



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:42 PM GMT

PDB ID : 1QAT
Title : 1-PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE PHOSPHODI-
ESTERASE DELTA COMPLEX WITH SAMARIUM (III) CHLORIDE
Authors : Grobler, J.A.; Hurley, J.H.
Deposited on : 1996-08-02
Resolution : 3.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

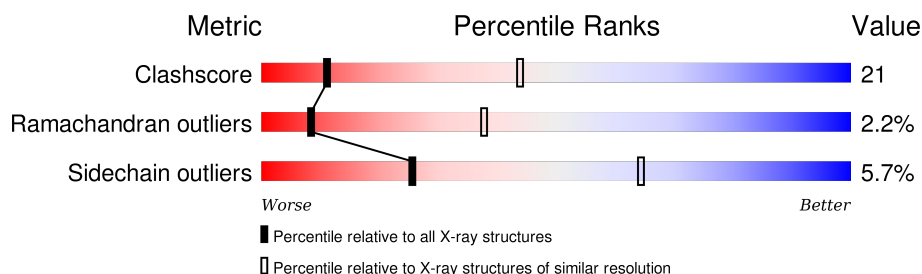
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	622	
1	B	622	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8022 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 PHOSPHOLIPASE C DELTA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4018	2536	704	756	22			
1	B	507	Total	C	N	O	S	0	0	0
			3999	2526	701	750	22			

- Molecule 2 is SAMARIUM (III) ION (three-letter code: SM) (formula: Sm).

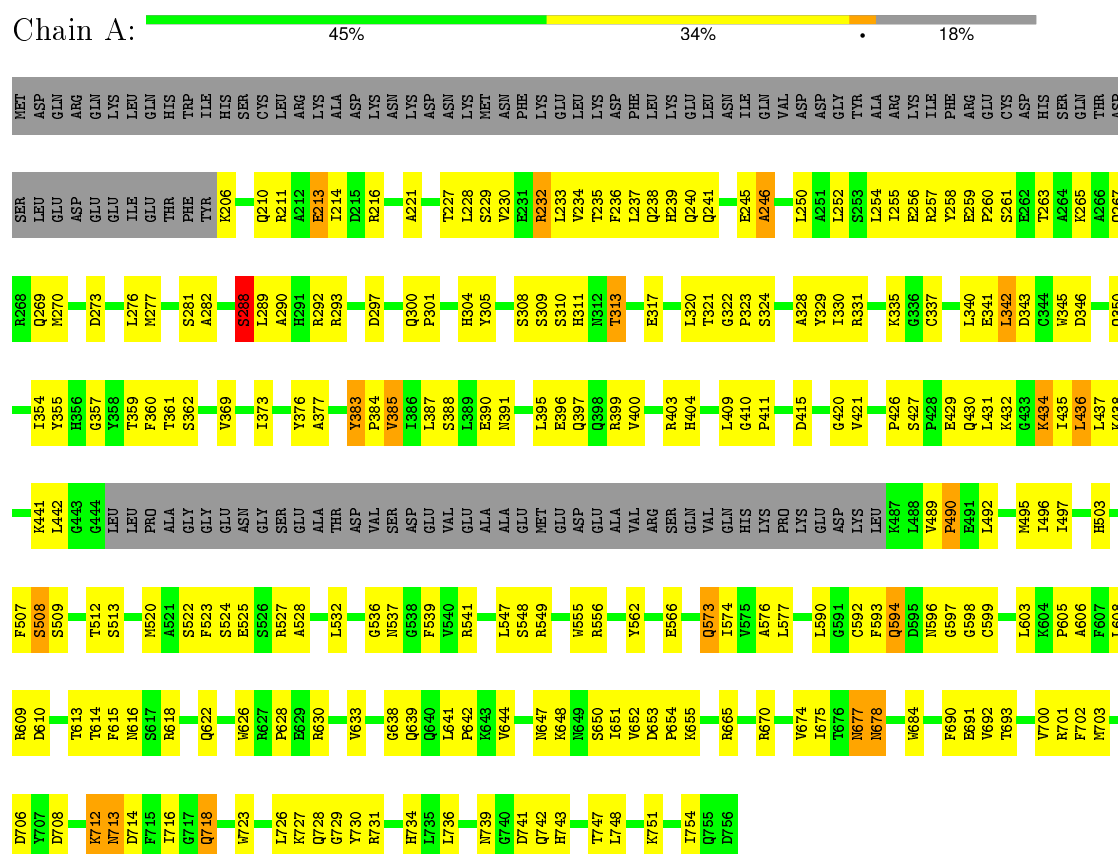
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Sm	0	0
			3	3		
2	A	2	Total	Sm	0	0
			2	2		

