
1:A:162:GLU:OE2	1:A:247:LYS:HD3	1.92	0.68
1:B:705:THR:HG22	4:B:2835:HOH:O	1.93	0.68
1:A:236:ASN:ND2	1:A:238:LYS:H	1.91	0.68
1:A:320:GLN:HE21	1:A:656:ARG:HH12	1.39	0.68
1:A:344:PRO:HG2	1:A:353:GLY:HA2	1.76	0.68
1:A:363:PHE:CD1	1:A:629:LEU:HD13	2.29	0.67
1:A:566:VAL:HG13	1:A:621:PRO:O	1.94	0.67
1:B:330:PHE:HZ	1:B:371:ILE:HD12	1.57	0.67
1:A:658:ASP:OD2	1:A:671:HIS:HD2	1.78	0.67
1:B:478:MET:HB3	1:B:494:ASN:HD21	1.60	0.67
1:B:436:ILE:HD12	1:B:448:TYR:HE2	1.60	0.66
1:B:312:ILE:HB	1:B:319:GLN:HG2	1.77	0.66
1:A:179:GLU:OE1	1:A:179:GLU:CA	2.40	0.65
1:B:176:MET:SD	4:B:2281:HOH:O	2.54	0.65
1:A:207:PRO:HA	1:A:214:ARG:HD3	1.78	0.65
1:B:462:ARG:HD2	1:B:530:GLU:OE1	1.96	0.65
1:B:325:ASN:HD21	1:B:655:ALA:HA	1.62	0.64
1:B:176:MET:HB3	4:B:2284:HOH:O	1.97	0.64
1:B:427:HIS:HD2	1:B:431:ASP:OD2	1.80	0.64
1:B:705:THR:HG23	1:B:706:TRP:CD1	2.33	0.63
1:A:142:SER:HA	1:A:297:HIS:CD2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:THR:HG21	4:B:2561:HOH:O	1.99	0.63
1:A:495:ASN:HD22	1:A:498:THR:H	1.47	0.62
1:B:325:ASN:HD22	1:B:678:ALA:CB	2.11	0.62
1:B:160:ASP:HB2	4:B:2244:HOH:O	2.00	0.62
1:A:196:ALA:HB1	1:A:229:ASN:HD21	1.65	0.61
1:B:604:ILE:HG21	1:B:690:ARG:NH1	2.15	0.61
1:B:105:LYS:HD3	1:B:106:ILE:N	2.16	0.60
1:B:274:LEU:C	1:B:274:LEU:HD23	2.27	0.60
1:A:1:MET:HG2	4:A:2663:HOH:O	2.02	0.59
1:B:157:ASN:ND2	1:B:159:SER:H	1.99	0.59
1:A:170:SER:CB	1:A:241:THR:HG22	2.32	0.59
1:B:436:ILE:HD11	4:B:2594:HOH:O	2.02	0.59
1:A:33:ASN:ND2	1:A:36:MET:H	2.00	0.59
1:A:127:GLU:OE2	1:A:132:ARG:HD2	2.02	0.59
1:A:276:ALA:O	1:A:280:GLN:HG3	2.02	0.59
1:B:361:GLU:CG	1:B:432:ILE:HD13	2.32	0.59
1:A:160:ASP:O	1:A:161:ALA:HB3	2.02	0.59
1:A:322:ILE:HD13	1:A:678:ALA:HB1	1.85	0.58
1:A:270:THR:CB	4:A:2337:HOH:O	2.50	0.58
1:A:426:ILE:HD13	1:A:467:ARG:HH12	1.67	0.58
1:A:143:VAL:H	1:A:297:HIS:HD2	1.52	0.58
1:B:176:MET:HE2	4:B:2042:HOH:O	2.02	0.58
1:B:325:ASN:ND2	1:B:678:ALA:CB	2.66	0.58
1:B:351:LYS:O	1:B:352:TYR:HB2	2.03	0.58
1:B:91:PRO:HG2	1:B:168:LYS:HB2	1.86	0.57
1:B:205:THR:O	1:B:214:ARG:HD2	2.05	0.57
1:A:495:ASN:ND2	1:A:498:THR:H	2.02	0.57
1:B:375:LYS:HE3	4:B:2526:HOH:O	2.04	0.57
