



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:55 AM GMT

PDB ID : 2ISD
Title : PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C-DELTA1 FROM RAT
Authors : Essen, L.-O.; Perisic, O.; Williams, R.L.
Deposited on : 1997-03-31
Resolution : 2.50 Å (reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

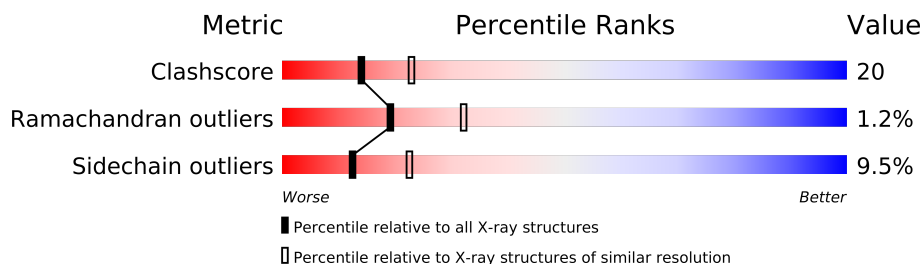
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	624	
1	B	624	

2 Entry composition i

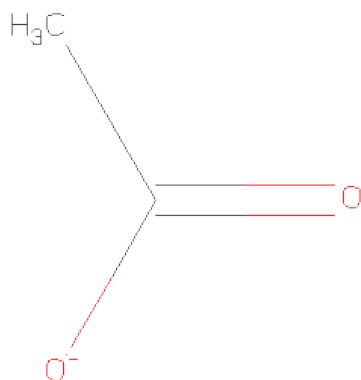
There are 3 unique types of molecules in this entry. The entry contains 9216 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	106	0	0
			4070	2573	709	766	22			
1	B	561	Total	C	N	O	S	104	0	0
			4465	2818	776	847	24			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	316	Total 316	O 316	0	0
3	B	357	Total 357	O 357	0	0

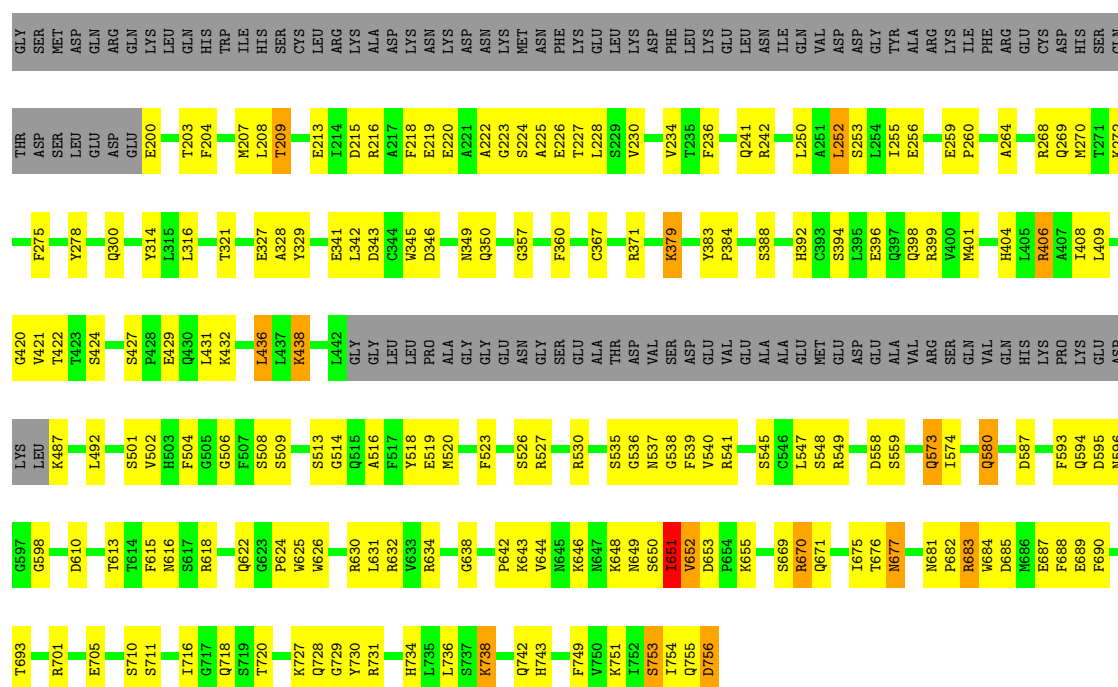
3 Residue-property plots

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.