3 Residue-property plots

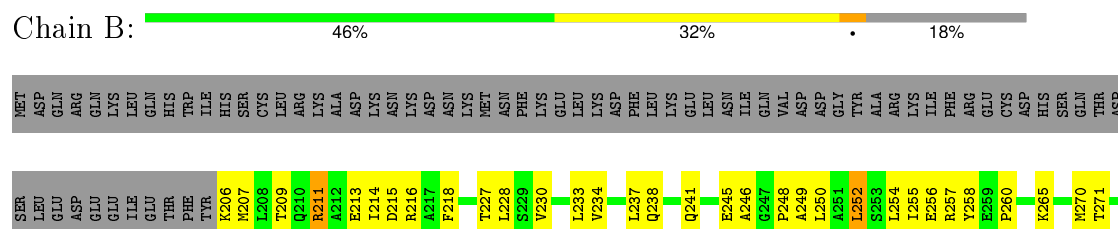
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: PHOSPHOLIPASE C DELTA-1



• Molecule 1: PHOSPHOLIPASE C DELTA-1



PRO	GLY	L445	Y355	L276
	THR	LEU	H356	M277
	SER	ALA	G357	S281
	G514	GLY	F360	A282
	M520	GLU	T361	D283
	F523	ASN	S362	S288
	S524	GLY	I364	L289
	E525	SER	V369	A290
	S526	GLU	V369	H291
	R527	THR	T373	R292
PRO	A528	ASP	A377	R293
	L532	SER		Q296
	G536	GLU	X383	D297
	M537	VAL	R384	Q300
	G538	GLU	V385	P301
	F539	ALA	I386	H304
	V540	ALA	L387	X306
	R541	GLU	S388	Y305
	L547	MET	L389	S309
	S548	GLU	E390	S310
PRO	R549	ASP	N391	H311
	M555	ALA	L395	N312
	R556	VAL	E396	T313
	T557	ARG	Q397	E317
	Y562	SER	I398	L320
	E566	GLN	V400	T321
	Q573	LYS	R403	G322
	I574	PRO	H404	P323
	V575	GLU	P411	S324
	A576	ASP	D415	
PRO	L577	LYS	V421	E327
	L590	L486		A328
	G591	R487	P426	Y329
	C592	L488	S427	L330
	F593	P490	A428	R331
	O594	E491	E429	
	D595	L492	Q430	E341
	M596		L431	L342
	G597	M495	R432	L343
	C598	I496	Q433	C344
PRO	C599	I497	H434	N345
	L603	X500	I435	D346
	R604		L436	G347
	P605	H503	L437	P348
	A606		K438	N349
	F607	F507	L442	Q350
	L608	S508	O443	E351
	R609	E509	P444	T354
	D610			
	T613			
W723	T614			
	F615			
	H616			
	S617			
	R618			
	D622			
	R630			
	V633			
	G638			
	D640			
W726	L641			
	P642			
	R643			
	V644			
	H645			
	K646			
	L647			
	R648			
	M649			
	S650			
W751	T651			
	V652			
	D653			
	P654			
	V674			
	L675			
	T676			
	H677			
	H678			
	V684			
W754	E691			
	V692			
	L699			
	V700			
	R701			
	F702			
	R703			
	D706			
	Y707			
	D708			
W756	S709			
	S710			
	I716			
	F717			
	Q718			

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.60Å 75.10Å 86.40Å 66.40° 85.60° 89.80°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.194 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8022	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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: SM

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	0.46	0/4111	0.76	3/5568 (0.1%)
1	B	0.46	0/4090	0.76	4/5539 (0.1%)
All	All	0.46	0/8201	0.76	7/11107 (0.1%)

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	B	0	2
All	All	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ARG	NE-CZ-NH1	14.31	127.46	120.30
1	A	331	ARG	NE-CZ-NH2	-13.87	113.36	120.30
1	B	331	ARG	NE-CZ-NH2	-12.49	114.06	120.30
1	B	331	ARG	NE-CZ-NH1	12.35	126.47	120.30
1	A	331	ARG	CD-NE-CZ	7.13	133.59	123.60
1	B	331	ARG	CD-NE-CZ	6.89	133.24	123.60
1	B	207	MET	CG-SD-CE	6.14	110.03	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	383	TYR	Sidechain
1	B	305	TYR	Sidechain
1	B	383	TYR	Sidechain

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	4018	0	3941	166	0
1	B	3999	0	3916	166	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
All	All	8022	0	7857	330	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 21.