1:B:319:GLN:HE21	1:B:319:GLN:CA	2.18	0.57
1:A:101:LEU:HD13	1:A:106:ILE:HD13	1.86	0.57
1:B:223:LEU:HD13	1:B:244:TYR:CE1	2.40	0.57
1:B:672:ILE:HA	1:B:675:MET:HG2	1.87	0.56
1:A:341:ASN:ND2	1:A:342:ILE:H	2.00	0.56
1:B:145:GLN:HE22	1:B:284:LYS:NZ	2.03	0.56
1:A:164:ASP:HB2	4:A:2208:HOH:O	2.04	0.56
1:A:697:HIS:HD2	1:A:742:ASP:OD1	1.89	0.56
1:A:205:THR:O	1:A:214:ARG:HD2	2.06	0.56
1:A:166:THR:OG1	1:A:245:THR:HG22	2.05	0.56
1:A:206:THR:HB	1:A:207:PRO:HD2	1.86	0.56
1:A:308:SER:HB3	1:A:371:ILE:HB	1.88	0.56
1:A:420:GLU:HG2	1:B:419:TRP:CZ2	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD11	1:A:120:LEU:HB2	1.87	0.56
1:A:179:GLU:CD	1:A:351:LYS:HG2	2.30	0.56
1:A:333:TYR:CZ	1:A:380:LEU:HD13	2.41	0.56
1:B:597:LEU:HD12	1:B:634:HIS:CE1	2.41	0.56
1:B:697:HIS:HD2	1:B:742:ASP:OD1	1.88	0.55
1:A:299:ALA:O	1:A:303:GLN:HG3	2.05	0.55
1:B:224:VAL:HB	1:B:257:GLU:HB2	1.88	0.55
1:B:2:LYS:HE3	4:B:2006:HOH:O	2.05	0.55
1:B:325:ASN:ND2	1:B:678:ALA:HB2	2.21	0.55
1:B:620:GLU:HB3	1:B:621:PRO:HD3	1.88	0.55
1:B:33:ASN:HD22	1:B:33:ASN:C	2.15	0.54
1:B:597:LEU:HD12	1:B:634:HIS:HE1	1.72	0.54
1:A:170:SER:HB2	1:A:241:THR:HG22	1.90	0.54
1:B:33:ASN:ND2	1:B:36:MET:H	2.06	0.53
1:B:657:LEU:HD22	1:B:662:TYR:HB2	1.90	0.53
1:B:695:GLN:NE2	1:B:742:ASP:HB2	2.24	0.53
1:B:329:LEU:HD22	1:B:368:TYR:OH	2.08	0.53
1:B:654:THR:HG23	1:B:655:ALA:N	2.24	0.53
1:A:145:GLN:HE22	1:A:284:LYS:NZ	2.08	0.52
1:B:142:SER:HA	1:B:297:HIS:CD2	2.45	0.52
1:A:224:VAL:HB	1:A:257:GLU:HB2	1.91	0.52
1:A:604:ILE:HG21	1:A:690:ARG:HH12	1.73	0.52
1:B:428:ARG:O	1:B:432:ILE:HG12	2.10	0.52
1:B:612:LYS:HE3	1:B:640:ASP:OD2	2.09	0.52
1:B:363:PHE:CD1	1:B:629:LEU:HD22	2.44	0.52
1:A:179:GLU:CG	1:A:351:LYS:HG2	2.38	0.52
1:A:142:SER:HA	1:A:297:HIS:HD2	1.73	0.52
1:A:510:LEU:HD13	1:A:535:GLN:HG2	1.92	0.51
1:B:495:ASN:HD22	1:B:498:THR:H	1.58	0.51
1:B:361:GLU:CD	1:B:361:GLU:H	2.18	0.51
1:A:39:ARG:NE	1:A:51:LEU:HB3	2.26	0.51
1:A:270:THR:HB	4:A:2337:HOH:O	2.09	0.51
1:B:427:HIS:CD2	1:B:431:ASP:OD2	2.62	0.51
1:A:128:ARG:CB	1:A:131:VAL:HG23	2.34	0.51
1:A:394:ASN:ND2	1:A:414:GLU:H	2.06	0.51
1:B:143:VAL:HG22	1:B:297:HIS:CD2	2.45	0.51