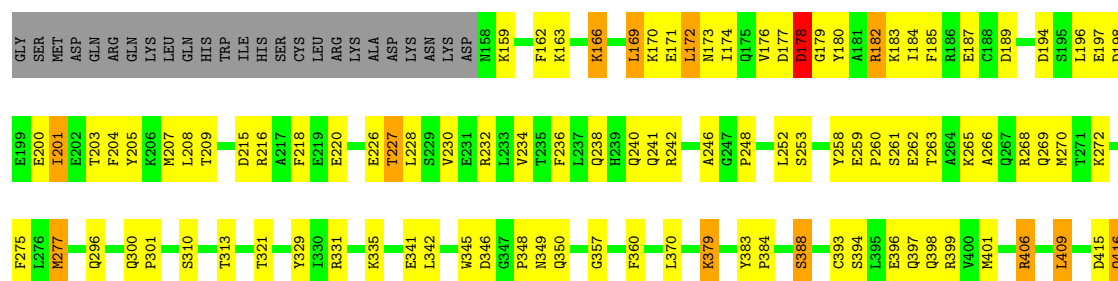
• Molecule 1: PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1

Chain A:



• Molecule 1: PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1

Chain B:



P417	L418	P426	S427	P428	E429	Q430	L431	K432	G433	K434	L435	L436	L437	K438	G439	K440	K441	L442	L445	LEU	PRO	ALA	GLY	GLY	GLY	GLY	ASN	GLY	SER	SER	GLU	ALA	THR	ASP	VAL	SER	SER	ASP	GLU	VAL	GLU	ALA	ALA	ALA	GLU	MET	GLU	ASP	ASP	ALA	VAL	ARG	SER	GLN	VAL	GLN	HIS	LYS	PRO	LYS	GLU
D484	K485	L486	K487	L488	L492	S493	D494	C499	K500	S501	F504	G505	G506	F507	S508	S509	P510	G511	T512	A516	F517	Y518	E519	M520	F523	S526	R527	S535	F539	S545	C546	S548	R549	I550	D558	S559	Q573	I574	Q580	D587	F593	Q594	D595	N596																	
G597	G598	P605	L608	R609	D610	P611	N612	T613	T614	F615	P624	W625	W626	R632	W633	R634	G638	V644	N645	K646	N647	K648	N649	S650	I651	V652	I657	Q671	T676	N677	F680	N681	P682	D685	N686	E687	F688	E689	R701	E705	D706	Y707	D708	S709	S710																
N713	I716	G717	Q718	S719	T720	Q728	G729	Y730	R731	H732	V733	H734	L735	L736	S737	K738	Q742	H743	L748	K751	I752	S753	I754	Q755	D756																																				

4 Data and refinement statistics

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

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	397.36 Å 397.36 Å 397.36 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50	Depositor
% Data completeness (in resolution range)	96.0 (15.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.227 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9216	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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: ACT