All (330) 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:206:LYS:HA	1:A:210:GLN:HG3	1.49	0.93
1:B:547:LEU:HD23	1:B:573:GLN:HG3	1.60	0.84
1:A:537:ASN:HD22	1:A:614:THR:HA	1.43	0.81
1:A:547:LEU:HD23	1:A:573:GLN:HG3	1.62	0.81
1:B:537:ASN:HD22	1:B:614:THR:HA	1.46	0.79
1:B:206:LYS:HA	1:B:209:THR:OG1	1.83	0.78
1:B:241:GLN:HE22	1:B:730:TYR:H	1.32	0.78
1:A:211:ARG:HB2	1:A:214:ILE:HB	1.65	0.76
1:B:309:SER:OG	1:B:574:ILE:HG23	1.86	0.76
1:A:350:GLN:HE22	1:A:396:GLU:HG3	1.52	0.75
1:B:350:GLN:HE22	1:B:396:GLU:HG3	1.52	0.74
1:B:648:LYS:HA	1:B:648:LYS:HE2	1.70	0.73
1:B:442:LEU:HG	1:B:488:LEU:HD23	1.69	0.72
1:B:245:GLU:HA	1:B:250:LEU:HD22	1.69	0.72
1:B:701:ARG:HE	1:B:718:GLN:HE21	1.36	0.72
1:B:548:SER:H	1:B:573:GLN:HE21	1.38	0.71
1:B:289:LEU:HD12	1:B:292:ARG:HG3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LYS:HD3	1:B:590:LEU:HD11	1.71	0.71
1:A:230:VAL:O	1:A:234:VAL:HG23	1.90	0.71
1:B:644:VAL:CG1	1:B:716:ILE:HG12	2.19	0.70
1:A:321:THR:HG22	1:A:360:PHE:HB2	1.72	0.69
1:A:335:LYS:HD3	1:A:590:LEU:HD11	1.74	0.69
1:B:211:ARG:NH1	1:B:276:LEU:HD11	2.07	0.69
1:B:566:GLU:HG2	1:B:618:ARG:HH21	1.56	0.69
1:B:321:THR:HG22	1:B:360:PHE:HB2	1.72	0.69
1:B:644:VAL:HG12	1:B:716:ILE:HG12	1.74	0.68
1:A:385:VAL:HG22	1:A:435:ILE:HG12	1.75	0.68
1:B:644:VAL:HG11	1:B:706:ASP:HB2	1.76	0.68
1:B:734:HIS:HA	1:B:747:THR:HG22	1.74	0.68
1:A:309:SER:OG	1:A:574:ILE:HG23	1.92	0.68
1:A:227:THR:CG2	1:A:269:GLN:HB3	2.24	0.68
1:A:228:LEU:HB2	1:A:270:MET:HB3	1.76	0.68
1:B:610:ASP:HB3	1:B:613:THR:HB	1.76	0.68
1:A:536:GLY:HA3	1:A:616:ASN:HD22	1.59	0.67
1:B:399:ARG:O	1:B:403:ARG:HG2	1.95	0.67
1:B:385:VAL:HG22	1:B:435:ILE:HG12	1.77	0.67
1:A:610:ASP:HB3	1:A:613:THR:HB	1.77	0.67
1:B:605:PRO:HD2	1:B:608:LEU:HD12	1.76	0.67
1:A:701:ARG:HE	1:A:718:GLN:HE21	1.42	0.66
1:A:548:SER:H	1:A:573:GLN:HE21	1.43	0.66
1:A:566:GLU:HG2	1:A:618:ARG:HH21	1.61	0.65
1:B:652:VAL:O	1:B:677:ASN:HA	1.97	0.65
1:A:238:GLN:HB3	1:A:246:ALA:HB3	1.79	0.65
1:B:536:GLY:HA3	1:B:616:ASN:HD22	1.61	0.65
1:A:395:LEU:O	1:A:399:ARG:HG3	1.97	0.64
1:A:399:ARG:O	1:A:403:ARG:HG2	1.98	0.64
1:A:734:HIS:HA	1:A:747:THR:HG22	1.78	0.64
1:B:324:SER:H	1:B:362:SER:HB3	1.62	0.64
1:A:324:SER:H	1:A:362:SER:HB3	1.61	0.64
1:B:703:MET:HG2	1:B:718:GLN:HB3	1.79	0.64
1:B:395:LEU:O	1:B:399:ARG:HG3	1.98	0.64
1:B:652:VAL:HG12	1:B:653:ASP:N	2.13	0.64
1:B:228:LEU:HB2	1:B:270:MET:HB3	1.79	0.64
1:A:605:PRO:HD2	1:A:608:LEU:HD12	1.80	0.64
1:B:593:PHE:O	1:B:598:GLY:HA2	1.98	0.63
1:B:437:LEU:HD12	1:B:495:MET:HB3	1.80	0.63
1:A:651:ILE:HB	1:A:677:ASN:OD1	1.98	0.63
1:A:238:GLN:HB3	1:A:246:ALA:CB	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:PHE:CD1	1:A:240:GLN:HG3	2.35	0.61
1:A:228:LEU:HD13	1:A:233:LEU:HD13	1.81	0.61
1:A:593:PHE:O	1:A:598:GLY:HA2	2.00	0.61
1:B:292:ARG:O	1:B:597:GLY:HA2	2.01	0.61
1:B:438:LYS:HE3	1:B:520:MET:HE2	1.81	0.61
1:A:437:LEU:HD12	1:A:495:MET:HB3	1.82	0.61
1:A:236:PHE:HD1	1:A:240:GLN:HG3	1.66	0.61