1:B:328:GLN:CB	1:B:675:MET:HE3	2.34	0.51
1:B:364:ALA:HA	1:B:676:THR:HG21	1.91	0.51
1:A:446:ASP:HB3	1:A:450:LEU:HD22	1.93	0.51
1:A:236:ASN:HD22	1:A:238:LYS:H	1.59	0.51
1:B:233:THR:HG22	4:B:2378:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:PHE:O	1:A:205:THR:HA	2.11	0.50
1:A:270:THR:OG1	4:A:2337:HOH:O	2.20	0.50
1:B:118:GLY:O	1:B:297:HIS:HE1	1.95	0.50
1:B:264:THR:OG1	1:B:266:ARG:HG2	2.11	0.50
1:A:91:PRO:HG2	1:A:168:LYS:HB2	1.94	0.50
1:A:33:ASN:HD21	1:A:36:MET:H	1.58	0.50
1:A:256:LEU:C	1:A:256:LEU:HD23	2.37	0.49
1:A:628:SER:HB3	1:A:674:SER:OG	2.12	0.49
1:B:604:ILE:HG21	1:B:690:ARG:HH11	1.77	0.49
1:B:630:SER:N	1:B:631:PRO:HD2	2.26	0.49
1:B:375:LYS:HG3	4:B:2526:HOH:O	2.12	0.49
1:A:363:PHE:CG	1:A:629:LEU:HD13	2.47	0.49
1:A:468:VAL:CG2	1:A:477:TYR:HB3	2.42	0.49
1:B:630:SER:O	1:B:634:HIS:HD2	1.95	0.49
1:A:132:ARG:H	1:A:159:SER:HB3	1.77	0.49
1:B:416:HIS:HE1	1:B:418:GLU:OE1	1.95	0.49
1:A:373:ASP:HB3	4:A:2409:HOH:O	2.11	0.48
1:B:85:VAL:HG13	1:B:173:ALA:HA	1.95	0.48
1:A:467:ARG:CZ	4:A:2469:HOH:O	2.59	0.48
1:B:171:ILE:HG22	1:B:201:ILE:HD12	1.95	0.48
1:A:101:LEU:N	1:A:101:LEU:HD23	2.27	0.48
1:A:690:ARG:HB3	1:A:690:ARG:CZ	2.43	0.48
1:A:25:GLN:CD	4:A:2039:HOH:O	2.57	0.48
1:A:365:PHE:HE2	1:A:439:TYR:HB2	1.78	0.48
1:A:1:MET:HG3	1:A:664:ASN:ND2	2.29	0.48
1:A:308:SER:CB	1:A:371:ILE:HB	2.43	0.47
1:A:345:LYS:HB2	1:A:353:GLY:HA3	1.94	0.47
1:A:419:TRP:HZ2	1:B:420:GLU:CG	2.24	0.47
1:A:419:TRP:CZ2	1:B:420:GLU:HG2	2.39	0.47
1:A:646:LYS:NZ	4:A:2652:HOH:O	2.45	0.47
1:A:33:ASN:C	1:A:33:ASN:HD22	2.20	0.47
1:B:359:ASP:OD2	1:B:629:LEU:HD11	2.15	0.47
1:A:425:GLU:HA	1:A:483:THR:O	2.14	0.47
1:B:319:GLN:HE21	1:B:319:GLN:HA	1.78	0.47
1:B:425:GLU:OE1	1:B:427:HIS:HE1	1.98	0.47
1:A:30:SER:CB	1:A:348:THR:HG22	2.45	0.47
1:A:300:ILE:HA	1:A:303:GLN:HE21	1.80	0.47
1:A:657:LEU:CD1	1:A:662:TYR:HB2	2.35	0.47
1:A:716:ARG:O	1:A:717:ASP:HB2	2.15	0.47
1:B:4:ILE:HG13	1:B:5:PHE:CD1	2.48	0.47
1:B:55:TYR:HB3	1:B:81:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ALA:HB1	1:B:379:ASN:ND2	2.30	0.47
1:A:1:MET:HG3	1:A:664:ASN:HD21	1.80	0.47