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	0.70	0/4165	0.79	3/5641 (0.1%)
1	B	0.69	0/4565	0.82	4/6174 (0.1%)
All	All	0.69	0/8730	0.81	7/11815 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	743	HIS	C-N-CD	-7.89	103.24	120.60
1	A	743	HIS	C-N-CD	-7.31	104.53	120.60
1	B	508	SER	N-CA-C	6.51	128.58	111.00
1	B	179	GLY	N-CA-C	-5.93	98.26	113.10
1	B	649	ASN	CB-CA-C	-5.46	99.47	110.40
1	A	420	GLY	N-CA-C	-5.21	100.09	113.10
1	A	514	GLY	N-CA-C	-5.02	100.56	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4070	0	3994	145	0
1	B	4465	0	4375	191	0
2	A	4	0	3	2	0
2	B	4	0	3	0	0
3	A	316	0	0	13	2
3	B	357	0	0	13	1
All	All	9216	0	8375	326	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (326) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:538:GLY:N	3:A:1031:HOH:O	1.97	0.98
1:B:176:VAL:HG21	1:B:208:LEU:HD11	1.42	0.98
1:B:644:VAL:HG23	1:B:645:ASN:H	1.29	0.98
1:A:200:GLU:HA	1:A:203:THR:HB	1.45	0.96
1:B:573:GLN:H	1:B:573:GLN:HE21	1.15	0.94
1:B:486:LEU:H	1:B:486:LEU:HD12	1.34	0.93
1:A:573:GLN:H	1:A:573:GLN:HE21	1.05	0.93
1:A:573:GLN:H	1:A:573:GLN:NE2	1.70	0.90
1:B:171:GLU:HG3	1:B:172:LEU:HD13	1.56	0.88
1:B:196:LEU:HD22	1:B:200:GLU:HB3	1.55	0.88
1:B:573:GLN:H	1:B:573:GLN:NE2	1.73	0.86
1:B:416:GLN:HG3	1:B:417:PRO:HD2	1.57	0.84
1:B:176:VAL:HG21	1:B:208:LEU:CD1	2.07	0.84
1:A:401:MET:HE2	1:A:492:LEU:HD11	1.60	0.84
1:A:241:GLN:HE22	1:A:730:TYR:H	1.22	0.83
1:A:383:TYR:HB3	1:A:384:PRO:HD2	1.61	0.82
1:B:383:TYR:HB3	1:B:384:PRO:HD2	1.61	0.82
1:A:520:MET:HE3	1:A:549:ARG:HB2	1.61	0.81
1:A:651:ILE:HD12	1:A:677:ASN:ND2	1.97	0.80
1:B:736:LEU:HD23	1:B:742:GLN:HA	1.65	0.79
1:B:234:VAL:O	1:B:238:GLN:HG3	1.83	0.78
1:B:238:GLN:HG2	1:B:246:ALA:CB	2.13	0.78
1:B:238:GLN:HG2	1:B:246:ALA:HB1	1.66	0.77
1:B:241:GLN:HE22	1:B:730:TYR:H	1.33	0.76
1:B:728:GLN:NE2	1:B:754:ILE:H	1.84	0.76
1:B:730:TYR:CE1	1:B:751:LYS:HD2	2.21	0.76
1:B:429:GLU:OE1	1:B:432:LYS:HE2	1.86	0.76
1:A:252:LEU:O	1:A:256:GLU:HG3	1.87	0.75
1:B:520:MET:HE3	1:B:549:ARG:HB2	1.69	0.74
1:B:438:LYS:HA	3:B:908:HOH:O	1.86	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:436:LEU:N	1:B:436:LEU:HD23	2.04	0.73
1:B:196:LEU:HD22	1:B:200:GLU:CB	2.18	0.73
1:A:200:GLU:HA	1:A:203:THR:CB	2.18	0.72
1:A:321:THR:HG22	1:A:360:PHE:HB2	1.71	0.71
1:B:227:THR:CG2	1:B:269:GLN:HB3	2.20	0.70
1:B:178:ASP:HB3	1:B:180:TYR:H	1.57	0.69
1:A:436:LEU:N	1:A:436:LEU:HD23	2.06	0.69
1:A:520:MET:CE	1:A:549:ARG:HB2	2.22	0.69
1:B:203:THR:O	1:B:207:MET:HG3	1.93	0.69
1:A:613:THR:HG22	1:A:615:PHE:H	1.58	0.69
1:A:670:ARG:HD3	3:A:909:HOH:O	1.92	0.69
1:B:509:SER:N	1:B:510:PRO:HD2	2.07	0.69
1:B:436:LEU:H	1:B:436:LEU:HD23	1.58	0.68
1:B:227:THR:HG21	1:B:269:GLN:HB3	1.74	0.68
1:B:706:ASP:O	1:B:713:ASN:HB3	1.93	0.68
1:B:171:GLU:CG	1:B:172:LEU:HD13	2.23	0.68
1:B:646:LYS:HG3	1:B:647:ASN:N	2.08	0.68
1:B:401:MET:HE2	1:B:492:LEU:HD11	1.74	0.68
1:B:708:ASP:HB2	3:B:1064:HOH:O	1.93	0.68
1:A:728:GLN:NE2	1:A:754:ILE:H	1.91	0.67
1:B:189:ASP:HB3	3:B:915:HOH:O	1.95	0.67
1:B:613:THR:HG22	1:B:615:PHE:H	1.60	0.66