1:B:373:ILE:O	1:B:377:ALA:HB2	2.01	0.61
1:B:300:GLN:HB2	1:B:305:TYR:CE1	2.36	0.61
1:B:256:GLU:HA	1:B:265:LYS:HE3	1.82	0.60
1:B:301:PRO:HD2	1:B:304:HIS:ND1	2.17	0.60
1:A:373:ILE:O	1:A:377:ALA:HB2	2.01	0.59
1:A:350:GLN:NE2	1:A:396:GLU:HG3	2.16	0.59
1:A:256:GLU:HA	1:A:265:LYS:HE3	1.82	0.59
1:B:426:PRO:HG2	1:B:431:LEU:HD11	1.84	0.59
1:A:642:PRO:HD2	1:A:716:ILE:HG22	1.84	0.59
1:A:227:THR:HG22	1:A:269:GLN:HB3	1.84	0.59
1:B:350:GLN:NE2	1:B:396:GLU:HG3	2.17	0.59
1:A:642:PRO:HG2	1:A:743:HIS:CE1	2.37	0.59
1:B:701:ARG:HE	1:B:718:GLN:NE2	2.00	0.59
1:B:536:GLY:HA3	1:B:616:ASN:ND2	2.17	0.58
1:A:300:GLN:HB2	1:A:305:TYR:CE2	2.38	0.58
1:A:692:VAL:HG21	1:A:723:TRP:CZ3	2.38	0.58
1:A:411:PRO:O	1:A:434:LYS:HE2	2.03	0.58
1:A:537:ASN:ND2	1:A:614:THR:HA	2.17	0.58
1:A:590:LEU:O	1:A:594:GLN:HG2	2.03	0.58
1:A:395:LEU:HD22	1:A:489:VAL:HG13	1.86	0.58
1:A:594:GLN:HE21	1:A:594:GLN:HA	1.69	0.58
1:A:729:GLY:O	1:A:751:LYS:HA	2.03	0.58
1:B:729:GLY:O	1:B:751:LYS:HA	2.02	0.58
1:A:652:VAL:O	1:A:677:ASN:HA	2.04	0.58
1:B:590:LEU:O	1:B:594:GLN:HG2	2.03	0.57
1:A:630:ARG:NH1	1:A:630:ARG:HB2	2.20	0.57
1:A:596:ASN:ND2	1:A:599:CYS:SG	2.77	0.57
1:B:311:HIS:HB2	1:B:576:ALA:HB1	1.86	0.57
1:B:594:GLN:HE21	1:B:594:GLN:HA	1.69	0.57
1:B:218:PHE:CE1	1:B:228:LEU:HG	2.40	0.57
1:B:728:GLN:NE2	1:B:754:ILE:H	2.03	0.57
1:B:411:PRO:O	1:B:434:LYS:HE2	2.04	0.57
1:B:610:ASP:O	1:B:613:THR:HG22	2.04	0.57
1:A:263:THR:O	1:A:267:GLN:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LEU:HD11	1:A:254:LEU:HD12	1.86	0.57
1:A:292:ARG:O	1:A:597:GLY:HA2	2.05	0.57
1:A:426:PRO:HG2	1:A:431:LEU:HD11	1.87	0.56
1:A:313:THR:HB	1:A:329:TYR:CE1	2.40	0.56
1:A:536:GLY:HA3	1:A:616:ASN:ND2	2.20	0.56
1:A:323:PRO:HA	1:A:362:SER:HB2	1.86	0.56
1:B:320:LEU:HD11	1:B:557:THR:HG21	1.88	0.56
1:B:548:SER:N	1:B:573:GLN:HE21	2.03	0.55
1:A:214:ILE:HG13	1:A:276:LEU:HD13	1.88	0.55
1:B:701:ARG:NE	1:B:718:GLN:HE21	2.03	0.55
1:B:652:VAL:HG12	1:B:653:ASP:H	1.69	0.55
1:A:429:GLU:O	1:A:432:LYS:HG3	2.05	0.55
1:B:429:GLU:O	1:B:432:LYS:HG3	2.05	0.55
1:B:633:VAL:HG11	1:B:702:PHE:HE2	1.73	0.54
1:A:400:VAL:HG12	1:A:404:HIS:CD2	2.42	0.54
1:B:537:ASN:ND2	1:B:614:THR:HA	2.20	0.54
1:A:301:PRO:HD2	1:A:304:HIS:ND1	2.23	0.54
1:B:323:PRO:HA	1:B:362:SER:HB2	1.89	0.54
1:B:537:ASN:O	1:B:541:ARG:HG3	2.09	0.53
1:B:728:GLN:HE21	1:B:754:ILE:H	1.56	0.53
1:B:727:LYS:HE3	1:B:731:ARG:NH2	2.23	0.53
1:B:246:ALA:H	1:B:250:LEU:HB2	1.73	0.53
1:A:227:THR:HG21	1:A:269:GLN:HB3	1.89	0.53
1:B:492:LEU:HA	1:B:495:MET:HE3	1.89	0.53
1:B:354:ILE:HD12	1:B:369:VAL:HG21	1.89	0.53
1:A:549:ARG:NH1	1:A:549:ARG:HG2	2.23	0.53
1:A:701:ARG:HE	1:A:718:GLN:NE2	2.06	0.53
1:B:258:TYR:OH	1:B:283:ASP:HB2	2.08	0.53
1:B:400:VAL:HG12	1:B:404:HIS:CD2	2.43	0.53
1:A:610:ASP:O	1:A:613:THR:HG22	2.08	0.53
1:B:313:THR:HB	1:B:329:TYR:CE2	2.43	0.53
1:A:537:ASN:O	1:A:541:ARG:HG3	2.09	0.53
1:A:420:GLY:H	1:B:349:ASN:ND2	2.07	0.53
1:B:230:VAL:O	1:B:234:VAL:HG23	2.09	0.53