1:B:361:GLU:HB2	1:B:435:ALA:HB2	1.97	0.47
1:A:646:LYS:HE3	4:A:2653:HOH:O	2.14	0.47
1:B:256:LEU:C	1:B:256:LEU:HD23	2.39	0.46
1:B:311:VAL:O	1:B:709:TYR:HA	2.14	0.46
1:B:699:ALA:N	1:B:700:PRO:HD3	2.30	0.46
1:A:414:GLU:HG2	1:A:422:THR:HG23	1.98	0.46
1:A:468:VAL:HG22	1:A:469:HIS:N	2.30	0.46
1:B:183:ASP:CG	1:B:183:ASP:O	2.59	0.46
1:B:518:GLN:O	1:B:522:LYS:HG3	2.15	0.46
1:A:4:ILE:HG13	1:A:5:PHE:CD1	2.51	0.46
1:B:22:LYS:O	1:B:26:GLU:HG3	2.15	0.46
1:B:119:VAL:CG1	1:B:138:GLN:HG3	2.45	0.46
1:B:701:PHE:CD1	1:B:701:PHE:C	2.94	0.46
1:A:166:THR:HG23	1:A:245:THR:HG22	1.96	0.46
1:B:369:LEU:HG	1:B:377:THR:HG21	1.98	0.46
1:B:291:GLU:CD	1:B:291:GLU:H	2.24	0.46
1:A:333:TYR:CZ	1:A:335:GLY:HA2	2.51	0.45
1:B:666:THR:O	1:B:666:THR:HG22	2.16	0.45
1:A:1:MET:HG3	1:A:664:ASN:OD1	2.15	0.45
1:B:312:ILE:O	1:B:319:GLN:HG2	2.16	0.45
1:B:33:ASN:C	1:B:33:ASN:ND2	2.74	0.45
1:B:478:MET:CB	1:B:494:ASN:HD21	2.27	0.45
1:B:145:GLN:HE22	1:B:284:LYS:HZ2	1.64	0.45
1:A:85:VAL:HG13	1:A:173:ALA:HA	1.99	0.45
1:A:416:HIS:HE1	1:A:418:GLU:OE1	2.00	0.45
1:A:468:VAL:HG23	1:A:478:MET:O	2.17	0.45
1:A:365:PHE:HE1	1:A:380:LEU:HB3	1.81	0.44
1:A:118:GLY:O	1:A:297:HIS:HE1	2.00	0.44
1:A:110:THR:O	1:A:122:ARG:HA	2.17	0.44
1:B:360:THR:HB	1:B:361:GLU:OE1	2.16	0.44
1:A:181:ASN:O	1:A:183:ASP:N	2.50	0.44
1:B:679:TRP:CE2	1:B:683:VAL:HG21	2.53	0.44
1:A:544:PRO:HB2	1:A:553:VAL:HB	2.00	0.44
1:A:623:THR:HG22	1:A:625:HIS:H	1.83	0.44
1:B:338:ALA:HB1	1:B:379:ASN:HD21	1.81	0.44
1:B:222:ARG:HH21	1:B:222:ARG:CG	2.31	0.44
1:B:657:LEU:C	1:B:657:LEU:HD13	2.43	0.44
1:A:280:GLN:NE2	4:A:2345:HOH:O	2.49	0.43
1:A:375:LYS:HG3	4:A:2411:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:ASN:OD1	1:B:578:GLN:HG3	2.18	0.43
1:A:170:SER:HB3	1:A:241:THR:HG22	2.00	0.43
1:A:170:SER:HA	1:A:221:MET:HE1	2.00	0.43
1:B:101:LEU:HD13	1:B:106:ILE:HD13	2.01	0.43
1:B:608:THR:OG1	1:B:611:GLN:HG3	2.18	0.43
1:A:145:GLN:HE22	1:A:284:LYS:HZ3	1.65	0.43
1:A:322:ILE:HD11	1:A:678:ALA:HB1	1.95	0.43
1:A:593:GLN:HB3	1:A:627:SER:HB3	2.00	0.43
1:B:447:SER:O	1:B:451:HIS:HD2	2.01	0.43
1:A:143:VAL:HG22	1:A:297:HIS:CD2	2.53	0.43
1:A:653:ARG:HD3	1:A:662:TYR:CE1	2.53	0.43