1:A:573:GLN:N	1:A:573:GLN:NE2	2.44	0.65
1:A:730:TYR:CE1	1:A:751:LYS:HD2	2.31	0.65
1:A:630:ARG:NH1	3:A:886:HOH:O	2.29	0.65
1:B:176:VAL:HG23	1:B:680:PHE:CD2	2.31	0.65
1:A:755:GLN:HG2	1:A:756:ASP:N	2.11	0.65
1:A:624:PRO:HD2	1:A:625:TRP:CE3	2.32	0.65
1:B:174:ILE:HG23	1:B:176:VAL:HB	1.78	0.64
1:A:350:GLN:OE1	1:A:396:GLU:HG3	1.98	0.64
1:B:348:PRO:HB2	1:B:349:ASN:ND2	2.12	0.64
1:B:634:ARG:HG3	1:B:687:GLU:HB2	1.79	0.64
1:A:504:PHE:CZ	1:A:506:GLY:HA2	2.33	0.64
1:B:350:GLN:HA	1:B:397:GLN:NE2	2.13	0.63
1:A:200:GLU:O	1:A:204:PHE:N	2.30	0.62
1:B:335:LYS:NZ	3:B:819:HOH:O	2.29	0.62
1:B:644:VAL:HG23	1:B:645:ASN:N	2.10	0.62
1:B:516:ALA:HB1	1:B:518:TYR:CE2	2.34	0.62
1:B:174:ILE:CG2	1:B:176:VAL:HB	2.30	0.62
1:B:205:TYR:O	1:B:209:THR:HG23	2.00	0.62
1:A:200:GLU:CA	1:A:203:THR:HB	2.24	0.62
1:A:227:THR:CG2	1:A:269:GLN:HB3	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:573:GLN:N	1:B:573:GLN:NE2	2.48	0.61
1:B:198:ASP:HA	1:B:201:ILE:HG13	1.83	0.61
1:A:651:ILE:HD12	1:A:677:ASN:HD21	1.64	0.61
1:B:171:GLU:O	1:B:172:LEU:HD22	2.01	0.60
1:B:172:LEU:O	1:B:174:ILE:HG13	2.01	0.60
1:B:196:LEU:O	1:B:201:ILE:HD11	2.01	0.60
1:A:516:ALA:HB3	1:A:519:GLU:HG3	1.83	0.60
1:A:379:LYS:HE2	3:A:916:HOH:O	2.00	0.60
1:A:429:GLU:OE1	1:A:432:LYS:HE2	2.01	0.60
1:A:215:ASP:OD1	1:A:272:LYS:NZ	2.30	0.60
1:A:632:ARG:HH22	1:B:406:ARG:CZ	2.15	0.60
1:B:185:PHE:CE1	1:B:196:LEU:HG	2.37	0.59
1:A:203:THR:O	1:A:207:MET:N	2.30	0.59
1:B:520:MET:CE	1:B:549:ARG:HB2	2.33	0.59
1:B:624:PRO:HD2	1:B:625:TRP:CE3	2.37	0.59
1:B:440:LYS:HA	3:B:764:HOH:O	2.02	0.59
1:B:718:GLN:NE2	1:B:720:THR:OG1	2.36	0.58
1:B:705:GLU:C	1:B:716:ILE:HD12	2.24	0.58
1:B:197:GLU:O	1:B:201:ILE:HG12	2.03	0.58
1:B:379:LYS:HE2	3:B:826:HOH:O	2.04	0.58
1:A:504:PHE:HB3	1:A:527:ARG:HH22	1.68	0.57
1:B:248:PRO:O	1:B:252:LEU:HB2	2.04	0.57
1:A:360:PHE:HE2	3:A:1013:HOH:O	1.87	0.57
1:A:718:GLN:NE2	1:A:720:THR:OG1	2.36	0.57
1:B:520:MET:HE3	1:B:549:ARG:CB	2.34	0.57
1:B:701:ARG:HE	1:B:718:GLN:HE21	1.51	0.57
1:B:728:GLN:HE21	1:B:753:SER:HA	1.70	0.57
1:A:622:GLN:HB2	1:B:445:LEU:HD13	1.87	0.56
1:B:162:PHE:CZ	1:B:182:ARG:HB2	2.40	0.56
1:B:216:ARG:O	1:B:220:GLU:HG3	2.05	0.56
1:A:343:ASP:HB3	3:A:821:HOH:O	2.04	0.56
1:A:622:GLN:CA	1:B:445:LEU:HD13	2.36	0.56
1:A:736:LEU:HD23	1:A:742:GLN:HA	1.88	0.56
1:B:701:ARG:HE	1:B:718:GLN:NE2	2.04	0.56
1:B:342:LEU:HD12	1:B:342:LEU:N	2.21	0.56
1:B:182:ARG:O	1:B:185:PHE:HB3	2.06	0.55
1:B:321:THR:HG22	1:B:360:PHE:HB2	1.88	0.55
1:B:547:LEU:HD23	1:B:573:GLN:HG3	1.87	0.55
1:B:215:ASP:OD1	1:B:272:LYS:NZ	2.30	0.55
1:A:219:GLU:O	1:A:223:GLY:N	2.36	0.55
1:A:642:PRO:HD2	1:A:716:ILE:CG2	2.37	0.55
1:B:729:GLY:O	1:B:751:LYS:HA	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:516:ALA:HB1	1:A:518:TYR:CE2	2.41	0.55
1:A:406:ARG:HH11	1:A:406:ARG:CG	2.19	0.55
1:B:548:SER:H	1:B:573:GLN:NE2	2.04	0.55
1:A:573:GLN:N	1:A:573:GLN:HE21	1.89	0.55
1:B:486:LEU:H	1:B:486:LEU:CD1	2.05	0.55
1:B:547:LEU:CD2	1:B:573:GLN:HG3	2.36	0.55
1:A:394:SER:O	1:A:398:GLN:HG3	2.07	0.54
1:A:327:GLU:OE1	1:A:327:GLU:HA	2.08	0.54