1:A:346:ASP:HA	1:A:397:GLN:OE1	2.09	0.53
1:B:630:ARG:HB2	1:B:630:ARG:NH1	2.25	0.52
1:B:596:ASN:ND2	1:B:599:CYS:SG	2.82	0.52
1:A:728:GLN:NE2	1:A:754:ILE:H	2.08	0.52
1:B:644:VAL:C	1:B:646:LYS:H	2.13	0.52
1:A:297:ASP:OD1	1:A:300:GLN:HG2	2.09	0.52
1:A:282:ALA:HB1	1:A:289:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:LEU:N	1:B:436:LEU:HD23	2.24	0.52
1:A:648:LYS:HE2	1:A:648:LYS:HA	1.90	0.52
1:A:237:LEU:HD23	1:A:241:GLN:HG3	1.92	0.52
1:B:692:VAL:HG21	1:B:723:TRP:CZ3	2.45	0.51
1:B:330:ILE:HG12	1:B:376:TYR:CD2	2.45	0.51
1:B:304:HIS:O	1:B:603:LEU:HD12	2.10	0.51
1:A:549:ARG:HG2	1:A:549:ARG:HH11	1.76	0.51
1:B:736:LEU:HA	1:B:742:GLN:HA	1.91	0.51
1:B:346:ASP:HA	1:B:397:GLN:OE1	2.11	0.51
1:A:206:LYS:HA	1:A:210:GLN:CG	2.30	0.51
1:A:703:MET:HG2	1:A:718:GLN:HB3	1.91	0.51
1:A:311:HIS:HB2	1:A:576:ALA:HB1	1.93	0.51
1:A:736:LEU:HA	1:A:742:GLN:HA	1.91	0.51
1:A:548:SER:N	1:A:573:GLN:HE21	2.07	0.51
1:B:644:VAL:HG21	1:B:706:ASP:OD2	2.10	0.51
1:B:547:LEU:CD2	1:B:573:GLN:HG3	2.36	0.51
1:A:211:ARG:HB3	1:A:213:GLU:OE2	2.10	0.51
1:B:211:ARG:HB2	1:B:213:GLU:OE2	2.10	0.51
1:A:638:GLY:HA2	1:A:748:LEU:HA	1.93	0.51
1:B:355:TYR:CZ	1:B:357:GLY:HA2	2.46	0.51
1:B:257:ARG:HD2	1:B:258:TYR:CZ	2.45	0.51
1:A:354:ILE:HD12	1:A:369:VAL:HG21	1.93	0.50
1:A:492:LEU:HA	1:A:495:MET:HE3	1.92	0.50
1:A:675:ILE:HG12	1:A:684:TRP:NE1	2.26	0.50
1:B:650:SER:O	1:B:651:ILE:HG13	2.11	0.50
1:A:523:PHE:HD1	1:A:527:ARG:HD3	1.76	0.50
1:B:395:LEU:HD22	1:B:489:VAL:HG13	1.94	0.50
1:A:300:GLN:HG3	1:A:603:LEU:HD11	1.94	0.50
1:A:727:LYS:HE3	1:A:731:ARG:NH2	2.27	0.50
1:A:396:GLU:O	1:A:400:VAL:HG23	2.11	0.49
1:B:297:ASP:OD1	1:B:300:GLN:HG2	2.12	0.49
1:B:444:GLY:HA2	1:B:500:LYS:HZ1	1.76	0.49
1:A:421:VAL:HG11	1:A:426:PRO:HD3	1.94	0.49
1:B:429:GLU:HA	1:B:432:LYS:HG3	1.93	0.49
1:A:547:LEU:CD2	1:A:573:GLN:HG3	2.38	0.49
1:A:429:GLU:HA	1:A:432:LYS:HG3	1.92	0.49
1:A:355:TYR:CZ	1:A:357:GLY:HA2	2.48	0.49
1:B:438:LYS:CE	1:B:520:MET:HE2	2.42	0.49
1:A:313:THR:O	1:A:328:ALA:HB1	2.12	0.49
1:A:436:LEU:N	1:A:436:LEU:HD23	2.28	0.49
1:B:396:GLU:O	1:B:400:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:ARG:HH11	1:A:618:ARG:HG3	1.76	0.49
1:A:290:ALA:O	1:A:293:ARG:HG2	2.13	0.48
1:B:427:SER:OG	1:B:430:GLN:HG3	2.13	0.48
1:A:630:ARG:HH11	1:A:630:ARG:HB2	1.78	0.48
1:B:234:VAL:O	1:B:238:GLN:HG2	2.13	0.48
1:A:258:TYR:CE1	1:A:281:SER:HB2	2.48	0.48
1:B:549:ARG:HG2	1:B:549:ARG:NH1	2.28	0.48
1:A:633:VAL:HG11	1:A:702:PHE:HE2	1.78	0.48
1:B:523:PHE:HD1	1:B:527:ARG:HD3	1.78	0.48
1:B:548:SER:H	1:B:573:GLN:NE2	2.10	0.48
1:A:701:ARG:NE	1:A:718:GLN:HE21	2.10	0.48
1:B:555:TRP:HE3	1:B:555:TRP:O	1.96	0.48
1:B:245:GLU:HA	1:B:250:LEU:CD2	2.43	0.48
1:B:438:LYS:CD	1:B:520:MET:HE2	2.44	0.48
1:A:642:PRO:HD2	1:A:716:ILE:CG2	2.44	0.48
1:B:675:ILE:HG12	1:B:684:TRP:NE1	2.29	0.48
1:B:345:TRP:CZ2	1:B:357:GLY:HA3	2.48	0.47
1:B:292:ARG:C	1:B:597:GLY:HA2	2.35	0.47
1:B:256:GLU:O	1:B:265:LYS:HE3	2.13	0.47