1:A:687:ALA:HA	1:A:700:PRO:CB	2.46	0.43
1:A:22:LYS:O	1:A:26:GLU:HG3	2.19	0.43
1:A:196:ALA:HB1	1:A:229:ASN:ND2	2.31	0.43
1:A:322:ILE:HD13	1:A:678:ALA:CB	2.48	0.43
1:A:15:HIS:HA	1:A:109:PHE:O	2.19	0.43
1:A:689:MET:HA	1:A:697:HIS:O	2.19	0.43
1:A:178:GLU:C	1:A:180:ALA:H	2.25	0.42
1:A:33:ASN:ND2	1:A:35:TYR:H	2.17	0.42
1:B:355:ALA:HB2	1:B:410:PHE:CE1	2.53	0.42
1:B:221:MET:HE3	1:B:242:THR:HG23	2.02	0.42
1:A:401:LYS:HE2	4:A:2466:HOH:O	2.19	0.42
1:A:212:THR:HB	1:A:213:PRO:HD2	2.02	0.42
1:A:449:VAL:HG13	1:A:450:LEU:HD13	2.02	0.42
1:B:461:SER:HB3	1:B:506:LEU:HD23	2.02	0.42
1:A:130:ALA:O	1:A:159:SER:HB2	2.19	0.42
1:B:361:GLU:HG3	1:B:432:ILE:HA	2.02	0.42
1:B:702:LEU:O	1:B:703:PRO:C	2.61	0.42
1:A:641:LEU:O	1:A:642:HIS:HB2	2.20	0.42
1:A:223:LEU:N	1:A:223:LEU:HD22	2.35	0.41
1:B:228:LYS:NZ	1:B:228:LYS:HB3	2.34	0.41
1:B:633:ILE:HD12	1:B:633:ILE:C	2.45	0.41
1:A:200:SER:HA	1:A:219:MET:O	2.20	0.41
1:A:710:THR:HA	1:A:722:VAL:O	2.20	0.41
1:A:733:LEU:CD2	1:A:753:ALA:HB2	2.51	0.41
1:A:80:LYS:NZ	4:A:2129:HOH:O	2.52	0.41
1:A:420:GLU:CD	1:A:420:GLU:H	2.26	0.41
1:B:186:PHE:O	1:B:205:THR:HA	2.20	0.41
1:A:39:ARG:HE	1:A:51:LEU:HB3	1.84	0.41
1:A:365:PHE:HZ	1:A:381:LEU:HG	1.86	0.41
1:A:671:HIS:O	1:A:675:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:THR:O	1:B:122:ARG:HA	2.21	0.41
1:B:157:ASN:HD21	1:B:159:SER:CB	2.33	0.41
1:B:204:LYS:HA	1:B:215:PHE:O	2.20	0.41
1:B:375:LYS:HG2	4:B:2211:HOH:O	2.21	0.41
1:A:182:TYR:O	1:A:183:ASP:C	2.63	0.41
1:A:698:TYR:OH	1:A:713:GLN:NE2	2.53	0.41
1:B:280:GLN:HG3	4:B:2428:HOH:O	2.19	0.41
1:A:1:MET:HG3	1:A:664:ASN:CG	2.46	0.41
1:B:689:MET:HA	1:B:697:HIS:O	2.20	0.41
1:A:160:ASP:O	1:A:161:ALA:CB	2.67	0.41
1:A:182:TYR:HD2	1:A:186:PHE:CZ	2.39	0.41
1:A:426:ILE:HD13	1:A:467:ARG:HH11	1.78	0.41
1:A:477:TYR:CD2	1:A:537:ILE:HA	2.56	0.41
1:A:478:MET:HB3	1:A:494:ASN:OD1	2.20	0.41
1:B:212:THR:HB	1:B:213:PRO:HD2	2.02	0.41
1:B:414:GLU:HG2	1:B:422:THR:HG23	2.02	0.41
1:A:204:LYS:HA	1:A:215:PHE:O	2.21	0.41
1:B:176:MET:HE3	4:B:2268:HOH:O	2.20	0.41
1:B:361:GLU:HA	1:B:365:PHE:CD1	2.56	0.41
1:A:22:LYS:HE2	1:A:42:PHE:CE1	2.55	0.40