1:B:348:PRO:HB2	1:B:349:ASN:HD22	1.73	0.54
1:A:227:THR:HG21	1:A:269:GLN:OE1	2.08	0.54
1:A:241:GLN:HE22	1:A:730:TYR:N	2.01	0.54
1:B:426:PRO:HB2	1:B:431:LEU:CD1	2.37	0.54
1:A:216:ARG:HG3	1:A:216:ARG:HH11	1.72	0.54
1:B:346:ASP:OD1	1:B:393:CYS:HA	2.08	0.53
1:B:416:GLN:CG	1:B:417:PRO:HD2	2.34	0.53
1:B:595:ASP:OD1	1:B:596:ASN:N	2.40	0.53
1:B:593:PHE:O	1:B:598:GLY:HA2	2.07	0.53
1:A:218:PHE:CE1	1:A:272:LYS:HA	2.43	0.53
1:B:500:LYS:NZ	3:B:958:HOH:O	2.39	0.53
1:B:205:TYR:CE1	1:B:209:THR:HG21	2.44	0.53
1:A:268:ARG:NE	3:A:904:HOH:O	2.30	0.53
1:B:163:LYS:HA	1:B:166:LYS:HB2	1.90	0.53
1:B:218:PHE:CE1	1:B:272:LYS:HA	2.44	0.52
1:A:504:PHE:HB3	1:A:527:ARG:NH2	2.24	0.52
1:A:346:ASP:OD2	1:A:394:SER:HB3	2.09	0.52
1:B:345:TRP:CZ2	1:B:357:GLY:HA3	2.45	0.52
1:B:486:LEU:HD12	1:B:486:LEU:N	2.14	0.52
1:B:379:LYS:HE3	3:B:954:HOH:O	2.10	0.52
1:A:689:GLU:OE2	1:B:494:ASP:OD2	2.29	0.51
1:B:272:LYS:O	1:B:275:PHE:HB3	2.10	0.51
1:A:587:ASP:OD2	2:A:5:ACT:O	2.28	0.51
1:B:383:TYR:HB3	1:B:384:PRO:CD	2.36	0.51
1:B:174:ILE:HG22	1:B:176:VAL:H	1.76	0.51
1:B:166:LYS:O	1:B:170:LYS:HG3	2.11	0.51
1:A:345:TRP:CZ2	1:A:357:GLY:HA3	2.46	0.51
1:A:622:GLN:HA	1:B:445:LEU:CD1	2.41	0.50
1:B:751:LYS:NZ	3:B:982:HOH:O	2.35	0.50
1:A:438:LYS:HE3	1:A:501:SER:OG	2.11	0.50
1:A:547:LEU:HD23	1:A:573:GLN:CG	2.41	0.50
1:A:670:ARG:HG3	1:A:690:PHE:CZ	2.46	0.50
1:A:272:LYS:O	1:A:275:PHE:HB3	2.12	0.50
1:A:547:LEU:HD23	1:A:573:GLN:HG3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:650:SER:HB3	3:B:868:HOH:O	2.11	0.50
1:B:227:THR:HG21	1:B:269:GLN:CD	2.31	0.50
1:A:216:ARG:HH21	1:A:683:ARG:HH22	1.59	0.50
1:A:227:THR:HG21	1:A:269:GLN:CD	2.32	0.50
1:A:230:VAL:O	1:A:234:VAL:HG23	2.12	0.50
1:B:730:TYR:C	1:B:731:ARG:HG2	2.31	0.50
1:A:593:PHE:O	1:A:598:GLY:HA2	2.11	0.49
1:B:523:PHE:N	1:B:523:PHE:CD1	2.80	0.49
1:A:558:ASP:O	1:A:559:SER:HB2	2.12	0.49
1:A:384:PRO:HG3	1:A:431:LEU:HB2	1.94	0.49
1:A:536:GLY:O	1:A:540:VAL:HG23	2.11	0.49
1:A:216:ARG:NH1	1:A:216:ARG:HG3	2.26	0.49
1:B:504:PHE:CZ	1:B:506:GLY:HA2	2.48	0.49
1:A:616:ASN:OD1	1:A:618:ARG:HB2	2.12	0.49
1:B:238:GLN:HG2	1:B:246:ALA:HB3	1.94	0.49
1:B:504:PHE:HB3	1:B:527:ARG:HH22	1.78	0.49
1:A:734:HIS:HE1	3:A:770:HOH:O	1.94	0.49
1:B:296:GLN:HA	3:B:907:HOH:O	2.13	0.49
1:A:651:ILE:HG22	1:A:677:ASN:C	2.33	0.49
1:A:350:GLN:HB3	3:A:1064:HOH:O	2.13	0.48
1:B:261:SER:O	1:B:265:LYS:HB2	2.13	0.48
1:A:729:GLY:O	1:A:751:LYS:HA	2.13	0.48
1:A:345:TRP:CZ2	1:A:392:HIS:CD2	3.02	0.48
1:B:184:ILE:HG22	1:B:204:PHE:CD2	2.48	0.48
1:B:701:ARG:NH2	1:B:718:GLN:HG3	2.28	0.48
1:A:255:ILE:HD13	1:A:268:ARG:O	2.13	0.48
1:B:441:LYS:NZ	1:B:493:SER:O	2.47	0.48
1:B:174:ILE:HG22	1:B:176:VAL:HG12	1.96	0.48
1:A:634:ARG:NH2	1:A:751:LYS:HD3	2.28	0.48
1:A:523:PHE:CD1	1:A:523:PHE:N	2.81	0.48
1:B:177:ASP:O	1:B:178:ASP:HB2	2.14	0.48
1:A:349:ASN:O	1:A:350:GLN:HB2	2.13	0.48
1:A:264:ALA:O	1:A:269:GLN:N	2.46	0.48
1:B:701:ARG:NE	1:B:718:GLN:HE21	2.12	0.48
1:B:196:LEU:CD2	1:B:200:GLU:HB3	2.34	0.47
1:B:736:LEU:CD2	1:B:742:GLN:HA	2.42	0.47
1:B:227:THR:CG2	1:B:228:LEU:N	2.77	0.47
1:B:587:ASP:HB3	1:B:718:GLN:NE2	2.29	0.47