1:A:728:GLN:HE21	1:A:754:ILE:H	1.62	0.47
1:B:643:LYS:O	1:B:645:ASN:N	2.47	0.47
1:B:528:ALA:O	1:B:532:LEU:HG	2.14	0.47
1:B:652:VAL:CG1	1:B:653:ASP:N	2.78	0.47
1:A:628:PRO:HB3	1:A:693:THR:HA	1.97	0.47
1:A:438:LYS:CD	1:A:520:MET:HE2	2.45	0.47
1:A:259:GLU:OE2	1:A:261:SER:HB3	2.15	0.47
1:A:438:LYS:HE3	1:A:520:MET:HE2	1.97	0.46
1:B:594:GLN:HE21	1:B:594:GLN:CA	2.28	0.46
1:B:643:LYS:H	1:B:643:LYS:HD2	1.81	0.46
1:A:562:TYR:CE1	1:A:577:LEU:HD23	2.51	0.46
1:B:241:GLN:N	1:B:241:GLN:HE21	2.14	0.46
1:A:594:GLN:HE21	1:A:594:GLN:CA	2.28	0.46
1:B:300:GLN:HB2	1:B:305:TYR:CZ	2.51	0.46
1:B:258:TYR:O	1:B:260:PRO:HD3	2.15	0.46
1:A:388:SER:HA	1:A:438:LYS:HB3	1.98	0.46
1:A:403:ARG:HG3	1:A:403:ARG:HH11	1.81	0.46
1:B:618:ARG:HG3	1:B:618:ARG:HH11	1.78	0.46
1:A:555:TRP:O	1:A:555:TRP:HE3	1.98	0.46
1:B:228:LEU:HD12	1:B:270:MET:HB3	1.97	0.45
1:B:369:VAL:O	1:B:373:ILE:HG13	2.16	0.45
1:B:313:THR:O	1:B:328:ALA:HB1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:TRP:CZ2	1:A:357:GLY:HA3	2.51	0.45
1:A:330:ILE:HG12	1:A:376:TYR:CD2	2.51	0.45
1:A:427:SER:OG	1:A:430:GLN:HG3	2.16	0.45
1:B:525:GLU:OE2	1:B:556:ARG:NE	2.49	0.45
1:B:289:LEU:HA	1:B:292:ARG:HG2	1.98	0.45
1:B:630:ARG:HB2	1:B:630:ARG:HH11	1.82	0.45
1:B:638:GLY:HA2	1:B:748:LEU:HA	1.99	0.45
1:B:415:ASP:C	1:B:497:ILE:HD11	2.37	0.45
1:A:441:LYS:HD2	1:A:496:ILE:O	2.17	0.45
1:B:642:PRO:HD3	1:B:746:ALA:HB2	1.97	0.45
1:A:508:SER:O	1:A:509:SER:HB2	2.16	0.45
1:B:707:TYR:CE2	1:B:709:SER:HA	2.51	0.45
1:B:606:ALA:HA	1:B:609:ARG:HE	1.82	0.45
1:B:383:TYR:HB3	1:B:384:PRO:HD2	1.99	0.45
1:B:290:ALA:O	1:B:293:ARG:HG2	2.17	0.45
1:A:383:TYR:HB3	1:A:384:PRO:HD2	1.99	0.44
1:B:214:ILE:HG13	1:B:276:LEU:HD13	1.99	0.44
1:B:403:ARG:HG3	1:B:403:ARG:HH11	1.82	0.44
1:B:317:GLU:HB2	1:B:323:PRO:HD2	1.98	0.44
1:A:256:GLU:HA	1:A:265:LYS:CE	2.47	0.44
1:A:525:GLU:OE2	1:A:556:ARG:NE	2.49	0.44
1:A:277:MET:O	1:A:281:SER:HB3	2.17	0.44
1:A:235:THR:O	1:A:239:HIS:HB3	2.18	0.44
1:A:712:LYS:HG2	1:A:713:ASN:H	1.81	0.44
1:B:652:VAL:CG1	1:B:653:ASP:H	2.28	0.44
1:B:388:SER:HA	1:B:438:LYS:HB3	2.00	0.44
1:A:706:ASP:O	1:A:713:ASN:HA	2.17	0.44
1:B:324:SER:N	1:B:362:SER:HB3	2.32	0.44
1:A:670:ARG:HG3	1:A:690:PHE:CZ	2.53	0.44
1:B:364:ILE:HD12	1:B:369:VAL:HG22	1.99	0.44
1:B:489:VAL:HG23	1:B:492:LEU:H	1.81	0.44
1:B:228:LEU:HD13	1:B:233:LEU:HD13	2.00	0.44
1:B:739:ASN:ND2	1:B:741:ASP:CG	2.72	0.44
1:B:248:PRO:O	1:B:252:LEU:HD12	2.16	0.44
1:A:214:ILE:HD13	1:A:214:ILE:HA	1.88	0.43
1:A:221:ALA:HB1	1:A:228:LEU:HD21	2.01	0.43
1:B:387:LEU:HD23	1:B:387:LEU:HA	1.71	0.43
1:B:227:THR:HG22	1:B:271:THR:HG22	1.99	0.43
1:A:300:GLN:HB2	1:A:305:TYR:CZ	2.54	0.43
1:B:347:GLY:HA3	1:B:351:GLU:O	2.18	0.43
1:B:487:LYS:HG2	1:B:487:LYS:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LEU:O	1:A:359:THR:HB	2.17	0.43
1:B:323:PRO:HA	1:B:362:SER:CB	2.48	0.43
1:A:237:LEU:O	1:A:241:GLN:HB2	2.19	0.43
1:A:257:ARG:HG2	1:A:257:ARG:O	2.18	0.43