1:B:574:ARG:HA	1:B:575:PRO:C	2.46	0.40
1:A:682:VAL:O	1:A:686:PHE:HB2	2.22	0.40
1:A:375:LYS:HE3	1:A:375:LYS:HB2	1.88	0.40
1:A:388:LEU:HD12	1:A:388:LEU:HA	1.94	0.40
1:A:657:LEU:HA	1:A:662:TYR:CD1	2.55	0.40
1:A:134:ALA:HB2	1:A:158:LEU:HD11	2.03	0.40
1:A:479:ILE:HB	1:A:499:ASN:HD21	1.86	0.40
1:B:188:ASP:OD2	1:B:206:THR:HG22	2.21	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	751/754 (100%)	725 (96%)	24 (3%)	2 (0%)	36	34
1	B	752/754 (100%)	732 (97%)	20 (3%)	0	100	100
All	All	1503/1508 (100%)	1457 (97%)	44 (3%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	ASP
1	A	182	TYR

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	117/647 (18%)	115 (98%)	2 (2%)	53	60
1	B	627/647 (97%)	616 (98%)	11 (2%)	51	58
All	All	744/1294 (58%)	731 (98%)	13 (2%)	53	60

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	179	GLU
1	B	33	ASN
1	B	51	LEU
1	B	222	ARG
1	B	233	THR
1	B	319	GLN
1	B	329	LEU
1	B	361	GLU
1	B	420	GLU
1	B	429	ASN
1	B	462	ARG
1	B	670	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	A	229	ASN
1	A	234	GLN
1	A	236	ASN
1	A	663	ASN
1	A	671	HIS
1	A	684	GLN
1	A	697	HIS
1	A	713	GLN
1	B	8	GLN
1	B	11	ASN
1	B	25	GLN
1	B	33	ASN
1	B	117	GLN
1	B	121	ASN
1	B	136	ASN
1	B	145	GLN
1	B	157	ASN
1	B	195	GLN
1	B	251	GLN
1	B	280	GLN
1	B	297	HIS
1	B	303	GLN
1	B	319	GLN
1	B	320	GLN
1	B	325	ASN
1	B	328	GLN
1	B	379	ASN
1	B	396	GLN
1	B	416	HIS
1	B	427	HIS
1	B	429	ASN
1	B	451	HIS
1	B	475	ASN
1	B	476	GLN
1	B	491	ASN
1	B	494	ASN
1	B	495	ASN
1	B	518	GLN
1	B	523	GLN
1	B	535	GLN

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Mol	Chain	Res	Type
1	B	554	GLN
1	B	578	GLN
1	B	611	GLN
1	B	634	HIS
1	B	664	ASN
1	B	684	GLN
1	B	695	GLN
1	B	697	HIS
1	B	713	GLN

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 3 ligands modelled in this entry, 2 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	$\# Z > 2$
3	PO4	B	1755	-	4,4,4	1.82	3 (75%)	6,6,6	0.46	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1755	PO4	P-O3	-2.12	1.48	1.54
3	B	1755	PO4	P-O4	-2.12	1.48	1.54
3	B	1755	PO4	P-O2	-2.01	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.