1:A:548:SER:H	1:A:573:GLN:NE2	2.13	0.47
1:B:258:TYR:HB3	1:B:277:MET:HB3	1.95	0.47
1:B:183:LYS:O	1:B:187:GLU:HG3	2.14	0.47
1:B:707:TYR:OH	1:B:709:SER:HB3	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:706:ASP:HB2	1:B:716:ILE:HD11	1.96	0.47
1:A:213:GLU:HG3	1:A:749:PHE:CD2	2.50	0.47
1:A:342:LEU:HD12	1:A:342:LEU:N	2.29	0.47
1:A:367:CYS:SG	1:A:371:ARG:NH2	2.87	0.47
1:B:259:GLU:OE1	1:B:270:MET:HA	2.14	0.47
1:B:300:GLN:HB3	1:B:301:PRO:CD	2.45	0.47
1:B:645:ASN:HB3	1:B:648:LYS:HD3	1.96	0.47
1:A:436:LEU:H	1:A:436:LEU:HD23	1.78	0.47
1:A:648:LYS:O	1:A:650:SER:N	2.47	0.47
1:B:638:GLY:O	1:B:681:ASN:HA	2.15	0.46
1:B:516:ALA:HB3	1:B:519:GLU:HG3	1.97	0.46
1:A:705:GLU:C	1:A:716:ILE:HD12	2.36	0.46
1:A:644:VAL:HG12	1:A:644:VAL:O	2.14	0.46
1:B:647:ASN:HB2	1:B:648:LYS:H	1.46	0.46
1:B:426:PRO:HB2	1:B:431:LEU:HD11	1.97	0.46
1:B:580:GLN:HG2	3:B:810:HOH:O	2.15	0.46
1:B:398:GLN:OE1	1:B:488:LEU:HD12	2.16	0.46
1:B:509:SER:N	1:B:510:PRO:CD	2.78	0.46
1:B:313:THR:HB	1:B:329:TYR:CE1	2.51	0.46
1:A:610:ASP:HB3	1:A:613:THR:OG1	2.16	0.46
1:A:222:ALA:HA	1:A:228:LEU:HD23	1.96	0.46
1:A:622:GLN:HA	1:B:445:LEU:HD11	1.97	0.46
1:A:655:LYS:NZ	1:A:671:GLN:OE1	2.43	0.46
1:B:734:HIS:HE1	3:B:828:HOH:O	1.99	0.46
1:B:263:THR:O	1:B:266:ALA:HB3	2.16	0.46
1:A:349:ASN:OD1	1:A:349:ASN:O	2.33	0.46
1:B:625:TRP:CD1	1:B:626:TRP:N	2.84	0.46
1:B:169:LEU:O	1:B:171:GLU:O	2.34	0.45
1:B:227:THR:HG21	1:B:269:GLN:OE1	2.15	0.45
1:B:645:ASN:OD1	1:B:648:LYS:HD2	2.15	0.45
1:A:632:ARG:NH2	1:B:406:ARG:CZ	2.79	0.45
1:B:701:ARG:HH21	1:B:718:GLN:HG3	1.80	0.45
1:A:227:THR:CG2	1:A:228:LEU:N	2.79	0.45
1:B:406:ARG:HH22	1:B:415:ASP:HB2	1.80	0.45
1:A:653:ASP:OD1	1:A:677:ASN:N	2.30	0.45
1:A:638:GLY:O	1:A:681:ASN:HA	2.16	0.45
1:B:418:LEU:HD11	1:B:431:LEU:CD2	2.46	0.45
1:B:632:ARG:NH1	1:B:689:GLU:OE1	2.50	0.45
1:A:626:TRP:CZ3	1:A:693:THR:HB	2.52	0.45
1:B:504:PHE:HB3	1:B:527:ARG:NH2	2.31	0.45
1:A:675:ILE:HG12	1:A:684:TRP:NE1	2.32	0.45
1:B:230:VAL:O	1:B:234:VAL:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:681:ASN:N	1:B:682:PRO:CD	2.80	0.44
1:A:595:ASP:OD1	1:A:596:ASN:N	2.47	0.44
1:B:406:ARG:HH11	1:B:406:ARG:CG	2.29	0.44
1:B:300:GLN:O	1:B:427:SER:HA	2.16	0.44
1:A:222:ALA:HA	1:A:228:LEU:CD2	2.47	0.44
1:A:406:ARG:CG	1:A:406:ARG:NH1	2.79	0.44
1:B:227:THR:HG23	1:B:269:GLN:HB3	1.96	0.44
1:B:442:LEU:HD21	1:B:488:LEU:O	2.17	0.44
1:B:632:ARG:HH21	1:B:755:GLN:CD	2.20	0.44
1:B:605:PRO:HD2	1:B:608:LEU:HD12	1.99	0.44
1:B:644:VAL:CG2	1:B:645:ASN:H	2.10	0.44
1:B:730:TYR:CZ	1:B:751:LYS:HD2	2.51	0.44
1:A:701:ARG:NH2	1:A:718:GLN:HG3	2.33	0.44
1:A:622:GLN:CB	1:B:445:LEU:HD13	2.47	0.44
1:A:259:GLU:OE1	1:A:270:MET:HA	2.17	0.44
1:A:670:ARG:HD3	3:A:850:HOH:O	2.17	0.44
1:B:610:ASP:O	1:B:613:THR:OG1	2.33	0.43
1:B:406:ARG:HH22	1:B:415:ASP:CB	2.30	0.43
1:B:394:SER:O	1:B:398:GLN:HG3	2.18	0.43
1:A:681:ASN:N	1:A:682:PRO:CD	2.80	0.43
1:B:396:GLU:O	1:B:399:ARG:HB2	2.18	0.43
1:A:730:TYR:C	1:A:731:ARG:HG2	2.38	0.43
1:B:198:ASP:O	1:B:201:ILE:HG13	2.19	0.43
1:A:341:GLU:C	1:A:342:LEU:HD12	2.39	0.43