1:B:237:LEU:HD13	1:B:250:LEU:HD23	2.01	0.43
1:A:317:GLU:HB2	1:A:323:PRO:HD2	2.00	0.43
1:A:654:PRO:HD2	1:A:675:ILE:O	2.17	0.43
1:A:308:SER:OG	1:A:337:CYS:HA	2.19	0.43
1:A:644:VAL:HG22	1:A:644:VAL:O	2.18	0.43
1:B:343:ASP:HA	1:B:390:GLU:HB3	2.01	0.43
1:A:492:LEU:HD23	1:A:495:MET:CE	2.48	0.43
1:A:700:VAL:HG21	1:A:726:LEU:HD22	2.00	0.43
1:A:343:ASP:HA	1:A:390:GLU:HB3	2.01	0.43
1:B:700:VAL:HG21	1:B:726:LEU:HD22	2.00	0.43
1:B:549:ARG:HG2	1:B:549:ARG:HH11	1.84	0.43
1:A:490:PRO:HD2	1:B:327:GLU:OE2	2.19	0.43
1:B:246:ALA:CB	1:B:249:ALA:HB3	2.49	0.42
1:A:258:TYR:CE1	1:A:281:SER:CB	3.02	0.42
1:A:507:PHE:O	1:A:508:SER:HB3	2.18	0.42
1:A:229:SER:OG	1:A:232:ARG:HB2	2.20	0.42
1:A:387:LEU:HD23	1:A:387:LEU:HA	1.66	0.42
1:B:341:GLU:C	1:B:342:LEU:HD12	2.40	0.42
1:A:730:TYR:CZ	1:A:751:LYS:HD2	2.54	0.42
1:B:674:VAL:HG21	1:B:707:TYR:CG	2.54	0.42
1:B:592:CYS:HB2	1:B:699:LEU:HD21	2.00	0.42
1:B:701:ARG:HH21	1:B:718:GLN:HG2	1.84	0.42
1:A:618:ARG:HG3	1:A:618:ARG:NH1	2.34	0.42
1:B:296:GLN:HG3	1:B:596:ASN:OD1	2.20	0.42
1:B:562:TYR:CE1	1:B:577:LEU:HD23	2.55	0.42
1:B:507:PHE:O	1:B:508:SER:HB2	2.20	0.42
1:A:292:ARG:C	1:A:597:GLY:HA2	2.39	0.42
1:A:245:GLU:HB2	1:A:250:LEU:HD22	2.02	0.42
1:A:324:SER:HB2	1:A:362:SER:O	2.20	0.42
1:A:341:GLU:C	1:A:342:LEU:HD12	2.41	0.42
1:B:537:ASN:HB3	1:B:615:PHE:O	2.20	0.41
1:A:340:LEU:HB2	1:A:387:LEU:CD2	2.50	0.41
1:A:739:ASN:ND2	1:A:741:ASP:CG	2.74	0.41
1:B:442:LEU:HD21	1:B:488:LEU:HB3	2.02	0.41
1:A:260:PRO:HG3	1:A:273:ASP:CB	2.50	0.41
1:A:528:ALA:O	1:A:532:LEU:HG	2.19	0.41
1:B:421:VAL:HG11	1:B:426:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:SER:HA	1:A:549:ARG:O	2.20	0.41
1:A:252:LEU:HD23	1:A:252:LEU:HA	1.89	0.41
1:B:310:SER:HB2	1:B:337:CYS:SG	2.60	0.41
1:A:606:ALA:HA	1:A:609:ARG:HE	1.86	0.41
1:B:618:ARG:HG3	1:B:618:ARG:NH1	2.35	0.41
1:A:304:HIS:O	1:A:603:LEU:HD12	2.21	0.41
1:B:645:ASN:O	1:B:647:ASN:N	2.53	0.41
1:A:255:ILE:O	1:A:259:GLU:HB3	2.21	0.41
1:B:218:PHE:HE1	1:B:228:LEU:HG	1.84	0.41
1:A:652:VAL:HG12	1:A:653:ASP:N	2.35	0.41
1:A:288:SER:HA	1:A:727:LYS:HD2	2.02	0.41
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.86	0.41
1:A:415:ASP:C	1:A:497:ILE:HD11	2.40	0.41
1:B:492:LEU:HD23	1:B:495:MET:CE	2.50	0.41
1:A:655:LYS:HB3	1:A:674:VAL:HG22	2.02	0.41
1:A:537:ASN:HB3	1:A:615:PHE:O	2.21	0.40
1:A:410:GLY:HA3	1:A:411:PRO:HD2	1.87	0.40
1:A:310:SER:HB2	1:A:337:CYS:SG	2.61	0.40
1:A:322:GLY:O	1:A:361:THR:HA	2.20	0.40
1:B:555:TRP:CE3	1:B:555:TRP:O	2.74	0.40
1:B:654:PRO:HD2	1:B:675:ILE:O	2.21	0.40
1:A:626:TRP:HH2	1:A:665:ARG:CZ	2.34	0.40
1:B:730:TYR:CZ	1:B:751:LYS:HD2	2.57	0.40
1:A:323:PRO:HA	1:A:362:SER:CB	2.50	0.40
1:A:654:PRO:HG2	1:A:678:ASN:O	2.20	0.40
1:B:255:ILE:HD13	1:B:255:ILE:HG21	1.85	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	505/622 (81%)	457 (90%)	37 (7%)	11 (2%)	8	38
1	B	501/622 (80%)	452 (90%)	38 (8%)	11 (2%)	8	38
All	All	1006/1244 (81%)	909 (90%)	75 (8%)	22 (2%)	8	38