1:B:657:ILE:HD13	1:B:671:GLN:HB3	2.01	0.43
1:B:341:GLU:C	1:B:342:LEU:HD12	2.38	0.43
1:A:631:LEU:O	1:A:689:GLU:HA	2.19	0.43
1:B:176:VAL:CG1	1:B:177:ASP:N	2.80	0.43
1:A:316:LEU:HD23	1:A:328:ALA:HB2	1.99	0.43
1:A:651:ILE:HB	1:A:677:ASN:ND2	2.33	0.43
1:A:314:TYR:HB3	1:A:329:TYR:CE2	2.54	0.43
1:A:396:GLU:O	1:A:399:ARG:HB2	2.19	0.42
1:A:227:THR:HG21	1:A:269:GLN:HB3	1.99	0.42
1:B:516:ALA:CB	1:B:518:TYR:CE2	3.00	0.42
1:B:379:LYS:O	1:B:379:LYS:HG3	2.17	0.42
1:B:426:PRO:HG2	1:B:431:LEU:HD11	2.00	0.42
1:B:558:ASP:O	1:B:559:SER:HB2	2.18	0.42
1:A:710:SER:OG	1:A:711:SER:N	2.52	0.42
1:A:209:THR:HG22	1:A:209:THR:O	2.19	0.42
1:A:537:ASN:CA	3:A:1031:HOH:O	2.67	0.42
1:A:404:HIS:O	1:A:408:ILE:HG13	2.19	0.42
1:A:218:PHE:CD1	1:A:272:LYS:HA	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:259:GLU:CD	1:A:260:PRO:HD2	2.39	0.42
1:A:530:ARG:HB2	1:A:530:ARG:CZ	2.45	0.42
1:B:196:LEU:HA	1:B:196:LEU:HD23	1.87	0.42
1:B:549:ARG:O	1:B:550:ILE:HD13	2.19	0.42
1:A:222:ALA:CB	1:A:228:LEU:HD23	2.50	0.42
1:B:580:GLN:HB2	1:B:580:GLN:HE21	1.47	0.42
1:A:730:TYR:CZ	1:A:751:LYS:HD2	2.55	0.42
1:B:624:PRO:HD2	1:B:625:TRP:CZ3	2.54	0.42
1:A:622:GLN:HB2	1:B:445:LEU:CD1	2.49	0.42
1:A:738:LYS:HG2	2:A:5:ACT:H3	2.02	0.41
1:A:727:LYS:HE2	3:A:939:HOH:O	2.20	0.41
1:B:445:LEU:HD23	1:B:445:LEU:HA	1.73	0.41
1:B:434:LYS:HD2	1:B:434:LYS:HA	1.90	0.41
1:A:502:VAL:HG11	1:A:519:GLU:HB3	2.01	0.41
1:B:259:GLU:OE2	1:B:260:PRO:HD2	2.20	0.41
1:B:409:LEU:HD12	1:B:409:LEU:HA	1.73	0.41
1:B:547:LEU:HD23	1:B:573:GLN:CG	2.51	0.41
1:B:416:GLN:HG3	1:B:417:PRO:CD	2.38	0.41
1:B:438:LYS:HE3	1:B:501:SER:OG	2.20	0.41
1:A:738:LYS:HE3	1:A:738:LYS:HB3	1.72	0.41
1:B:236:PHE:CD1	1:B:240:GLN:HG3	2.55	0.41
1:A:728:GLN:HE21	1:A:753:SER:HA	1.84	0.41
1:B:259:GLU:CD	1:B:260:PRO:HD2	2.41	0.41
1:B:236:PHE:CE1	1:B:240:GLN:HG3	2.56	0.41
1:B:610:ASP:HA	1:B:611:PRO:HD2	1.78	0.41
1:A:622:GLN:CA	1:B:445:LEU:CD1	2.99	0.41
1:B:436:LEU:N	1:B:436:LEU:CD2	2.79	0.41
1:A:236:PHE:HA	3:A:866:HOH:O	2.19	0.41
1:A:687:GLU:HG2	1:A:688:PHE:N	2.36	0.41
1:B:388:SER:OG	1:B:438:LYS:HD3	2.22	0.41
1:A:516:ALA:CB	1:A:518:TYR:CZ	3.04	0.41
1:B:733:VAL:HB	1:B:748:LEU:HB2	2.02	0.41
1:A:300:GLN:O	1:A:427:SER:HA	2.20	0.41
1:A:537:ASN:O	1:A:541:ARG:HG3	2.22	0.40
1:B:196:LEU:HD22	1:B:200:GLU:HB2	2.02	0.40
1:A:670:ARG:HG3	1:A:690:PHE:CE1	2.56	0.40
1:A:436:LEU:CD2	1:A:436:LEU:N	2.80	0.40
1:B:580:GLN:HG3	1:B:580:GLN:H	1.18	0.40
1:A:547:LEU:CD2	1:A:573:GLN:HG3	2.51	0.40
1:B:197:GLU:O	1:B:200:GLU:HB2	2.22	0.40
1:A:580:GLN:HG3	1:A:580:GLN:H	0.97	0.40
1:A:669:SER:C	1:A:670:ARG:HG2	2.42	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:370:LEU:HA	1:B:370:LEU:HD23	1.84	0.40
1:A:250:LEU:O	1:A:253:SER:OG	2.32	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:889:HOH:O	3:A:889:HOH:O[52_555]	2.00	0.20
3:A:990:HOH:O	3:B:966:HOH:O[24_555]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/624 (82%)	468 (92%)	34 (7%)	7 (1%)	16	27
1	B	557/624 (89%)	509 (91%)	42 (8%)	6 (1%)	21	34
All	All	1066/1248 (85%)	977 (92%)	76 (7%)	13 (1%)	19	32

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	646	LYS
1	B	178	ASP
1	B	647	ASN
1	A	209	THR
1	A	649	ASN
1	A	651	ILE
1	B	173	ASN
1	B	648	LYS
1	B	644	VAL
1	A	225	ALA
1	A	421	VAL
1	B	512	THR
1	A	652	VAL

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	448/545 (82%)	410 (92%)	38 (8%)	15	28
1	B	492/545 (90%)	441 (90%)	51 (10%)	10	18
All	All	940/1090 (86%)	851 (90%)	89 (10%)	12	22

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	LEU
1	A	220	GLU
1	A	224	SER
1	A	226	GLU
1	A	242	ARG
1	A	252	LEU
1	A	278	TYR
1	A	379	LYS
1	A	388	SER
1	A	406	ARG
1	A	409	LEU
1	A	422	THR
1	A	424	SER
1	A	436	LEU
1	A	438	LYS
1	A	487	LYS
1	A	508	SER
1	A	509	SER
1	A	513	SER
1	A	526	SER
1	A	535	SER
1	A	539	PHE
1	A	545	SER
1	A	573	GLN
1	A	574	ILE
1	A	580	GLN
1	A	594	GLN
1	A	643	LYS
1	A	651	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	652	VAL
1	A	670	ARG
1	A	676	THR
1	A	677	ASN
1	A	683	ARG
1	A	685	ASP
1	A	738	LYS
1	A	753	SER
1	A	756	ASP
1	B	159	LYS
1	B	166	LYS
1	B	169	LEU
1	B	172	LEU
1	B	178	ASP
1	B	182	ARG
1	B	194	ASP
1	B	201	ILE
1	B	226	GLU
1	B	227	THR
1	B	232	ARG
1	B	242	ARG
1	B	253	SER
1	B	262	GLU
1	B	268	ARG
1	B	277	MET
1	B	310	SER
1	B	331	ARG
1	B	379	LYS
1	B	388	SER
1	B	406	ARG
1	B	409	LEU
1	B	416	GLN
1	B	436	LEU
1	B	438	LYS
1	B	484	ASP
1	B	486	LEU
1	B	499	CYS
1	B	509	SER
1	B	526	SER
1	B	535	SER
1	B	539	PHE
1	B	545	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	573	GLN
1	B	574	ILE
1	B	580	GLN
1	B	594	GLN
1	B	613	THR
1	B	614	THR
1	B	646	LYS
1	B	648	LYS
1	B	650	SER
1	B	651	ILE
1	B	652	VAL
1	B	676	THR
1	B	677	ASN
1	B	685	ASP
1	B	710	SER
1	B	738	LYS
1	B	753	SER
1	B	756	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	312	ASN
1	A	573	GLN
1	A	580	GLN
1	A	594	GLN
1	A	639	GLN
1	A	677	ASN
1	A	718	GLN
1	A	728	GLN
1	A	734	HIS
1	A	743	HIS
1	B	210	GLN
1	B	241	GLN
1	B	312	ASN
1	B	349	ASN
1	B	573	GLN
1	B	594	GLN
1	B	639	GLN
1	B	677	ASN
1	B	718	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	728	GLN
1	B	734	HIS
1	B	743	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	A	5	-	1,3,3	3.31	1 (100%)	0,3,3	0.00	-
2	ACT	B	5	-	1,3,3	3.24	1 (100%)	0,3,3	0.00	-

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
2	ACT	A	5	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACT	B	5	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5	ACT	CH3-C	3.31	1.53	1.48
2	B	5	ACT	CH3-C	3.24	1.53	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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