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	512	THR
1	A	513	SER
1	A	647	ASN
1	B	444	GLY
1	B	644	VAL
1	B	646	LYS
1	A	508	SER
1	A	246	ALA
1	A	650	SER
1	A	677	ASN
1	A	678	ASN
1	B	677	ASN
1	B	678	ASN
1	B	709	SER
1	B	710	SER
1	A	442	LEU
1	A	288	SER
1	A	712	LYS
1	B	281	SER
1	B	288	SER
1	B	650	SER
1	B	443	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	441/544 (81%)	416 (94%)	25 (6%)	25	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	437/544 (80%)	412 (94%)	25 (6%)	25	64
All	All	878/1088 (81%)	828 (94%)	50 (6%)	25	64

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	GLU
1	A	216	ARG
1	A	232	ARG
1	A	288	SER
1	A	313	THR
1	A	342	LEU
1	A	385	VAL
1	A	391	ASN
1	A	434	LYS
1	A	436	LEU
1	A	490	PRO
1	A	503	HIS
1	A	524	SER
1	A	539	PHE
1	A	573	GLN
1	A	592	CYS
1	A	594	GLN
1	A	622	GLN
1	A	639	GLN
1	A	641	LEU
1	A	691	GLU
1	A	708	ASP
1	A	713	ASN
1	A	714	ASP
1	A	718	GLN
1	B	211	ARG
1	B	215	ASP
1	B	216	ARG
1	B	252	LEU
1	B	254	LEU
1	B	277	MET
1	B	283	ASP
1	B	342	LEU
1	B	385	VAL
1	B	391	ASN
1	B	434	LYS

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Mol	Chain	Res	Type
1	B	436	LEU
1	B	490	PRO
1	B	503	HIS
1	B	524	SER
1	B	539	PHE
1	B	592	CYS
1	B	594	GLN
1	B	622	GLN
1	B	639	GLN
1	B	641	LEU
1	B	643	LYS
1	B	691	GLU
1	B	708	ASP
1	B	718	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	350	GLN
1	A	391	ASN
1	A	503	HIS
1	A	515	GLN
1	A	537	ASN
1	A	573	GLN
1	A	594	GLN
1	A	596	ASN
1	A	718	GLN
1	A	724	ASN
1	A	728	GLN
1	A	743	HIS
1	B	210	GLN
1	B	241	GLN
1	B	349	ASN
1	B	350	GLN
1	B	391	ASN
1	B	503	HIS
1	B	515	GLN
1	B	537	ASN
1	B	573	GLN
1	B	594	GLN
1	B	596	ASN
1	B	718	GLN

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Mol	Chain	Res	Type
1	B	728	GLN
1	B	743	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.